What are EDMs?

pre-distance matrix (or dissimilarity matrix)

ia an $n \times n$ symmetric matrix $D = (d_{ij})$ with nonnegative elements and zero diagonal

Euclidean distance matrix (EDM)

is a pre-distance matrix such that there exists points $x^1, x^2, \ldots, x^n$ in $\mathbb{R}^r$ such that

$$d_{ij} = \|x^i - x^j\|^2, \quad i, j = 1, 2, \ldots, n.$$

The smallest value of r is called **the embedding dimension** of D. (r is always $\leq n - 1$)

EDM Completion

The Problem

Given a partial symmetric matrix A with certain elements specified, the Euclidean distance matrix completion problem (EDMCP) consists in finding the unspecified elements of A that make A a EDM.

WHY?

e.g.:

- shape of enzyme determines chemical function; Once shape known, then proper drug can be designed (molecular conformation).

- protein folding; multidimensional scaling; etc...

Approximate EDMCP

weighted, closest Euclidean distance matrix problem

let: A be a pre-distance matrix; H be an $n \times n$ symmetric matrix with nonnegative elements; the objective function

$$f(D) := \|H \circ (A - D)\|_F^2,$$

Then

$$(CDM_0) \quad \mu^* := \begin{array}{cc} \min & f(D) \\ \text{subject to} & D \in \mathcal{E}, \end{array}$$

where $\mathcal{E}$ denotes the cone of EDMs.

DISTANCE GEOMETRY

Characterization of EDM

A pre-distance matrix D is a EDM
if and only if
D is negative semidefinite on
$M_v := \left\{x \in \mathbb{R}^n : x^t v = 0\right\} = \{v\}^\perp$,
where we set $v = e$, the vector of all ones.

orthogonal projection onto M_v,

Define $V\ n \times (n-1)$, full column rank such that $V^t v = 0$. Then

$$J := VV^\dagger = I - \frac{vv^t}{\|v\|^2}$$

is the orthogonal projection onto M_v, where $V^\dagger$ denotes Moore-Penrose generalized inverse.

Linear Transformations/subspaces

centered and hollow subspaces

$$\begin{aligned} \mathcal{S}_C &:= \{B \in \mathcal{S}^n : Be = 0\}, \\ \mathcal{S}_H &:= \{D \in \mathcal{S}^n : \operatorname{diag}(D) = 0\}. \end{aligned}$$

two linear operators

$$\mathcal{K}(B) := \operatorname{diag}(B)\, e^t + e \operatorname{diag}(B)^t - 2B,$$

$$\mathcal{T}(D) := -\tfrac{1}{2} JDJ.$$

The operator $-2\mathcal{T}$ is an orthogonal projection onto $\mathcal{S}_C$.
THEOREM The linear operators satisfy
$\mathcal{K}(\mathcal{S}_C) = \mathcal{S}_H, \qquad \mathcal{T}(\mathcal{S}_H) = \mathcal{S}_C,$
and $\mathcal{K}_{|\mathcal{S}_C}$ and $\mathcal{T}_{|\mathcal{S}_H}$ are inverses of each other.

Characterization of EDMs

Using $\mathcal{T}$

A hollow matrix D is EDM if and only if
$B = \mathcal{T}(D) \succeq 0$ (positive semidefinite)

Using $\mathcal{K}$

D is EDM if and only if
$D = \mathcal{K}(B)$, for some B with $Be = 0$ and $B \succeq 0$.
THEN: embedding dimension r EQUALS rank B.
with $B = XX^t$, then coordinates of points $x^1, x^2, \ldots, x^n$ that generate D are given in rows of X
and $Be = 0$ implies origin coincides with centroid of points.

Loss of Slater CQ

Difficulty

The cone of EDMs, $\mathcal{E}_n$, has empty interior. And
$D \in \mathcal{E}_n \implies \mathcal{K}^\dagger(D)e = 0$

Project on Minimal Face

V full column rank $n-1$ with $V^T e = 0$

$$V \cdot V^t : \mathcal{S}_{n-1} \to \mathcal{S}_n \cap \mathcal{S}_C$$

Define the composite operators

$$\mathcal{K}_V(X) := \mathcal{K}(VXV^t),$$

$$\mathcal{T}_V(D) := V^\dagger \mathcal{T}(D)(V^\dagger)^t = -\tfrac{1}{2} V^\dagger D (V^\dagger)^t.$$

Properties of $\mathcal{K}_V, \mathcal{T}_V$

$$\mathcal{K}_V(\mathcal{S}^{n-1}) = \mathcal{S}_H,$$
$$\mathcal{T}_V(\mathcal{S}_H) = \mathcal{S}^{n-1},$$

and $\mathcal{K}_V$ and $\mathcal{T}_V$ are inverses of each other on these two spaces.

$$\begin{aligned} \mathcal{K}_V(\mathcal{S}_+^{n-1}) &= \mathcal{E}_n, \\ \mathcal{T}_V(\mathcal{E}_n) &= \mathcal{S}_+^{n-1}. \end{aligned}$$

Summary

objective function

$$f(X) := \|H \circ (A - \mathcal{K}_V(X))\|_F^2$$
$$= \|H \circ \mathcal{K}_V(B - X)\|_F^2,$$

where $B = \mathcal{T}_V(A)$.
($\mathcal{K}_V$ and $\mathcal{T}_V$ are both linear transformations)

(Re)Define the closest EDM problem

$$(CDM) \quad \begin{array}{rll} \mu^* := & \min & f(X) \\ & \text{subject to} & \mathcal{A}X = b \\ & & X \succeq 0. \end{array}$$