Facial reduction for Euclidean distance matrix problems

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Outline

1. Euclidean Distance Matrices
2. Facial Reduction
3. Facial Reduction for EDM Completion
4. Noisy EDM Completion

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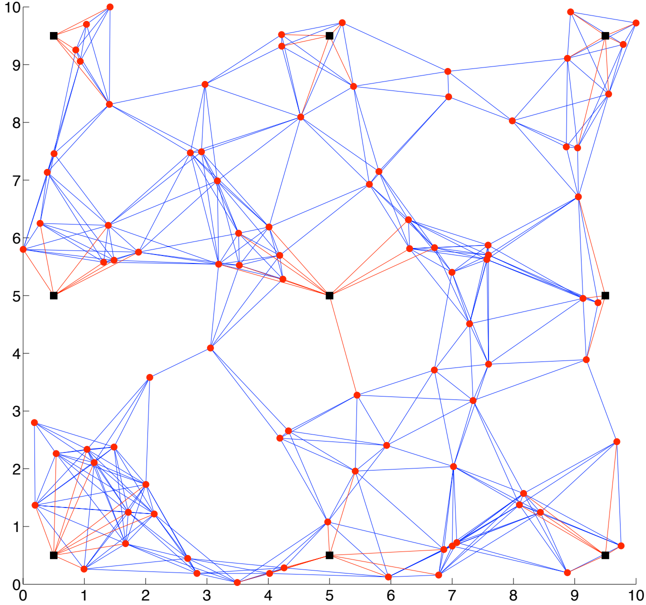
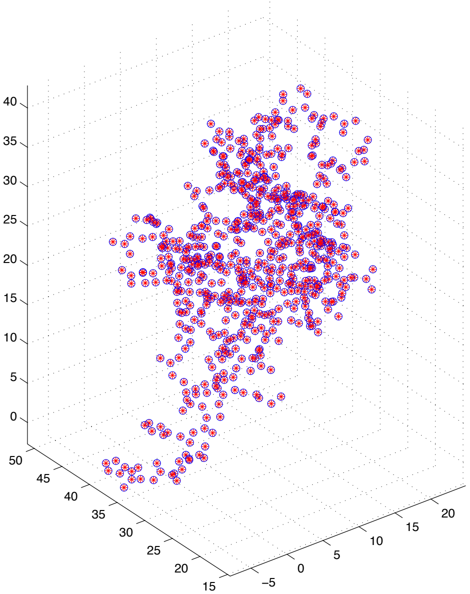
Sensor Network Localization



Protein Structure Determination



Euclidean Distance Matrices

Euclidean distance matrices (EDMs)

- An $n \times n$ matrix D is an EDM if

$$\exists p_1, \ldots, p_n \in \mathbb{R}^k : D_{ij} = \|p_i - p_j\|_2^2 \tag{1}$$

- The embedding dimension of D:

$$\dim(D) = \min\{k : (1) \text{ holds}\}$$

- $\mathcal{E}^n =$ the set of all $n \times n$ EDMs

EDM completion

$$\begin{array}{ll} \text{find} & D \in \mathcal{E}^n \\ \text{such that} & D_{ij} = \bar{D}_{ij}, \quad \forall ij \in E \\ & \dim(D) \leq k \end{array}$$

Euclidean Distance Matrices

EDMs and semidefinite matrices

- Let $p_1, \ldots, p_n \in \mathbb{R}^k$ and D be their EDM
- Let $Y \in \mathcal{S}^n$ be the Gram matrix:

$$Y_{ij} = \langle p_i, p_j \rangle, \quad \forall ij$$

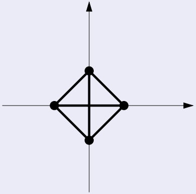
- Then Y is a semidefinite matrix: $Y \in \mathcal{S}^n_+$

$$\begin{aligned} D_{ij} &= \|p_i - p_j\|_2^2 \\ &= \langle p_i, p_i \rangle - 2\langle p_i, p_j \rangle + \langle p_j, p_j \rangle \\ &= Y_{ii} - 2Y_{ij} + Y_{jj} \\ &=: \mathcal{K}(Y)_{ij} \end{aligned}$$

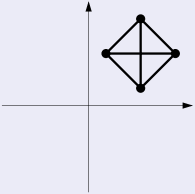
- Therefore: $\mathcal{K}(\mathcal{S}^n_+) = \mathcal{E}^n$

Euclidean Distance Matrices

Translation invariant: $D = D'$ but $Y \neq Y'$



$D = \mathcal{K}(Y)$



$D' = \mathcal{K}(Y')$

Centered matrices: $\mathcal{S}_c^n := \{Y \in \mathcal{S}^n : Ye = 0\}$, $e = \begin{bmatrix} 1 & \cdots & 1 \end{bmatrix}^T$

- $\mathcal{K}\colon \mathcal{S}_+^n \cap \mathcal{S}_c^n \to \mathcal{E}^n$ is a linear bijection whose inverse is given by

$$\mathcal{K}^\dagger(D) = -\frac{1}{2} J \operatorname{offDiag}(D) J, \quad J = I - \frac{1}{n} ee^T$$

- If $D \in \mathcal{E}^n$, then $\dim(D) = \operatorname{rank}(\mathcal{K}^\dagger(D))$

Euclidean Distance Matrices

EDM completion

$$\begin{array}{ll} \text{find} & Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_c \\ \text{such that} & \mathcal{K}(Y)_{ij} = \bar{D}_{ij}, \quad \forall ij \in E \\ & \operatorname{rank}(Y) \leq k \end{array}$$

- non-convex and NP-hard

Semidefinite relaxation

$$\begin{array}{ll} \text{find} & Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_c \\ \text{such that} & \mathcal{K}(Y)_{ij} = \bar{D}_{ij}, \quad \forall ij \in E \end{array}$$

- convex and solvable in polynomial-time by an interior-point method
- only problems of small size can be solved efficiently
- highly degenerate: not strictly feasible
- facial reduction $\Rightarrow$ a much smaller equivalent problem

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Facial Reduction

Face of a convex cone K

- We say a convex cone $F \subseteq K$ is a face of K (denoted $F \trianglelefteq K$) if

$$x, y \in F \quad \text{whenever} \quad x, y \in K \ \text{ and } \ \frac{1}{2}(x+y) \in F$$

- The minimal face of K containing $S \subseteq K$ is

$$\operatorname{face}(S) := \bigcap_{S \subseteq F \trianglelefteq K} F$$

- We say that $F \trianglelefteq K$ is exposed if there exists ϕ such that

$$F = K \cap \{\phi\}^\perp$$

Facial Reduction

A simple example

$$\begin{array}{lccccccccc} \text{minimize} & 2x_1 & + & 6x_2 & - & x_3 & - & 2x_4 & & \\ \text{subject to} & x_1 & + & x_2 & + & x_3 & + & x_4 & = & 1 \\ & x_1 & - & x_2 & - & x_3 & & & = & -1 \\ & x_1 & , & x_2 & , & x_3 & , & x_4 & \geq & 0 \end{array}$$

- Summing the constraints:

$$2x_1 + x_4 = 0 \quad \Rightarrow \quad x_1 = x_4 = 0$$

Restrict problem to the face $\left\{x \in \mathbb{R}^4_+ : x_1 = x_4 = 0\right\}$

$$\begin{array}{lccccc} \text{minimize} & 6x_2 & - & x_3 & & \\ \text{subject to} & x_2 & + & x_3 & = & 1 \\ & x_2 & , & x_3 & \geq & 0 \end{array}$$

Facial Reduction

Linear programming

$$\text{(LP)} \qquad \boxed{\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax = b \\ & x \in \mathbb{R}^n_+ \end{array}}$$

Certificate of non-strict feasibility

- Suppose $\exists y \in \mathbb{R}^m$ such that $0 \neq A^T y \geq 0$ and $b^T y = 0$
- If $Ax = b$ and $x \geq 0$, then

$$\begin{aligned} y^T A x = y^T b \quad &\implies \quad (A^T y)^T x = 0 \\ &\implies \quad x_i = 0, \quad \forall i \in \operatorname{supp}(A^T y) \end{aligned}$$

- Therefore, the feasible set of (LP) is contained in the face

$$\mathbb{R}^n_+ \cap \{A^T y\}^\perp = \left\{ x \in \mathbb{R}^n_+ : x_i = 0, \forall i \in \operatorname{supp}(A^T y) \right\}$$

Facial Reduction

Semidefinite programming

$$\text{(SDP)} \qquad \boxed{\begin{array}{ll} \text{minimize} & \langle C, X\rangle \\ \text{subject to} & \mathcal{A}X = b \\ & X \in \mathcal{S}^n_+ \end{array}}$$

Certificate of non-strict feasibility

- Suppose $\exists y \in \mathbb{R}^m$ such that $0 \neq \mathcal{A}^* y \succeq 0$ and $b^T y = 0$
- If $\mathcal{A}X = b$ and $X \succeq 0$, then

$$\begin{aligned} y^T \mathcal{A}X = y^T b \quad &\implies \quad \langle \mathcal{A}^* y, X\rangle = 0 \\ &\implies \quad X(\mathcal{A}^* y) = (\mathcal{A}^* y)X = 0 \end{aligned}$$

- Therefore, the feasible set of (SDP) is contained in the face

$$\mathcal{S}^n_+ \cap \{\mathcal{A}^* y\}^\perp = \left\{X \in \mathcal{S}^n_+ : \text{range}(X) \subseteq \text{null}(A^* y)\right\}$$

Facial Reduction

Faces of the semidefinite cone

Let $Q = \begin{bmatrix} U & V \end{bmatrix} \in \mathbb{R}^{n \times n}$ be orthogonal and

$$F := \left\{ X \in \mathcal{S}^n_+ : \text{range}(X) \subseteq \text{range}(U) \right\} \trianglelefteq \mathcal{S}^n_+.$$

Then

$$F = U \mathcal{S}^k_+ U^T.$$

Semidefinite facial reduction [Borwein & Wolkowicz (1981)]

$$\left\{ X \in \mathcal{S}^n_+ : \langle A_i, X \rangle = b_i, \forall i \right\} \subseteq U \mathcal{S}^k_+ U^T$$

Then substituting $X = UZU^T$, (SDP) is equivalent to:

$$\begin{array}{ll} \text{minimize} & \langle C, UZU^T \rangle \\ \text{subject to} & \langle A_i, UZU^T \rangle = b_i, \quad \forall i \\ & Z \in \mathcal{S}^k_+ \end{array}$$

Facial Reduction

Faces of the semidefinite cone

Let $Q = \begin{bmatrix} U & V \end{bmatrix} \in \mathbb{R}^{n \times n}$ be orthogonal and

$$F := \left\{ X \in \mathcal{S}^n_+ : \operatorname{range}(X) \subseteq \operatorname{range}(U) \right\} \trianglelefteq \mathcal{S}^n_+.$$

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Semidefinite facial reduction [Borwein & Wolkowicz (1981)]

$$\left\{ X \in \mathcal{S}^n_+ : \langle A_i, X \rangle = b_i, \forall i \right\} \subseteq U \mathcal{S}^k_+ U^T$$

Then substituting $X = UZU^T$, (SDP) is equivalent to:

$$\boxed{\begin{array}{ll} \text{minimize} & \langle U^T C U, Z \rangle \\ \text{subject to} & \langle U^T A_i U, Z \rangle = b_i, \quad \forall i \\ & Z \in \mathcal{S}^k_+ \end{array}}$$

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Facial Reduction for EDM Completion

Theorem: Facial reduction for EDM [K. & Wolkowicz (2010)]

Let $D \in \mathcal{E}^p$ with $\dim(D) = k$,

$$\mathcal{F} := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_c : \mathcal{K}(Y)_{ij} = D_{ij}, \forall i, j = 1, \ldots, p \right\},$$

the columns of $\bar{U} \in \mathbb{R}^{p \times (k+1)}$ form a basis for $\operatorname{range}\left(\begin{bmatrix} \mathcal{K}^\dagger(D) & e \end{bmatrix}\right)$, and

$$U := \begin{bmatrix} \bar{U} & 0 \\ 0 & I_{n-p} \end{bmatrix}.$$

Then

$$\operatorname{face}(\mathcal{F}) = \left(U \mathcal{S}^{n-p+k+1}_+ U^T \right) \cap \mathcal{S}^n_c.$$

Facial Reduction for EDM Completion

Theorem: Constraint reduction [K. & Wolkowicz (2010)]

- Let $D \in \mathcal{E}^p$ with $\dim(D) = k$,

$$\mathcal{F} := \left\{ Y \in \mathcal{S}_+^n \cap \mathcal{S}_c^n : \mathcal{K}(Y)_{ij} = D_{ij}, \forall i,j = 1,\ldots,p \right\},$$

  and U be defined as in the previous theorem.
- Let $\beta \subseteq \{1,\ldots,p\}$ such that $\dim(D[\beta,\beta]) = k$.
- Then

$$\mathcal{F} = \left\{ Y \in \left(U\mathcal{S}_+^{n-p+k+1} U^T \right) \cap \mathcal{S}_c^n : \mathcal{K}(Y)_{ij} = D_{ij}, \forall i,j \in \beta \right\}.$$

Example : $n = 1000$, $p = 100$, $|\beta| = 3$

variables : $1000 \rightsquigarrow 903$, constraints : $4950 \rightsquigarrow 3$

Facial Reduction for EDM Completion

Algorithm for computing the face

$$\mathcal{F} := \left\{ Y \in \mathcal{S}_+^n \cap \mathcal{S}_c^n : \mathcal{K}(Y)_{ij} = D_{ij}, \forall ij \in E \right\}$$

- Find some cliques α_i in the graph
- Let $F_i := \left(U_i \mathcal{S}_+^{n-|\alpha_i|+t_i+1} U_i^T \right) \cap \mathcal{S}_c^n$ be the corresponding faces
- Compute $U \in \mathbb{R}^{n \times (t+1)}$ full column rank such that

$$\text{range}(U) = \bigcap_i \text{range}(U_i)$$

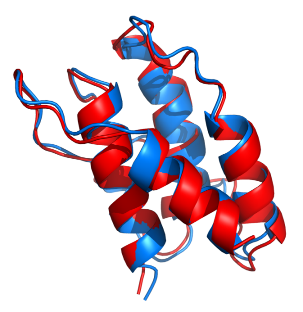
- Then:

$$\mathcal{F} \subseteq \left(U \mathcal{S}_+^{t+1} U^T \right) \cap \mathcal{S}_c^n$$

Facial Reduction for EDM Completion

Protein structure determination

- Protein 2L30 from the PDB
- 393 cliques: 269 2D + 124 3D
- SDP size: 1867 $\rightsquigarrow$ 512
- equality constraints: 7143 $\rightsquigarrow$ 1492



Babak Alipanahi, Nathan Krislock, Ali Ghodsi, Henry Wolkowicz, Logan Donaldson, and Ming Li. (2012)
Determining protein structures from NOESY distance constraints by semidefinite programming. *Journal of Computational Biology*.

Facial Reduction for EDM Completion

Theorem: EDM completion [K. & Wolkowicz (2010)]

Let D be a partial EDM and

- $\mathcal{F} := \left\{ Y \in \mathcal{S}_+^n \cap \mathcal{S}_c^n : \mathcal{K}(Y)_{ij} = D_{ij}, \forall ij \in E \right\}$
- $\mathcal{F} \subseteq \left(U\mathcal{S}_+^{t+1} U^T \right) \cap \mathcal{S}_c^n = (UV)\mathcal{S}_+^t (UV)^T$

If $\exists \bar{Y} \in \mathcal{F}$ and β is a clique with $\dim(D[\beta, \beta]) = t$, then:

- $\bar{Y} = (UV)\bar{Z}(UV)^T$, where $\bar{Z}$ is the unique solution of

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

- $\bar{D} := \mathcal{K}(\bar{P}\bar{P}^T) \in \mathcal{E}^n$ is the unique completion of D, where

$$\bar{P} := UV\bar{Z}^{1/2} \in \mathbb{R}^{n \times t}$$

Note: In this case, an SDP solver is not required.

Facial Reduction for EDM Completion

Face representation approach

n	R	Time	RMSD (%R)
10000	0.06	8 s	2e-10
20000	0.03	17 s	7e-10
60000	0.015	1 m 53 s	5e-9
100000	0.011	5 m 46 s	8e-7

Point representation approach

n	R	Time	RMSD (%R)
10000	0.06	6 s	1e-12
20000	0.03	14 s	3e-12
60000	0.015	1 m 27 s	6e-12
100000	0.011	3 m 55 s	9e-12

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Noisy EDM Completion

Multiplicative noise model

$$d_{ij} = \|p_i - p_j\|_2(1 + \sigma\varepsilon_{ij}), \quad \text{for all } ij \in E$$

- ε_{ij} is normally distributed with mean 0 and standard deviation 1
- $\sigma \geq 0$ is the *noise factor*
- $D_{ij} = d_{ij}^2$

Point representation approach (no refinement used)

n	σ	R	Time	RMSD (%R)
10000	1e-6	0.04	5 s	0.002
10000	1e-4	0.04	5 s	0.25
10000	1e-2	0.04	5 s	500

Noisy EDM Completion

Exposing vector representation of faces

- Recall we had faces in primal form:

$$F_i = \left(U_i \mathcal{S}_+^{n-|\alpha_i|+t_i+1} U_i^T \right) \cap \mathcal{S}_c^n$$

- The exposing vector Φ_i for the face F_i gives a dual representation:

$$F_i = \mathcal{S}_+^n \cap \{\Phi_i\}^\perp$$

- The intersection of the faces can be easily computed by

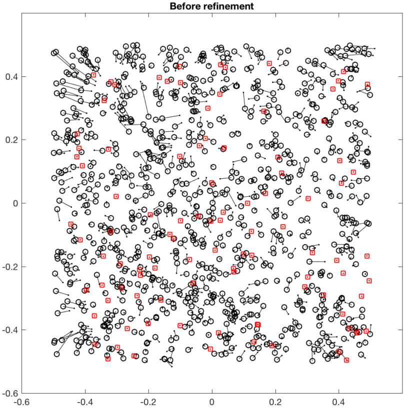
$$F := \bigcap_i F_i = \mathcal{S}_+^n \cap \left\{ \sum_i \Phi_i \right\}^\perp$$

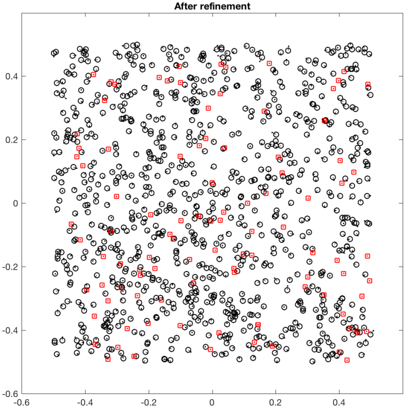
Noisy EDM Completion

Exposing Vector Algorithm

- For each clique α
  - $Y_\alpha :=$ nearest pos. semidef. rank-r matrix to $\mathcal{K}^\dagger(D[\alpha,\alpha])$
  - $\Phi_\alpha :=$ exposing vector of face$(\{Y_\alpha\})$ extended to $\mathcal{S}^n$ by adding zeros
- $\Phi :=$ nearest pos. semidef. rank-$(n-r-1)$ matrix to $\sum_\alpha \Phi_\alpha$
- Let $U \in \mathbb{R}^{n\times r}$, such that $U^T e = 0$, be eigenvectors of Φ for the smallest r eigenvalues
- Solve $\min \left\{ \sum_{ij\in E} |\mathcal{K}(UZU^T)_{ij} - D_{ij}|^2 : Z \in \mathcal{S}^r_+ \right\}$
- Return $P = UZ^{1/2}$

Noisy EDM Completion





Noisy EDM Completion

Exposing Vector Algorithm + Refinement (10% anchors)

Specifications			Time		RMSD (%R)	
n	σ	R	initial	refine	initial	refine
2000	0.0	0.20	1 s	0.1 s	0.0	0.0
2000	0.1	0.20	1 s	2 s	3.9	1.0
2000	0.2	0.20	1 s	2 s	8.1	2.0
2000	0.3	0.20	1 s	2 s	12.5	3.0
4000	0.0	0.16	4 s	0.3 s	0.0	0.0
4000	0.1	0.16	4 s	6 s	3.6	0.9
4000	0.2	0.16	4 s	6 s	7.3	1.7
4000	0.3	0.16	4 s	6 s	11.2	2.6
10000	0.05	0.10	12 s	14 s	1.8	0.4
15000	0.05	0.10	29 s	20 s	1.6	0.3
20000	0.05	0.10	54 s	44 s	1.5	0.3

Summary

- EDM problems are highly degenerate due to non-strict-feasibility
- Facial reduction is a powerful technique for taking advantage of this degeneracy
- The exposing vector approach is a very effective approach for noisy EDM problems