# Taking advantage of Degeneracy in Cone Optimization with Applications to Sensor Network Localization and Molecular Conformation 

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## Outline

## Part I: Sensor Network Localization, SNL, Henry Wolkowicz

- exploiting implicit degeneracy
- solving huge problems
- high accuracy (low rank) solutions
(With: N. Krislock, F. Rendl)


## Part II: Preprocessing and Reduction for Degenerate Semidefinite Programs, Y-L (Vris) Cheung

- backward stable preprocessing technique using rank-revealing rotations
- (strict) complementarity and duality gaps
(With: S. Schurr and H. Wolkowicz)


## Part I: Sensor Network Localization, SNL, Problem (Exploiting (Implicit) Degeneracy)

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

- $n$ ad hoc wireless sensors (nodes) to locate in $\mathbb{R}^{r}$, ( $r$ is embedding dimension;
sensors $\left.p_{i} \in \mathbb{R}^{r}, i \in V:=1, \ldots, n\right)$
- $m$ of the sensors are anchors, $p_{i}, i=n-m+1, \ldots, n$ ) (positions known, using e.g. GPS)
- pairwise distances $D_{i j}=\left\|p_{i}-p_{j}\right\|^{2}, i j \in E$, are known within radio range $R>0$
- 

$$
P^{T}=\left[\begin{array}{lll}
p_{1} & \ldots & p_{n}
\end{array}\right]=\left[\begin{array}{ll}
X^{\top} & A^{T}
\end{array}\right] \in \mathbb{R}^{r \times n}
$$

## Applications

> Horst Stormer (Nobel Prize, Physics, 1998), "21 Ideas for the 21st Century", Business Week. 8/23-30, 1999

Untethered micro sensors will go anywhere and measure anything - traffic flow, water level, number of people walking by, temperature. This is developing into something like a nervous system for the earth, a skin for the earth. The world will evolve this way.

## Tracking Humans/Animals/Equipment/Weather

- geographic routing; data aggregation; topological control; soil humidity; earthquakes and volcanos; weather and ocean currents; radiation levels.
- military; tracking of goods; vehicle positions; surveillance; random deployment in inaccessible terrains.
- brain scans


## Underlying Graph Realization/Partial EDM NP-Hard

## Graph

- node set $\mathcal{V}=\{1, \ldots, n\}$
- edge set $(i, j) \in \mathcal{E} ; \omega_{i j}=\left\|p_{i}-p_{j}\right\|^{2}$ known approximately
- The anchors form a clique (complete subgraph)
- Realization of $\mathcal{G}$ in $\Re^{r}$ : a mapping of node $v_{i} \rightarrow p_{i} \in \Re^{r}$ with squared distances given by $\omega$.

Corresponding Partial Euclidean Distance Matrix, EDM

$$
D_{i j}=\left\{\begin{array}{cl}
d_{i j}^{2} & \text { if }(i, j) \in \mathcal{E} \\
0 & \text { otherwise (unknown distance) }
\end{array}\right.
$$

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

## Sensor Localization Problem/Partial EDM



## Molecular Conformation: $r=3$, no anchors

## Distance Geometry Description

From Experimental data, e.g. NMR spectroscopy
(1) a list of distances (lower and upper bounds on the distances between pairs of atoms)
(2) chirality constraints (chirality of its rigid quadruples of atoms)

## Connections to Semidefinite Programming (SDP)

## , Cone of (symmetric) SDP matrices in <br> inner product $\langle A, B\rangle=$ trace $A B$ <br> Löwner (psd) partial order $A \succeq B, A \succ B$

$D=\mathcal{K}(B) \in \mathcal{E}^{n}, B=\mathcal{K}^{\dagger}(D) \in \mathcal{S}^{n} \cap S_{C}$

## (centered Be

$P^{T}=\left[\begin{array}{llll}p_{1} & p_{2} & \ldots & p_{n}\end{array}\right] \in \mathcal{M}^{r \times n} ;$
$B:=P P^{T} \in \mathcal{S}_{+}^{n}$ (Gram matrix of inner products);
$\operatorname{rank} B=r$; let $D \in \mathcal{E}^{n}$ corresponding EDM ; $e=\left(\begin{array}{lll}1 & \ldots & 1\end{array}\right)^{T}$

$$
\begin{aligned}
\left(\text { to } D \in \mathcal{E}^{n}\right) \quad D & =\left(\left\|p_{i}-p_{j}\right\|_{2}^{2}\right)_{i, j=1}^{n} \\
& =\left(p_{i}^{T} p_{i}+p_{j}^{T} p_{j}-2 p_{i}^{T} p_{j}\right)_{i, j=1}^{n} \\
& =\operatorname{diag}(B) e^{T}+e \operatorname{diag}(B)^{T}-2 B \\
& =: \mathcal{\mathcal { D } _ { e } ( B ) - 2 B} \\
& \left.=: \mathcal{K}(B) \quad \text { (from } B \in \mathcal{S}_{+}^{n}\right) .
\end{aligned}
$$

## Euclidean Distance, EDM, and Semidefinite, SDP, Matrices

Moore-Penrose Generalized Inverse

$$
\begin{aligned}
B \succeq 0 & \Longrightarrow \quad D=\mathcal{K}(B)=\operatorname{diag}(B) e^{T}+e \operatorname{diag}(B)^{T}-2 B \in \mathcal{E} \\
D \in \mathcal{E} & \left.\Longrightarrow \quad B=\mathcal{K}^{\dagger}(D)=-\frac{1}{2} J(\text { offDiag }) J\right) \succeq 0, D e=0
\end{aligned}
$$

## Theorem (Schoenberg, 1935)

A (hollow) matrix $D$ with $\operatorname{diag}(D)=0\left(D \in S_{H}\right)$ is a
Euclidean distance matrix
if and only if

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

And

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

## Linear Transformations:

- allow: $\mathcal{D}_{v}(B):=\operatorname{diag}(B) v^{T}+v \operatorname{diag}(B)^{T}$;

$$
\mathcal{D}_{v}(y):=y v^{\top}+v y^{\top}
$$

- adjoint $\mathcal{K}^{*}(D)=2(\operatorname{Diag}(D e)-D)$.
- $\mathcal{K}$ is $1-1$, onto between centered $\&$ hollow subspaces
$\mathcal{S}_{C}:=\left\{B \in \mathcal{S}^{n}: B e=0\right\} ;$
$\mathcal{S}_{H}:=\left\{D \in \mathcal{S}^{n}: \operatorname{diag}(D)=0\right\}=\mathcal{R}($ offDiag $)$
- $J:=I-\frac{1}{n} e e^{T}$ (orthogonal projection onto $M:=\{e\}^{\perp}$ );
- $\mathcal{T}(D):=-\frac{1}{2} \operatorname{JoffDiag}(D) J \quad\left(=\mathcal{K}^{\dagger}(D)\right)$


## Popular Techniques; SDP Relax.; Highly Degen.

Nearest, Weighted, SDP Approx. (relax/discard rank B)

- $\min _{B \succeq 0, B \in \Omega}\|H \circ(\mathcal{K}(B)-D)\| ;$ rank $B=r$; typical weights: $H_{i j}=1 / \sqrt{D_{i j}}$, if $i j \in E$.
- 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 $B \mathrm{~s}$ )


## Instead: (Shall) Take Advantage of Degeneracy!

(1) given clique $\alpha,|\alpha|=k$; with corresp. principal EDM block $D[\alpha]$; and embed. dim. $=t \leq r<k$
(2) IMPLIES a restriction on rank of corresp. Gram matrix: rank $\left(\mathcal{K}^{\dagger}(D[\alpha])\right)=t \leq r$
(3) IMPLIES a restriction on rank of principal block of main Gram matrix: $\operatorname{rank}(B[\alpha]) \leq \operatorname{rank}\left(\mathcal{K}^{\dagger}(D[\alpha])\right)+1$
(9) IMPLIES $\operatorname{rank} B=\operatorname{rank}\left(\mathcal{K}^{\dagger}(D)\right) \leq n-(k-t-1)$
(6) IMPLIES Slater's CQ (strict feasibility) fails

## Semidefinite Cone, Faces

## Faces of cone $K$

- $F \subseteq K$ is a face of $K$, denoted $F \unlhd K$, if

$$
\left(x, y \in K, \frac{1}{2}(x+y) \in F\right) \Longrightarrow(\operatorname{cone}\{x, y\} \subseteq F)
$$

- $F \triangleleft K$, if $F \unlhd K, F \neq K ; F$ is proper face if $\{0\} \neq F \triangleleft K$.
- $F \unlhd K$ is exposed if: intersection of $K$ with a hyperplane.
- face $(S)$ denotes smallest face of $K$ that contains set $S$.
- if $S$ is convex set, $F$ is a face

is a Facially Exposed Cone
All faces are exposed.


## Facial Structure of SDP Cone; Equivalent SUBSPACES

Face $F \unlhd S^{n}$ Equivalence to $\mathcal{R}(U)$ Subspace of $\mathbb{R}^{n}$
$F \unlhd \mathcal{S}_{+}^{n}$ determined by range of any $S \in$ relint $F$,
i.e. let $S=U \Gamma U^{\top}$ be compact spectral decomposition; $\Gamma \in \mathcal{S}_{++}^{t}$ is diagonal matrix of pos. eigenvalues; $F=U \mathcal{S}_{+}^{t} U^{T}$
( $F$ associated with $\mathcal{R}(U)$ )

$$
\operatorname{dim} F=t(t+1) / 2
$$

face $F$ representation by subspace $\mathcal{L}$
(subspace) $\mathcal{L}=\mathcal{R}(T), T$ is $n \times t$ full column, then:

$$
F:=T \mathcal{S}_{+}^{t} T^{T} \unlhd \mathcal{S}_{+}^{n}, \quad \text { relint }(F)=T \mathcal{S}_{++}^{t} T^{T}
$$

## Basic Single Clique/Facial Reduction



Given $\bar{D}$; find a corresponding $B \succeq 0$; find the corresponding face; find the corresponding subspace.
if $\alpha=1: k$; embedding dim embdim ( $\bar{D}$ )

$$
D=\left[\begin{array}{ll}
\bar{D} & \cdot \\
\cdot & .
\end{array}\right],
$$

## THEOREM 1: Single Clique/Facial Reduction

Let: $\bar{D}:=D[1: k] \in \mathcal{E}^{k}, k<n$, $\operatorname{embdim}(\bar{D})=t \leq r$;
$B:=\mathcal{K}^{\dagger}(\bar{D})=\bar{U}_{B} S \bar{U}_{B}^{T}, \bar{U}_{B} \in \mathcal{M}^{k \times t}, \bar{U}_{B}^{T} \bar{U}_{B}=I_{t}, S \in \mathcal{S}_{++}^{t} ;$
$U_{B}:=\left[\begin{array}{ll}\bar{U}_{B} & \frac{1}{\sqrt{k}} e\end{array}\right] \in \mathcal{M}^{k \times(t+1)}, U:=\left[\begin{array}{cc}U_{B} & 0 \\ 0 & I_{n-k}\end{array}\right]$, and
$\left[\begin{array}{ll}V & \frac{U^{T} e}{\left\|U^{T} e\right\|}\end{array}\right] \in \mathcal{M}^{n-k+t+1}$ orthogonal. Then:

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

Note that the minimal face is defined by the subspace $\mathcal{L}=\mathcal{R}(U V)$. 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.

## Facial Reduction for Disjoint Cliques

## Corollary from Basic Theorem

let $\alpha_{1}, \ldots, \alpha_{\ell} \subseteq 1: n$ pairwise disjoint sets, wlog:
$\alpha_{i}=\left(k_{i-1}+1\right): k_{i}, k_{0}=0, \alpha:=\bigcup_{i=1}^{\ell} \alpha_{i}=1:|\alpha|$ let
$\bar{U}_{i} \in \mathbb{R}^{\left|\alpha_{i}\right| \times\left(t_{i}+1\right)}$ with full column rank satisfy $e \in \mathcal{R}\left(\bar{U}_{i}\right)$ and

$$
U_{i}:=\begin{gathered}
k_{i-1} \\
\left|\alpha_{i}\right| \\
n-k_{i}
\end{gathered}\left[\begin{array}{ccc}
k_{i-1} & t_{i}+1 & n-k_{i} \\
1 & 0 & 0 \\
0 & \bar{U}_{i} & 0 \\
0 & 0 & l
\end{array}\right] \in \mathbb{R}^{n \times\left(n-\left|\alpha_{i}\right|+t_{i}+1\right)}
$$

The minimal face is defined by $\mathcal{L}=\mathcal{R}(U)$ :

$$
\begin{aligned}
& \begin{array}{llll}
t_{1}+1 & \ldots & t_{\ell}+1 & n-|\alpha|
\end{array} \\
& U:=\begin{array}{c}
\left|\alpha_{1}\right| \\
\vdots \\
\left|\alpha_{\ell}\right| \\
n-|\alpha|
\end{array}\left[\begin{array}{cccc}
\bar{U}_{1} & \ldots & 0 & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & \bar{U}_{\ell} & 0 \\
0 & \ldots & 0 & 1
\end{array}\right] \in \mathbb{R}^{n \times(n-|\alpha|+t+1)}, \\
& \text { where } t:=\sum_{i=1}^{\ell} t_{i}+\ell-1 \text {. And } e \in \mathcal{R}(U) \text {. }
\end{aligned}
$$

## Sets for Intersecting Cliques/Faces



For each clique $|\alpha|=k$, we get a corresponding face/subspace ( $k \times r$ matrix) representation. We now see how to handle two cliques, $\alpha_{1}, \alpha_{2}$, that intersect.

## Two (Intersecting) Clique Reduction/Subsp. Repres.

THEOREM 2: Clique/Facial Intersection Using Subspace Intersection
$\left\{\alpha_{1}, \alpha_{2} \subseteq 1: n_{;} \quad k:=\left|\alpha_{1} \cup \alpha_{2}\right|\right.$
For $i=1,2: \bar{D}_{i}:=D\left[\alpha_{i}\right] \in \mathcal{E}^{k_{i}}$, embedding dimension $t_{i}$;
$B_{i}:=\mathcal{K}^{\dagger}\left(\bar{D}_{i}\right)=\bar{U}_{i} S_{i} \bar{U}_{i}^{\top}, \bar{U}_{i} \in \mathcal{M}^{k_{i} \times t_{i}}, \bar{U}_{i}^{T} \bar{U}_{i}=I_{t_{i}}, S_{i} \in \mathcal{S}_{++}^{t_{i}} ;$ $U_{i}:=\left[\begin{array}{ll}\bar{U}_{i} & \frac{1}{\sqrt{k_{i}}} e\end{array}\right] \in \mathcal{M}^{k_{i} \times\left(t_{i}+1\right)} ;$ and $\bar{U} \in \mathcal{M}^{k \times(t+1)}$ satisfies

$$
\mathcal{R}(\bar{U})=\mathcal{R}\left(\left[\begin{array}{cc}
U_{1} & 0 \\
0 & I_{\bar{k}_{3}}
\end{array}\right]\right) \cap \mathcal{R}\left(\left[\begin{array}{cc}
I_{\bar{k}_{1}} & 0 \\
0 & U_{2}
\end{array}\right]\right) \text {, with } \bar{U}^{T} \bar{U}=I_{t+1}
$$

## cont...

## Two (Intersecting) Clique Reduction, cont. . .

THEOREM 2 Nosing. Clique/Facial Inters. cont. . .
cont. . . with
$\mathcal{R}(\bar{U})=\mathcal{R}\left(\left[\begin{array}{cc}U_{1} & 0 \\ 0 & \bar{k}_{k_{3}}\end{array}\right]\right) \cap \mathcal{R}\left(\left[\begin{array}{cc}c_{k_{1}} & 0 \\ 0 & U_{2}\end{array}\right]\right)$, with $\bar{U}^{T} \bar{U}=I_{t+1}$
let: $U:=\left[\begin{array}{cc}\bar{U} & 0 \\ 0 & I_{n-k}\end{array}\right] \in \mathcal{M}^{n \times(n-k+t+1)}$ and
$\left[\begin{array}{ll}V & \frac{U^{\top} e}{\left\|U^{\top} e\right\|}\end{array}\right] \in \mathcal{M}^{n-k+t+1}$ be orthogonal. Then
$\underline{\underline{\bigcap_{i=1}^{2} \text { face } \mathcal{K}^{\dagger}\left(\mathcal{E}^{n}\left(\alpha_{i}, \bar{D}_{i}\right)\right)}}=\left(U \mathcal{S}_{+}^{n-k+t+1} U^{\top}\right) \cap \mathcal{S}_{C}$
$=(U V) \mathcal{S}_{+}^{n-k+t}(U V)^{T}$

## Expense/Work of (Two) Clique/Facial Reductions

## Subspace Intersection for Two Intersecting Cliques/Faces

Suppose:

$$
U_{1}=\left[\begin{array}{cc}
U_{1}^{\prime} & 0 \\
U_{1}^{\prime \prime} & 0 \\
0 & 1
\end{array}\right] \quad \text { and } \quad U_{2}=\left[\begin{array}{cc}
1 & 0 \\
0 & U_{2}^{\prime \prime} \\
0 & U_{2}^{\prime}
\end{array}\right]
$$

Then:

$$
U:=\left[\begin{array}{c}
U_{1}^{\prime} \\
U_{1}^{\prime \prime} \\
U_{2}^{\prime}\left(U_{2}^{\prime \prime}\right)^{\dagger} U_{1}^{\prime \prime}
\end{array}\right] \quad \text { or } \quad U:=\left[\begin{array}{c}
U_{1}^{\prime}\left(U_{1}^{\prime \prime}\right)^{\dagger} U_{2}^{\prime \prime} \\
U_{2}^{\prime \prime} \\
U_{2}^{\prime}
\end{array}\right]
$$

$\left(Q_{1}=:\left(U_{1}^{\prime \prime}\right)^{\dagger} U_{2}^{\prime \prime}, Q_{2}=\left(U_{2}^{\prime \prime}\right)^{\dagger} U_{1}^{\prime \prime}\right.$ orthogonal/rotation)
(Efficiently) satisfies

$$
\mathcal{R}(U)=\mathcal{R}\left(U_{1}\right) \cap \mathcal{R}\left(U_{2}\right)
$$

## Two (Intersecting) Clique Reduction Figure



Completion: missing distances can be recovered if desired.

## Two (Intersecting) Clique Explicit Delayed Completion

## COR. Intersection with Embedding Dim. r/Completion

Hypotheses of Theorem 2 holds. Let $\bar{D}_{i}:=D\left[\alpha_{i}\right] \in \mathcal{E}^{k_{i}}$, 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 $\left[\begin{array}{ll}\bar{V} & \frac{\bar{U}^{\top} e}{\left\|U^{T} e\right\|}\end{array}\right] \in \mathcal{M}^{t+1}$
be orthogonal. Let $Z:=\left(J \bar{U}_{\beta} \bar{V}\right)^{\dagger} B\left(\left(J \bar{U}_{\beta} \bar{V}\right)^{\dagger}\right)^{\top}$. 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
$\left(J \bar{U}_{\beta} \bar{V}\right) Z\left(J \bar{U}_{\beta} \bar{V}\right)^{T}=B$, and the exact completion is

$$
D[\gamma]=\mathcal{K}\left(P P^{T}\right) \text { where } P:=U V Z^{\frac{1}{2}} \in \mathbb{R}^{|\gamma| \times r}
$$

## Completing SNL (Delayed use of Anchor Locations)

## Rotate to Align the Anchor Positions

- Given $P=\left[\begin{array}{l}P_{1} \\ P_{2}\end{array}\right] \in \mathbb{R}^{n \times r}$ such that $D=\mathcal{K}\left(P P^{T}\right)$
- Solve the orthogonal Procrustes problem:

$$
\begin{array}{cc}
\min & \left\|A-P_{2} Q\right\| \\
\text { s.t. } & Q^{T} Q=I
\end{array}
$$

$P_{2}^{T} A=U \Sigma V^{T}$ SVD decomposition; set $Q=U V^{T}$;
(Golub/Van Loan, Algorithm 12.4.1)

- Set $X:=P_{1} Q$


## Algorithm: Four Cases

Non-rigid

## ALGOR: clique union; facial reduct.; delay compl.

Initialize: Find initial set of cliques.

$$
C_{i}:=\left\{j:\left(D_{p}\right)_{i j}<(R / 2)^{2}\right\}, \quad \text { for } i=1, \ldots, n
$$

## Iterate

- For $\left|C_{i} \cap C_{j}\right| \geq r+1$, do Rigid Clique Union
- For $\left|C_{i} \cap \mathcal{N}(j)\right| \geq r+1$, do Rigid Node Absorption
- For $\left|C_{i} \cap C_{j}\right|=r$, do Non-Rigid Clique Union (lower bnds)
- For $\left|C_{i} \cap \mathcal{N}(j)\right|=r$, do Non-Rigid Node Absorp. (lower bnds)


## Finalize

When $\exists$ a clique containing all anchors, use computed facial representation and positions of anchors to solve for $X$

## 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

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

$n$ \# of Sensors Located

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

## Results - N Huge SDPs Solved

## Large-Scale Problems

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

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

$\mathcal{E}_{n}($ density of $\mathcal{G})=\pi R^{2} ; M=\mathcal{E}_{n}(|E|)=\pi R^{2} N$ (\# constraints)
Size of SDP Problems:

$$
\begin{aligned}
& M=\left[\begin{array}{lllll}
3,078,915 & 12,315,351 & 27,709,309 & 76,969,790
\end{array}\right] \\
& N=10^{9}\left[\begin{array}{llll}
0.2000 & 0.8000 & 1.8000 & 5.0000
\end{array}\right]
\end{aligned}
$$

## Locally Recover Exact EDMs

## Nearest EDM

- Given clique $\alpha$; corresp. EDM $D_{\epsilon}=D+N_{\epsilon}, N_{\epsilon}$ noise
- we need to find the smallest face containing $\mathcal{E}^{n}(\alpha, D)$.
- $\left\{\begin{array}{cl}\min & \left\|\mathcal{K}(X)-D_{\epsilon}\right\| \\ \text { s.t. } & \operatorname{rank}(X)=r, X e=0, X \succeq 0 \\ & X \succeq 0 .\end{array}\right.$
- Eliminate the constraints: $V e=0, V^{\top} V=I$,
$\mathcal{K}{ }_{V}(X):=\mathcal{K}\left(V X V^{T}\right):$

$$
\begin{array}{cl}
U_{r}^{*} \in \underset{\operatorname{argmin}}{ } & \frac{1}{2}\left\|\mathcal{K}_{V}\left(U U^{T}\right)-D_{\epsilon}\right\|_{F}^{2} \\
\text { s.t. } & U \in M^{(n-1) r} .
\end{array}
$$

The nearest EDM is $D^{*}=\mathcal{K}_{v}\left(U_{r}^{*}\left(U_{r}^{*}\right)^{T}\right)$.

## Solve Overdetermined Nonlin. Least Squares Prob.

Newton (expensive) or Gauss-Newton (less accurate)

$$
F(U):=u s 2 \operatorname{vec}\left(\mathcal{K}_{V}\left(U U^{T}\right)-D_{\epsilon}\right), \quad \min _{U} f(U):=\frac{1}{2}\|F(U)\|^{2}
$$

## Derivatives: gradient and Hessian

$$
\begin{gathered}
\nabla f(U)(\Delta U)=\left\langle 2\left(\mathcal{K}_{V}^{*}\left[\mathcal{K}_{V}\left(U U^{T}\right)-D_{\epsilon}\right]\right) U, \Delta U\right\rangle \\
\nabla^{2} f(U)=2 \operatorname{vec}\left(\mathcal{L}_{U}^{*} \mathcal{K}_{V}^{*} \mathcal{K}_{V} \mathcal{S}_{\Sigma} \mathcal{L}_{U}+\mathcal{K}_{V}^{*}\left(\mathcal{K}_{V}\left(U U^{T}\right)-D_{\epsilon}\right)\right) \text { Mat } \\
\text { where } \mathcal{L} U(\cdot)=\cdot U^{T} ; \quad \mathcal{S}_{\Sigma}(U)=\frac{1}{2}\left(U+U^{T}\right)
\end{gathered}
$$

## random noisy probs; $r=2, m=9, n f=1 e-6$

- Using only Rigid Clique Union, preliminary results:



## Summary Part I

- 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 constraint qualification (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
- Without using an SDP-solver (eg. SeDuMi or SDPT3), we quickly compute the exact solution to the SDP relaxation


## Thanks for your attention!

# Taking advantage of Degeneracy in Cone Optimization with Applications to Sensor Network Localization and Molecular Conformation 

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Tues. July 19, 3-5PM, Room:14


