Euclidean Distance Matrices + SDP

$D \in S^n$ is an EDM if $\exists p_1, \dots, p_n \in \mathbb{R}^d$ s.t.

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

The smallest such d is called the embedding dimension of D, denoted $\mathrm{embdim}(D)$.

Let $Y \in S^n$ s.t. $Y_{ij} = p_i^T p_j$, $\forall ij$. (Gram matrix)

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

$\therefore$ $\mathcal{K} : S^n \to S^n$ is linear and satisfies

$$\underbrace{\mathcal{K}(S_+^n)}_{\text{p.s.d. cone}} = \underbrace{\mathcal{E}^n}_{\text{EDM cone}},$$

but not one-to-one, since translating the points gives the same EDM, but a different Gram matrix.

$\therefore$ we centre the points at the origin:

$$\sum_{i=1}^n p_i = 0 \quad (\text{equivalently, } Ye = 0).$$

Then
$$\mathcal{K}(S_+^n \cap S_c^n) = \mathcal{E}^n \quad \text{and} \quad \mathcal{K}^\dagger(\mathcal{E}^n) = S_+^n \cap S_c^n,$$

where $S_c^n := \{Y \in S^n : Ye = 0\}$.

Moreover,

$$\operatorname{embdim}(D) = \operatorname{rank}(\mathcal{K}^{\dagger}(D)), \quad \forall D \in \mathcal{E}^n.$$

EDM completion

Suppose D_{ij} only known for $ij \in E$.

The minimum rank EDM completion problem is:

$$\begin{array}{ll} \min & \operatorname{embdim}(\bar{D}) \\ \text{s.t.} & \bar{D}_{ij} = D_{ij}, \ \forall ij \in E \\ & \bar{D} \in \mathcal{E}^n \end{array} \equiv \begin{array}{ll} \min & \operatorname{rank}(Y) \\ \text{s.t.} & \mathcal{K}(Y)_{ij} = D_{ij}, \ \forall ij \in E \\ & Y \in S_+^n \cap S_c^n. \end{array}$$

Applications

① Molecular conformation from NMR

$$\left[\begin{array}{ll} \text{find} & Y \in S_+^n \cap S_c^n \\ \text{s.t.} & \mathcal{K}(Y)_{ij} = D_{ij}, \ \forall ij \in E \\ & \cancel{\operatorname{rank}(Y) = 3} \end{array}\right]$$

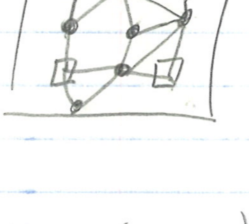
$$\left[\begin{array}{ll} \text{find} & p_1, \ldots, p_n \in \mathbb{R}^3 \\ \text{s.t.} & \|p_i - p_j\|^2 = D_{ij}, \ \forall ij \in E \end{array}\right]$$

Determine the atom positions from the partial distance information

② Sensor network localization

$$\left[\begin{array}{ll} \text{find} & X \in \mathbb{R}^{n \times 2} \\ \text{s.t.} & \mathcal{K}\left(\begin{bmatrix} X \\ A \end{bmatrix}\begin{bmatrix} X \\ A \end{bmatrix}^T\right)_{ij} = D_{ij}, \\ & \forall ij \in E \end{array}\right]$$

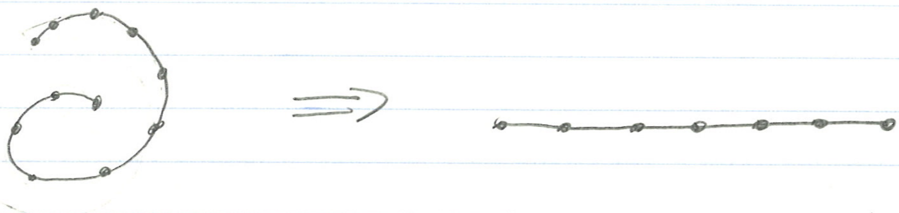
$$\left[\begin{array}{ll} \text{find} & x_1, \ldots, x_n \in \mathbb{R}^2 \\ \text{s.t.} & \|x_i - x_j\|^2 = D_{ij}, \ \forall ij \in E_x \\ & \|x_i - a_j\|^2 = D_{ij}, \ \forall ij \in E_a \end{array}\right]$$



$$\left[\begin{array}{ll} \text{find} & Y \in S_+^{n+m} \\ \text{s.t.} & \mathcal{K}(Y)_{ij} = D_{ij}, \ \forall ij \in E \\ & Y_{22} = AA^T \\ & \cancel{\operatorname{rank}(Y) = 2} \end{array}\right]$$

$a_1, \ldots, a_m \in \mathbb{R}^2$ are <u>anchors</u> (positions known)

③ Nonlinear dimensionality reduction
a.k.a. nonlinear PCA
a.k.a. manifold unfolding



$x_1, \dots, x_n \in \mathbb{R}^D$. $p_1, \dots, p_n \in \mathbb{R}^d$

Maximum Variance Unfolding (MVU):

$$\left[\begin{array}{ll} \max & \operatorname{trace}(Y) \\ \text{s.t.} & K(Y)_{ij} = D_{ij}, \ \forall ij \in E \\ & Y \in S^n_+ \cap S^n_c \end{array}\right]$$

<u>Note:</u> $Y_{ij} = p_i^T p_j \Rightarrow \operatorname{trace}(Y) = \sum_{i=1}^n \|p_i\|^2$.

<u>Semidefinite Facial Reduction</u>

Let $F := \{ Y \in S^n_+ \cap S^n_c : K(Y)_{ij} = D_{ij}, \ \forall ij \in E \}$.

If $F \subseteq U S^k_+ U^T \leftarrow$ a <u>face</u> of S^n_+
then we get a smaller equivalent problem using the substitution

$$Y = U Z U^T, \quad Z \in S^k_+ .$$

Noisy distances

If $d_{ij} = \|p_i - p_j\|(1+\sigma\varepsilon_{ij})$ $\forall ij \in E$ [Mult. noise model]

where ε_{ij} is random with normal distribution ($\substack{\text{mean}=0 \\ \text{std. dev.}=1}$).

Then the maximum likelihood positions are the opt. sol'n of the nonlinear least-squares problem:

$$\boxed{\begin{aligned} \min \quad & \sum_{ij\in E} v_{ij}^2 \\ \text{s.t.} \quad & \|p_i - p_j\|^2 (1+v_{ij})^2 = d_{ij}^2, \ \forall ij \in E \\ & \sum_{i=1}^{n} p_i = 0 \\ & p_1, \ldots, p_n \in \mathbb{R}^d \end{aligned}}$$