Semidefinite Programming and Matrix Completions

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OUTLINE

1. Short intro. to SDP
2. SDP and positive definite matrix completions
3. Euclidean distance matrix (EDM) completions
4. New characterization for EDM;
   solving large sparse problems

(Advantages of using $X - \mu Z^{-1} = 0$ form of perturbed complementary slackness.)

SDP BACKGROUND and NOTATION

Semidefinite Programming
looks just like
Linear Programming

$$
\textbf{(PSDP)} \qquad \begin{array}{rlll} p^* = & \max & \operatorname{trace} CX & (\langle C, X\rangle) \\ & \text{s.t.} & \mathcal{A}X = b & (\text{linear}) \\ & & X \succeq 0, \quad (X \in \mathcal{P}) & (\text{nonneg}) \end{array}
$$

$\preceq$ denotes the Löwner partial order

$A \preceq B$ if $B - A \succeq 0$

$\mathcal{S}^n$ denotes $n \times n$ symmetric matrices

$$\mathcal{A} : \mathcal{S}^n \rightarrow \Re^m$$

$$(\mathcal{A}X)_i = \operatorname{trace}(A_i X), \text{ for given } A_i \in \mathcal{S}^n$$

$\mathcal{P}$ - cone of positive semidefinite matrices

replaces

$\Re^n_+$ - nonnegative orthant

---

adjoint operator, $\quad \mathcal{A}^* y = \sum_i y_i A_i$

$$\langle \mathcal{A}^* y, X \rangle = \langle y, \mathcal{A}X \rangle, \quad \forall X, y$$

payoff function, player Y to player X (Lagrangian)

$$L(X,y) := \operatorname{trace}(CX) + y^t(b - \mathcal{A}X)$$

$$p^* = \max_{X \succeq 0} \min_y L(X,y) \leq d^* := \min_y \max_{X \succeq 0} L(X,y)$$

dual obtained from optimal strategy of competing player Y;
use *hidden constraint* $C - \mathcal{A}^* y \preceq 0$

$$(\mathbf{DSDP}) \quad \begin{array}{rll} d^* = & \min & b^t y \\ & \text{s.t.} & \mathcal{A}^* y \succeq C \end{array}$$

for the primal

$$(\mathbf{PSDP}) \quad \begin{array}{rll} p^* = & \max & \operatorname{trace} CX \\ & \text{s.t.} & \mathcal{A}X = b \\ & & X \succeq 0 \end{array}$$

Characterization of optimality for the
dual pair X, y (slack $Z \succeq 0$)

$$\begin{aligned} \mathcal{A}^* y - Z &= C && \text{dual feasibility} \\ \mathcal{A} X &= b && \text{primal feasibility} \\ Z X &= 0 && \text{complementary slackness} \end{aligned}$$

$$ZX = \mu I \qquad \text{perturbed}$$

Forms the basis for:

interior point methods
(primal simplex method, dual simplex method)

Positive Definite Completions of Partial Hermitian Matrices

- $\mathcal{G}(V, E)$ finite undirected graph
- $A(\mathcal{G})$ is a $\mathcal{G}$-partial matrix (a_{ij} defined iff $\{i, j\} \in E$)
- $A(\mathcal{G})$ is a $\mathcal{G}$-partial positive matrix if $a_{ij} = \overline{a_{ji}}, \forall \{i, j\} \in E$ and all existing principal minors are positive.
- with $\mathcal{J} = (V, \bar{E}), E \subset \bar{E}$ a $\mathcal{J}$-partial matrix $B(\mathcal{J})$ extends the $\mathcal{G}$-partial matrix $A(\mathcal{G})$ if $b_{ij} = a_{ij}, \forall \{i, j\} \in E$
- $\mathcal{G}$ is positive completable if every $\mathcal{G}$-partial positive matrix can be extended to a positive definite matrix.

$\mathcal{G}$ is **chordal** if there are no minimal cycles of length ≥ 4. (every cycle of length ≥ 4 has a chord)

THEOREM (Grone, Johnson, Sa, Wolkowicz)
$\mathcal{G}$ is positive completable iff $\mathcal{G}$ is chordal. ∎

equivalently - strict feasibility for SDP:

$$\begin{aligned} \operatorname{trace} E_{ij} P &= a_{ij}, \quad \forall \{i,j\} \in E \\ P &\succ 0 \end{aligned}$$

where $E_{ij} = e_i e_j^t + e_j e_k^t$

Approximate Positive Semidefinite Completions

(with Charlie Johnson
and Brenda Kroschel)

given:

$H = H^t \geq 0$ a real, nonnegative (elementwise) **symmetric matrix of weights**, with positive diagonal elements $H_{ii} > 0, \ \forall i$;
and $A = A^*$ the **given partial Hermitian matrix**
(i.e. some elements approximately fixed; others free; for notational purposes, assume free elements set to 0 if not specified.)

$||A||_F = \sqrt{\operatorname{trace} A^* A}$ *Frobenius norm*, $\circ$ denotes *Hadamard product.*

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

weighted, best approximate, completion problem

$$(AC) \qquad \begin{array}{rcc} \mu^* := & \min & f(P) \\ & \text{subject to} & KP = b \\ & & P \succeq 0, \end{array}$$

where $K : \mathcal{H}^n \to \mathcal{C}^m$ linear operator

Lagrangian:

$$L(P, y, \Lambda) = f(P) + \langle y, b - KP \rangle - \operatorname{trace} \Lambda P$$

Dual problem:

$$(DAC) \quad \begin{array}{ll} \max & f(P) + \langle y, b - KP \rangle - \operatorname{trace} \Lambda P \\ \text{subject to} & \nabla f(P) - K^* y - \Lambda = 0 \\ & \Lambda \succeq 0. \end{array}$$

THEOREM The matrix $\bar{P} \succeq 0$ and vector-matrix $\bar{y}, \bar{\Lambda} \succeq 0$ solve AC and DAC if and only if

$$\begin{array}{rc} K\bar{P} = b & \text{primal feas.} \\ 2H^{(2)} \circ (\bar{P} - A) - K^* \bar{y} - \bar{\Lambda} = 0 & \text{dual feas.} \\ \operatorname{trace} \bar{\Lambda}\bar{P} = 0 & \text{compl. slack.} \end{array}$$

$\blacksquare$

For simplicity and sparsity, discard linear operator K and replace with appropriate weights in H.

Use (*square*) perturbed optimality conditions.

$$\begin{aligned} 2H^{(2)} \circ (P - A) - \Lambda = 0 &\quad \text{dual feasibility} \\ -P + \mu\Lambda^{-1} = 0 &\quad \text{perturbed C.S.} \end{aligned}$$

Linearization of second equation
and solve for h and l

$$h = \mu\Lambda^{-1} - \mu\Lambda^{-1} l \Lambda^{-1} - P$$

$$l = \frac{1}{\mu}\{-\Lambda(P+h)\Lambda\} + \Lambda$$

Dual Step First:
(if many elements of P are free)

We can eliminate the primal step h and solve for the dual step l.

$$\begin{aligned} l &= 2H^{(2)} \circ h + \left(2H^{(2)} \circ (P - A) - \Lambda\right) \\ &= 2H^{(2)} \circ \left(\mu\Lambda^{-1} - \mu\Lambda^{-1} l \Lambda^{-1} - P\right) \\ &\qquad + (2H^{(2)} \circ (P - A) - \Lambda). \end{aligned}$$

Equivalently, we get the Newton equation

$$2H^{(2)} \circ (\mu\Lambda^{-1} l \Lambda^{-1}) + l = 2H^{(2)} \circ (\mu\Lambda^{-1} - A) - \Lambda.$$

l, Λ have same sparsity pattern as H,
order is number of nonzeros/2 in H.

dim	toler	Hdens./infty	Apsd	cond(A)	Hpd	min/max	iters
60	10^{-6}	.01/.001	yes	79.7	no	15/23	16.8
65	10^{-6}	.015/.001	yes	49.9	yes	18/24	21.3
83	10^{-6}	.007/.001	no	235.1	no	24/29	25.5
85	10^{-5}	.008/.001	yes	94.7	no	11/17	13.1
85	10^{-6}	.0075/.001	no	299.9	no	23/27	25.2
87	10^{-6}	.006/.001	yes	74.2	yes	14/19	16.9
89	10^{-6}	.006/.001	no	179.3	no	23/28	15.2
110	10^{-6}	.007/.001	yes	172.3	yes	15/20	17.8
155	10^{-6}	.01/0	yes	643.9	yes	14/18	15.3
655	10^{-6}	.017/0	yes	1.4	no	14/14	14.
755	10^{-6}	.002/0	yes	1.5	no	15/15	15.

data for dual-step-first (20 problems per test for $n \leq 155$; one otherwise):
dimension; tolerance for duality gap;
density of nonzeros in H/ density of infinite values in H;
positive semidefiniteness of A; condition number of A; positive definiteness of H;

(only one test for: 655,755)

Euclidean Distance Matrix Completion Problem

(with Abdo Alfakih)

What are EDMs?

—–

A **pre-distance matrix** (or dissimilarity matrix):

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

—–

A (squared) **Euclidean distance matrix** (EDM):

• a pre-distance matrix such that there exists points $x^1, x^2, \ldots, x^n$ in $\Re^r$ 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 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.:

• The shape of an enzyme determines it chemical function. Once the shape is known, then the proper drug can be designed.

• distance geometry on molecules: Atoms are points in space with pairwise distances; find a set of points which yield those distances.

For approximate EDMCP:

A is a pre-distance matrix, H is an $n \times n$ symmetric weight matrix,

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

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

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

DISTANCE GEOMETRY A *pre-distance matrix* D is a EDM if and only if D is negative semidefinite on

$$M := \left\{ x \in \Re^n : x^t e = 0 \right\},$$

where e is the vector of all ones.

Define **centered** and **hollow** subspaces

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

Define 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

$$\mathcal{K}(\mathcal{S}_C) = \mathcal{S}_H,$$
$$\mathcal{T}(\mathcal{S}_H) = \mathcal{S}_C,$$

and $\mathcal{K}_{|\mathcal{S}_C}$ and $\mathcal{T}_{|\mathcal{S}_H}$ are inverses of each other. ■

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

D is EDM
if and only if
$D = \mathcal{K}(B)$, for some B with $Be = 0$ and $B \succeq 0$.

In this case the embedding dimension r is given by the rank of B. Moreover if $B = XX^t$, then the coordinates of the points $x^1, x^2, \ldots, x^n$ that generate D are given by the rows of X and, since $Be = 0$, it follows that the origin coincides with the centroid of these points.

For Projection: V $n \times (n-1)$, full column rank with $V^t e = 0$.

$$J := VV^{\dagger} = I - \frac{ee^t}{n}$$

is orthogonal projection onto M, where $V^{\dagger}$ denotes Moore-Penrose generalized inverse.

The cone of EDMs, $\mathcal{E}$, has empty interior. This can cause problems for interior-point methods.

$$V \cdot V : \mathcal{S}_{n-1} \to \mathcal{S}_n$$

$$V \cdot V : \mathcal{P}_{n-1} \to \mathcal{P}_n$$

Define the composite operators

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

and

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

LEMMA

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

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

COROLLARY

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

∎

Summary

(Re)Define the closest EDM problem:

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

where $B = \mathcal{T}_V(A)$.

($\mathcal{K}_V$ and $\mathcal{T}_V$ are both linear operators)

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

THEOREM Suppose that Slater's condition holds. Then $\bar{X} \succeq 0$, and $\bar{y}$, $\bar{\Lambda} \succeq 0$ solve (CDM) and (DCDM), respectively, if and only if the following three equations hold.

$$\begin{array}{rcl} \mathcal{A}(\bar{X}) = b & & \text{prim. feas.} \\ 2\mathcal{K}_V^*(H^{(2)} \circ \mathcal{K}_V(\bar{X} - B)) - \mathcal{A}^*\bar{y} - \bar{\Lambda} = 0 & & \text{dual feas.} \\ \operatorname{trace} \bar{\Lambda}\bar{X} = 0 & & \text{C.S.} \end{array}$$

■

LEMMA Let H be an $n \times n$ symmetric matrix with nonnegative elements and 0 diagonal such that the graph of H is connected. Then

$$\mathcal{K}_V^*(H^{(2)} \circ \mathcal{K}_V(I)) \succ 0,$$

where $I \in \mathcal{S}_{n-1}$ is the identity matrix. ■

equating $\Lambda = \mu X^{-1}$ and multiplying through by X

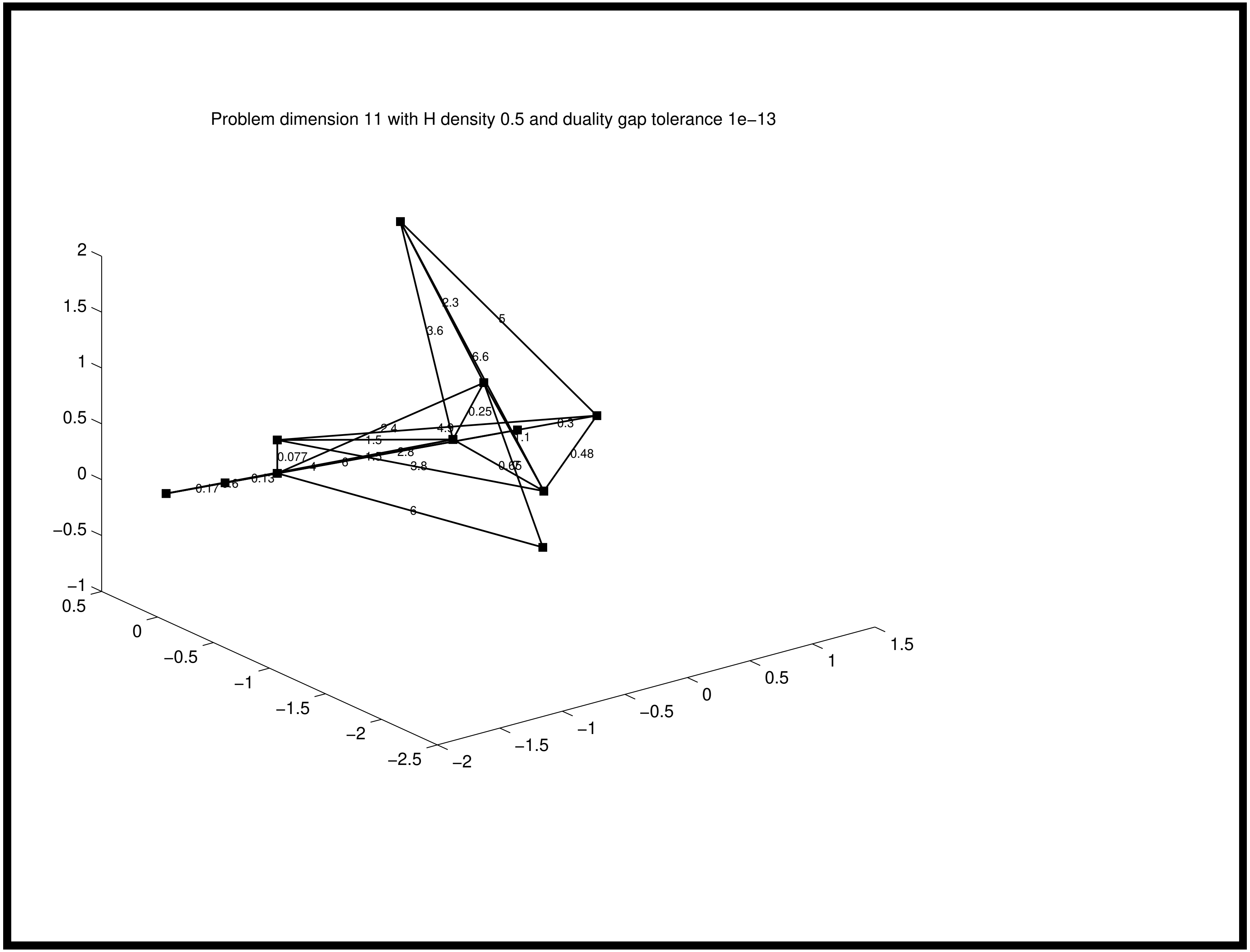
optimality conditions, $F := \begin{pmatrix} F_d \\ F_c \end{pmatrix} = 0$,

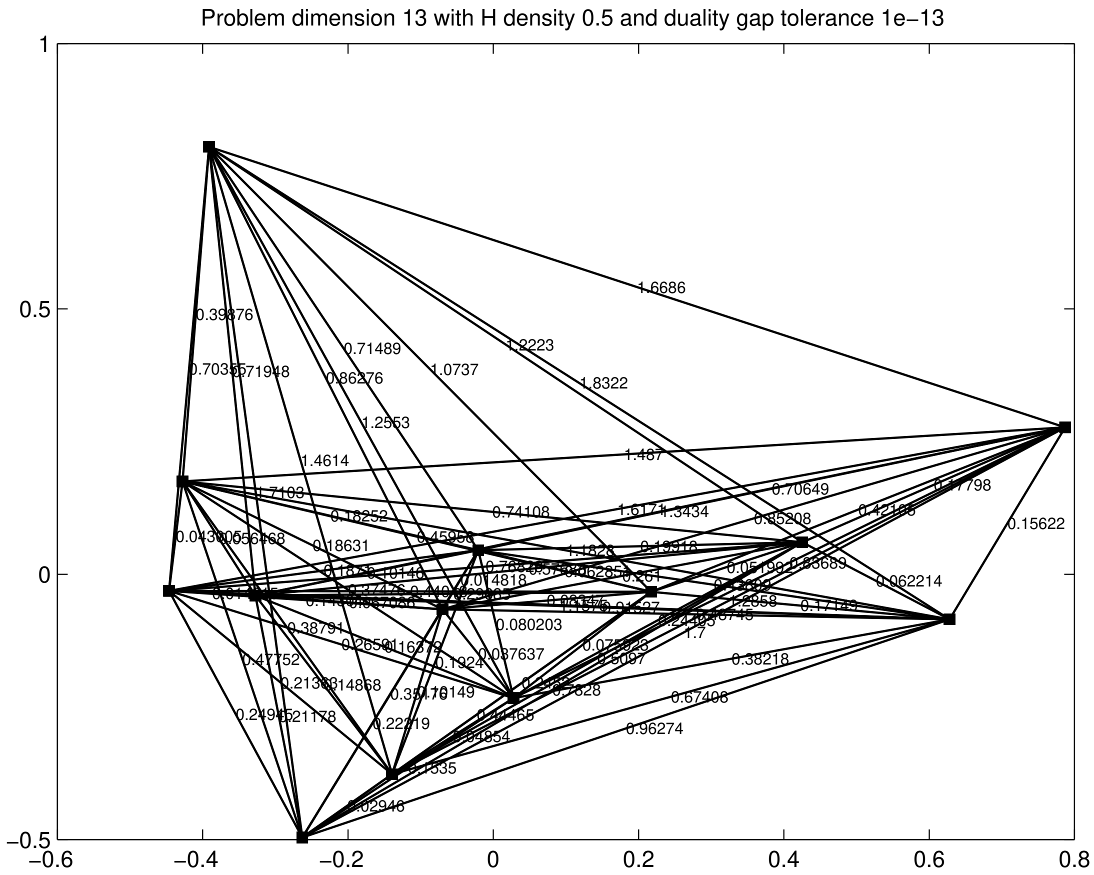
$$\begin{array}{rcll} 2\mathcal{K}_V^* \left(H^{(2)} \circ \mathcal{K}_V(X) \right) - C - \Lambda & = & 0 & \text{dual feas.} \\ \Lambda X - \mu I & = & 0 & \text{pert. C.S.,} \end{array}$$

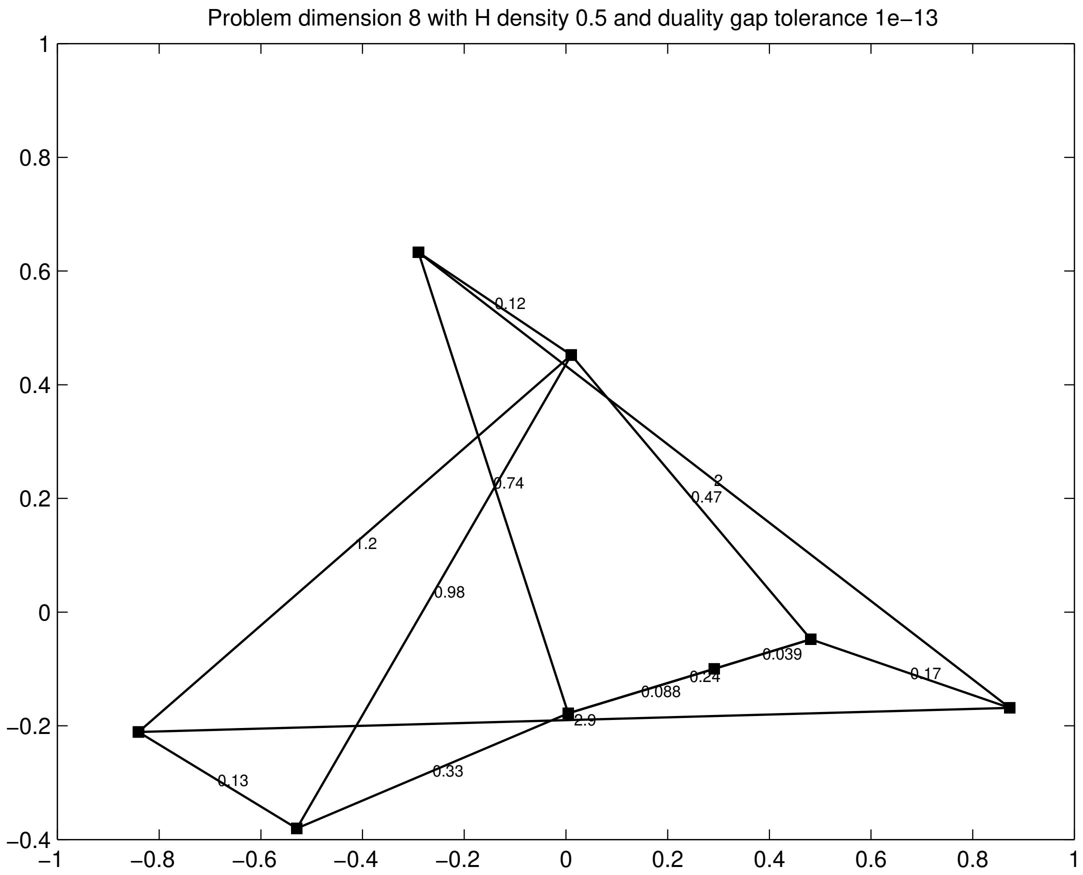
(an OVERDETERMINED nonlinear system since ΛX not symmetric)

estimate of the barrier parameter

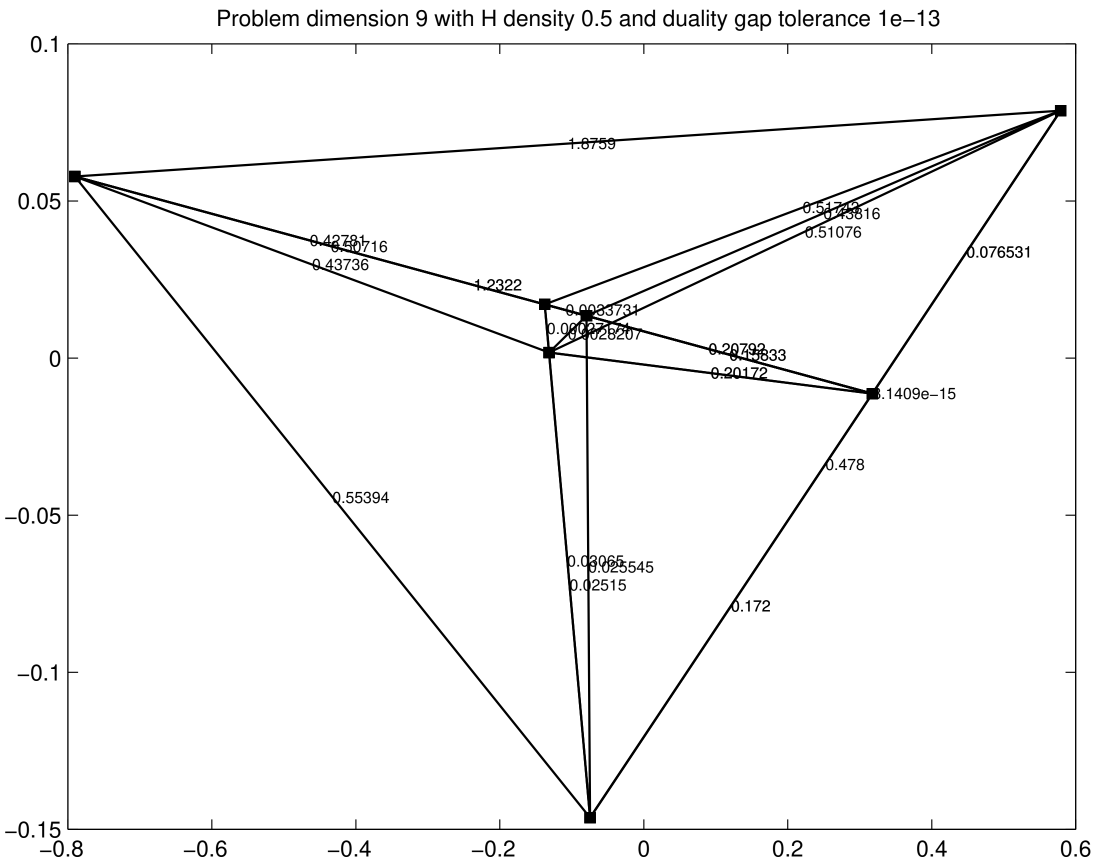
$$\mu = \frac{1}{n-1} \text{ trace } \Lambda X$$


Problem dimension 11 with H density 0.5 and duality gap tolerance 1e−13
2.3
5
3.6
6.6
0.25
2.4
4.3
0.3
1.5
1.1
0.077
2.8
0.48
4
6
1.5
3.8
0.65
0.13
6
2
1.5
1
0.5
0
−0.5
−1
0.5
0
−0.5
−1
−1.5
−2
−2.5
−2
−1.5
−1
−0.5
0
0.5
1
1.5


Problem dimension 13 with H density 0.5 and duality gap tolerance 1e−13
1
0.5
0
−0.5
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1.6686
1.2223
1.8322
0.71489
1.0737
0.86276
1.2553
1.4614
1.487
0.70649
0.15622
0.74108
0.85208
0.062214
0.080203
0.38218
0.67406
0.96274
0.18631
0.47752
0.22219
0.18252



Problem dimension 8 with H density 0.5 and duality gap tolerance 1e−13
0.12
0.74
2
0.47
1.2
0.98
0.039
0.24
0.17
0.088
2.9
0.33
0.13
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1


Problem dimension 9 with H density 0.5 and duality gap tolerance 1e−13
0.1
0.05
0
−0.05
−0.1
−0.15
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
1.8759
0.51076
0.076531
0.43736
1.2322
0.0033731
0.0028207
0.20172
0.478
0.55394
0.025545
0.02515
0.172

Larger Models

Instead of projecting and reducing the dimension to get Slater's condition, add a variable and increase the dimension.

Lemma 1 *Let*

$$\begin{array}{rcl}\mathcal{F} & := & \{X \in \mathcal{S}^n : v^T e = 0 \quad \Rightarrow \quad v^T X v \leq 0\}, \\ \mathcal{F}_0 & := & \{X \in \mathcal{S}^n : X - \alpha e e^t \preceq 0, \quad \textit{for some } \alpha \geq 0\}, \\ \mathcal{F}_1 & := & \{X \in \mathcal{S}^n : X - \alpha e e^t \preceq 0, \quad \forall\ \alpha \geq \bar{\alpha}, \\ & & \qquad \textit{for some } \bar{\alpha} \geq 0\}.\end{array}$$

Then

$$\mathrm{ri}\,(\mathcal{F}) \subset \mathcal{F}_0 = \mathcal{F}_1 \subset \mathcal{F} \subset \overline{\mathcal{F}_0}. \tag{1}$$

Proof. Suppose that $\bar{X} \in \mathrm{ri}\,(\mathcal{F})$ (i.e. $v^T e = 0, v \neq 0 \Rightarrow v^T \bar{X} v < 0$) but $\bar{X} \notin \mathcal{F}_0$. Then, for each $\alpha \geq 0$, there exists w_α with $||w_\alpha|| = 1$, such that $w_\alpha \to \bar{w}$, as $\alpha \to \infty$ and

$$w_\alpha^T(\bar{X} - \alpha e e^t) w_\alpha > 0, \quad \forall\, \alpha \geq 0,$$

i.e.

$$w_\alpha^T \bar{X} w_\alpha > \alpha w_\alpha^T e e^t w_\alpha, \quad \forall\, \alpha \geq 0.$$

Since w_α converges and the left-hand-side of the above inequality must be finite, this implies that $e^t \bar{w} = \bar{w}^T \bar{X} \bar{w} = 0$, a contradiction. Therefore, $\mathrm{ri}\,(\mathcal{F}) \subset \mathcal{F}_0$. That $\mathcal{F}_0 = \mathcal{F}_1$ is clear.

Now suppose that $\bar{X} - \alpha e e^t \preceq 0,\ \alpha \geq 0$. Let $v^T e = 0$. Then $0 \geq v^T(\bar{X} - \alpha e e^t) v = v^T \bar{X} v$, i.e. $\mathcal{F}_0 \subset \mathcal{F}$. The final inclusion comes from the first and the fact that $\mathcal{F}$ is closed. ∎

Corollary 1 *Let*

$$\begin{aligned}
\mathcal{E} &:= \{X \in \mathcal{S}_H : v^T e = 0 \quad \Rightarrow \quad v^T X v \leq 0\}, \\
\mathcal{E}_0 &:= \{X \in \mathcal{S}_H : X - \alpha e e^t \preceq 0, \quad \textit{for some } \alpha\}, \\
\mathcal{E}_1 &:= \{X \in \mathcal{S}_H : X - \alpha e e^t \preceq 0, \quad \forall\ \alpha \geq \bar{\alpha}, \\
&\qquad \textit{for some } \bar{\alpha}\}.
\end{aligned}$$

Then

$$\mathcal{E} = \mathcal{E}_0 = \mathcal{E}_1. \tag{2}$$

Proof. (Similar to Lemma 1.) For closure, suppose $0 \neq X_k \in \mathcal{E}_0$, i.e. $\operatorname{diag}(X_k) = 0, X_k \preceq \alpha_k E$, for some α_k; and, suppose $X_k \rightarrow \bar{X}$. Since X_k is hollow it has exactly one positive eigenvalue which must be smaller than α_k. However, since X_k converges to $\bar{X}$, $\bar{X} \leq \lambda_{\max}(\bar{X})E$, where $\lambda_{\max}(\bar{X})$ is the largest eigenvalue of $\bar{X}$. ∎

let: $E = ee^t$; $f(P) := \|H \circ (A-P)\|_F^2$;
$\mathcal{K}$ lin. operator with constraint $\operatorname{diag}(P) = 0$.
primal problem is:

$$(\mathrm{CDM}) \quad \begin{array}{lll} \mu^* := & \min & f(P) \\ & \text{subject to} & \alpha E - P \succeq 0 \end{array}$$

and **dual problem (DCDM)** is

$$\begin{array}{lll} \nu^* := & \max & f(P) + \langle y, b - KP \rangle - \operatorname{trace} \Lambda(\alpha E - P) \\ & \text{subject to} & \nabla_P f(P) - \mathcal{K}^* y + \Lambda = 0 \\ & & -\operatorname{trace} \Lambda E = 0 \\ & & \Lambda \succeq 0. \end{array}$$

(Slater's holds for primal but fails for dual.)

(perturbed) Optimality Conditions are:

$$
\begin{array}{rl}
\operatorname{diag}(P) = 0 & \text{primal feas.} \\
\left.\begin{array}{r} 2H^{(2)} \circ (P - A) - \operatorname{Diag}(y) + \Lambda = 0 \\ -\operatorname{trace} \Lambda E = 0 \end{array}\right\} & \text{dual feas.} \\
-(\alpha E - P) + \mu \Lambda^{-1} = 0, & \text{pert. C.S.}
\end{array}
$$

0.0.1 On a New Characterization of EDMs

The above application for EDM uses

$$D = \lambda E - P, \; P \succeq 0, \; \operatorname{diag} P = \lambda e, \; \lambda \geq 0;$$

this raises the **question**:

> **which** *Euclidean distance matrices* D *can be expressed as* $D = \lambda(E - C)$ *for some nonnegative scalar* λ *and some correlation matrix* C*, where* E *is the matrix of all ones.*

We **show (and characterize)** that the cones

$$\operatorname{cone}(E - \mathcal{E}_n) \subsetneq \overline{\operatorname{cone}(E - \mathcal{E}_n)} = \mathcal{D}_n,$$

where $\mathcal{E}_n$ is the elliptope (set of correlation matrices) and $\mathcal{D}_n$ is the (closed convex) cone of Euclidean distance matrices.

The characterization is given using the Gale transform of the points generating D. We also show that given points $p^1, p^2, \ldots, p^n \in \mathcal{R}^r$, for any scalars $\lambda_1, \lambda_2, \ldots, \lambda_n$ such that

$$\sum_{j=1}^{n} \lambda_j \, p^j = 0, \qquad \sum_{j=1}^{n} \lambda_j = 0,$$

we have

$$\sum_{j=1}^{n} \lambda_j \, \|p^i - p^j\|^2 = \alpha \text{ for all } i = 1, \ldots, n,$$

for some scalar α independent of i.

Recall:

- $n \times n$ matrix $D = (d_{ij})$ is *Euclidean distance matrix (EDM)* if

$$\exists \quad p^1, p^2, \ldots, p^n \in \mathcal{R}^r, \text{ such that } \|p^i - p^j\|^2 = d_{ij}, \quad \forall i, j$$

- dimension of smallest Euclidean space containing $p^1, p^2, \ldots, p^n$ is the *embedding dimension* of D.
- D (hollow) EDM $\iff$ D negative semidefinite on $e^\perp$
- the set of $n \times n$ EDM matrices is a closed convex cone, $\mathcal{D}_n$

Since $\mathcal{E}_n$ denotes set of $n \times n$ *correlation matrices*, i.e., set of positive semidefinite symmetric matrices whose diagonal is equal to e, we are using the well known fact [**?**] that $\mathcal{D}_n$ is the tangent cone of $\mathcal{E}_n$ at E, the matrix of all ones, i.e.,

$$\mathcal{D}_n = \overline{\text{cone } (E - \mathcal{E}_n)} = \overline{\{\lambda(E - C) : \lambda \geq 0, C \in \mathcal{E}_n\}}, \tag{3}$$

where $\bar{\cdot}$ denotes closure.

In general, it is difficult to determine whether the generated cone of a set, $cone(C)$ is closed, though there are sufficient conditions, e.g. C is convex and compact and 0 is not in C.

- Let V be $n \times (n-1)$ such that

$$V^T e = 0\,, \quad V^T V = I_{n-1}\,. \tag{4}$$

- orthogonal projection on $M = e^\perp$, denoted by J, is $J := VV^T = I - ee^T/n$.

- D hollow is EDM $\iff B := -\frac{1}{2}\, JDJ \succeq 0$

- embedding dimension of D is equal, r, rank of B.

- the points $p^1, p^2, \ldots, p^n$ that generate D are given by the rows of the $n \times r$ matrix P where $B := PP^T$.

- since $Be = 0$, centroid of the points p^i, $i = 1, \ldots, n$ coincides with the origin

Let $p^1, p^2, \ldots, p^n$ be points in $\mathcal{R}^r$ whose centroid coincides with the origin, and are not contained in a proper hyperplane. Then

$$P := \begin{bmatrix} {p^1}^T \\ {p^2}^T \\ \vdots \\ {p^n}^T \end{bmatrix}$$

is of rank r. Let $B = PP^T$. Then it follows that the EDM matrix D generated by p^i, $i = 1, \ldots, n$ is given by

$$D = \operatorname{diag} Be^T + e \left(\operatorname{diag} B\right)^T - 2B. \tag{5}$$

- Let $\bar{r} = n - 1 - r$ and

$$Z \text{ be } n \times \bar{r}, \text{ full column rank with, } P^T Z = 0, e^T Z = 0$$

- ${z^i}^T$ denotes the i-th row of Z. i.e.,

$$Z^T := \left[z^1 \mid z^2 \mid \ldots \mid z^n \right].$$

- z^i is called Gale transform of p^i; Z is called a *Gale matrix* corresponding to D.
- The columns of Z represent the *affine dependence relations* among the points $p^1, p^2, \ldots, p^n$, i.e., among the rows of P.

Main Results

Theorem 1 *Let D be a Euclidean distance matrix and let Z be a Gale matrix corresponding to D. Then, the columns of DZ are proportional to e.*

Equivalently

Theorem 2 *Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be coefficients, not all zero, of the affine dependence equation of the points $p^1, p^2, \ldots, p^n$, in $\mathcal{R}^r$, i.e.,*

$$\sum_{j=1}^{n} \lambda_j p^j = 0, \quad \sum_{j=1}^{n} \lambda_j = 0.$$

Then

$$\sum_{j=1}^{n} \lambda_j \, \|p^i - p^j\|^2 = \alpha \textit{ for all } i = 1, \ldots, n,$$

for some scalar α independent of i.

Theorem 3 *Let D be a Euclidean distance matrix and let Z be a Gale matrix corresponding to D. Then* **the following are equivalent***:*

1. $$D = \lambda(E - C), \tag{6}$$

   for some nonnegative scalar λ and some correlation matrix C;

2. $$DZ = 0. \tag{7}$$

Proof of the Main Results

Lemma 2 *Let D be a Euclidean distance matrix and let $B = -\frac{1}{2}JDJ$. Then:*

1.

$$-\frac{1}{2}V^T DV = V^T BV;$$

2.

$$\mathcal{N}(V^T DV) = \mathcal{N}(P^T V).$$

Proof. The first part follows directly from (5) and the definition of V. This yields the second part since $B = PP^T$ and $\mathcal{N}(V^T BV) = \mathcal{N}(V^T PP^T V) = \mathcal{N}(P^T V)$. ■

Lemma 3 *Let D be a Euclidean distance matrix and let U be the matrix whose columns form an orthonormal basis of the null space of $V^T DV$. Then VU is a Gale matrix corresponding to D.*

Proof. It follows from Lemma 2 that $P^T VU = V^T DVU = 0$ and from the definition of V in (4) that $e^T VU = 0$. Hence, the columns of VU form an orthonormal basis for the null space of $\begin{bmatrix} P^T \\ e^T \end{bmatrix}$. ■

Proof of Theorem 1. Let Z be a Gale matrix corresponding to D. Then It follows from Lemma 3 that $VU = ZQ$ for some nonsingular $\bar{r} \times \bar{r}$ matrix Q. Thus $V^T DZ = V^T DVUQ^{-1} = 0$. Hence, the columns of DZ are proportional to e. $\blacksquare$

Proof of Theorem 3. $D = \lambda(E - C)$ for some nonnegative scalar λ and some correlation matrix C if and only if $E - \frac{1}{\lambda} D$ is positive semidefinite. Let $Q = [\frac{e}{\sqrt{n}} \; V]$. Then, $E - D/\lambda \succeq 0$ if and only if $Q^T \; (E - D/\lambda) \; Q \succeq 0$. But

$$Q^T \; (E - D/\lambda) \; Q = \begin{bmatrix} n - \frac{1}{\lambda \, n} \, e^T D e & -\frac{1}{\lambda \sqrt{n}} \, e^T D V \\ -\frac{1}{\lambda \sqrt{n}} \, V^T D e & -\frac{1}{\lambda} \, V^T D V \end{bmatrix}.$$

Recall that $V^T(-D)V \succeq 0$ follows from Lemma 2. Let W and U be the matrices whose columns form an orthonormal basis for the range space and null space of $V^T(-D)V$, respectively.

Hence, $V^T(-D)V = W\Lambda W^T$, where Λ is the diagonal matrix of the positive eigenvalues of $V^T(-D)V$. Let $Q' = \begin{bmatrix} 1 & 0 & 0 \\ 0 & W & U \end{bmatrix}$. Then, $E - D/\lambda$ is positive semidefinite if and only if

$$\begin{aligned} R &= {Q'}^T Q^T (E - D/\lambda) Q Q' \\ &= \begin{bmatrix} n - \frac{1}{\lambda n} e^T D e & -\frac{1}{\lambda\sqrt{n}} e^T D V W & -\frac{1}{\lambda\sqrt{n}} e^T D V U \\ -\frac{1}{\lambda\sqrt{n}} W^T V^T D e & \frac{1}{\lambda}\Lambda & 0 \\ -\frac{1}{\lambda\sqrt{n}} U^T V^T D e & 0 & 0 \end{bmatrix} \succeq 0. \end{aligned} \tag{8}$$

Now for sufficiently large λ the submatrix

$$\begin{bmatrix} n - \frac{1}{\lambda\, n}\, e^T De & -\frac{1}{\lambda\,\sqrt{n}}\, e^T DVW \\ -\frac{1}{\lambda\,\sqrt{n}}\, W^T V^T De & \frac{1}{\lambda}\,\Lambda \end{bmatrix}$$

is positive definite.

Thus $E - D/\lambda$ is positive semidefinite if and only if $e^T DVU = e^T DZ = 0$. But it follows from Theorem 1 that $e^T DZ = 0$ if and only if $DZ = 0$ and the result follows. ∎

Given the two Euclidean distance matrices:

$$D_1 = \begin{bmatrix} 0 & 1 & 4 \\ 1 & 0 & 1 \\ 4 & 1 & 0 \end{bmatrix}, \qquad D_2 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix},$$

Gale matrices Z_1, Z_2 corresponding to D_1, D_2, resp. are:

$$Z_1^T = [1 \ -2 \ 1], \quad Z_2^T = [1 \ 0 \ -1],$$

Now $D_1 Z_1 = 2e$ and $D_2 Z_2 = 0$. Then: $D_2 = E - C_2$, where

$$C_2 = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \succeq 0.$$

However, there exists no $\lambda \geq 0$ such that $D_1 = \lambda(E - C_1)$ for some correlation matrix C_1.