Taking Advantage of Degeneracy in Cone Optimization: with Applications to Sensor Network Localization and Molecular Conformation

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February 28, 2013

Motivation: Loss of Slater CQ/Facial reduction

- optimization algorithms rely on the KKT system;
  and require that some constraint qualification (CQ) holds
  (Slater's CQ for convex conic optimization)

- However, surprisingly many conic opt, SDP relaxations,
  instances arising from applications (QAP, GP, strengthened MC, SNL, POP, Molecular Conformation)
  do not satisfy Slater's CQ/are degenerate

- lack of Slater's CQ results in: unbounded dual solutions;
  theoretical and numerical difficulties,
  in particular for *primal-dual interior-point methods*.

- solution:
  - theoretical *facial reduction* *(Borwein, W.'81[2])*
  - preprocess for regularized smaller problem (Cheung, Schurr, W.'11[4])
  - take advantage of degeneracy
    (Krislock, W.'10[7]; Krislock, Rendl, W.'10[6])

Outline: Regularization/Facial Reduction

1. Preprocessing/Regularization
   - Abstract convex program
     - LP case
     - CP case
   - Cone optimization/SDP case
2. Applications: QAP, GP, SNL, Molecular conformation ...
   - SNL; highly (implicit) degenerate/low rank solutions

Background/Abstract convex program

$$\text{(ACP)} \quad \inf_x f(x) \text{ s.t. } g(x) \preceq_K 0, x \in \Omega$$

where:

- $f : \mathbb{R}^n \to \mathbb{R}$ convex; $g : \mathbb{R}^n \to \mathbb{R}^m$ is K-convex
  - $K \subset \mathbb{R}^m$ closed convex cone; $\Omega \subseteq \mathbb{R}^n$ convex set
  - $a \preceq_K b \iff b - a \in K$
  - $g(\alpha x + (1-\alpha y)) \preceq_K \alpha g(x) + (1-\alpha) g(y)$, $\forall x, y \in \mathbb{R}^n, \forall \alpha \in [0,1]$

Slater's CQ: $\exists \hat{x} \in \Omega$ s.t. $g(\hat{x}) \in -\operatorname{int} K$ $\quad (g(x) \prec_K 0)$

- guarantees strong duality
- essential for efficiency/stability in primal-dual interior-point methods

Case of Linear Programming, LP

Primal-Dual Pair: $A, m \times n$ / $\mathcal{P} = \{1, \dots, n\}$ constr. matrix/set

$$\text{(LP-P)} \quad \begin{array}{ll} \max & b^\top y \\ \text{s.t.} & A^\top y \le c \end{array} \qquad \text{(LP-D)} \quad \begin{array}{ll} \min & c^\top x \\ \text{s.t.} & Ax = b, \ x \ge 0. \end{array}$$

Slater's CQ for (LP-P) / Theorem of alternative

$\exists \hat{y}$ s.t. $c - A^\top \hat{y} > 0$, $\quad \left((c - A^\top \hat{y})_i > 0, \forall i \in \mathcal{P} = \mathcal{P}^< \right)$

iff

$$Ad = 0, \ c^\top d = 0, \ d \ge 0 \implies d = 0 \qquad (*)$$

implicit equality constraints: $i \in \mathcal{P}^=$

Finding solution $0 \ne d^*$ to $(*)$ with max number of non-zeros determines

$$d_i^* > 0 \quad \implies (c - A^\top y)_i = 0, \forall y \in \mathcal{F}^y \quad (i \in \mathcal{P}^=)$$

Rewrite implicit-equalities to equalities/ Regularize LP

Facial Reduction: $A^\top y \leq_f c$; minimal face $f \trianglelefteq \mathbb{R}^n_+$

$$(\text{LP}_{reg}\text{-P}) \quad \begin{array}{ll} \max & b^\top y \\ \text{s.t.} & (A^<)^\top y \leq c^< \\ & (A^=)^\top y = c^= \end{array} \qquad (\text{LP}_{reg}\text{-D}) \quad \begin{array}{ll} \min & (c^<)^\top x^< + (c^=)^\top x^= \\ \text{s.t.} & \begin{bmatrix} A^< & A^= \end{bmatrix} \begin{pmatrix} x^< \\ x^= \end{pmatrix} = b \\ & x^< \geq 0, x^= \text{ free} \end{array}$$

Mangasarian-Fromovitz CQ (MFCQ) holds

(after deleting redundant equality constraints!)

$$\left(\exists \hat{y} : \quad \underset{(A^<)^\top \hat{y} < c^<}{\underline{i \in \mathcal{P}^<}} \quad \underset{(A^=)^\top \hat{y} = c^=}{\underline{i \in \mathcal{P}^=}} \right) \qquad (A^=)^\top \text{ is onto}$$

MFCQ holds iff dual optimal set is compact

Numerical difficulties if MFCQ fails; in particular for interior point methods! Modelling issue?

Facial Reduction

Linear Programming Example, $x \in \mathbb{R}^5$

$$\begin{array}{ll} \min & \begin{pmatrix} 2 & 6 & -1 & -2 & 7 \end{pmatrix} x \\ \text{s.t.} & \begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & -1 & -1 & 0 & 1 \end{bmatrix} x = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\ & x \geq 0 \end{array}$$

Sum the two constraints:

$$2x_1 + x_4 + x_5 = 0 \implies x_1 = x_4 = x_5 = 0.$$

yields the equivalent simplified problem in a smaller face

$$\begin{array}{ll} \min & \begin{pmatrix} 6 & -1 \end{pmatrix} \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} \\ \text{s.t.} & \begin{bmatrix} 1 & 1 \end{bmatrix} \begin{pmatrix} x_2 \\ x_3 \end{pmatrix} = 1 \\ & x_2, x_3 \geq 0, x_1 = x_4 = x_5 = 0 \end{array}$$

Case of ordinary convex programming, CP

$$\text{(CP)} \qquad \sup_y \; b^\top y \text{ s.t. } g(y) \leq 0,$$

where

- $b \in \mathbb{R}^m$; $g(y) = (g_i(y)) \in \mathbb{R}^n$, $g_i : \mathbb{R}^m \to \mathbb{R}$ convex $\forall i \in \mathbb{P}$
- Slater's CQ: $\exists \hat{y}$ s.t. $g_i(\hat{y}) < 0, \forall i$ (implies MFCQ)
- Slater's CQ fails implies implicit equality constraints exist, i.e.:
  $\mathcal{P}^= := \{i \in \mathcal{P} : g(y) \leq 0 \implies g_i(y) = 0\} \neq \emptyset$
  Let $\mathcal{P}^< := \mathcal{P} \backslash \mathcal{P}^=$ and
  $g^< := (g_i)_{i \in \mathcal{P}^<}, g^= := (g_i)_{i \in \mathcal{P}^=}$

Rewrite implicit equalities to *equalities*/ Regularize CP

(CP) is equivalent to $g(y) \preceq_f 0$, f is minimal face

$$(\mathrm{CP_{reg}}) \qquad \begin{array}{ll} \sup & b^\top y \\ \text{s.t.} & g^<(y) \leq 0 \\ & y \in \mathcal{F}^= \end{array} \qquad \text{or } (g^=(y) = 0)$$

where $\mathcal{F}^= := \{y : g^=(y) = 0\}$. Then

$\mathcal{F}^= = \{y : g^=(y) \leq 0\}$, so is a convex set!

Slater's CQ holds for (CP_{reg}) $\exists \hat{y} \in \mathcal{F}^= : g^<(\hat{y}) < 0$

modelling issue again?

Faithfully convex case

Faithfully convex function f (Rockafellar70 [8])

f affine on a line segment only if affine on complete line containing the segment (e.g. analytic convex functions)

$\mathcal{F}^= = \{y : g^=(y) = 0\}$ is an affine set

Then:

$\mathcal{F}^= = \{y : Vy = V\hat{y}\}$ for some $\hat{y}$ and full-row-rank matrix V.

Then MFCQ holds for

$$(\mathrm{CP_{reg}}) \qquad \begin{array}{rrcl} \sup & b^\top y & & \\ \text{s.t.} & g^<(y) & \leq & 0 \\ & Vy & = & V\hat{y} \end{array}$$

Semidefinite Programming, SDP

$K = \mathcal{S}^n_+ = K^*$ nonpolyhedral cone!

$$\text{(SDP-P)} \quad v_P = \sup_{y \in \mathbb{R}^m} b^\top y \text{ s.t. } g(y) := \mathcal{A}^* y - c \preceq_{\mathcal{S}^n_+} 0$$

$$\text{(SDP-D)} \quad v_D = \inf_{x \in \mathcal{S}^n} \langle c, x \rangle \text{ s.t. } \mathcal{A}x = b,\ x \succeq_{\mathcal{S}^n_+} 0$$

where

- PSD cone $\mathcal{S}^n_+ \subset \mathcal{S}^n$ symm. matrices
- $c \in \mathcal{S}^n$, $b \in \mathbb{R}^m$
- $\mathcal{A} : \mathcal{S}^n \to \mathbb{R}^m$ is a linear map, with adjoint $\mathcal{A}^*$

Slater's CQ/Theorem of Alternative

Assume that $\exists \tilde{y}$ s.t. $c - \mathcal{A}^* \tilde{y} \succeq 0$.

$$\exists \hat{y} \text{ s.t. } s = c - \mathcal{A}^* \hat{y} \succ 0$$

holds iff

$$\mathcal{A}d = 0,\ \langle c, d \rangle = 0,\ d \succeq 0 \implies d = 0 \qquad (*)$$

Faces of Cones - Useful for Charact. of Opt.

Face

A convex cone F is a face of K, denoted $F \trianglelefteq K$, if
$x, y \in K$ and $x + y \in F \implies x, y \in F$
($F \triangleleft K$ proper face)

Conjugate Face

If $F \trianglelefteq K$, the conjugate face (or complementary face) of F is
$F^c := F^\perp \cap K^* \trianglelefteq K^*$
If $x \in \mathrm{ri}(F)$, then $F^c = \{x\}^\perp \cap K^*$.

Minimal Faces

$f_P := \text{face}\, \mathcal{F}_P^s \trianglelefteq K$, $\mathcal{F}_P^s$ is primal feasible set
$f_D := \text{face}\, \mathcal{F}_D^x \trianglelefteq K^*$, $\mathcal{F}_D^x$ is dual feasible set

Regularization Using Minimal Face

Borwein-W.'81 [2], $f_P = \text{face}\,\mathcal{F}_P^S$

(SDP-P) is equivalent to the regularized

$$\text{(SDP}_{reg}\text{-P)} \qquad v_{RP} := \sup_y \{\langle b, y\rangle \ : \ \mathcal{A}^* y \preceq_{f_P} c\}$$

(slack $s = c - \mathcal{A}^* y \in f_p$)

Lagrangian Dual DRP Satisfies Strong Duality:

$$\text{(SDP}_{reg}\text{-D)} \quad v_{DRP} := \inf_x \{\langle c, x\rangle \ : \ \mathcal{A} x = b, \ x \succeq_{f_P^*} 0\}$$

$$= v_P = v_{RP}$$

and v_{DRP} is attained.

SDP Regularization process

Alternative to Slater CQ

$$\mathcal{A}d = 0,\ \langle c, d\rangle = 0,\ 0 \neq d \succeq_{\mathcal{S}^n_+} 0 \qquad (*)$$

Determine a proper face $f \lhd \mathcal{S}^n_+$

Let d solve $(*)$ with $d = Pd_+P^\top$, $d_+ \succ 0$, and $[P\ Q] \in \mathbb{R}^{n\times n}$ orthogonal. Then

$$\begin{aligned} c - \mathcal{A}^*y \succeq_{\mathcal{S}^n_+} 0 &\implies \langle c - \mathcal{A}^*y, d^*\rangle = 0 \\ &\implies \mathcal{F}^s_P \subseteq \mathcal{S}^n_+ \cap \{d^*\}^\perp = Q\mathcal{S}^{\bar{n}}_+ Q^\top \lhd \mathcal{S}^n_+ \end{aligned}$$

(implicit rank reduction, $\bar{n} < n$)

Regularizing SDP

- at most $n-1$ iterations to satisfy Slater's CQ.
- to check Theorem of Alternative

$$\mathcal{A}d = 0, \ \langle c, d\rangle = 0, \ 0 \neq d \succeq_{\mathcal{S}^n_+} 0, \qquad (*)$$

use auxiliary problem

$$(AP) \qquad \min_{\delta, d} \ \delta \ \text{ s.t. } \left\| \begin{bmatrix} \mathcal{A}d \\ \langle c, d\rangle \end{bmatrix} \right\|_2 \leq \delta, \quad \text{trace}(d) = \sqrt{n}, \quad d \succeq 0.$$

- Both (AP) and its dual satisfy Slater's CQ.

Regularizing SDP

Minimal face containing $\mathcal{F}_P^s := \{s : s = c - \mathcal{A}^* y \succeq 0\}$

$$f_P = Q \mathcal{S}_+^{\bar{n}} Q^\top$$

for some $n \times n$ orthogonal matrix $U = [P \; Q]$

(SPD-P) is equivalent to

$$\sup_y \; b^\top y \text{ s.t. } g^{\prec}(y) \preceq 0, \; g^{=}(y) = 0,$$

where

$$g^{\prec}(y) := Q^\top (\mathcal{A}^* y - c) Q$$

$$g^{=}(y) := \begin{bmatrix} P^\top (\mathcal{A}^* y - c) P \\ P^\top (\mathcal{A}^* y - c) Q + Q^\top (\mathcal{A}^* y - c) P \end{bmatrix}.$$

Slater's CQ holds for the reduced program:
$\exists \hat{y}$ s.t. $g^{\prec}(y) \prec 0$ and $g^{=}(y) = 0$.

Conclusion Part I

- Minimal representations of the data regularize (P); use min. face f_P (and/or implicit rank reduction)
- goal: a backwards stable preprocessing algorithm to handle (feasible) conic problems for which Slater's CQ (almost) fails

Part II: Applications of SDP where Slater's CQ fails

Instances of SDP relaxations of NP-hard combinatorial optimization problems with row and column sum and $0, 1$ constraints

- Quadratic Assignment (Zhao-Karish-Rendl-W.'96 [10])
- Graph partitioning (W.-Zhao'99 [9])

Low rank problems

- Sensor network localization (SNL) problem (Krislock-W.'10[7], Krislock-Rendl-W.'10[6])
- Molecular conformation (Burkowski-Cheung-W.'11 [3])
- general SDP relaxation of low-rank matrix completion problem

SNL (K-W10[7],K-R-W10[6])

Highly (implicit) degenerate/low-rank problem

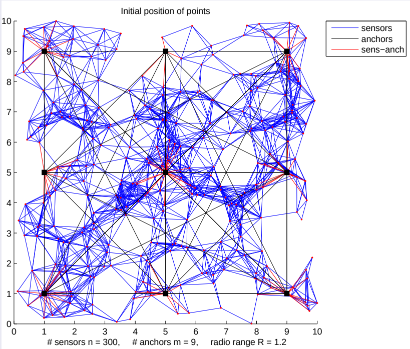
- high (implicit) degeneracy translates to low rank solutions
- fast, high accuracy solutions

SNL - a Fundamental Problem of Distance Geometry; easy to describe - dates back to Grasssmann 1886

- r : embedding dimension
- n ad hoc wireless sensors $p_1, \ldots, p_n \in \mathbb{R}^r$ to locate in $\mathbb{R}^r$;
- m of the sensors $p_{n-m+1}, \ldots, p_n$ are anchors (positions known, using e.g. GPS)
- pairwise distances $D_{ij} = \|p_i - p_j\|^2, ij \in E$, are known within radio range $R > 0$
- $$P^\top = \begin{bmatrix} p_1 & \ldots & p_n \end{bmatrix} = \begin{bmatrix} X^\top & A^\top \end{bmatrix} \in \mathbb{R}^{r \times n}$$

Sensor Localization Problem/Partial EDM

Sensors ○ and Anchors ■



Underlying Graph Realization/Partial EDM NP-Hard

Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \omega)$

- node set $\mathcal{V} = \{1, \dots, n\}$
- edge set $(i,j) \in \mathcal{E}$; $\omega_{ij} = \|p_i - p_j\|^2$ known approximately
- The anchors form a clique (complete subgraph)
- Realization of $\mathcal{G}$ in $\mathbb{R}^r$: a mapping of nodes $v_i \mapsto p_i \in \mathbb{R}^r$ with squared distances given by ω.

Corresponding Partial Euclidean Distance Matrix, EDM

$$D_{ij} = \begin{cases} d_{ij}^2 & \text{if } (i,j) \in \mathcal{E} \\ 0 & \text{otherwise (unknown distance)}, \end{cases}$$

$d_{ij}^2 = \omega_{ij}$ are known squared Euclidean distances between sensors p_i, p_j; anchors correspond to a clique.

Connections to Semidefinite Programming (SDP)

$D = \mathcal{K}(B) \in \mathcal{E}^n$, $B = \mathcal{K}^\dagger(D) \in \mathcal{S}^n \cap \mathcal{S}_C$ (centered $Be = 0$)

$P^\top = \begin{bmatrix} p_1 & p_2 & \dots & p_n \end{bmatrix} \in \mathcal{M}^{r \times n}$;
$B := PP^\top \in \mathcal{S}^n_+$ (Gram matrix of inner products);
$\operatorname{rank} B = r$; let $D \in \mathcal{E}^n$ corresponding EDM; $e = \begin{pmatrix} 1 & \dots & 1 \end{pmatrix}^\top$

$$
\begin{array}{rcl}
\text{(to } D \in \mathcal{E}^n\text{)} \quad D & = & \left(\|p_i - p_j\|_2^2\right)_{i,j=1}^n \\
& = & \left(p_i^T p_i + p_j^T p_j - 2p_i^T p_j\right)_{i,j=1}^n \\
& = & \boxed{\operatorname{diag}(B)\, e^\top + e \operatorname{diag}(B)^\top - 2B} \\
& =: & \mathcal{D}_e(B) - 2B \\
& =: & \mathcal{K}(B) \quad \text{(from } B \in \mathcal{S}^n_+\text{)}.
\end{array}
$$

Euclidean Distance Matrices and Semidefinite Matrices

Moore-Penrose Generalized Inverse $\mathcal{K}^\dagger$

$$B \succeq 0 \quad \Longrightarrow \quad D = \mathcal{K}(B) = \operatorname{diag}(B)e^\top + e\operatorname{diag}(B)^\top - 2B \in \mathcal{E}$$

$$D \in \mathcal{E} \quad \Longrightarrow \quad B = \mathcal{K}^\dagger(D) = -\frac{1}{2} J \operatorname{offDiag}(D) J \succeq 0, \; De = 0$$

Theorem (Schoenberg, 1935)

A (hollow) matrix D (with $\operatorname{diag}(D) = 0, D \in S_H$) is a Euclidean distance matrix
if and only if

$$B = \mathcal{K}^\dagger(D) \succeq 0.$$

And

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

Popular Techniques; SDP Relax.; Highly Degen.

Nearest, Weighted, SDP Approx. (relax/discard $\operatorname{rank} B$)

- $\min_{B \succeq 0} \|H \circ (\mathcal{K}(B) - D)\|$; $\operatorname{rank} B = r$;
  typical weights: $H_{ij} = 1/\sqrt{D_{ij}}$, if $ij \in E$, $H_{ij} = 0$ otherwise.
- with rank constraint: a non-convex, NP-hard program
- SDP relaxation is convex, BUT: expensive/low accuracy/implicitly highly degenerate (cliques restrict ranks of feasible Bs)

Instead: (Shall) Take Advantage of Degeneracy!

clique $\alpha, |\alpha| = k$ (corresp. $D[\alpha]$) with embed. dim. $= t \leq r < k$
$\implies \operatorname{rank} \mathcal{K}^\dagger(D[\alpha]) = t \leq r \implies \operatorname{rank} B[\alpha] \leq \operatorname{rank} \mathcal{K}^\dagger(D[\alpha]) + 1$
$\implies \operatorname{rank} B = \operatorname{rank} \mathcal{K}^\dagger(D) \leq n - \boxed{(k - t - 1)} \implies$
Slater's CQ (strict feasibility) fails

Basic Single Clique/Facial Reduction

Matrix with Fixed Principal Submatrix

For $Y \in \mathcal{S}^n$, $\alpha \subseteq \{1, \dots, n\}$: $Y[\alpha]$ denotes principal submatrix formed from rows & cols with indices α.

$\bar{D} \in \mathcal{E}^k$, $\alpha \subseteq 1{:}n$, $|\alpha| = k$

Define $\mathcal{E}^n(\alpha, \bar{D}) := \left\{D \in \mathcal{E}^n : D[\alpha] = \bar{D}\right\}$.

Given $\bar{D}$; find a corresponding $B \succeq 0$; find the corresponding face; find the corresponding subspace.

if $\alpha = 1:k$; embedding dim $\operatorname{embdim}(\bar{D}) = t \leq r$

$$D = \begin{bmatrix} \bar{D} & \cdot \\ \cdot & \cdot \end{bmatrix}.$$

BASIC THEOREM for Single Clique/Facial Reduction

THEOREM 1: Single Clique/Facial Reduction

Let: $\bar{D} := D[1:k] \in \mathcal{E}^k$, $k < n$, $\text{embdim}\,(\bar{D}) = t \leq r$;
$B := \mathcal{K}^\dagger(\bar{D}) = \bar{U}_B S \bar{U}_B^\top$, $\bar{U}_B \in \mathcal{M}^{k\times t}$, $\bar{U}_B^\top \bar{U}_B = I_t$, $S \in \mathcal{S}_{++}^\top$;
$U_B := \begin{bmatrix} \bar{U}_B & \frac{1}{\sqrt{k}}e \end{bmatrix} \in \mathcal{M}^{k\times(t+1)}$, $U := \begin{bmatrix} U_B & 0 \\ 0 & I_{n-k} \end{bmatrix}$, and
$\begin{bmatrix} V & \frac{U^\top e}{\|U^\top e\|} \end{bmatrix} \in \mathcal{M}^{n-k+t+1}$ orthogonal. Then:

$$\begin{aligned} \text{face}\,\mathcal{K}^\dagger\left(\mathcal{E}^n(1:k,\bar{D})\right) &= \left(U\mathcal{S}_+^{n-k+t+1}U^\top\right) \cap \mathcal{S}_C \\ &= (UV)\mathcal{S}_+^{n-k+t}(UV)^\top \end{aligned}$$

Note that the minimal face is defined by the subspace $\mathcal{L} = \mathcal{R}\,(UV)$. We add $\frac{1}{\sqrt{k}}e$ to represent $\mathcal{N}\,(\mathcal{K}\,)$; then we use V to eliminate e to recover a centered face.

Expense/Work of (Two) Clique/Facial Reductions

Subspace Intersection for Two Intersecting Cliques/Faces

Suppose:

$$U_1 = \begin{bmatrix} U_1' & 0 \\ U_1'' & 0 \\ 0 & I \end{bmatrix} \quad \text{and} \quad U_2 = \begin{bmatrix} I & 0 \\ 0 & U_2'' \\ 0 & U_2' \end{bmatrix}$$

Then:

$$U := \begin{bmatrix} U_1' \\ U_1'' \\ U_2'(U_2'')^\dagger U_1'' \end{bmatrix} \quad \text{or} \quad U := \begin{bmatrix} U_1'(U_1'')^\dagger U_2'' \\ U_2'' \\ U_2' \end{bmatrix}$$

($Q_1 =: (U_1'')^\dagger U_2'', Q_2 = (U_2'')^\dagger U_1''$ orthogonal/rotation)
(Efficiently) satisfies

$$\mathcal{R}(U) = \mathcal{R}(U_1) \cap \mathcal{R}(U_2)$$

Two (Intersecting) Clique Explicit Delayed Completion

COR. Intersection with Embedding Dim. r/Completion

Hypotheses of Theorem 2 holds. Let $\bar{D}_i := D[\alpha_i] \in \mathcal{E}^{k_i}$, for $i = 1, 2$, $\beta \subseteq \alpha_1 \cap \alpha_2, \gamma := \alpha_1 \cup \alpha_2, \bar{D} := D[\beta], B := \mathcal{K}^\dagger(\bar{D}), \quad \bar{U}_\beta := \bar{U}(\beta, :)$, where $\bar{U} \in \mathcal{M}^{k \times (t+1)}$ satisfies intersection equation of Theorem 2. Let $\begin{bmatrix} \bar{V} & \frac{\bar{U}^\top e}{\|\bar{U}^\top e\|} \end{bmatrix} \in \mathcal{M}^{t+1}$ be orthogonal. Let $\boxed{Z := (J\bar{U}_\beta \bar{V})^\dagger B ((J\bar{U}_\beta \bar{V})^\dagger)^\top}$. If the embedding dimension for $\bar{D}$ is r, THEN $t = r$ in Theorem 2, and $Z \in \mathcal{S}^r_+$ is the unique solution of the equation $(J\bar{U}_\beta \bar{V}) Z (J\bar{U}_\beta \bar{V})^\top = B$, and the exact completion is

$$\boxed{D[\gamma] = \mathcal{K}\left(PP^\top\right)} \quad \text{where} \quad \boxed{P := UVZ^{\frac{1}{2}} \in \mathbb{R}^{|\gamma| \times r}}$$

Completing SNL (Delayed use of Anchor Locations)

Rotate to Align the Anchor Positions

- Given $P = \begin{bmatrix} P_1 \\ P_2 \end{bmatrix} \in \mathbb{R}^{n \times r}$ such that $D = \mathcal{K}(PP^\top)$
- Solve the orthogonal Procrustes problem:

$$\begin{array}{ll} \min & \|A - P_2 Q\| \\ \text{s.t.} & Q^\top Q = I \end{array}$$

$P_2^\top A = U\Sigma V^\top$ SVD decomposition; set $Q = UV^\top$; (Golub/Van Loan79[5], Algorithm 12.4.1)

- Set $X := P_1 Q$

Summary: Facial Reduction for Cliques

- Using the basic theorem: each clique corresponds to a Gram matrix/corresponding subspace/corresponding face of SDP cone (implicit rank reduction)
- In the case where two cliques intersect, the union of the cliques correspond to the (efficiently computable) intersection of the corresponding faces/subspaces
- Finally, the positions are determined using a Procrustes problem

Results - Data for Random Noisless Problems

- 2.16 GHz Intel Core 2 Duo, 2 GB of RAM
- Dimension $r = 2$
- Square region: $[0, 1] \times [0, 1]$
- $m = 9$ anchors
- Using only Rigid Clique Union and Rigid Node Absorption
- Error measure: Root Mean Square Deviation

$$\text{RMSD} = \left(\frac{1}{n} \sum_{i=1}^{n} \|p_i - p_i^{\text{true}}\|^2 \right)^{1/2}$$

Results - Large n (SDP size $O(n^2)$)

n # of Sensors Located

n # sensors \ R	0.07	0.06	0.05	0.04
2000	2000	2000	1956	1374
6000	6000	6000	6000	6000
10000	10000	10000	10000	10000

CPU Seconds

# sensors \ R	0.07	0.06	0.05	0.04
2000	1	1	1	3
6000	5	5	4	4
10000	10	10	9	8

RMSD (over located sensors)

n # sensors \ R	0.07	0.06	0.05	0.04
2000	$4e-16$	$5e-16$	$6e-16$	$3e-16$
6000	$4e-16$	$4e-16$	$3e-16$	$3e-16$
10000	$3e-16$	$5e-16$	$4e-16$	$4e-16$

Results - N Huge SDPs Solved

Large-Scale Problems

# sensors	# anchors	radio range	RMSD	Time
20000	9	.025	$5e-16$	25s
40000	9	.02	$8e-16$	1m 23s
60000	9	.015	$5e-16$	3m 13s
100000	9	.01	$6e-16$	9m 8s

Size of SDPs Solved: $N = \binom{n}{2}$ (# vrbls)

$\mathcal{E}_n(\text{density of } \mathcal{G}) = \pi R^2$; $M = \mathcal{E}_n(|E|) = \pi R^2 N$ (# constraints)

Size of SDP Problems:

$M = \left[3,078,915 \quad 12,315,351 \quad 27,709,309 \quad 76,969,790\right]$

$N = 10^9 \left[0.2000 \quad 0.8000 \quad 1.8000 \quad 5.0000\right]$

Molecular conformation

- protein structure prediction problems;
- work with Babak et. al.11[1];
- side chain packing.

(see pages 8-22 in alternate pdf file)

Summary Part II

- Instances of degeneracy/failurs of Slater's CQ occur in many applications
- SDP relaxation of SNL is highly (implicitly) degenerate: The feasible set of this SDP is restricted to a low dim. face of the SDP cone, causing the Slater's CQ (strict feasibility) to fail
- We take advantage of this degeneracy by finding explicit representations of intersections of faces of the SDP cone corresponding to unions of intersecting cliques
- <u>Without</u> using an SDP-solver (eg. SeDuMi or SDPT3), we quickly compute the exact solution to the SDP relaxation

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Thanks for your attention!

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February 28, 2013