On Euclidean Distance Matrices and Spherical Configurations.

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Outline

- Survey of EDMs:
  - Characterizations.
  - Properties.
  - Classes of EDMs: Spherical and Nonspherical.
  - EDM Inverse Eigenvalue Problem.
- Spherical Configurations
  - Yielding and Nonyielding Entries.
  - Unit Spherical EDMs which differ in 1 entry.
  - Two-Distance Sets.

Definition

- An $n \times n$ matrix D is an EDM if there exist points $p^1, \ldots, p^n$ in some Euclidean space such that:

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- The dimension of the affine span of the generating points of an EDM D is called the embedding dimension of D.
- An EDM D is spherical if its generating points lie on a hypersphere. Otherwise, it is nonspherical.

Important Vectors in EDM Theory

- e the vector of all 1's in $\mathbb{R}^n$ and $V : V^T e = 0$ and $V^T V = I_{n-1}$.

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- w where $Dw = e$. Some times we set $w = D^\dagger e$.
- s where $e^T s = 1$. Vector s fixes the origin. Two important choices: $s = e/n$ and $s = 2w$.

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- $B = \mathcal{T}(D)$ is the Gram matrix of the generating points of D. Note that $Bs = 0$.
- Given B, generating points of D are given by the rows of P, where $B = PP^T$.

Proof

Define:

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- $\mathcal{T} : S_h^n \to S_s^n : \mathcal{T}(D) = -\frac{1}{2}(I - es^T)D(I - se^T)$
  $\mathcal{K} : S_s^n \to S_h^n : \mathcal{K}(B) = \text{diag}(B)e^T + e(\text{diag}(B))^T - 2B$.

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  $\mathcal{K} : S^n_s \to S^n_h : \mathcal{K}(B) = \operatorname{diag}(B)e^T + e(\operatorname{diag}(B))^T - 2B$.
- Theorem [Critchley '88]:

$$\mathcal{T}|_{S^n_h} = (\mathcal{K}|_{S^n_s})^{-1} \text{ and } \mathcal{K}|_{S^n_s} = (\mathcal{T}|_{S^n_h})^{-1}.$$

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- $d_{ij} = ||p^i - p^j||^2 = B_{ii} + B_{jj} - 2B_{ij}$, where $B = PP^T$. Thus $D = \mathcal{K}(B)$ and $D \in S_h^n$ is an EDM iff $B = \mathcal{T}(D) \succeq 0$.

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- $X = V^TBV$ is called the projected Gram matrix. Moreover, $X \succeq 0$ and of rank r iff $B \succeq 0$ and of rank r.
- Define [A. , Khandani and Wolkowicz '99]:
  $\mathcal{K}_V(X) = \mathcal{K}(VXV^T)$ and
  $\mathcal{T}_V(D) = V^T\mathcal{T}(D)V = -V^TDV/2$. Then the cone of EDMs of order n is the image of the PSD cone of order $n-1$ under $\mathcal{K}_V$.

Restatement of the Basic Characterization

- Theorem [AlHomidan and Fletcher '95, A. et al '99] Let D be a real symmetric matrix with zero diagonal. Then D is an EDM iff
$$X = \mathcal{T}_V(D) = -\frac{1}{2}V^T DV \succeq 0.$$
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Moreover, the embedding dimension of $D = \text{rank } X$.
- Let $U^T = [-e_{n-1} \; I_{n-1}]$. Then
Theorem [AlHomidan and Wolkowicz '05] Let
$D = \begin{bmatrix} 0 & d^T \\ d & \bar{D} \end{bmatrix}$ be an $n \times n$ real symmetric matrix with zero diagonal. Then D is an EDM iff
$$ed^T + de^T - \bar{D} \succeq 0.$$
- This is equivalent to setting $s = e^1$, i.e., $p^1 = 0$.

Characterization of $0 - 1$ EDMs

- Theorem [A. '18] Let A be the adjacency matrix of a simple graph G. Then A is an EDM if and only if G is a complete multipartite graph.

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  Salter condition may not hold.
- [A. , Khandani and Wolkowicz '99]

$$\begin{array}{ll} \min & \|H \circ \mathcal{K}_V(\mathcal{T}_V(A) - X)\|_F^2 \\ \text{subject to} & X \succeq 0. \end{array}$$

Other Characterizations

- Theorem [Crouzeix and Ferland '82] Let D be a real symmetric matrix with zero diagonal. Assume that D has exactly one positive eigenvalue. Then D is an EDM iff there exists $w \in \mathbb{R}^n$ such that $Dw = e$ and $e^T w \geq 0$.

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- Whether $e^T w = 0$ or $e^T w > 0$ has geometrical significance as will be seen later.

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- Theorem [Hayden and Wells '88, Fiedler '94] Let D be a real sym matrix with zero diagonal. Then D is an EDM iff its Cayley-Menger matrix M has exactly one positive eigenvalue, in which case, rank $M = r + 2$, where r is the embedding dimension of D.

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- Theorem [A.'19] Let M be the Cayley-Menger matrix of an EDM D. Then:
  D is spherical of radius $\rho \leq 1$ iff M is an EDM.
  D is spherical of radius $\rho = 1$ iff M is a nonspherical EDM.

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- Let V denote the volume of the simplex defined by $p^1, \ldots, p^n$. Then

$$\begin{aligned} V^2 &= \frac{(-1)^n}{2^{n-1}((n-1)!)^2} \det \begin{bmatrix} 0 & e^T \\ e & D \end{bmatrix}. \\ &= \frac{n}{((n-1)!)^2} \det\left(X = \mathcal{T}_V(D)\right). \end{aligned}$$

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- Let ${z^i}^T$ denote the ith row of Z. z^i is Gale Transform of p^i.

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- $\text{rank}(D) = r + 1$ or $r + 2$ independent of n.

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- $\exists$ scalar β: $\beta ee^T - D \succeq 0$ [Neumaier '81, Tarazaga et al '96]
  Moreover, $\beta_{\min} = 2\rho^2$.

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- $e^T w > 0$, where $Dw = e$. $\rho^2 = 1/(2e^T w)$. [Gower '82 '85].
- $\exists a$: $Pa = J\text{diag}(B)/2$ where $B = -JDJ/2$. a is center of sphere and $\rho^2 = a^T a + e^T De/(2n^2)$ [Tarazaga et al '96].

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- The EDM cone is the closure of the set of spherical EDMs.
- The interior of the EDM cone is made up of spherical EDMs, while its boundary is made up of both spherical and nonspherical EDMs.

Examples of Spherical EDMs: 1- Regular EDMs

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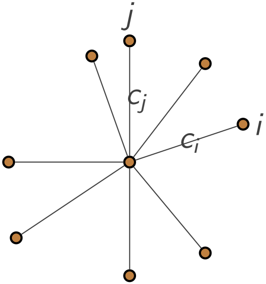
- Theorem [A. '18] Let D be an $n \times n$ EDM and let $\lambda > -\alpha_1 > \cdots > -\alpha_k$ be the distinct eigenvalues of D. Then $\exists$ polynomial $f(D)$: $f(D) = ee^T$ iff D is regular, in which case

$$f(D) = n \frac{\prod_{i=1}^{k}(D + \alpha_i I)}{\prod_{i=1}^{k}(e^T De/n + \alpha_i)}.$$

$f(D)$ is called the Hoffman polynomial of D.

2- Cell Matrices



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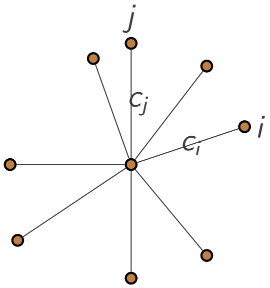

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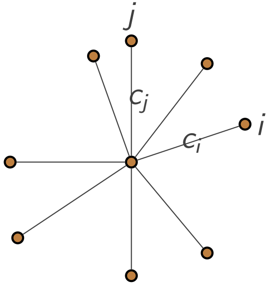

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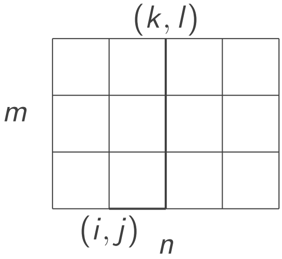
- Theorem [Jaklic and Modic '10] Cell matrices are spherical EDMs.
- Let s denote the number of 0 entries of $c \in \mathbb{R}^n$, $c \geq 0$. Then the embedding dimension of D is

$$r = \begin{cases} n-1 & \text{if } s = 0 \text{ or } s = 1, \\ n-s & \text{otherwise.} \end{cases}$$

3-Manhattan Distance Matrices on Grids

Consider a rectangular grid of unit squares with m row and n columns. Let $d_{ij,kl} = |i - k| + |j - l|$.



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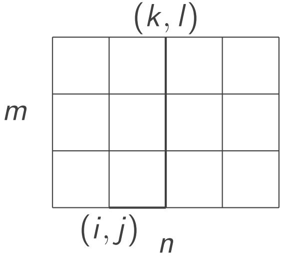

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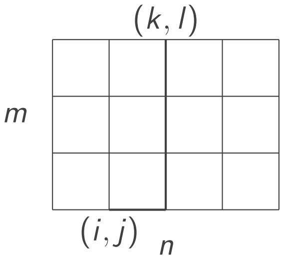

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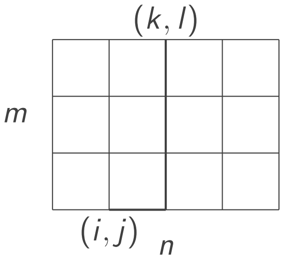

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- Theorem [A.] D is a spherical EDM with $\rho^2 = (n + m - 2)/4$.
- QAP library (Nugent): [Mettlemann and Peng '10] $\frac{1}{2}(n + m - 2)ee^T - D \succeq 0$.

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- The vertices p^i's of the Hypercube Q_r are all points in $\mathbb{R}^r$ whose entries are 0 or 1.
- Let $d_{ij} = \sum_{k=1}^{r} |p_k^i - p_k^j|$.
- D is a regular EDM of embedding dimension r and of radius $\rho = \sqrt{r}/2$.

4-Hamming Distance Matrices on the Cube

- The vertices p^i's of the Hypercube Q_r are all points in $\mathbb{R}^r$ whose entries are 0 or 1.
- Let $d_{ij} = \sum_{k=1}^{r} |p_k^i - p_k^j|$.
- D is a regular EDM of embedding dimension r and of radius $\rho = \sqrt{r}/2$.
- Theorem [Graham and Winkler '85] Let $p^1, \ldots, p^{r+1}$ of Q_r form a simplex. Then the det of the submatrix of D induced by these points is:

$$(-1)^r r 2^{r-1}.$$

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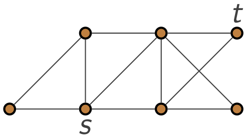
Consider a graph G where each edge is a unit resistor.



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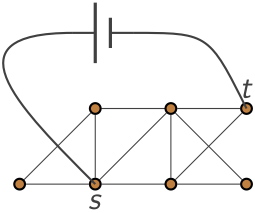

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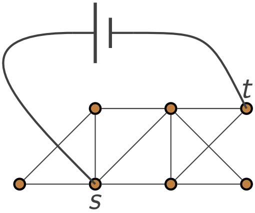

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- Let L denote the Laplacian of G. Then

$$\Omega = \mathcal{K}(L^\dagger) = \text{diag}(L^\dagger)e^T + e(\text{diag}(L^\dagger))^T - 2L^\dagger.$$

Ω is a spherical EDM since embedding dim $= n - 1$.

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- rank$(D)= r+2$. [Gower '85].
- $e^T w = 0$, where $Dw = e$. [Gower '82 '85].

EDM Inverse Eigenvalue Problem

- Given $\lambda_1 > 0 \geq \lambda_2 \geq \cdots \geq \lambda_n$, where $\sum_{i=1}^{n} \lambda_i = 0$. Does there exist an EDM whose eigenvalues are these λ_i's?

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- Theorem [Hayden et al '99] Given such λ_i's, let $\Lambda = \text{Diag}(\lambda_1, \ldots, \lambda_n)$. Then $D = H\Lambda H^T/n$ is a regular EDM, where $H = [e\ \bar{H}]$ is a Hadamard matrix.

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- It is an open conjecture that there exists H_n for all $n = 4k$. The smallest n in doubt is $n = 668$.

Yielding Entries of an EDM

- Let D be an EDM and let E^{kl} be the matrix with 1's in (k, l)th and (l, k)th positions and 0's elsewhere.
- Let $l_{kl} \leq 0$ and $u_{kl} \geq 0$ such that $D + tE^{kl}$ is EDM iff $l_{kl} \leq t \leq u_{kl}$.

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- D is in general position in $\mathbb{R}^r$ if every $r + 1$ of its generating points are affinely independent.
- Corollary [A. '18] Let D be an EDM of embedding dimension $r = n - 2$. If D is in general position, then every entry of D is yielding.

Determining Yielding Intervals

- Let $B = -JDJ/2 = PP^T$, then $B^\dagger = P(P^TP)^{-2}P^T$. Let $B^\dagger = SS^T$, i.e., $S = P(P^TP)^{-1}$. Let ${s^i}^T$ denote the ith row of S.

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$$\underline{\theta} = \frac{2}{(s^k)^T s^l - ||s^k||\ ||s^l||} \text{ and } \overline{\theta} = \frac{2}{(s^k)^T s^l + ||s^k||\ ||s^l||}.$$

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- Theorem [A. '19] Let D be an $n \times n$ EDM of embedding dimension r and let $B = -JDJ/2$. Assume that d_{kl} is yielding. If $r = n - 1$ or if $r \leq n - 2$ and $z^k = z^l = 0$. Then the yielding interval of d_{kl} is

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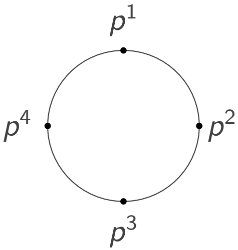
$$[l_{kl}, u_{kl}] = \begin{cases} [\theta_c, 0] & \text{if } c > 0, \\ [0, \theta_c] & \text{if } c < 0. \end{cases}$$

Example

$$D = \begin{bmatrix} 0 & 2 & 4 & 2 \\ 2 & 0 & 2 & 4 \\ 4 & 2 & 0 & 2 \\ 2 & 4 & 2 & 0 \end{bmatrix}$$



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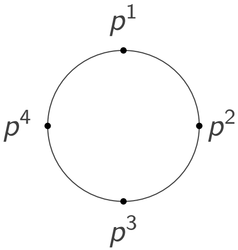

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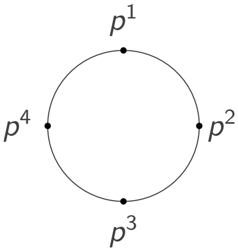

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Unit Spherical EDMs

Let D be a spherical EDM of $\rho = 1$. Define:
$T_{kl}^{\leq} = \{t \in [l_{kl}, u_{kl}] : D + tE^{kl}$ is a spherical EDM of $\rho \leq 1\}$.

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- Theorem [A. '19] Let D be a unit spherical EDM and let $\tilde{z}^i$ denote the ith row of $\tilde{Z}$. Then $T^{\leq}_{kl} = \{0\}$ iff $\tilde{z}^k$ is not parallel to $\tilde{z}^l$. i.e., $\nexists c \neq 0$: $w_k = cw_l$ and $z^k = cz^l$.

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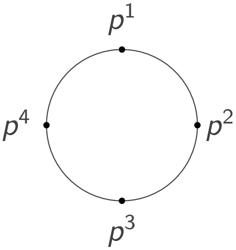

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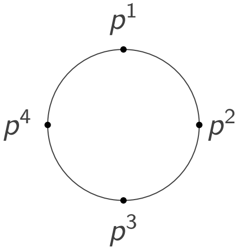

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- $\tilde{z}^1 = \tilde{z}^3 = \begin{bmatrix} 1/8 \\ 1 \end{bmatrix}$ and $\tilde{z}^2 = \begin{bmatrix} 1/8 \\ -1 \end{bmatrix}$.
- $T^{\leq}_{12} = \{0\}$ and $T^{\leq}_{13} = [l_{13}, u_{13}]$.

- If $\tilde{z}^k$ is parallel to $\tilde{z}^l$, then $T_{kl}^{\leq}$ may or may not be equal to $[l_{kl}, u_{kl}]$. Moreover, $T_{kl}^{\leq}$ can be expressed in terms of $\underline{\theta}$, $\overline{\theta}$ or θ_c and 0.

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- $T^{=}_{kl} = \{t \in T^{\leq}_{kl} : D + tE^{kl}$ is a spherical EDM of $\rho = 1\}$.
- Theorem [A. '19] Let D be a unit spherical EDM of embedding dimension r and assume that $\tilde{z}^k = c\tilde{z}^l$ for some $c \neq 0$.
  1. If $w_k = w_l = 0$, or $w_k \neq 0$ and $z^k \neq 0$, then $T^{=}_{kl} = T^{\leq}_{kl}$.
  2. Otherwise, if $w_k = cw_l \neq 0$ and either $r = n - 1$ or $z^k = z^l = 0$, then

$$T^{=}_{kl} = \begin{cases} \{0\} & \text{if } ||s^k||^2 = c^2||s^l||^2, \\ \{0, \theta_c\} & \text{otherwise.} \end{cases}$$

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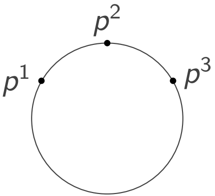

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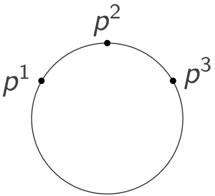

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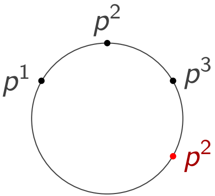

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- Question 2: Can two different graphs have the same β?
- Musin '18 proved that the answer to Question 1 is yes and the configuration is unique. However, his proof is not constructive.

- Let A and $\bar{A}$ denote, respectively, the adjacency matrices of G and its complement $\bar{G}$. Then
  Q1: Does there exist a unit spherical EDM D such that
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- Example: graphs $G_n = \overline{C_n}$ all have $\lambda_1(\bar{A}) = 2$. Hence, they have the same $\beta = 3$.

Proof:

- For a unit spherical EDM D, let $s = 2w$, then $e^T s = 1$. Let B denote the Gram matrix such that $Bw = 0$. Then $2B = 2ee^T - D$.

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- Now for $D = 2A + (2 + 2\delta)\bar{A}$, we have $B = I - \delta\bar{A}$. Hence, we need to find δ such that

$$I - \delta\bar{A} \succeq 0 \text{ and } Bw = w - \delta\bar{A}w = 0.$$

Proof:

- For a unit spherical EDM D, let $s = 2w$, then $e^T s = 1$. Let B denote the Gram matrix such that $Bw = 0$. Then $2B = 2ee^T - D$.
- Now for $D = 2A + (2 + 2\delta)\bar{A}$, we have $B = I - \delta\bar{A}$. Hence, we need to find δ such that

$$I - \delta\bar{A} \succeq 0 \text{ and } Bw = w - \delta\bar{A}w = 0.$$

- Hence,

$$\delta \leq \frac{1}{\lambda_1(\bar{A})} \text{ and } \delta \geq \frac{1}{\lambda_1(\bar{A})}.$$

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