Semidefinite Representations and Facial Reduction *

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Abstract

In this paper we extend a recent algorithm for solving the sensor network localization problem ($\boldsymbol{SNL}$) to include instances with facial reduction to include the intersection of more than two faces. In particular, we continue to exploit the implicit degeneracy in the semidefinite programming ($\boldsymbol{SDP}$) relaxation of $\boldsymbol{SNL}$.

This is a preliminary working paper, and is a work in progress.

Contents

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1 Introduction

In this paper we derive and test an algorithm for solving large scale sensor localization problems ($\boldsymbol{SNL}$) using simultaneous intersections of faces.

The $\boldsymbol{SNL}$ problem consists in locating sensors using the fact that some of the sensors are anchors for which the locations are given, and that the distances between sensors within a given *radio range* are (approximately) known. Our algorithm extends the results in [19].

Following the approach in [19], we then exploit the implicit degeneracy in the semidefinite programming ($\boldsymbol{SDP}$) relaxation of $\boldsymbol{SNL}$. This involves finding the subspace representation of the faces of the semidefinite cone $\mathcal{S}^n_+$ corresponding to the faces of the Euclidean distance matrix cone $\mathcal{E}^n$. We repeatedly find the intersection of faces by finding the intersection of the subspace representations. We delay the completion of the original $\boldsymbol{EDM}$ till the end, i.e., after we find the $\boldsymbol{EDM}$ completion from the data, we finalize by rotating the problem using the original positions of the anchors.

2 Background

The $\boldsymbol{SNL}$ problem has recently attracted a lot of interest; see, for example, [5, 23, 24, 25, 17]. See also the webpage www.convexoptimization.com/dattorro/sensor_network_localization.html and the recent thesis [18]. Nie [23] using sums of squares also includes an error analysis. Noisy distances are handled in [4] using a combination of regularization and refinement.

3 Notation and Preliminary Results

We let $\mathcal{M}^{m\times n}$ denote the vector space of $m\times n$ real matrices equipped with the *trace inner product*, $\langle A,B\rangle = \operatorname{trace} A^TB$; let $\mathcal{M}^n := \mathcal{M}^{n\times n}$ and let $\mathcal{S}^n$ denote the subspace of *real symmetric* $n\times n$ *matrices*; $\mathcal{S}^n_+$ and $\mathcal{S}^n_{++}$ denote the cone of positive semidefinite and positive definite matrices, respectively; $A\succeq B$ and $A\succ B$ denote the Löwner partial order, $A-B\in\mathcal{S}^n_+$ and $A-B\in\mathcal{S}^n_{++}$, respectively; $\mathcal{R}(\mathcal{L})$ and $\mathcal{N}(\mathcal{L})$ denote the range space and null space of the linear transformation $\mathcal{L}$, respectively; we let e denote the vector of ones of appropriate dimension; and we use the MATLAB notation $1{:}n = \{1,\dots,n\}$. For $M\in\mathcal{M}^n$, we let $\mathcal{S}_\Sigma(M) = \frac{1}{2}(M+M^T)\in\mathcal{S}^n$ denote the *sum symmetrization*. Thus, $\mathcal{S}_\Sigma\colon\mathcal{M}^n\to\mathcal{S}^n$ represents the orthogonal projection onto $\mathcal{S}^n$. The adjoint of $\mathcal{S}_\Sigma$ is given by $\mathcal{S}_\Sigma{}^*(S)=S$, for all $S\in\mathcal{S}^n$. For $M\in\mathcal{M}^{mn}$, we let $\mathcal{S}_\Pi(M) = MM^T\in\mathcal{S}^n$ denote the *product symmetrization*.

For a subset S, let $\operatorname{cone}(S)$ denotes the convex cone generated by the set S. A subset $F\subseteq K$ is a *face of the cone* K, denoted $F\trianglelefteq K$, if

$$\left(x,y\in K,\ \frac{1}{2}(x+y)\in F\right) \implies (\operatorname{cone}\{x,y\}\subseteq F)\,.$$

If $F \trianglelefteq K$, but is not equal to K, we write $F \triangleleft K$. If $\{0\} \neq F \triangleleft K$, then F is a *proper face* of K. For $S \subseteq K$, we let face(S) denote the smallest face of K that contains S. A face $F \trianglelefteq K$ is an *exposed face* if it is the intersection of K with a hyperplane. The cone K is *facially exposed* if every face $F \trianglelefteq K$ is exposed.

The cone of positive semidefinite matrices $\mathcal{S}^n_+$ is facially exposed. A face $F \trianglelefteq \mathcal{S}^n_+$ can be characterized using the range or the nullspace of any matrix S in the relative interior of the face. If $S \in \operatorname{relint} F$, and $S = UD_SU^T$ is the compact spectral decomposition of S with the diagonal matrix of eigenvalues $D_S \in \mathcal{S}^t_{++}$, then

$$F = U\mathcal{S}^t_+U^T. \tag{3.1}$$

We let $\mathcal{S}_H \subseteq \mathcal{S}^n$ denote the space of *hollow matrices*; i.e., the set of symmetric matrices with zero diagonal. Let $D \in \mathcal{S}_H$. If there exist points $p_1, \dots, p_n \in \mathbb{R}^r$ such that

$$D_{ij} = \|p_i - p_j\|_2^2, \quad i, j = 1, \dots, n, \tag{3.2}$$

then D is called a *Euclidean distance matrix*, denoted $\boldsymbol{EDM}$. Note that we work with *squared distances*. The smallest value of r such that (3.2) holds is called the *embedding dimension* of D. The set of $\boldsymbol{EDM}$ matrices forms a closed convex cone in $\mathcal{S}^n$, denoted $\mathcal{E}^n$. If we are given a partial $\boldsymbol{EDM}$, $D_p \in \mathcal{E}^n$, let $\mathcal{G} = (N, E, \omega)$ be the corresponding simple graph on the nodes $N = 1{:}n$ whose edges E correspond to the known entries of D_p, with $(D_p)_{ij} = \omega^2_{ij}$, for all $(i,j) \in E$.

Definition 3.1. *For $Y \in \mathcal{S}^n$ and $\alpha \subseteq 1{:}n$, we let $Y[\alpha]$ denote the corresponding* principal submatrix *formed from the rows and columns with indices α. If, in addition, $|\alpha| = k$ and $\bar{Y} \in \mathcal{S}^k$ is given, then we define*

$$\mathcal{S}^n(\alpha, \bar{Y}) := \left\{Y \in \mathcal{S}^n : Y[\alpha] = \bar{Y}\right\}, \quad \mathcal{S}^n_+(\alpha, \bar{Y}) := \left\{Y \in \mathcal{S}^n_+ : Y[\alpha] = \bar{Y}\right\}.$$

Definition 3.2. *Given $D \in \mathcal{E}^n$ and $\alpha \subseteq 1{:}n$, let $B := \mathcal{K}^\dagger(D[\alpha]) = P_\alpha P_\alpha^T$, where P is full column rank. Then the rows of P are called a representation of the points in the subset α.*

The subset of matrices in $\mathcal{S}^n$ with the top left $k \times k$ block fixed is

$$\mathcal{S}^n(1{:}k, \bar{Y}) = \left\{Y \in \mathcal{S}^n : Y = \left[\begin{array}{c|c} \bar{Y} & \cdot \\ \hline \cdot & \cdot \end{array}\right]\right\}. \tag{3.3}$$

Similarly, if the principal submatrix $\bar{D} \in \mathcal{E}^k$ is given, for index set $\alpha \subseteq 1{:}n$, with $|\alpha| = k$, we define

$$\mathcal{E}^n(\alpha, \bar{D}) := \left\{D \in \mathcal{E}^n : D[\alpha] = \bar{D}\right\}. \tag{3.4}$$

The subset of matrices in $\mathcal{E}^n$ with the top left $k \times k$ block fixed is

$$\mathcal{E}^n(1{:}k, \bar{D}) = \left\{D \in \mathcal{E}^n : D = \left[\begin{array}{c|c} \bar{D} & \cdot \\ \hline \cdot & \cdot \end{array}\right]\right\}. \tag{3.5}$$

We are given a subset (including the distances between anchors) of the (squared) distances from (3.2). This forms a partial $\boldsymbol{EDM}, D_p$. We intend to solve the $\boldsymbol{EDM}$ *completion problem*, i.e. finding the missing entries of D_p to complete the $\boldsymbol{EDM}$. This completion problem can be solved by finding a set of points $p_1, \dots, p_n \in \mathbb{R}^r$ satisfying (3.2), where r is the embedding dimension of the partial $\boldsymbol{EDM}, D_p$. Equivalently, we solve the graph realizability problem with dimension r, i.e. we finding positions in $\mathbb{R}^r$ for the vertices of a graph such that the inter-distances of these positions satisfy the given edge lengths of the graph.

Let $Y \in \mathcal{M}^n$ be an $n \times n$ real matrix and $y \in \mathbb{R}^n$ a vector. We let $\operatorname{diag}(Y)$ denote the vector in $\mathbb{R}^n$ formed from the diagonal of Y. Then $\operatorname{Diag}(y) = \operatorname{diag}^*(y)$ denotes the diagonal matrix in $\mathcal{M}^n$ with the vector y along its diagonal; Diag is the adjoint of diag. The operator offDiag can then be defined as $\operatorname{offDiag}(Y) := Y - \operatorname{Diag}(\operatorname{diag} Y)$; let $\operatorname{us2vec} : \mathcal{S}^n \to \mathbb{R}^{n(n-1)/2}$ where $\operatorname{us2vec}(D)$ is $\sqrt{2}$ times the vector in $\mathbb{R}^{n(n-1)/2}$ formed from the strictly upper triangular part of D taken columnwise; the adjoint is $\operatorname{us2Mat} = \operatorname{us2vec}^*$ and $\operatorname{us2Mat}(d) \in \mathcal{S}_H$ takes $\frac{1}{\sqrt{2}}$ times the vector $d \in \mathbb{R}^{n(n-1)/2}$ and forms the matrix in $\mathcal{S}_H$. Note that $\operatorname{us2Mat} = \operatorname{us2vec}^\dagger$, i.e. $\operatorname{us2vec}\operatorname{us2Mat} = I$; and us2Mat is an isometry from $\mathbb{R}^{n(n-1)/2}$ to $\mathcal{S}_H$.

For $P^T = \begin{bmatrix} p_1 & p_2 & \dots & p_n \end{bmatrix} \in \mathcal{M}^{r \times n}$, where p_j, $j = 1, \dots, n$, are the points used in (3.2), let $Y := PP^T$, and let D be the corresponding $\boldsymbol{EDM}$ satisfying (3.2). The following linear operators $\mathcal{K}$ and $\mathcal{D}_e$ provide the connection between $\boldsymbol{SDP}$ and $\boldsymbol{EDM}$.

$$
\begin{array}{rcl}
\mathcal{K}(Y) & := & \mathcal{D}_e(Y) - 2Y \\
& := & \operatorname{diag}(Y)\, e^T + e \operatorname{diag}(Y)^T - 2Y \\
& = & \left(p_i^T p_i + p_j^T p_j - 2 p_i^T p_j\right)_{i,j=1}^n \\
& = & \left(\|p_i - p_j\|_2^2\right)_{i,j=1}^n \\
& = & D.
\end{array}
\tag{3.6}
$$

By abuse of notation, we also allow $\mathcal{D}_v$ to act on a vector; that is, $\mathcal{D}_v(y) := yv^T + vy^T$. Note that

$$
\mathcal{K}(Y) = 2\,\mathcal{S}_\Sigma(\operatorname{diag}(Y)e^T) - 2Y = 2(\mathcal{S}_\Sigma(\cdot e^T)\operatorname{diag})(Y) - 2Y. \tag{3.7}
$$

Therefore, the adjoint of $\mathcal{K}$ acting on $D \in \mathcal{S}^n$ is

$$
\begin{array}{rcl}
\mathcal{K}^*(D) & = & 2(\mathcal{S}_\Sigma(\cdot e^T)\operatorname{diag})^*(D) - 2D \\
& = & 2\operatorname{diag}^*(\cdot e^T)^*(\mathcal{S}_\Sigma)^*(D) - 2D \\
& = & 2\operatorname{Diag}(\cdot e)(D) - 2D \\
& = & 2(\operatorname{Diag}(De) - D).
\end{array}
\tag{3.8}
$$

Moreover,

$$
\begin{array}{rcl}
\mathcal{K}^*\,\mathcal{K}(Y) & = & 2(\operatorname{Diag}(\mathcal{K}(Y)e) - \mathcal{K}(Y)) \\
& = & -2(\mathcal{K}(Y) - \operatorname{Diag}(v)),
\end{array}
\tag{3.9}
$$

where $v = \mathcal{K}(Y)e$, i.e. we write it this way to emphasize that we simply subtract the row sums from the diagonal of $\mathcal{K}(Y)$.

The linear operator $\mathcal{K}$ is one-one and onto between the *centered* and *hollow* subspaces of $\mathcal{S}^n$, which are defined as

$$
\begin{array}{rcll}
\mathcal{S}_C & := & \{Y \in \mathcal{S}^n : Ye = 0\} & \text{(zero row sums)}, \\
\mathcal{S}_H & := & \{D \in \mathcal{S}^n : \operatorname{diag}(D) = 0\} & = \mathcal{R}(\operatorname{offDiag}).
\end{array}
\tag{3.10}
$$

Let $J := J_k := I - \frac{1}{k}ee^T$ denote the orthogonal projection onto the subspace $\{e\}^\perp$, and define the linear operator $\mathcal{T}(D) := -\frac{1}{2}J\operatorname{offDiag}(D)J$. (We use J when the dimension is clear.) Then we have the following relationships.

Proposition 3.3. *([1]) The linear operator $\mathcal{T}$ is the generalized inverse of the linear operator $\mathcal{K}$; that is, $\mathcal{K}^\dagger = \mathcal{T}$. Moreover:*

$$\begin{array}{rl} \mathcal{R}(\mathcal{K}) = \mathcal{S}_H; & \mathcal{N}(\mathcal{K}) = \mathcal{R}(\mathcal{D}_e); \\ \mathcal{R}(\mathcal{K}^*) = \mathcal{R}(\mathcal{T}) = \mathcal{S}_C; & \mathcal{N}(\mathcal{K}^*) = \mathcal{N}(\mathcal{T}) = \mathcal{R}(\mathrm{Diag}); \end{array} \tag{3.11}$$

$$\mathcal{S}^n = \mathcal{S}_H \oplus \mathcal{R}(\mathrm{Diag}) = \mathcal{S}_C \oplus \mathcal{R}(\mathcal{D}_e). \tag{3.12}$$

Theorem 3.4. *([1]) The linear operators $\mathcal{T}$ and $\mathcal{K}$ are one-to-one and onto mappings between the cone $\mathcal{E}^n \subset \mathcal{S}_H$ and the face of the semidefinite cone $\mathcal{S}^n_+ \cap \mathcal{S}_C$. That is,*

$$\mathcal{T}(\mathcal{E}^n) = \mathcal{S}^n_+ \cap \mathcal{S}_C \quad \textit{and} \quad \mathcal{K}(\mathcal{S}^n_+ \cap \mathcal{S}_C) = \mathcal{E}^n.$$

Let $D_p \in \mathcal{S}^n$ be a *partial* ***EDM*** with embedding dimension r and let $H \in \mathcal{S}^n$ be the 0–1 matrix corresponding to the known entries of D_p. One can use the substitution $D = \mathcal{K}(Y)$, where $Y \in \mathcal{S}^n_+ \cap \mathcal{S}_C$, in the ***EDM*** completion problem

$$\begin{array}{rc} \text{Find} & D \in \mathcal{E}^n \\ \text{s.t.} & H \circ D = D_p \end{array}$$

to obtain the ***SDP*** relaxation

$$\begin{array}{rc} \text{Find} & Y \in \mathcal{S}^n_+ \cap \mathcal{S}_C \\ \text{s.t.} & H \circ \mathcal{K}(Y) = D_p \end{array}.$$

This relaxation does not restrict the rank of Y and may yield a solution with embedding dimension that is too large, if $\mathrm{rank}\,(Y) > r$. A clique $\gamma \subseteq 1{:}n$ in the graph $\mathcal{G}$ corresponds to a subset of sensors for which the distances $\omega_{ij} = \|p_i - p_j\|_2$ are known, for all $i, j \in \gamma$; equivalently, the clique corresponds to the principal submatrix $D_p[\gamma]$ of the partial ***EDM*** matrix D_p, where all the elements of $D_p[\gamma]$ are known. Moreover, solving ***SDP*** problems with rank restrictions is NP-HARD. However, we work on faces of $\mathcal{S}^n_+$ described by $U\mathcal{S}^t_+U^T$, with $t \leq n$. In order to find the face with the smallest dimension t, we must have the correct knowledge of the matrix U. In this paper, we obtain information on U using the cliques in the graph of the partial ***EDM***.

Suppose that

$$V^T e = 0 \text{ and } \begin{bmatrix} e & V \end{bmatrix} \text{ is nonsingular.} \tag{3.13}$$

We now introduce the composite operators

$$\mathcal{K}_V(X) \quad := \quad \mathcal{K}(VXV^T), \tag{3.14}$$

and

$$\mathcal{T}_V(D) \quad := \quad V^\dagger \mathcal{T}(D)(V^T)^\dagger = -\tfrac{1}{2} V^\dagger J \,\mathrm{offDiag}(D) J (V^T)^\dagger. \tag{3.15}$$

Lemma 3.5 ([2, 1])**.** *Suppose that V satisfies the definition in (3.13). Then*

$$\begin{array}{c} \mathcal{K}_V(\mathcal{S}_{n-1}) = \mathcal{S}_H, \\ \mathcal{T}_V(\mathcal{S}_H) = \mathcal{S}_{n-1}, \end{array}$$

and $\mathcal{K}_V = \mathcal{T}_V^\dagger$.

From (3.13) and (3.6) we get that

$$\mathcal{K}_V^*(D) \;=\; V^T \mathcal{K}^*(D) V \tag{3.16}$$

is the adjoint operator of $\mathcal{K}_V$. The following corollary summarizes useful relationships between $\mathcal{E}$, the cone of Euclidean distance matrices of order n, and $\mathcal{P}$, the cone of positive semidefinite matrices of order $n-1$.

Corollary 3.6 ([2, 1])**.** *Suppose that V is defined as in (3.13). Then:*

$$\begin{aligned} \mathcal{K}_V(\mathcal{P}) &= \mathcal{E}, \\ \mathcal{T}_V(\mathcal{E}) &= \mathcal{P}. \end{aligned}$$

4 Facial Geometry

Let $\bar{D}$ be an $n \times n$ *partial* Euclidean distance matrix with associated graph $G = (V, E)$. In particular, we have that

$$V = 1{:}n \quad \text{and} \quad E = \left\{ ij : \bar{D}_{ij} \text{ is specified} \right\}.$$

Let $\mathcal{F}$ be the corresponding set of feasible centred Gram matrices Y; that is,

$$\mathcal{F} := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : \mathcal{K}(Y)_{ij} = \bar{D}_{ij}, \forall ij \in E \right\}.$$

Let $\alpha \subseteq 1{:}n$ be a subset of the nodes of the graph G. We define the feasible set of centred Gram matrices Y that agree with the distances on the subgraph induced by the nodes in α as

$$\mathcal{F}_\alpha := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : \mathcal{K}(Y)_{ij} = \bar{D}_{ij}, \forall ij \in E \cap (\alpha \times \alpha) \right\}.$$

Note that $\mathcal{F} \subseteq \mathcal{F}_\alpha$.

Let $\alpha_1, \alpha_2 \subseteq 1{:}n$ and let

$$\operatorname{face}(\mathcal{F}_{\alpha_i}) = U_i \mathcal{S}_+^{n-|\alpha_i|+d_i+1} U_i^T,$$

for $i = 1, 2$.

4.1 Mixed dimension face intersection lemma

Suppose that $0 \neq f_i \lhd \mathcal{S}^n_+, i = 1, 2$ are proper faces. We would like to study the intersection of these two faces. Let

$$d_i = \dim f_i,\ G_i \in \operatorname{relint} f_i,\ 0 \neq v_i \in \mathcal{N}(G_i),\ Q_i^T e = v_i,\ Q_i \in \mathcal{O}_n,\ i = 1, 2.$$

By using the rotations $f_i \leftarrow Q f_i Q^T$, we can ensure that

$$e \in \mathcal{N}(G_i),\ G_i \in \mathcal{S}_C,\ f_i \subseteq \mathcal{S}_C,\ i = 1, 2.$$

Therefore, if needed, we can assume that the G_i are appropriate centered Gram matrices. In addition, we can factor a Gram matrix ????$G \in f_1 \cap f_2$???? as

$$G = U \begin{bmatrix} G_{11} & G_{12} \\ G_{12}^T & G_{22} \end{bmatrix} U^T, \quad U = \begin{array}{c} \\ |\alpha_1 \backslash \alpha_2| \\ |\alpha_1 \cap \alpha_2| \\ |\alpha_2 \backslash \alpha_1| \end{array} \begin{array}{c} \begin{array}{cc} d_1+1 & |\alpha_2 \backslash \alpha_1| \end{array} \\ \begin{bmatrix} U^{11} & 0 \\ U^{12} & 0 \\ 0 & I_{22} \end{bmatrix} \end{array} = \begin{array}{c} \\ |\alpha_1| \\ |\alpha_2 \backslash \alpha_1| \end{array} \begin{array}{c} \begin{array}{cc} d_1+1 & |\alpha_2 \backslash \alpha_1| \end{array} \\ \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{22} \end{bmatrix} \end{array},$$

?????check out the details???? i.e. any two faces can be factored this way to get a special structure for the intersection?????

????connection to Kronecker canonical form???? e.g., [21] and so we can do this for an arbitrary pair of faces???? how????

We now consider the special case where each G_i has a decomposition as above with a U that has a identity matrix block.

Lemma 4.1. *For $i = 1, 2$, let d_i be a nonnegative integer, $\alpha_i \subseteq 1{:}n$, and $\bar{U}_i \in \mathbb{R}^{|\alpha_i| \times (d_i+1)}$. Let*

$$U_1 := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_1\cap\alpha_2| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_1{+}1 & |\alpha_2\backslash\alpha_1| \end{array} \\ \begin{bmatrix} U_1^{11} & 0 \\ U_1^{12} & 0 \\ 0 & I_{22} \end{bmatrix} \end{array} := \begin{array}{c} \\ |\alpha_1| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_1{+}1 & |\alpha_2\backslash\alpha_1| \end{array} \\ \begin{bmatrix} \bar{U}_1 & 0 \\ 0 & I_{22} \end{bmatrix} \end{array}, \tag{4.1}$$

$$U_2 := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_1\cap\alpha_2| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} |\alpha_1\backslash\alpha_2| & d_2{+}1 \end{array} \\ \begin{bmatrix} I_{11} & 0 \\ 0 & U_2^{12} \\ 0 & U_2^{22} \end{bmatrix} \end{array} := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_2| \end{array} \!\!\begin{array}{c} \begin{array}{cc} |\alpha_1\backslash\alpha_2| & d_2{+}1 \end{array} \\ \begin{bmatrix} I_{11} & 0 \\ 0 & \bar{U}_2 \end{bmatrix} \end{array}. \tag{4.2}$$

For $i = 1, 2$, let $k_i := \dim\left(\operatorname{null}\left(U_i^{12}\right)\right)$ and $Z_i \in \mathbb{R}^{(d_i+1)\times k_i}$ satisfy

$$\operatorname{range}(Z_i) = \operatorname{null}(U_i^{12}).$$

- *If* $\operatorname{range}(U_2^{12}) \subseteq \operatorname{range}(U_1^{12})$ *and*

$$U := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_2| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_2{+}1 & k_1 \end{array} \\ \begin{bmatrix} U_1^{11}\left(U_1^{12}\right)^{\dagger} U_2^{12} & U_1^{11} Z_1 \\ \bar{U}_2 & 0 \end{bmatrix} \end{array}, \tag{4.3}$$

  then $\operatorname{range}(U) = \operatorname{range}(U_1) \cap \operatorname{range}(U_2)$.

- *If* $\operatorname{range}(U_1^{12}) \subseteq \operatorname{range}(U_2^{12})$ *and*

$$U := \begin{array}{c} \\ |\alpha_1| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_1{+}1 & k_2 \end{array} \\ \begin{bmatrix} \bar{U}_1 & 0 \\ U_2^{22}\left(U_2^{12}\right)^{\dagger} U_1^{12} & U_2^{22} Z_2 \end{bmatrix} \end{array}, \tag{4.4}$$

  then $\operatorname{range}(U) = \operatorname{range}(U_1) \cap \operatorname{range}(U_2)$.

If $\operatorname{range}(U_1^{12}) = \operatorname{range}(U_2^{12})$, *then*

$$d_1 + k_2 = d_2 + k_1. \tag{4.5}$$

Proof. Let U be given by equation (4.3). Suppose that $x \in \operatorname{range}(U_1) \cap \operatorname{range}(U_2)$. Then

$$x = \begin{bmatrix} U_1^{11} v_1 \\ U_1^{12} v_1 \\ v_2 \end{bmatrix} = \begin{bmatrix} w_1 \\ U_2^{12} w_2 \\ U_2^{22} w_2 \end{bmatrix}, \tag{4.6}$$

for some $v = [v_1; v_2] \in \mathbb{R}^{d_1+1+|\alpha_2\backslash\alpha_1|}$ and $w = [w_1; w_2] \in \mathbb{R}^{|\alpha_1\backslash\alpha_2|+d_2+1}$. Therefore, we have that

$$v_1 \in \left(U_1^{12}\right)^\dagger U_2^{12} w_2 + \operatorname{null}\left(U_1^{12}\right),$$

so $v_1 = \left(U_1^{12}\right)^\dagger U_2^{12} w_2 + Z_1 z_1$, for some $z_1 \in \mathbb{R}^{k_1}$. Thus,

$$x = \begin{bmatrix} U_1^{11}\left(U_1^{12}\right)^\dagger U_2^{12} w_2 + U_1^{11} Z_1 z_1 \\ U_2^{12} w_2 \\ U_2^{22} w_2 \end{bmatrix} = U \begin{bmatrix} w_2 \\ z_1 \end{bmatrix}, \tag{4.7}$$

so $x \in \operatorname{range}(U)$. Now suppose that $x \in \operatorname{range}(U)$. Then there exist $w_2 \in \mathbb{R}^{d_2+1}$ and $z_1 \in \mathbb{R}^{k_1}$ satisfying equation (4.7). Let

$$\begin{aligned} v_1 &:= \left(U_1^{12}\right)^\dagger U_2^{12} w_2 + Z_1 z_1, \\ v_2 &:= U_2^{22} w_2, \\ w_1 &:= U_1^{11} v_1. \end{aligned}$$

Since $\operatorname{range}\left(U_2^{12}\right) \subseteq \operatorname{range}\left(U_1^{12}\right)$ and $\operatorname{range} Z_1 = \operatorname{null}\left(U_1^{12}\right)$, we have

$$U_1^{12} v_1 = U_1^{12}\left(U_1^{12}\right)^\dagger U_2^{12} w_2 + U_1^{12} Z_1 z_1 = U_2^{12} w_2.$$

Therefore, equation (4.6) holds, so $x \in \operatorname{range}(U_1) \cap \operatorname{range}(U_2)$. Thus,

$$\operatorname{range}(U) = \operatorname{range}(U_1) \cap \operatorname{range}(U_2).$$

A similar argument gives the same result when U is given by equation (4.4).

Finally, suppose $\operatorname{range}(U_1^{12}) = \operatorname{range}(U_2^{12})$. Then

$$d_1 + 1 = \dim(\operatorname{null}(U_1^{12})) + \operatorname{rank}(U_1^{12}) = k_1 + \operatorname{rank}(U_1^{12})$$

and

$$d_2 + 1 = \dim(\operatorname{null}(U_2^{12})) + \operatorname{rank}(U_2^{12}) = k_2 + \operatorname{rank}(U_2^{12})$$

implies that $d_2 + 1 - k_2 = d_1 + 1 - k_1$. Therefore, $d_2 + k_1 = d_1 + k_2$. $\square$

Lemma 4.2. *For $i = 1, 2$, let d_i be a nonnegative integer, $\alpha_i \subseteq 1{:}n$, and $\bar{U}_i \in \mathbb{R}^{|\alpha_i|\times(d_i+1)}$. Let*

$$U_1 := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_1\cap\alpha_2| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_1{+}1 & |\alpha_2\backslash\alpha_1| \end{array} \\ \begin{bmatrix} U_1^{11} & 0 \\ U_1^{12} & 0 \\ 0 & I \end{bmatrix} \end{array} := \begin{array}{c} \\ |\alpha_1| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} d_1{+}1 & |\alpha_2\backslash\alpha_1| \end{array} \\ \begin{bmatrix} \bar{U}_1 & 0 \\ 0 & I \end{bmatrix} \end{array}, \tag{4.8}$$

$$U_2 := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_1\cap\alpha_2| \\ |\alpha_2\backslash\alpha_1| \end{array} \!\!\begin{array}{c} \begin{array}{cc} |\alpha_1\backslash\alpha_2| & d_2{+}1 \end{array} \\ \begin{bmatrix} I & 0 \\ 0 & U_2^{12} \\ 0 & U_2^{22} \end{bmatrix} \end{array} := \begin{array}{c} \\ |\alpha_1\backslash\alpha_2| \\ |\alpha_2| \end{array} \!\!\begin{array}{c} \begin{array}{cc} |\alpha_1\backslash\alpha_2| & d_2{+}1 \end{array} \\ \begin{bmatrix} I & 0 \\ 0 & \bar{U}_2 \end{bmatrix} \end{array}. \tag{4.9}$$

Let $\mathcal{F}_i, i = 1, 2$ denote the corresponding two faces. Then there exists matrices $Q_i, i = 1, 2$, each with linearly independent columns such that

$$\cap_{i=1,2} \operatorname{range}(U_i) = \operatorname{range}(U_j Q_j), j = 1, 2.$$

Equivalently, the intersection of the two faces is represented by either choice of $(U_j Q_j), j = 1, 2$.

Proof. The intersection of the two faces is represented by the matrix X in the relative interior where the range of X is given by the intersection of the two ranges, i.e.

$$X = U_i Q_i D_i Q_i^T U_i^T, D_i \succ 0, i = 1, 2,$$

for appropriate matrices Q_i. This means we can represent the face with either representation of the appropriate range space. $\square$

4.1.1 Determining k_1 and k_2

For a Euclidean distance matrix $\hat{D} \in \mathcal{S}^n$, we define the *embedding dimension* of $\hat{D}$ as

$$\operatorname{embdim}(\hat{D}) := \min \left\{ d : \exists p_1, \ldots, p_n \in \mathbb{R}^d \ni \|p_i - p_j\|_2^2 = \hat{D}_{ij}, \forall ij \right\}.$$

For a *partial* Euclidean distance matrix D, we define the *maximum embedding dimension* as

$$\operatorname{maxdim}(D) := \max \left\{ \operatorname{rank}(Y) : Y \in \mathcal{S}_+^n \cap \mathcal{S}_C^n \ni \mathcal{K}(Y)_{ij} = D_{ij}, \forall ij \in E \right\},$$

where $E := \{ij : D_{ij} \text{ is "specified"}\}$.

Let $\alpha \subseteq 1{:}n$ and

$$\operatorname{face} \left\{ Y \in \mathcal{S}_+^n : H[\alpha] \circ \mathcal{K}(Y[\alpha]) = H[\alpha] \circ D[\alpha] \right\} := U \mathcal{S}^{n-|\alpha|+d+1} U^T,$$

where

$$U\left[\alpha, 1{:}(d+1)\right] := \bar{U} \in \mathbb{R}^{|\alpha| \times (d+1)}, \tag{4.10}$$

$$U\left[\bar{\alpha}, (d+2){:}(n - |\alpha| + d + 1)\right] := I \in \mathcal{S}^{n-|\alpha|}. \tag{4.11}$$

$$U_\beta := \bar{U}\left[\beta, :\right]$$

4.2 Alternate/Direct Approach Using SVD

We start off with the equation for the unknown vectors y.

$$U_1 x = U_2 y = U_3 z.$$

We let

$$U_i = u_i s_i v_i^T, i = 1, 2, 3$$

denote the SVD for the matrices. Therefore, the system for y becomes:

$$u_1 s_1 v_1 x = u_2 s_2 v_2 y = u_3 s_3 v_3 z;$$

$$s_1 v_1 x = u_1^T u_2 s_2 v_2 y = u_1^T u_3 s_3 v_3 z.$$

In this example, all the cliques are the same size, 4. The embedding dimension is 2. Therefore we lose $4 - 2 - 1 = 1$ rank in the clique reduction for each clique, i.e. the dimension of each face is $7 - 1 = 6$. Therefore, each U_i is 7×6 and is full column rank. In fact, by construction the U_i have orthogonal columns and so singular values are all 1 except for one which is 0. Therefore, $s_1 v_1$ has a zero bottom row. We get:

$$x = (s_1 v_1)^\dagger u_1^T u_2 s_2 v_2 y = (s_1 v_1)^\dagger u_1^T u_3 s_3 v_3 z, \quad b_2 y = 0, b_3 z = 0,$$

where b_i denotes the last row of $u_1^T u_i s_i v_i, i = 2, 3$. We can substitute using bases for the orthogonal complements of the b_i

$$x = (s_1 v_1)^\dagger u_1^T u_2 s_2 v_2 P_2 \bar{y} = (s_1 v_1)^\dagger u_1^T u_3 s_3 v_3 P_3 \bar{z}.$$

We can repeat this step to find $\bar{y}$ in terms of $\bar{z}$, e.g. by using the SVD $(s_1 v_1)^\dagger u_1^T u_2 s_2 v_2 P_2 = \bar{u}\bar{s}\bar{v}$. Therefore, we get

$$\bar{u}\bar{s}\bar{v}\bar{y} = (s_1 v_1)^\dagger u_1^T u_3 s_3 v_3 P_3 \bar{z}.$$

Again, $\bar{s}$ has a zero bottom row. This gives us a new constraint on $\bar{z}$. We can substitute using a basis for the range of the orthogonal complement of the bottom row of $\bar{u}^T (s_1 v_1)^\dagger u_1^T u_3 s_3 v_3 P_3$, call it $\bar{b}_3$ and the basis $\bar{P}_3$. This yields the equation

$$\bar{y} = (\bar{s}\bar{v})^\dagger \bar{u}^T (s_1 v_1)^\dagger u_1^T u_3 s_3 v_3 P_3 \bar{P}_3 \hat{z}.$$

5 Clique Reduction

We now present several techniques for reducing an $\boldsymbol{EDM}$ completion problem using cliques in the graph. This extends the results presented in [10, 9, 19]. In particular, we modify the approach in [19] for combining two cliques.

The following two technical lemmas are given in [19].

Lemma 5.1 ([19]). *Let $B \in \mathcal{S}^n$, $Bv = 0$, $v \neq 0$, $y \in \mathbb{R}^n$ and $\bar{Y} := B + \mathcal{D}_v(y)$. If $\bar{Y} \succeq 0$, then*

$$y \in \mathcal{R}(B) + \operatorname{cone}\{v\}.$$

□

Lemma 5.2 ([19]). *Let $Y \in \mathcal{S}^k_+$ and $\bar{U} \in \mathcal{M}^{k\times t}$ with $\bar{U}$ having full column rank. If* face $\{\bar{Y}\} \trianglelefteq$ *(resp.=) $\bar{U}\mathcal{S}^t_+\bar{U}^T$, then*

$$\operatorname{face} \mathcal{S}^n_+(1{:}k, \bar{Y}) \trianglelefteq \ \textit{(resp.=)} \ \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{n-k} \end{bmatrix} \mathcal{S}^{n-k+t}_+ \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{n-k} \end{bmatrix}^T. \tag{5.1}$$

Proof. The result in [19] assumes that $\bar{U}^T\bar{U} = I$. The extension to $\bar{U}$ having full column rank follows from taking the compact QR-factorization $U = QR$, where $Q^T Q = I$ and R is nonsingular. □

We can now find an expression for the face defined by a given clique in the graph. Without loss of generality, we can assume that $\alpha = 1{:}k \subseteq 1{:}n$, $|\alpha| = k$.

Theorem 5.3 ([19]). *Let $D \in \mathcal{E}^n$, with embedding dimension r. Let $\alpha := 1{:}k$, $\bar{D} := D[\alpha] \in \mathcal{E}^k$ with embedding dimension t, and $B := \mathcal{K}^\dagger(\bar{D}) = \bar{U}_B S \bar{U}_B^T$, where $\bar{U}_B \in \mathcal{M}^{k\times t}$, $\bar{U}_B$ having full column rank, and $S \in \mathcal{S}^t_{++}$. Furthermore, let $U_B := \begin{bmatrix} \bar{U}_B & \frac{1}{\sqrt{k}}e \end{bmatrix} \in \mathcal{M}^{k\times(t+1)}$, $U := \begin{bmatrix} U_B & 0 \\ 0 & I_{n-k} \end{bmatrix}$, and let $\begin{bmatrix} V & \frac{U^T e}{\|U^T e\|} \end{bmatrix} \in \mathcal{M}^{n-k+t+1}$ be orthogonal. Then*

$$\operatorname{face} \mathcal{K}^\dagger\left(\mathcal{E}^n(1{:}k, \bar{D})\right) = \left(U\mathcal{S}^{n-k+t+1}_+ U^T\right) \cap \mathcal{S}_C = (UV)\mathcal{S}^{n-k+t}_+ (UV)^T. \tag{5.2}$$

Proof. As in Lemma 5.2, the result in [19] assumes that $\bar{U}^T\bar{U} = I$. The extension follows as in the proof of the Lemma. $\square$

In Theorem 5.3 we can make various choices for S and thus change the choice of $\bar{U}_B$. An interesting choice for $\bar{U}_B$ allows for a representation for the points in the clique.

Corollary 5.4. *Let $D, r, \alpha, \bar{D}, t$ be defined as in Theorem 5.3. Let $B := \mathcal{K}^\dagger(\bar{D}) = P_B P_B^T$, where $P_B \in \mathcal{M}^{k\times t}$ is full column rank. Furthermore, let Q be orthogonal, $U_B := \begin{bmatrix} P_B Q & \frac{1}{\sqrt{k}}e \end{bmatrix} \in \mathcal{M}^{k\times(t+1)}$, $U := \begin{bmatrix} U_B & 0 \\ 0 & I_{n-k}\end{bmatrix}$, and let $\begin{bmatrix} V & \frac{U^Te}{\|U^Te\|}\end{bmatrix} \in \mathcal{M}^{n-k+t+1}$ be orthogonal. Then (5.2) holds, and the rows of P_BQ provide a relative representation of the points in the clique α, i.e.*

$$\mathcal{K}((P_BQ)(P_BQ)^T) = D[\alpha].$$

Proof. We just need to use $S = I_t = QQ^T$ in the expression for B in the hypothesis of Theorem 5.3; e.g. we could use the compact spectral decomposition $B = UDU^T$ and set $P_B = UD^{1/2}$. Then $\mathcal{K}((P_BQ)(P_BQ)^T) = \mathcal{K}(P_B(P_B^T) = \mathcal{K}(B) = D[\alpha]$. $\square$

The following result provides expressions for the face for the union of two cliques.

Theorem 5.5 ([19]). *Let $D \in \mathcal{E}^n$ with embedding dimension r and define the sets of positive integers*

$$\begin{array}{c} \alpha_1 := 1{:}(\bar{k}_1 + \bar{k}_2), \quad \alpha_2 := (\bar{k}_1 + 1){:}(\bar{k}_1 + \bar{k}_2 + \bar{k}_3) \subseteq 1{:}n, \\ k_1 := |\alpha_1| = \bar{k}_1 + \bar{k}_2, \quad k_2 := |\alpha_2| = \bar{k}_2 + \bar{k}_3, \\ k := \bar{k}_1 + \bar{k}_2 + \bar{k}_3. \end{array} \tag{5.3}$$

For $i = 1, 2$, let $\bar{D}_i := D[\alpha_i] \in \mathcal{E}^{k_i}$ with embedding dimension t_i, and $B_i := \mathcal{K}^\dagger(\bar{D}_i) = \bar{U}_i S_i \bar{U}_i^T$, where $\bar{U}_i \in \mathcal{M}^{k_i\times t_i}$, $\bar{U}_i^T\bar{U}_i = I_{t_i}$, $S_i \in \mathcal{S}^{t_i}_{++}$, and $U_i := \begin{bmatrix} \bar{U}_i & \frac{1}{\sqrt{k_i}}e\end{bmatrix} \in \mathcal{M}^{k_i\times(t_i+1)}$. Let t and $\bar{U} \in \mathcal{M}^{k\times(t+1)}$ satisfy

$$\mathcal{R}(\bar{U}) = \mathcal{R}\left(\begin{bmatrix} U_1 & 0 \\ 0 & I_{\bar{k}_3}\end{bmatrix}\right) \cap \mathcal{R}\left(\begin{bmatrix} I_{\bar{k}_1} & 0 \\ 0 & U_2\end{bmatrix}\right), \text{ with } \bar{U}^T\bar{U} = I_{t+1}. \tag{5.4}$$

Let $U := \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{n-k}\end{bmatrix} \in \mathcal{M}^{n\times(n-k+t+1)}$ and $\begin{bmatrix} V & \frac{U^Te}{\|U^Te\|}\end{bmatrix} \in \mathcal{M}^{n-k+t+1}$ be orthogonal. Then

$$\bigcap_{i=1}^{2} \operatorname{face} \mathcal{K}^\dagger\left(\mathcal{E}^n(\alpha_i, \bar{D}_i)\right) = \left(U\mathcal{S}_+^{n-k+t+1}U^T\right) \cap \mathcal{S}_C = (UV)\mathcal{S}_+^{n-k+t}(UV)^T. \tag{5.5}$$

$\square$

5.1 Rigidity and Primal-Dual Approach

First, we summarize the definitions and characterizations of global and universal rigidity in terms of the matrix Ω and its co-rank.

We then present our algorithm of facial reduction for the Gram matrix as simultaneously building the conjugate face for the rigidity matrix.

5.2 Nonsingular Reduction with Intersection Embedding Dimension r

We need the following technical result on the intersection of two structured subspaces.

Lemma 5.6 ([19]). *Let*

$$U_1 := \begin{bmatrix} U_1' \\ U_1'' \end{bmatrix}, \quad U_2 := \begin{bmatrix} U_2'' \\ U_2' \end{bmatrix}, \quad \hat{U}_1 := \begin{bmatrix} U_1^{11} & 0 \\ U_1^{12} & 0 \\ 0 & I \end{bmatrix}, \quad \hat{U}_2 := \begin{bmatrix} I & 0 \\ 0 & U_2^{12} \\ 0 & U_2^{22} \end{bmatrix}$$

be appropriately blocked with $U_1^{12}, U_2^{12} \in \mathcal{M}^{k \times l}$ full column rank and $\mathcal{R}(U_1^{12}) = \mathcal{R}(U_2^{12})$. Furthermore, let

$$\bar{U}_1 := \begin{bmatrix} U_1' \\ U_1'' \\ U_2'(U_2'')^\dagger U_1'' \end{bmatrix}, \quad \bar{U}_2 := \begin{bmatrix} U_1'(U_1'')^\dagger U_2'' \\ U_2'' \\ U_2' \end{bmatrix}. \tag{5.6}$$

Then $\bar{U}_1$ and $\bar{U}_2$ are full column rank and satisfy

$$\mathcal{R}(\hat{U}_1) \cap \mathcal{R}(\hat{U}_2) = \mathcal{R}\left(\bar{U}_1\right) = \mathcal{R}\left(\bar{U}_2\right).$$

Moreover, if $e_l \in \mathbb{R}^l$ is the l^{th} standard unit vector, and $U_i e_l = \alpha_i e$, for some $\alpha_i \neq 0$, for $i = 1, 2$, then $\bar{U}_i e_l = \alpha_i e$, for $i = 1, 2$. □

The following key result shows that we can complete the distances in the union of two cliques provided that their intersection has embedding dimension equal to r.

Theorem 5.7 ([19]). *Let the hypotheses of Theorem 5.5 hold. Let*

$$\beta \subseteq \alpha_1 \cap \alpha_2, \quad \bar{D} := D[\beta], \quad B := \mathcal{K}^\dagger(\bar{D}), \quad \bar{U}_\beta := \bar{U}[\beta, :],$$

where $\bar{U} \in \mathcal{M}^{k \times (t+1)}$ satisfies equation (5.4). Let $\begin{bmatrix} \bar{V} & \frac{\bar{U}^T e}{\|\bar{U}^T e\|} \end{bmatrix} \in \mathcal{M}^{t+1}$ be orthogonal. Let

$$Z := (J\bar{U}_\beta \bar{V})^\dagger B ((J\bar{U}_\beta \bar{V})^\dagger)^T. \tag{5.7}$$

If the embedding dimension for $\bar{D}$ is r, then $t = r$, $Z \in \mathcal{S}_{++}^r$ is the unique solution of the equation

$$(J\bar{U}_\beta \bar{V}) Z (J\bar{U}_\beta \bar{V})^T = B, \tag{5.8}$$

and

$$D[\alpha_1 \cup \alpha_2] = \mathcal{K}\left((\bar{U}\bar{V}) Z (\bar{U}\bar{V})^T\right). \tag{5.9}$$

□

The following result shows that if we know the minimal face of $\mathcal{S}_+^n$ containing $\mathcal{K}^\dagger(D)$, and we know a small submatrix of D, then we can compute a set of points in $\mathbb{R}^r$ that generate D by solving a small equation.

Corollary 5.8 ([19]). *Let $D \in \mathcal{E}^n$ with embedding dimension r, and let $\beta \subseteq 1{:}n$. Let $U \in \mathcal{M}^{n \times (r+1)}$ satisfy*

$$\operatorname{face} \mathcal{K}^\dagger(D) = \left(U \mathcal{S}_+^{r+1} U^T\right) \cap \mathcal{S}_C,$$

let $U_\beta := U[\beta, :]$, and let $\begin{bmatrix} V & \frac{U^T e}{\|U^T e\|} \end{bmatrix} \in \mathcal{M}^{r+1}$ be orthogonal. If $D[\beta]$ has embedding dimension r, then

$$(JU_\beta V) Z (JU_\beta V)^T = \mathcal{K}^\dagger(D[\beta])$$

has a unique solution $Z \in \mathcal{S}_{++}^r$, and $D = \mathcal{K}(PP^T)$, where $P := UVZ^{1/2} \in \mathbb{R}^{n \times r}$. □

We now show that we can combine two cliques using the relative point representations of each.

Theorem 5.9. *Let the hypotheses of Theorem 5.5 hold, and following Corollary 5.4, for* $i = 1, 2$*, let* $B_i = P_i P_i^T$ *be full column rank factorizations, so that the rows of* P_i *provide relative positions for the points in the cliques* α_i*; and partition*

$$P_1 := \begin{bmatrix} P_1' \\ P_1'' \end{bmatrix}, \quad P_2 := \begin{bmatrix} P_2'' \\ P_2' \end{bmatrix}, \quad \hat{P}_1 := \begin{bmatrix} P_1^{11} & 0 \\ P_1^{12} & 0 \\ 0 & I \end{bmatrix}, \quad \hat{P}_2 := \begin{bmatrix} I & 0 \\ 0 & P_2^{12} \\ 0 & P_2^{22} \end{bmatrix}.$$

Furthermore, let

$$\bar{P}_1 := \begin{bmatrix} P_1' \\ P_1'' \\ P_2'(P_2'')^\dagger P_1'' \end{bmatrix}, \quad \bar{P}_2 := \begin{bmatrix} P_1'(P_1'')^\dagger P_2'' \\ P_2'' \\ P_2' \end{bmatrix}. \tag{5.10}$$

If the embedding dimension of $\bar{D}$ *is* r*, then:* $t = r$*;* $Q_1 := (P_1'')^\dagger P_2''$ *and* $Q_2 := (P_2'')^\dagger P_1''$ *are both orthogonal;* $\bar{P}_1$ *and* $\bar{P}_2$ *are full column rank and their rows provide relative representations for the points in the union of the cliques* $\alpha_i, i = 1, 2$*, i.e.*

$$D[\alpha_1 \cup \alpha_2] = \mathcal{K}(\bar{P}_i \bar{P}_i^T), \quad i = 1, 2. \tag{5.11}$$

Proof. From Lemma 5.6, we have that $\mathcal{R}(\bar{P}_1) = \mathcal{R}(\bar{P}_2)$. Therefore, $\mathcal{R}(P_1'') = \mathcal{R}(P_2'')$. This means that we can apply the projections on these ranges and get that

$$P_2''(P_2'')^\dagger P_1'' = P_1''; \quad P_1''(P_1'')^\dagger P_2'' = P_2''.$$

Therefore, $\bar{P}_1$ is obtained using $Q_1 = (P_1'')^\dagger P_2''$ and the multiplication $P_1 Q_1$. Similarly, $\bar{P}_2$ is obtained using $Q_2 = (P_2'')^\dagger P_1''$ and the multiplication $P_2 Q_2$.

Since

$$P_i e = 0, \quad \bar{D} = \mathcal{K}(P_i''(P_i'')^T), \qquad i = 1, 2,$$

We get that both $Q_i, i = 1, 2$ are orthogonal. □

Remark 5.10. *Note that there can be many ways to find the full column rank factorizations* $B_i = P_i P_i^T$ *in Theorem 5.9, e.g.: the compact spectral decomposition; the partial Cholesky factorization; or the compact QR factorization.*

5.3 Degenerate Case I

We now show that we can combine three cliques using the relative point representations of each. ?????? but the intersections are degenerate ????? We first note the effect of a permutation of the points P on the Gram matrix $B = PP^T$ and the EDM $D = \mathcal{K}(B)$, i.e., let Π be an $n \times n$ permutation matrix. Then ΠP denotes a permutation of the order of the points, nodes. We see:

$$\Pi B \Pi^T = (\Pi P)(\Pi P)^T, \quad \mathcal{K}(\Pi B \Pi^T) = \operatorname{diag}(\Pi B \Pi^T)e^T + e \operatorname{diag}(\Pi B \Pi^T)^T - 2\Pi B \Pi^T = \Pi D \Pi^T. \tag{5.12}$$

The following result provides expressions for the face for the union of three cliques.

Theorem 5.11. *Let $D \in \mathcal{E}^n$ with embedding dimension r and define the sets of positive integers*

$$
\begin{array}{l}
\alpha = \alpha_1 \cup \alpha_2 \cup \alpha_3 = \alpha_{11} \cup \alpha_{12} \cup \alpha_{22} \cup \alpha_{23} \cup \alpha_{33} \cup \alpha_{13} = 1:n, \\
\alpha_1 = \alpha_{11} \cup \alpha_{12} \cup \alpha_{13}, \alpha_2 = \alpha_{12} \cup \alpha_{22} \cup \alpha_{23} = k_{11}+1 : k_{23}, \alpha_3 = \alpha_{23} \cup \alpha_{33} \cup \alpha_{13} = k_{22}+1 : k_{13}, \\
\alpha_{11} = 1{:}k_{11}, \quad \alpha_{12} = (k_{11}+1){:}k_{12}, \quad \alpha_{22} = (k_{12}+1){:}k_{22}, \\
\qquad \alpha_{23} = (k_{22}+1){:}k_{23}, \quad \alpha_{33} = (k_{23}+1){:}k_{33}, \quad \alpha_{13} = (k_{33}+1){:}k_{13}, \\
1 < k_{11} < k_{12} < k_{22} < k_{23} < k_{33} < k_{13} = n.
\end{array}
\tag{5.13}
$$

Let

$$
P = P[\alpha] = P[\{1, \ldots, k_{11}, \ldots, k_{12}, \ldots, k_{22}, \ldots, k_{23}, \ldots, k_{33}, \ldots, k_{13}\}] \in \mathcal{M}^{n \times r}
$$

denote the matrix with corresponding n points. For $i = 1, 2, 3$, let $\bar{D}_i := D[\alpha_i] \in \mathcal{E}^{|\alpha_i|}$ with embedding dimension t_i, and $B_i := \mathcal{K}^\dagger(\bar{D}_i) = \bar{U}_i S_i \bar{U}_i^T$, where $\bar{U}_i \in \mathcal{M}^{|\alpha_i| \times t_i}$, $\bar{U}_i^T \bar{U}_i = I_{t_i}$, $S_i \in \mathcal{S}^{t_i}_{++}$, and $U_i := \begin{bmatrix} \bar{U}_i & \frac{1}{\sqrt{|\alpha_i|}} e \end{bmatrix} \in \mathcal{M}^{|\alpha_i| \times (t_i+1)}$. Let $\Pi_i, i = 1, 2, 3$ denote the permutations that return the original ordering in P:

$$
\begin{array}{l}
P = \Pi_1 P[\{1 : k_{12}, (k_{33}+1) : k_{13}, (k_{12}+1) : k_{33}\}], \\
P = \Pi_2 P[\{(k_{11}+1) : k_{23}, 1 : k_{11}, (k_{23}+1) : k_{1,3}\}], \\
P = \Pi_3 P[\{(k_{22}+1) : k_{13}, 1 : k_{22}\}].
\end{array}
$$

Let t and $\bar{U} \in \mathcal{M}^{n \times (t+1)}$ satisfy $\bar{U}^T \bar{U} = I_{t+1}$ and

$$
\begin{array}{rcl}
\mathcal{R}(\bar{U}) & = & \mathcal{R}\left(\Pi_1 \begin{bmatrix} U_1 & 0 \\ 0 & I_{n-|\alpha_1|} \end{bmatrix}\right) \cap \mathcal{R}\left(\begin{bmatrix} I_{|\alpha_{11}|} & 0 & 0 \\ 0 & U_2 & 0 \\ 0 & 0 & I_{|\alpha_{33} \cup \alpha_{13}|} \end{bmatrix}\right) \cap \mathcal{R}\left(\begin{bmatrix} I_{n-|\alpha_3|} & 0 \\ 0 & U_3 \end{bmatrix}\right) \\
& = & \cap_{i=1}^3 \mathcal{R}\left(\Pi_i \begin{bmatrix} U_i & 0 \\ 0 & I_{n-|\alpha_i|} \end{bmatrix}\right)
\end{array}
\tag{5.14}
$$

????still have to fix up n here to get proper subset of points?????also ???k????t???? Let $U := \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{n-k} \end{bmatrix} \in \mathcal{M}^{n \times (n-k+t+1)}$ and $\begin{bmatrix} V & \frac{U^T e}{\|U^T e\|} \end{bmatrix} \in \mathcal{M}^{n-k+t+1}$ be orthogonal. Then

$$
\bigcap_{i=1}^{3} \operatorname{face} \mathcal{K}^\dagger\left(\mathcal{E}^n(\alpha_i, \bar{D}_i)\right) = \left(U \mathcal{S}_+^{n-k+t+1} U^T\right) \cap \mathcal{S}_C = (UV) \mathcal{S}_+^{n-k+t} (UV)^T. \tag{5.15}
$$

□

Remark 5.12. *Let the hypotheses of Theorem 5.11 hold, and following Corollary 5.4, for $i = 1, 2, 3$, let $B_i = P_i P_i^T$ be full column rank factorizations, so that the rows of P_i provide relative positions for the points in the cliques α_i; and partition*

$$
P_1 := \begin{bmatrix} P_1^{11} \\ P_1^{12} \\ P_1^{13} \end{bmatrix}, \quad P_2 := \begin{bmatrix} P_2^{12} \\ P_2^{22} \\ P_2^{23} \end{bmatrix}, \quad P_3 := \begin{bmatrix} P_3^{23} \\ P_3^{33} \\ P_3^{13} \end{bmatrix},
$$

so that the matrices P_i are $k_i \times r$ with $k_i > 2r, \forall i$ and the pairs of points

$$
\left(P_1^{12}, P_2^{12}\right), \left(P_2^{23}, P_3^{23}\right), \left(P_1^{13}, P_3^{13}\right), \tag{5.16}
$$

coincide with the intersections of the cliques $(\alpha_1\cap\alpha_2),(\alpha_2\cap\alpha_3),(\alpha_1\cap\alpha_3)$, *respectively. And, these matrices in* (5.16) *are all nonsingular. We have* $P_i^Te=0,\forall i$. *Let*

$$U_i=\begin{bmatrix}P_i & e\end{bmatrix},\hat U_i=\begin{bmatrix}U_i & 0\\ 0 & I_{n-|\alpha_i|}\end{bmatrix},V_i=\begin{bmatrix}e^T\\ -I\end{bmatrix},\quad \forall i.$$

Then

$$\mathcal{R}\left(\hat U_i\right)=\mathcal{R}\left(\begin{bmatrix}P_i & 0 & \left(1-\frac{n}{|\alpha_i|}\right)e & e\\ 0 & V_i & e & e\end{bmatrix}\right)=\mathcal{R}\left(\begin{bmatrix}P_i & 0 & \left(1-\frac{n}{|\alpha_i|}\right)e & e\\ 0 & e^T & 1 & 1\\ 0 & -I_{n-|\alpha_i|-1} & e & e\end{bmatrix}\right). \tag{5.17}$$

Moreover, the last column e *of* $\hat V_i=\begin{bmatrix}P_i & 0 & \left(1-\frac{n}{|\alpha_i|}\right)e & e\\ 0 & e^T & 1 & 1\\ 0 & -I_{n-|\alpha_i|-1} & e & e\end{bmatrix}$ *is orthogonal to the other columns in* $\hat V_i$. *Therefore, we can ignore the column of ones and we need only find the intersection of the ranges of the three matrices, respectively,* $\Pi_i\hat V_i, i=1,2,3$; *each has six blocks of rows:*

$$\begin{bmatrix}P_1^{11} & 0 & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\\ \boxed{P_1^{12}} & 0 & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & \begin{bmatrix}e^T\\ -I\end{bmatrix} & \begin{bmatrix}e^T\\ 0\end{bmatrix} & \begin{bmatrix}e^T\\ 0\end{bmatrix} & e\\ 0 & 0 & -I & 0 & e\\ 0 & 0 & 0 & -I & e\\ \boxed{\boxed{\boxed{P_1^{13}}}} & 0 & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\end{bmatrix},\quad \begin{bmatrix}\begin{bmatrix}e^T\\ -I\end{bmatrix} & 0 & \begin{bmatrix}e^T\\ 0\end{bmatrix} & \begin{bmatrix}e^T\\ 0\end{bmatrix} & e\\ 0 & \boxed{P_2^{12}} & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & P_2^{22} & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & \boxed{\boxed{P_2^{23}}} & 0 & 0 & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & 0 & -I & 0 & e\\ 0 & 0 & 0 & -I & e\end{bmatrix},$$
$$\begin{bmatrix}\begin{bmatrix}e^T\\ -I\end{bmatrix} & \begin{bmatrix}e^T\\ 0\end{bmatrix} & \begin{bmatrix}e^T\\ 0\end{bmatrix} & 0 & e\\ 0 & -I & 0 & 0 & e\\ 0 & 0 & -I & 0 & e\\ 0 & 0 & 0 & \boxed{\boxed{P_3^{23}}} & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & 0 & 0 & P_3^{33} & \left(1-\frac{n}{|\alpha_1|}\right)e\\ 0 & 0 & 0 & \boxed{\boxed{\boxed{P_3^{13}}}} & \left(1-\frac{n}{|\alpha_1|}\right)e\end{bmatrix}. \tag{5.18}$$

We have put boxes around the blocks that overlap/coincide. We immediately get the three homogeneous (block) equations

$$\begin{bmatrix}P_1^{12} & -P_2^{12} & & \delta_1 e & -\delta_2 e & \\ & P_2^{23} & -P_3^{23} & & \delta_2 e & -\delta_3 e\\ P_1^{13} & & -P_3^{13} & \delta_1 e & & -\delta_3 e\end{bmatrix}\begin{pmatrix}x_1^1\\ x_2^2\\ x_3^4\\ x_1^5\\ x_2^5\\ x_3^5\end{pmatrix}=0.$$

We now use block Gaussian elimination on this system. We assume that we order the cliques appropriately to choose the blocks with the best condition numbers first as the pivot blocks.

$$\begin{bmatrix} I & -(P_1^{12})^{-1}P_2^{12} & & \delta_1(P_1^{12})^{-1}e & -\delta_2(P_1^{12})^{-1}e & & \\ & P_2^{23} & -P_3^{23} & & \delta_2 e & -\delta_3 e & \\ & P_1^{13}(P_1^{12})^{-1}P_2^{12} & -P_3^{13} & \delta_1 e - P_1^{13}\delta_1(P_1^{12})^{-1}e & \delta_2 P_1^{13}(P_1^{12})^{-1}e & & -\delta_3 e \end{bmatrix}$$

$$\begin{bmatrix} I & & -(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-1}P_3^{23} & \delta_1(P_1^{12})^{-1}e & -\delta_2(P_1^{12})^{-1}e + \delta_2(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-1}e & -\delta_3(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-} \\ & I & -(P_2^{23})^{-1}P_3^{23} & & \delta_2(P_2^{23})^{-1}e & -\delta_3(P_2^{23})^{-1}e \\ & & \boxed{P_1^{13}(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-1}P_3^{23} - P_3^{13}} & \delta_1 e - P_1^{13}\delta_1(P_1^{12})^{-1}e & \delta_2 P_1^{13}(P_1^{12})^{-1}e - \delta_2 P_1^{13}(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-1}e & \end{bmatrix}$$

Then the union of the three cliques is rigid if and only if

$$\boxed{P_1^{13}(P_1^{12})^{-1}P_2^{12}(P_2^{23})^{-1}P_3^{23} - P_3^{13}} \quad \textit{is nonsingular}$$

(proof is that: it is iff the dimension of the nullspace is 3????)

Furthermore, let

$$\bar{P}_1 := \begin{bmatrix} P_1' \\ P_1'' \\ P_2'(P_2'')^\dagger P_1'' \end{bmatrix}, \quad \bar{P}_2 := \begin{bmatrix} P_1'(P_1'')^\dagger P_2'' \\ P_2'' \\ P_2' \end{bmatrix}. \tag{5.19}$$

If the embedding dimension of $\bar{D}$ is r, then: $t = r$; $Q_1 := (P_1'')^\dagger P_2''$ and $Q_2 := (P_2'')^\dagger P_1''$ are both orthogonal; $\bar{P}_1$ and $\bar{P}_2$ are full column rank and their rows provide relative representations for the points in the union of the cliques $\alpha_i, i = 1, 2$, i.e.

$$D[\alpha_1 \cup \alpha_2] = \mathcal{K}(\bar{P}_i \bar{P}_i^T), \quad i = 1, 2. \tag{5.20}$$

Proof. ?????? not a proof ??? after a remark???? From Lemma 5.6, we have that $\mathcal{R}(\bar{P}_1) = \mathcal{R}(\bar{P}_2)$. Therefore, $\mathcal{R}(P_1'') = \mathcal{R}(P_2'')$. This means that we can apply the projections on these ranges and get that

$$P_2''(P_2'')^\dagger P_1'' = P_1''; \quad P_1''(P_1'')^\dagger P_2'' = P_2''.$$

Therefore, $\bar{P}_1$ is obtained using $Q_1 = (P_1'')^\dagger P_2''$ and the multiplication $P_1 Q_1$. Similarly, $\bar{P}_2$ is obtained using $Q_2 = (P_2'')^\dagger P_1''$ and the multiplication $P_2 Q_2$.

Since

$$P_i e = 0, \quad \bar{D} = \mathcal{K}(P_i''(P_i'')^T), \qquad i = 1, 2,$$

We get that both $Q_i, i = 1, 2$ are orthogonal. $\square$

5.4 Nearest EDM

Suppose that we have a clique α corresponding to the ***EDM*** $\bar{D}$. Then we can find the smallest face containing $\mathcal{E}^n(\alpha, \bar{D})$ using $B = \mathcal{K}^\dagger(\bar{D})$; see [19]. We now consider the case when we are given a possibly noisy ***EDM*** and we would like to find a best approximation, or the nearest ***EDM*** , i.e. we want to find a best approximation of $B = \mathcal{K}^\dagger(\bar{D})$ with the correct rank r. For this purpose, we let $D \in \mathcal{E}^n$ with embedding dimension r, and suppose that $D_\epsilon = D + N_\epsilon \in \mathcal{S}_H \cap \mathcal{N}$, where the off diagonal elements of the rows of the error matrix $N_\epsilon \in \mathcal{S}_H$ are independently and identically distributed with zero mean and the same variance. We now look for the best approximation to the given noisy distance matrix $D_\epsilon (= \bar{D})$. For example, we could do this in two steps: we first find the least squares solution $B_\epsilon = \mathcal{K}^\dagger(D_\epsilon)$, which may not be positive semidefinite and may have the wrong rank; we then use the truncated spectral decomposition $B_\epsilon = \mathcal{K}^\dagger(D_\epsilon) \approx U_\epsilon \Sigma_\epsilon U_\epsilon^T$, where $U_\epsilon^T U_\epsilon = I_r$, $\Sigma_\epsilon \in \mathcal{S}_{++}^r$. We could then use the approximation $\mathcal{K}(U_\epsilon \Sigma_\epsilon U_\epsilon^T) \approx D_\epsilon$, i.e.

$$D_\epsilon \approx \mathcal{K}(U_\epsilon \Sigma_\epsilon U_\epsilon^T), \qquad \text{where } B_\epsilon = \mathcal{K}^\dagger(D_\epsilon) \approx U_\epsilon \Sigma_\epsilon U_\epsilon^T,\ U_\epsilon^T U_\epsilon = I_r, \text{ and } \Sigma_\epsilon \in \mathcal{S}_{++}^r. \tag{5.21}$$

Alternatively, we could solve the ***SDP***

$$\begin{array}{rl} \min & \|\mathcal{K}(X) - D_\epsilon\| \\ \text{s.t.} & \operatorname{rank}(X) = r \\ & Xe = 0 \\ & X \succeq 0. \end{array} \tag{5.22}$$

We could introduce V as in Corollary 3.6, eliminate the constraints. We get the following.

Problem 5.4.1. *The unconstrained nearest **EDM** problem with embedding dimension r is*

$$\begin{array}{rcll} U_r^* & \in & \operatorname{argmin} & \frac{1}{2}\left\|\mathcal{K}_V(UU^T) - D_\epsilon\right\|_F^2 \\ & & s.t. & U \in M^{(n-1)r}. \end{array} \tag{5.23}$$

*The nearest **EDM** is $D^* = \mathcal{K}_V(U_r^*(U_r^*)^T)$.*

5.5 Clique Reductions Algorithm

In [19], we presented an algorithm for exact ***SNL*** given exact data. We now outline this algorithm and extend to include new cases. The algorithm in [19] considered/handled four different cases:

1. Rigid clique intersection:

2. Non-rigid clique intersection:

3. Rigid node absorption:

4. Non-rigid node absorption:

Each of these cases made use of the essential fact that we knew the embedding dimension is r and that the operation resulted in a unique face of dimension r from the intersection of two faces. This resulted in a very successful algorithm. However, the algorithm could fail when the graph is very sparse. This is due to the fact that the intersection process did not result in a unique face of proper dimension.

In the case that we end up with more than one clique after applying the above four techniques, we now extend it to allow the intersection of faces to have dimension $> r$. For example, the singular intersections with the application of lower bounds may not yield a unique solution, so we let the solution be in a higher dimension. This still reduces the dimension of the current face of the problem.

6 Localization using Dimensionality Reduction

The approach for the nearest $\boldsymbol{EDM}$ in Section 5.4 concentrated on finding the best approximation of the Gram matrix X with the correct rank r, e.g., (5.22). This involves solving a nonlinear nearest matrix optimization problem. We could delay the restriction to the best rank, and obtain X with higher rank, i.e., we could delay fixing the rank r till the end. (????done in section ???? with facial reductions also reducing rank???)

We now study an alternate approach that finds the localization for cliques and then postpones further localizations in order to find all the locations, all of P, in one step. This uses dimensionality reductions with a linear projection.

Lemma 6.1. *Let α be a clique corresponding to the possibly noisy $\boldsymbol{EDM}$ $\bar{D} = D[\alpha]$ with $|\alpha| = k$. Let $B \cong \mathcal{K}^\dagger(\bar{D})$ with $B = YY^T \succeq 0$ an approximate Gram matrix for this clique, where*

$$Y = U \begin{bmatrix} \Sigma_{r_Y} \\ 0 \end{bmatrix} V^T = U_1 \Sigma_{r_Y} V^T \in \mathbb{R}^{k \times r_Y}$$

is full column rank with its SVD, and $U = \begin{bmatrix} U_1 U_2 \end{bmatrix}$ is partitioned appropriately. Then, an optimal least squares approximation for the linear dimensionality reducing transformation is

$$L_\alpha^* = Y^\dagger JP[\alpha, :] \in \operatorname{argmin} \|JP[\alpha, :] - YL_\alpha\|. \tag{6.1}$$

And, the best $P_\alpha := P[\alpha, :] \in C$ is found explicitly from the data Y using

$$\min_{P_\alpha \in C} \|(I - YY^\dagger)JP_\alpha\|.$$

In addition, the projection $I - YY^\dagger = I - U_1 U_1^T$; and, if $Y^T e = 0$ (centered), then $(I - YY^\dagger)J = J - U_1 U_1^T$.

Proof. The proof is immediate, since this is the Frobenius norm. For completeness, we use the SVD of Y and see that

$$\begin{array}{rcl}
\min_{L_\alpha} \|JP[\alpha, :] - YL_\alpha\|_F^2 & = & \min\limits_{L_\alpha} \|JP[\alpha, :] - U \begin{bmatrix} \Sigma_{r_Y} \\ 0 \end{bmatrix} (V^T L_\alpha)\|_F^2 \\
& = & \min\limits_{L_\alpha} \|U^T JP[\alpha, :] - \begin{bmatrix} \Sigma_{r_Y} \\ 0 \end{bmatrix} (V^T L_\alpha)\|_F^2 \\
& = & \min\limits_{L_\alpha} \| \begin{bmatrix} \Sigma_{r_Y}^{-1} & 0 \end{bmatrix} U^T JP[\alpha, :] - (V^T L_\alpha)\|_F^2 \\
& = & \min\limits_{L_\alpha} \|V \begin{bmatrix} \Sigma_{r_Y}^{-1} & 0 \end{bmatrix} U^T JP[\alpha, :] - L_\alpha\|_F^2.
\end{array}$$

The final expression is found by substituting for L_α in (6.1). □

6.1 Global Localization

The above Lemma 6.1 allows one to find the explicit expression for the dimension reduction linear transformation $\mathcal{L}_\alpha$ implicitly in terms of the unknown points $P[\alpha, :]$. Therefore, if $\mathcal{A}$ is a set of cliques, then we can find the set of points in the union of all the rows of $P[\alpha, :], \alpha \in \mathcal{A}$ all at once.

$$\min_{P_\alpha \in C_\alpha, \alpha \in \mathcal{A}} \sum_{\alpha \in \mathcal{A}} \|(J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T) P_\alpha\|^2.$$

The objective function is convex and *partially separable*, see e.g., [15, 16, 8, 7, 6, 26]. Therefore, these special techniques can be used to exploit the sparsity if one can properly choose the constraint sets C_α. However, by using simple choices for C_α, we now present two methods of obtaining *explicit* optimal solutions.

Now let $S_\alpha \in \{0,1\}^{|\alpha|\times n}$ be the *selection matrix* that chooses the appropriate rows of P so that

$$P_\alpha = S_\alpha P.$$

Therefore, with $Q_\alpha := R_\alpha S_\alpha := \left(J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T\right) S_\alpha$, we get

$$Q_\alpha^T Q_\alpha = S_\alpha^T (R_\alpha^T R_\alpha) S_\alpha = S_\alpha^T (J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T) S_\alpha,$$

and

$$\begin{array}{rcl} \sum_{\alpha\in\mathcal{A}} \|(J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T) P_\alpha\|^2 & = & \sum_{\alpha\in\mathcal{A}} \|(J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T) S_\alpha P\|^2 \\ & = & \sum_{\alpha\in\mathcal{A}} \|Q_\alpha P\|^2 \\ & = & \operatorname{trace} \sum_{\alpha\in\mathcal{A}} P^T Q_\alpha^T Q_\alpha P \\ & = & \langle P, \sum_{\alpha\in\mathcal{A}} Q_\alpha^T Q_\alpha P \rangle. \end{array}$$

This is a quadratic form in P. The corresponding positive semidefinite matrix is

$$Q := \sum_{\alpha\in\mathcal{A}} Q_\alpha^T Q_\alpha \quad = \quad \begin{bmatrix} S_{\alpha_1} \\ S_{\alpha_2} \\ \dots \\ S_{\alpha_k} \end{bmatrix}^T \begin{bmatrix} R_{\alpha_1} & 0 & 0 & \dots & 0 \\ 0 & R_{\alpha_2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \\ \dots & \dots & \dots & \dots & \\ 0 & \dots & 0 & \dots & R_{\alpha_k} \end{bmatrix} \begin{bmatrix} S_{\alpha_1} \\ S_{\alpha_2} \\ \dots \\ S_{\alpha_k} \end{bmatrix}. \tag{6.2}$$

6.1.1 Orthogonality Constrained Localization

An optimal solution of points P can be assumed centered $Pe = 0$. Since $Qe = 0$ (e is an eigenvector with eigenvalue 0), without further normalization, we get $P = 0$ as the trivial optimal solution. First, for normalization, we add an orthogonality constraint on P.

Theorem 6.2. *The solution for the points P of the localization problem for all the cliques at once using the program*

$$\min_{P^T P = I, Pe = 0} \sum_{\alpha\in\mathcal{A}} \|(J_\alpha - (U_\alpha)_1 (U_\alpha)_1^T) S_\alpha P\|^2 \tag{6.3}$$

is found by forming the full rank factorization

$$PP^T = B = \sum_{i=1}^{r} \lambda_i v_i v_i^T$$

using the r smallest <u>*positive*</u> *eigenvalues and corresponding orthonormal eigenvectors $\lambda_i, v_i, i = 1, \dots, r$ of the matrix of the quadratic form Q given in* (6.2)*.*

Proof. We eliminate the smallest eigenvalue as it is zero and choose the next r smallest. The result follows immediately from applying a theorem of Fan [14] (also [22, Ch 9.B]) to the quadratic form in the objective function in (6.3). □

6.1.2 Trace Constrained Localization

The orthogonal normalization $P^TP = I_r$ in (6.3) appears to be quite arbitrary. Without any normalization, the optimal solution is $P = 0$. The normalization constraint forces the optimal solution to have $\operatorname{rank} P = 3$.

An alternative P can be found by solving using a weaker normalization from a trace constraint, yielding a homogeneous trust region subproblem. Rather than the $t(r) := r(r+1)/2$ constraint of the normalization, the trace constraint is a single constraint and so we can expect an optimal solution of $\operatorname{rank} P = 1$????. with better optimal value????

Theorem 6.3. *The solution for the points P of the localization problem for all the cliques at once using the program*

$$\min_{\operatorname{trace} P^TP=1, Pe=0} \sum_{\alpha\in\mathcal{A}} \|(J_\alpha - (U_\alpha)_1(U_\alpha)_1^T)S_\alpha P\|^2 \tag{6.4}$$

is found using the Rayleigh quotient to be

??????

using the smallest <u>*positive*</u> *eigenvalue and corresponding normalized eigenvector v of the matrix of the quadratic form Q given in* (6.2). *??????? i.e. all possible combinations of the eigenvectors of the Kronecker product:* $\operatorname{Mat}(e_i \otimes v)$*, where v is the eigenvector corresponding to the smallest eigenvalue other than* 0 *of*

Proof. The constraint $Pe = 0$ forces the solution to be orthogonal to the 0 eigenvalue. As in Theorem 6.2, the objective function is a quadratic form with the matrix Q, i.e., we can use the Kronecker product and the vectorization of P (by columns) and get the equivalent objective function

$$\min_{\operatorname{trace} P^TP=1} \operatorname{trace} P^TQP = \min_{\|\operatorname{vec} P\|=1} (\operatorname{vec} P)^T(I_r \otimes Q)(\operatorname{vec} P).$$

Let $Q = UDU^T$ be the spectral decomposition. The Lagrangian is $\operatorname{trace} P^TQP - \lambda(P^TP - 1)$ with stationarity condition

$$0 = QP - \lambda P = UD(U^TP) - \lambda P,$$

or $D(U^TP) - \lambda(U^TP) = 0$. We choose the smallest eigenvalue and corresponding eigenvector of Q (equivalently of D). ???? does Q have multiple smallest eigenvalue corresponding to smallest clique????? ☐

7 Generating/Testing Instances

The ***SNL*** is closely related to the molecular distance geometry problem; see, for example, [13, 12, 11, 3]. In particular, the *Extended Geometric Build-up Algorithm, (EGBA)* is presented in [13]. This algorithm, for $r = 3$ starts with a clique made up of 4 atoms, and then builds up the size of the clique by adding one atom at a time. They include a discussion on how to avoid the build up of round-off error. See [20] for information on generating instances for the molecular distance geometry problem.

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