Robust Algorithms for Large Sparse Semidefinite Programming (SDP)

with Applications to the Nearest Euclidean Distance Matrix Problem

Henry Wolkowicz

hwolkowicz@uwaterloo.ca

Department of Combinatorics and Optimization

University of Waterloo

Toulouse 2004

First Joint Canada-France meeting of the Mathematical Sciences

Robust Algorithms for Large Sparse Semidefinite Programming (SDP)

Friday July 15, 2004.

OUTLINE

- Background on SDP; Notation and Motivation
- Robust, ('non-interior') path-following algorithm for SDP
  (outline of GN PCG method using LP)
- Application to Nearest Euclidean Distance Matrix Problem
- Numerics (Comparisons with a dual algorithm)

Notation and Motivation

$$
\text{(SDP)} \qquad \begin{array}{rl} \min & f(X) \\ \text{subject to} & \mathcal{A}X = b \\ & X \succeq 0, \end{array}
$$

where:

$$
\begin{array}{rl}
f : \mathcal{S}^n \to \mathbb{R} & \text{convex function} \\
\mathcal{S}^n & n \times n \text{ real symmetric matrices} \\
X (\succeq) \succ 0 & \text{denotes positive (semi)definite} \\
\mathcal{A} : \mathcal{S}^n \to \mathbb{R}^m & \text{linear transformation}
\end{array}
$$

$$
\left(\quad (\mathcal{A}X)_i = \langle A_i, X \rangle = \operatorname{trace} A_i X, \quad A_i = A_i^T, i = 1 \ldots n) \quad \right)
$$

Linear Primal-Dual Pair of SDPs

(looks/behaves like Linear Program, LP)

$$
\text{(PSDP)} \qquad \begin{array}{ll} \min & \langle C, X \rangle = \operatorname{trace} CX \\ \text{subject to} & \mathcal{A}X = b \\ & X \succeq 0 \end{array}
$$

$$
\text{(SDP)} \qquad \begin{array}{ll} \max & b^T y \\ \text{subject to} & \mathcal{A}^* y + Z = C \\ & Z \succeq 0 \end{array}
$$

adjoint operator: $\mathcal{A}^* y = \sum_{i=1}^m y_i A_i$

(some of the) APPLICATIONS

- Relaxations of **hard combinatorial problems**: e.g. max-cut; graph partitioning; quadratic assignment problem; max-clique.
- **NLP** e.g.: quasi-Newton updates that preserve positive definiteness; Trust region algorithms for large scale minimization; Extended SQP techniques for constrained minimization.
- Partial Hermitian **matrix completion problems** and Euclidean distance matrix completion problems.
- **Engineering problems** such as: Ricatti equations; min-max eigenvalue problems; matrix norm minimization; eigenvalue localization.

SIMILARITIES to LP: (i) Duality

payoff function, player Y to player X (Lagrangian)

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

Optimal (worst case) strategy for player X:

$$p^* = \max_{X \succeq 0} \min_{y} L(X, y)$$

Using the *hidden constraint* $b - \mathcal{A}X = 0$,
recovers primal problem.

apply adjoint

$$\begin{aligned} L(X,y) &= \operatorname{trace}(CX) + y^t(b - \mathcal{A}X) \\ &= b^t y + \operatorname{trace}\,(C - \mathcal{A}^* y)\, X \end{aligned}$$

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

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

Hidden Constraint: $C - \mathcal{A}^* y \preceq 0$

exploit *Hidden Constraint*

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

dual obtained from optimal strategy of competing player, Y.
Hidden Constraint: $C - \mathcal{A}^* y \preceq 0$ yields the dual

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

for the primal

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

Characterization of Optimality

primal-dual pair X, y (slack $Z \succeq 0$)

$A^* y - Z = C$ dual feasibility

$AX = b$ primal feasibility

$ZX = 0$ complementary slackness

$ZX = \mu I$ perturbed C.S., $\mu > 0$

Basis for methods:

- primal simplex (maintain: primal feas. & compl. slack.)
- dual simplex (maintain: dual feas. & compl. slack.)
- interior point (maintain: primal feas. & dual feas.)

SDP Application: (Direct) Max-Cut Relaxation

Graph $G = (E, V)$; $|V| = n$ (nodes); w_{ij} weights on edges;

$$\max \ \frac{1}{2} \sum_{i<j} w_{ij}(1 - x_i x_j), \quad x \in \{\pm 1\}^n.$$

Equate $x_i = 1$ with i in set $\mathcal{I}$ and $x_i = -1$ otherwise.
Equivalent problem: homogeneous (± 1)-*QQP*

$$\mu^* := \max \ q(x) := x^t Q x = \operatorname{trace} Q x x^T, \quad x \in \{\pm 1\}^n.$$

REPLACE $x \in \{\pm 1\}^n$ WITH CONSTRAINTS $x_i^2 = 1$??!!

LIFTING : $\quad X = x x^t$

Relax the rank-1 condition on X to get linear SDP.

$$\mu^* \leq \max\{\operatorname{trace} QX : \operatorname{diag}(X) = e, X \succeq 0\}$$

SDP from general quadratic approx? (Lagr. Relax.!)

$$q_i(y) := \frac{1}{2} y^t Q_i y + y^t b_i + c_i, \; y \in \Re^n$$

$$\begin{array}{rrll} & q^* = & \min & q_0(y) \\ (\textbf{QQP}) & & \text{s.t.} & q_i(y) \leq 0 \\ & & & i = 1, \ldots m \end{array}$$

Lagrangian : $\quad L(y,x) \; = \; q_0(y) + \sum_{i=1}^m x_i q_i(y)$

or equivalently

$$\begin{array}{rcll} L(y,x) & = & \frac{1}{2} y^t (Q_0 + \sum_{i=1}^m x_i Q_i) y & \text{(quadratic in } y\text{)} \\ & & + y^t (b_0 + \sum_{i=1}^m x_i b_i) & \text{(linear in } y\text{)} \\ & & + (c_0 + \sum_{i=1}^m x_i c_i) & \text{(constant in } y\text{)} \end{array}$$

Weak Duality

follows from definition of dual program and hidden constraints:

$$d^* = \max_{x \geq 0} \min_y L(y, x) \leq q^* = \min_y \max_{x \geq 0} L(y, x).$$

Now homogenize; multiply linear term by new variable y_0

$$y_0 y^t (b_0 + \sum_{i=1}^m x_i b_i), \quad y_0^2 = 1.$$

and add new constraint to Lagrangian (Lagrange multiplier t)

$$t(y_0^2 - 1)$$

Homogenization

$$
\begin{aligned}
d^* &= \max_{x\geq 0} \min_{y} \quad L(y,x) \\
&= \max_{x\geq 0} \min_{y_0^2=1} \quad \tfrac{1}{2} y^t (Q_0 + \textstyle\sum_{i=1}^m x_i Q_i) y \quad + t y_0^2 \\
&\qquad + y_0 y^t (b_0 + \textstyle\sum_{i=1}^m x_i b_i) \\
&\qquad + (c_0 + \textstyle\sum_{i=1}^m x_i c_i) \quad - t \\
&= \max_{x\geq 0, t} \min_{y} \quad \tfrac{1}{2} y^t (Q_0 + \textstyle\sum_{i=1}^m x_i Q_i) y \quad + t y_0^2 \\
&\qquad + y_0 y^t (b_0 + \textstyle\sum_{i=1}^m x_i b_i) \\
&\qquad + (c_0 + \textstyle\sum_{i=1}^m x_i c_i) \quad - t
\end{aligned}
$$

hidden semidefinite constraint yields SDP

Apply Hidden SDP Constraint (Hessian psd)

$$B := \begin{pmatrix} 0 & b_0^t \\ b_0 & Q_0 \end{pmatrix} \text{ and } A : \Re^{m+1} \rightarrow \mathcal{S}_{n+1}$$

$$A \begin{pmatrix} t \\ x \end{pmatrix} := - \begin{bmatrix} t & \sum_{i=1}^m x_i b_i^t \\ \sum_{i=1}^m x_i b_i & \sum_{i=1}^m x_i Q_i \end{bmatrix}$$

$$\text{Lagrangian psd} \quad : \qquad B - A \begin{pmatrix} t \\ x \end{pmatrix} \succeq 0.$$

NOTE There is NO hidden constraint on the Q_i **if all** q_i **are convex.** Better algorithms exist for the convex case, e.g. proximal methods, using quadratic cones, ...

Dual of Dual → SDP Relaxation

dual program is equivalent to SDP (with $c_0 = 0$)

$$
(\mathbf{D}) \qquad \begin{array}{rll} d^* = & \sup & -t + \sum_{i=1}^m x_i c_i \\ & \text{s.t.} & A \begin{pmatrix} t \\ x \end{pmatrix} \preceq B \\ & & x \in \Re^m, t \in \Re \end{array}
$$

As in LP, dual of dual is obtained from optimal strategy of the competing player:

$$
(\mathbf{DD}) \qquad \begin{array}{rll} d^* = & \inf & \operatorname{trace} BU \\ & \text{s.t.} & A^*U = \begin{pmatrix} -1 \\ c \end{pmatrix} \\ & & U \succeq 0. \end{array}
$$

Tractable Relaxations

In some sense, Lagrangian relaxation is **best tractable relaxation**.
There are *higher order* relaxations:
e.g. from $X = xx^T$ from max-cut relaxation (from $x_j^2 = 1$)

$$\text{2nd LIFTING}: \quad x_i x_j^2 x_k = x_i x_k, \quad Y = \begin{pmatrix} 1 \\ \operatorname{svec} X \end{pmatrix} \begin{pmatrix} 1 & \operatorname{svec} X \end{pmatrix}$$

Public domain software: e.g. NEOS
URL: www-neos.mcs.anl.gov

(Perturbed) Optimality Conditions

For *barrier parameter* $\mu > 0$:

$$F_\mu(X, y, Z) := \begin{pmatrix} \mathcal{A}^* y + Z - C \\ \mathcal{A}X - b \\ ZX - \mu I \end{pmatrix} = 0 \qquad \begin{pmatrix} \text{dual feasibility} \\ \text{primal feasibility} \\ \text{pert. compl. slack.} \end{pmatrix}$$

For SDP:

$$F_\mu : \mathcal{S}^n \times \Re^m \times \mathcal{S}^n \rightarrow \mathcal{S}^n \times \Re^m \times \mathcal{M}^n$$

i.e. overdetermined nonlinear system

(Non) Interior Path-Following

Illustration/Motivation on LP Case

$$
(\text{LP}) \qquad \begin{array}{rll} p^* := & \min & c^T x \quad (\text{or } \langle c, x\rangle) \\ & \text{s.t.} & Ax = b \\ & & x \geq 0 \quad (\text{or } x \succeq 0) \end{array}
$$

$$
(\text{DLP}) \qquad \begin{array}{rll} d^* := & \max & b^T y \\ & \text{s.t.} & A^T y + z = c \\ & & z \geq 0 \quad (\text{or } z \succeq 0) \end{array}
$$

Assume: $A \in \Re^{m \times n}$ full rank (onto); LP, DLP strictly feasible

dual log-barrier problem; parameter $\mu > 0$

$$
\begin{array}{rll}
d_\mu^* := & \max & b^T y + \mu \sum_{j=1}^n \log z_j \quad (+\mu \log\det(z)) \\
& \text{s.t.} & A^T y + z = c \qquad (A^T \cong A^*) \\
& & z > 0 \qquad (z \succ 0).
\end{array}
$$

stationary point of the Lagrangian / optimality conditions

$$
F_\mu(x,y,z) = \begin{pmatrix} A^T y + z - c \\ Ax - b \\ X - \mu Z^{-1} \end{pmatrix} = 0, \qquad \begin{array}{l} x, z > 0, \quad (\succ 0) \\ X = \text{Diag}\,(x) \\ Z = \text{Diag}\,(z) \end{array}
$$

central path:= set of solutions $(x_\mu, y_\mu, z_\mu), \mu > 0$

Jacobian Ill-conditioning

As $\mu \to 0$, Jacobian $F'_\mu(x,y,z)$ ill-conditioned near central path
Cure/Fix: Make nonlinear equations *less nonlinear*, i.e.
preconditioning for Newton type methods;

premultiply by block-diag matrix with blocks (I, I, Z):

$$F_\mu(x,y,z) \leftarrow \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & Z \end{pmatrix} F_\mu(x,y,z) = \begin{pmatrix} A^T y + z - c \\ Ax - b \\ ZX - \mu I \end{pmatrix} =: \begin{pmatrix} R_d \\ r_p \\ R_{ZX} \end{pmatrix}$$

recovers modern primal-dual optimality paradigm

Exploited Special Structure

linearization for the Newton direction

$$\Delta s = \begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix}$$

$$F'_\mu(x, y, z)\Delta s = \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & 0 & X \end{pmatrix} \Delta s = -F_\mu(x, y, z).$$

Overdetermined system in SDP case

$$\mathcal{S}^n \times \Re^m \times \mathcal{S}^n \rightarrow \mathcal{S}^n \times \Re^m \times \mathcal{M}^n$$

apply symmetrization; undoes preconditioning

$$\begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & \mathcal{S} \end{pmatrix} \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & 0 & X \end{pmatrix}$$

e.g. last equation after symmetrization:
$ZX + XZ - 2\mu I = 0$ (AHO search direction)

Reduction/Block-Elimination $\rightarrow$ Normal Equations

Step 1 (Eliminate Δz from row 3):

$$\begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -X & 0 & I \end{pmatrix} \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & 0 & X \end{pmatrix} = \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & -XA^T & 0 \end{pmatrix}.$$

Define:

$$P_Z := \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -X & 0 & I \end{pmatrix}, \quad K := \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & -XA^T & 0 \end{pmatrix}.$$

with right-hand side

$$-\begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -X & 0 & I \end{pmatrix} \begin{pmatrix} R_d \\ r_p \\ R_{ZX} - \mu e \end{pmatrix} = \begin{pmatrix} -R_d \\ -r_p \\ XR_d - R_{ZX} \end{pmatrix}$$

Step 2: Eliminate Δx from row 2

(and scale row 3)

$$F_n := P_n K \quad := \begin{pmatrix} I & 0 & 0 \\ 0 & I & -AZ^{-1} \\ 0 & 0 & Z^{-1} \end{pmatrix} \begin{pmatrix} 0 & A^T & I \\ A & 0 & 0 \\ Z & -XA^T & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & A^T & I_n \\ 0 & AZ^{-1}XA^T & 0 \\ I_n & -Z^{-1}XA^T & 0 \end{pmatrix}$$

$AZ^{-1}XA^T$ can have:

- uniformly bounded condition number, e.g. Güler et al 1993
- structured singularity, e.g. S. Wright 95,97/ M. Wright 1999

But $\mathrm{cond}(F_n) \to \infty$

The right-hand side becomes

$$-P_n P_Z \begin{pmatrix} R_d \\ r_p \\ R_{ZX} \end{pmatrix} = \begin{pmatrix} -R_d \\ -r_p + A(x - Z^{-1}XR_d - \mu Z^{-1}e) \\ Z^{-1}XR_d - x + \mu Z^{-1}e \end{pmatrix}$$

Ill-conditioning

Proposition The condition number of $F_n^T F_n$ diverges to infinity if $x(\mu)_i / z(\mu)_i$ diverges to infinity, for some i, as μ converges to 0. The condition number of $(F'_\mu)^T F'_\mu$ is uniformly bounded if there exists a unique primal-dual solution.

PROOF: Note that

$$F_n^T F_n = \begin{pmatrix} I_n & -Z^{-1}XA^T & 0 \\ -AXZ^{-1} & (AA^T + (AZ^{-1}XA^T)^2 + AZ^{-2}X^2A^T) & A \\ 0 & A^T & I_n \end{pmatrix}.$$

By interlacing of eigenvalues, ... ■

Corollary The condition number of F_n is at least $O(1/\mu)$. ■

EXAMPLE

$$A = \begin{pmatrix} 1 & 1 \end{pmatrix}, c = \begin{pmatrix} -1 \\ 1 \end{pmatrix}, b = 1,$$

$$x^* = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, y^* = -1, z^* = \begin{pmatrix} 0 \\ 2 \end{pmatrix};$$

initial points:

$$x = \begin{pmatrix} 9.183012e-001 \\ 1.356397e-008 \end{pmatrix}, z = \begin{pmatrix} 2.193642e-008 \\ 1.836603e+000 \end{pmatrix},$$

$$y = -1.163398e+000.$$

residuals and duality gap:

$$\|r_b\| = 0.081699, \|R_d\| = 0.36537, \mu = x^T z/n = 2.2528e-008$$

5 decimals rounding before/after arithmetic

centering with $\sigma = .1$

BUT: residuals are NOT order μ.

search directions found

using : full matrix F'_μ and backsolve matrix F_n

$$\begin{pmatrix} \Delta x \\ \Delta y \\ \Delta z \end{pmatrix} = \begin{pmatrix} 8.17000e-02 \\ -1.35440e-08 \\ 1.63400e-01 \\ -2.14340e-08 \\ 1.63400e-01 \end{pmatrix} ; \quad \begin{pmatrix} -6.06210e+01 \\ -1.35440e-08 \\ 1.63400e-01 \\ 0.00000e+00 \\ 1.63400e-01 \end{pmatrix}$$

error in Δy is small;
but error after backsubstitution for $(\Delta x)_1$ is large.

$$\begin{pmatrix} AZ^{-1}XA^T \\ -Z^{-1}XA^T \end{pmatrix} = \begin{pmatrix} 4.18630e+07 \\ -4.18630e+07 \\ -7.38540e-09 \end{pmatrix}$$

Alternate Second Step; Stable Reduction

Assuming! $A = [I_m \; E]$.

Partition diagonal matrix Z, X using vectors

$$z = \begin{pmatrix} z_m \\ z_v \end{pmatrix}, x = \begin{pmatrix} x_m \\ x_v \end{pmatrix}, XA^T = \begin{pmatrix} X_m \\ X_v E^T \end{pmatrix}$$

$$F_s := P_s K = \begin{pmatrix} I_n & 0 & 0 & 0 \\ 0 & I_m & 0 & 0 \\ 0 & -Z_m & I_m & 0 \\ 0 & 0 & 0 & I_v \end{pmatrix} \begin{pmatrix} 0 & 0 & A^T & I_n \\ I_m & E & 0 & 0 \\ Z_m & 0 & -X_m & 0 \\ 0 & Z_v & -X_v E^T & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & A^T & I_n \\ I_m & E & 0 & 0 \\ 0 & -Z_m E & -X_m & 0 \\ 0 & Z_v & -X_v E^T & 0 \end{pmatrix}.$$

The right-hand side becomes

$$-P_s P_Z \begin{pmatrix} A^T y + z - c \\ Ax - b \\ ZXe - \mu e \end{pmatrix} = -P_s \begin{pmatrix} R_d \\ r_p \\ -XR_d + ZXe - \mu e \end{pmatrix}$$

$$= \begin{pmatrix} -R_d \\ -r_p \\ -Z_m r_p - X_m (R_d)_m + Z_m X_m e - \mu e \\ -X_v (R_d)_v + Z_v X_v e - \mu e \end{pmatrix}$$

Summary: Path-following;

NOT Interior-point

• staying interior is a heuristic for staying within a neighbourhood of the central path
• staying interior is required for numerical accuracy when solving the *current* ill-conditioned reduced systems

(Nearest) Euclidean Distance Matrix Completion using SDP

Given:

pre-distance matrix $A \in \mathcal{S}^n$ (nonnegative with zero diagonal)

weight matrix $H \in \mathcal{S}^n$:

$$\text{(NEDM)} \quad \mu^* = \min \frac{1}{2}\|H \circ (A - D)\|_F^2 \text{ subject to: } D \in \text{EDM}$$

$\text{EDM} = \{D = (d_{ij}) \in \mathcal{S}^n : d_{ij} = \|x_i - x_j\|^2,$ for some $x_i \in \Re^k\}$, k is *embedding dimension*

$\circ$ denotes Hadamard (elementwise) matrix product

Applications

e.g. molecular conformation problems in chemistry; multidimensional scaling and multivariate analysis problems in statistics; genetics, geography, ...

Mixed-Cone Formulation

direct approach using a mixed SDP and second-order (or Lorentz) cone problem:

$$\begin{array}{ll} \min & \alpha \\ \text{s.t.} & Y = H \circ (\mathcal{L}(X) - A), \; \|Y\|_F \leq \alpha \\ & X \in \mathcal{S}^{n-1}, Y \in \mathcal{S}^n, X \in \text{SDP} \end{array}$$

where $X \in SDP \Rightarrow \mathcal{L}(X) \in \text{EDM}$
(Public domain software packages are available, but problem size becomes large)

Connection between SDP and EDM

$$B = [x_1\ x_2\ \ldots\ x_n], \quad k \times n$$

$$D_{ij} = \|x_i - x_j\|^2 = -2x_i^T x_j + \|x_i\|^2 + \|x_j\|^2$$

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

With $X = B^T B \succeq 0$

Operator Notation:

us2vec , us2Mat , svec , sMat

$$x = \operatorname{svec}(X) \in \mathbb{R}^{\binom{n+1}{2}}, \qquad X = \operatorname{sMat}(x)$$

$\sqrt{2}$ times vector (columnwise) from upper-triang of X.
$\binom{n+1}{2} = n(n+1)/2$; $\sqrt{2}$ guarantees isometry.
$\operatorname{sMat} := \operatorname{svec}^{-1}$ mapping into $\mathcal{S}^n$
adjoint transformation $\operatorname{sMat}^* = \operatorname{svec}$:

$$\begin{aligned} \langle \operatorname{sMat}(v), S\rangle &= \operatorname{trace} \operatorname{sMat}(v) S \\ &= v^T \operatorname{svec}(S) = \langle v, \operatorname{svec}(S)\rangle \end{aligned}$$

Characterization of EDM using SDP

$$D \text{ is EDM} \quad (\subset \mathcal{S}^n)$$

iff

$$D = \mathcal{L}(X) := \begin{pmatrix} 0 & \operatorname{diag}(X)^T \\ \operatorname{diag}(X) & \operatorname{diag}(X)e^T + e\operatorname{diag}(X)^T - 2X \end{pmatrix},$$

$$\text{for some } X \succeq 0, X \in \mathcal{S}^{n-1}$$

(e is vector of ones)

$$\mathcal{L} : \mathcal{S}^{n-1} \to \mathcal{S}^n, \quad \mathcal{L}(\mathcal{S}_+^{n-1}) = \text{EDM}$$

adjoint/generalized inverse

with partition:

$$D = \begin{bmatrix} \alpha & d^T \\ d & \bar{D} \end{bmatrix},$$

where $\alpha \in \mathbb{R}$

$$\mathcal{L}^*(D) = 2\left(\mathrm{Diag}\,(d) + \mathrm{Diag}\,(\bar{D}e) - \bar{D}\right)$$

$$\mathcal{L}^\dagger(D) = \frac{1}{2}\left(de^T + ed^T - \bar{D}\right)$$

$$\mathcal{L}^*, \mathcal{L}^\dagger : \mathcal{S}^n \to \mathcal{S}^{n-1}, \quad \mathcal{L}^\dagger(EDM) = \mathcal{S}_+^{n-1}$$

Duality and Optimality Conditions

(using $X = \mathrm{sMat}\,(x) + I$) an equivalent problem is:

$$\mu^* := \min \frac{1}{2}\|H \circ (A - \mathcal{L}(X))\|_F^2 \quad \text{subject to} \quad X \succeq 0$$

strong (Lagrangian) duality holds (Slater's holds for primal and holds for dual if the graph is complete)

$$\mu^* = \nu^* := \max_{\Lambda \succeq 0} \min_X \frac{1}{2}\|H \circ (A - \mathcal{L}(X))\|_F^2 - \mathrm{trace}\,\Lambda X$$

Wolfe dual and optimality conditions

With

$$C := \mathcal{L}^*(H^{(2)} \circ A),$$

optimality conditions are:

$$\begin{array}{rcll} X & := & \mathrm{sMat}\,(x) \succeq 0 & \text{(primal feasibility)} \\ \Lambda & := & \mathcal{L}^* \left\{ H^{(2)} \circ (\mathcal{L}(X)) \right\} - C, \;\; \Lambda \succeq 0 & \text{(dual feasibility)} \\ \Lambda X & := & 0 & \text{(compl. slack.)} \end{array}$$

equivalent dual problem:

$$\text{(0.1)} \qquad \begin{array}{rl} \max & \frac{1}{2}\|H \circ (A - \mathcal{L}(X))\|_F^2 - \operatorname{trace} \Lambda X \\ \text{subject to} & \Lambda = \mathcal{L}^* \left\{ H^{(2)} \circ (\mathcal{L}(X)) \right\} - C \\ & \Lambda \succeq 0. \end{array}$$

Bilinear System

eliminate Λ
exact primal-dual feasibility during iterations
full rank Jacobian at optimality.
single bilinear (perturbed) equation in x;
$F_\mu(x) : \mathbb{R}^{\binom{n}{2}} \longrightarrow \mathcal{M}^{n-1}$

$$F_\mu(x) := \left[\mathcal{L}^* \left\{ H^{(2)} \circ (\mathcal{L}(X)) \right\} - C \right] X - \mu I = 0$$

typical SDP - overdetermined system of bilinear equations
current approach is to symmetrize - which results in
ill-conditioning! from rank deficient Jacobian at optimality.
BUT, here, no symmetrization used;
solve using (an inexact) Gauss-Newton method - with PCG

Linearization

Let $\mathcal{W}(x) := \mathcal{L}^* \left\{ H^{(2)} \circ (\mathcal{L}(x)) \right\}$

Linearization for search direction Δx at current $x = \mathrm{svec}\,(X)$:

$$F'_\mu(x)\Delta x = [\mathcal{W}(x) - C]\,\Delta x + [\mathcal{W}(\Delta x)]\,X$$

This is a linear, full rank, overdetermined system.

Our search direction Δx is its (approx.) least squares solution.

Algorithm: p-d i-e-p framework

- **Initialization:**
  - •• **Input data:** a pre-distance $n \times n$ matrix A
  - •• **Positive tolerances:**

$$\epsilon_1 \text{ (stopping)}, \ \epsilon_2 \text{ (lss accuracy)}, \ \epsilon_3 \text{ (crossover)},$$

  - •• **Find initial strictly feasible points:** both $X^0, \Lambda^0 := (\mathcal{W}(X) - C) \succ 0; \mu > 0$
  - •• **Set initial parameters:**

$$\text{gap} = \text{trace}\, \Lambda^0 X^0; \ \ \mu = \text{gap}/n; \ \ \text{objval} = f(X^0); \ \ k = 0.$$

Algorithm continued 1

- **while** $\min\{\frac{\text{gap}}{\text{objval}+1}, \text{objval}\} > \epsilon_1$
  - •• **solve lss for search direction** (accuracy $\epsilon_2 \min\{\mu, 1\}$)

$$F'_{\sigma\mu}(x^k)\left(\Delta x^k\right) = -F_{\sigma\mu}(x^k),$$

where σ_k centering, $\mu_k = \frac{1}{n}\text{trace}\,(\mathcal{W}(X^k) - C)X^k$

$$X^{k+1} = X^k + \alpha_k \Delta X^k, \quad \alpha_k > 0,$$

so that both $X^{k+1}, (\mathcal{W}(X^{k+1}) - C) \succeq 0$
($\alpha_k = 1$ after the crossover.)

  - •• **update**

$$k \leftarrow k+1 \qquad \text{and then}$$

Algorithm continued 2

- **while** $\min\{\frac{\text{gap}}{\text{objval}+1}, \text{objval}\} > \epsilon_1$
  - •• **solve lss for search direction**

    ...
  - •• **update**

$$k \leftarrow k+1 \quad \text{and then}$$

$$\sigma_k \quad \left(\text{set } \sigma_k = 0 \text{ if } \min\{\frac{\text{gap}}{\text{objval}+1}, \text{objval}\} < \epsilon_3\right)$$

- **end (while)**.
- **Conclusion:** $D = \mathcal{L}(X) \in \text{EDM}$ is approx. to A

Crossover

After the **crossover**, centering $\sigma = 0$ and steplength $\alpha = 1$, we get q-quadratic convergence; allows for *warm starts*.

Long steps can be taken *beyond* the positivity boundary. (tests show improved convergence rates)

Preconditioning

$$(\Lambda + \mathcal{X}\mathcal{W})\, P^{-1}(\widehat{\Delta x}) = -F_\mu(x),$$

where

$$\widehat{\Delta x} = P(\Delta x)$$

Diagonal Preconditioning

Optimal scaling Dennis and W. (1993) full rank matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$, with condition number $\omega(K) := n^{-1}\operatorname{trace}(K)/\det(K)^{1/n}$, the optimal scaling

$$\min \omega((AD)^T(AD)) \quad \text{subject to: } D \text{ positive and diagonal}$$

solution: $d_{ii} = 1/\|A_{:i}\|_2, i = 1, \ldots, n$
explicit expressions for preconditioner
inexpensive

Explicit Preconditioning

diagonal operator P; evaluate using columns of $F'_\mu(v)$.
$k \cong (i,j),\ 1 \le i < j \le n$, strictly upper triangular part

$$\begin{array}{rcl} \|(\Lambda + \mathcal{X}\mathcal{W})(e_k)\|_F^2 & = & \|\Lambda(e_k)\|_F^2 + \|(\mathcal{W}(e_k))X\|_F^2 \\ & & + \langle \Lambda(E_{ij}), (\mathcal{W}(E_{ij}))X \rangle , \end{array}$$

where

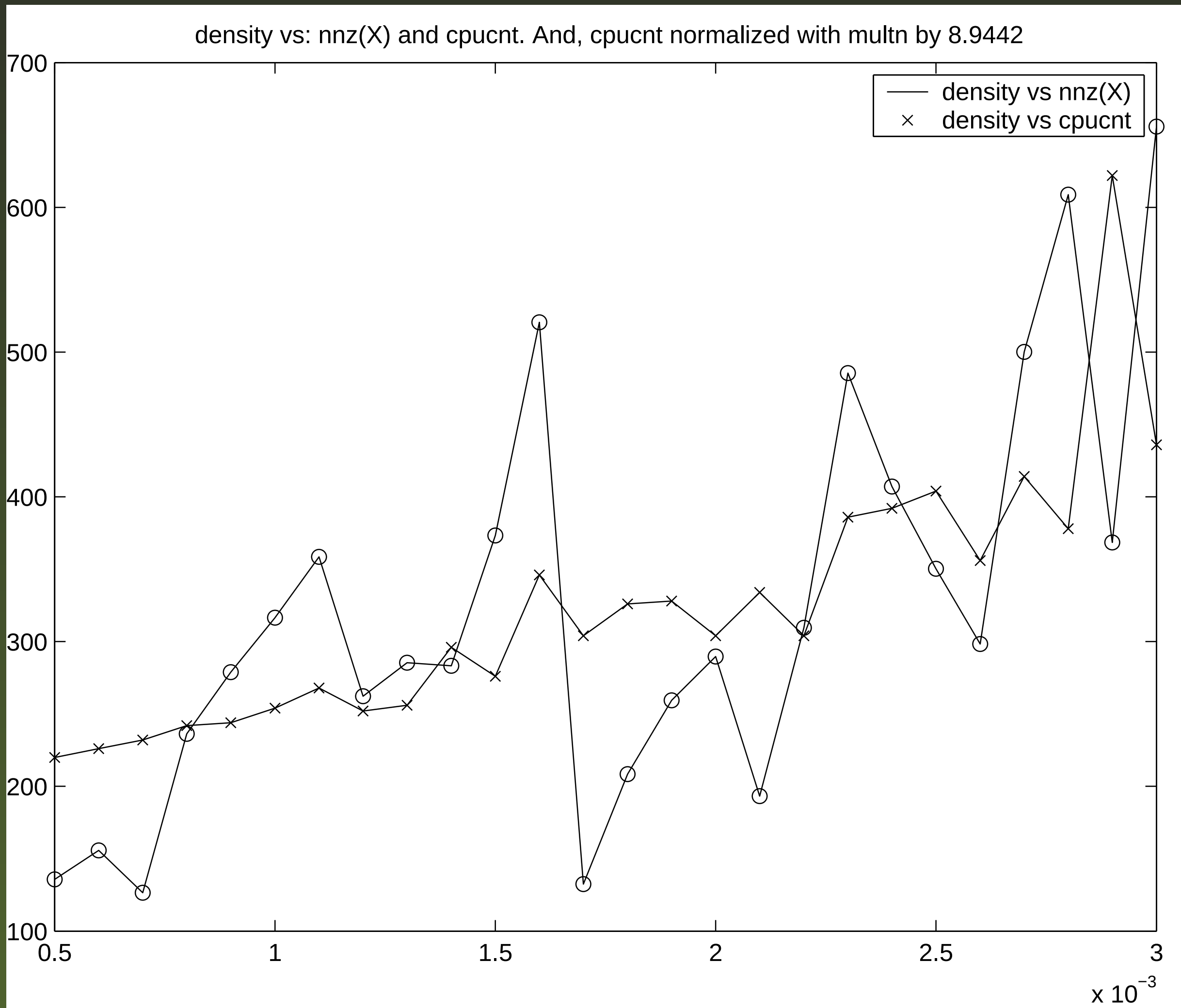
$$\Lambda(e_k) \;=\; \begin{cases} \frac{1}{\sqrt{2}}\left(\Lambda_{:i}e_j^T + \Lambda_{:j}e_i^T\right), & \text{if } i < j \\ \left(\Lambda_{:i}e_i^T\right), & \text{if } i = j. \end{cases}$$

and $\mathcal{X}\mathcal{W}$ ..... inexpensive - 50% reduction in LSQR iterations

Numerical Tests

Pentium 4; MATLAB 6.5; 1 GIG RAM.
crossover heuristic: relative duality gap $< .1$.
Stopping criteria (relative duality gap) $< \epsilon_1 = 1e-10$.
(But - average accuracy attained $1e-13$, q-quadratic convergence.)

density .0005:.001:.003, CPU times and nnz(Λ), n=200



Conclusion

Gauss-Newton direction:

- Advantages/Disadvantages:
  - Robust, warm starts are simple, longer steps
  - exact primal and dual feasibility at each iteration
  - Can apply CG-type approaches
  - q-quadratic convergence
  - scale-invariant on the right
- Future:
  - Need large sparse QR efficient as Cholesky
  - predictor-corrector

EDM Completion Problem, EDMC

- given certain fixed elements of a EDM matrix A
- the other elements are unknown (free)
- complete this matrix to an EDM

$$\mathcal{S} = \{(i,j) : A_{i,j} = \frac{1}{\sqrt{2}} b_k \text{ is known, fixed, } i < j\}, \ |S| = m,$$

$$(\text{EDMC}) \qquad \begin{array}{rcl} \mu^* := & \min & f(X) := \frac{1}{2}\|X\|_F^2 \\ & \text{subject to} & \mathcal{A}(X) = b \\ & & X \succeq 0, \end{array}$$

constraint $\mathcal{A} = \mathcal{I} \cdot \mathcal{L} : \mathcal{S}^{n-1} \rightarrow \mathbb{R}^{|S|}$ yields interpolation conditions

$$\mathcal{A}(X)_{ij} = \operatorname{trace} E_{ij} \mathcal{L}(X) = b_k, \quad \forall k \cong (ij) \in S,$$

Duality/Optimality for EDMC

- strict convexity, coercivity implies compact level sets
- EDMC attained and no duality gap (actually primal and dual attainment)

Lagrangian dual

$$\mu^* = \nu^* := \max_{\Lambda \succeq 0, y \in \mathbb{R}^{|S|}} \min_X \frac{1}{2}\|X\|_F^2 + y^T(b - \mathcal{A}(X)) - \operatorname{trace} \Lambda X$$

characterization of optimality

THEOREM Suppose that the feasible set of EDMC is not the empty set. Then the optimal solution of EDMC is $D = \mathcal{L}\left([\mathcal{A}^*(y)]_+\right)$, where y is the unique solution of the single equation

$$\mathcal{A}\left([\mathcal{A}^*(y)]_+\right) = b,$$

and B_+ denotes the projection of the symmetric matrix $B \in \mathcal{S}^{n-1}$ onto the cone $\mathcal{P}_{n-1}$.

Proof

optimality conditions after differentiation

$$
\begin{aligned}
X = \mathcal{A}^*(y) + \Lambda \succeq 0, \quad \Lambda \succeq 0, & \qquad \text{dual feasibility} \\
\mathcal{A}(X) = b & \qquad \text{primal feasibility} \\
\Lambda X = 0 & \qquad \text{complementary slackness}
\end{aligned}
$$

This means that $\mathcal{A}^*(y) = X - \Lambda$, where both $X \succeq 0, \Lambda \succeq 0$, and $\Lambda X = 0$. Therefore the three symmetric matrices $W = \mathcal{A}^*(y), X, \Lambda$ are mutually diagonalizable. We write $X = P D_X P^T$, $\Lambda = P D_\Lambda P^T$, i.e. we conclude that $W = \mathcal{A}^*(y) = P\left(D_X - D_\Lambda\right)P^T$, $D_X D_\Lambda = 0$. Therefore $[\mathcal{A}^*(y)]_+ = P D_X P^T = X$. ■

Efficient/Explicit Solution if $y \geq 0$

large class (generic?) can be solved in polytime.

COROLLARY The linear operator $\mathcal{A}$ is onto and $\mathcal{A}\mathcal{A}^*$ is nonsingular. Suppose that $y = (\mathcal{A}\mathcal{A}^*)^{-1}b \in \mathbb{R}^m_+$. Then

$$D = \mathcal{L}\left(\mathcal{A}^*(y)\right)$$

is the unique solution of EDMC .

PROOF: That $\mathcal{A}$ is onto follows from the definitions.
If $y \geq 0$, then the matrix $\mathcal{I}(y) \geq 0$ with 0 diagonal. Therefore, $X = \mathcal{L}^*(\mathcal{I}(y))$ is diagonally dominant with nonnegative diagonal, i.e. $X \succeq 0$ by Gersgorin's disk theorem. This implies that D is a distance matrix and it satisfies the interpolation conditions, i.e. it satisfies the optimality conditions in the Theorem. ■

Numerics: dim vs dens with $\#$ of failures in 100 tests

though $y = \mathcal{A}^{\dagger} b \geq 0$ does not hold in general, we still get a distance matrix D, i.e. $\mathcal{A}^*(y) \succeq 0$.

$n = 10 : 10 : 100$; density $.1 : .1 : .8$.

$n \backslash$density	.1	.2	.3	.4	.5	.6	.7	.8
10	19	27	29	25	32	27	20	38
20	6	20	23	22	27	21	28	28
30	8	8	9	9	11	16	17	24
40	2	2	6	5	14	17	20	17
50	2	0	2	8	7	8	15	12
60	1	1	1	1	3	8	15	11
70	2	0	3	1	5	7	6	15
80	1	0	0	4	2	4	9	9
90	1	0	0	1	3	2	5	6
100	0	0	0	0	1	6	5	5