Semidefinite Facial Reduction for Euclidean Distance Matrix Completion

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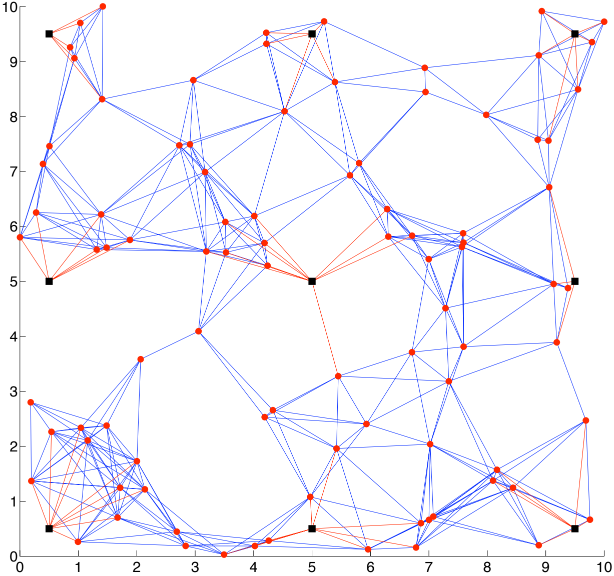
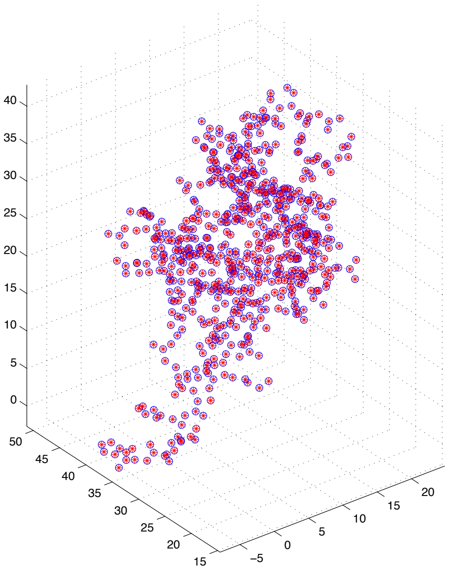
Sensor Network Localization



Molecular Conformation



Previous Work I

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Semidefinite programming for ad hoc wireless sensor network localization.
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Pratik Biswas, Tzu-Chen Liang, Kim-Chuan Toh, Ta-Chung Wang, and Yinyu Ye.
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IEEE Transactions on Automation Science and Engineering, 3:360–371, 2006.

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A distributed SDP approach for large-scale noisy anchor-free graph realization with applications to molecular conformation.
SIAM Journal on Scientific Computing, 30(3):1251–1277, 2008.

Previous Work II

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Sunyoung Kim, Masakazu Kojima, and Hayato Waki.
Exploiting sparsity in SDP relaxation for sensor network localization.
SIAM Journal on Optimization, 20(1):192–215, 2009.

Ting Pong and Paul Tseng.
(Robust) Edge-based semidefinite programming relaxation of sensor network localization.
Mathematical Programming, 2010.
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Explicit sensor network localization using semidefinite representations and facial reductions.
To appear in SIAM Journal on Optimization, 2010.

Summary

- We developed a theory of semidefinite facial reduction for the EDM completion problem
- Using this theory, we can transform the SDP relaxations into much smaller equivalent problems
- We developed a highly efficient algorithm for EDM completion:
  - SDP solver not required
  - can solve problems with up to 100,000 sensors in a few minutes on a laptop computer
  - obtained very high accuracy for noiseless problems
  - our running times are highly competitive with other SDP-based codes

Outline

1. Euclidean Distance Matrices
   - Introduction
   - Euclidean Distance Matrices and Semidefinite Matrices

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1. Euclidean Distance Matrices
   - Introduction
   - Euclidean Distance Matrices and Semidefinite Matrices
2. Facial Reduction
   - Semidefinite Facial Reduction
3. Results
   - Facial Reduction Theory for EDM Completion
   - Numerical Results
   - Noisy Problems

Outline

Introduction

Euclidean Distance Matrices

- An $n \times n$ matrix D is an EDM if $\exists p_1, \ldots, p_n \in \mathbb{R}^r$

$$D_{ij} = \|p_i - p_j\|^2, \qquad \text{for all } i, j = 1, \ldots, n$$

- $\mathcal{E}^n :=$ set of all $n \times n$ EDMs

Embedding Dimension of $D \in \mathcal{E}^n$

$$\mathrm{embdim}(D) := \min \left\{ r : \exists p_1, \ldots, p_n \in \mathbb{R}^r \text{ s.t. } D_{ij} = \|p_i - p_j\|^2, \text{ for all } i, j \right\}$$

Introduction

Partial Euclidean Distance Matrices

D is a partial EDM in $\mathbb{R}^r$ if

- every entry D_{ij} is either “specified” or “unspecified”, $\operatorname{diag}(D) = 0$
- for all $\alpha \subseteq \{1, \dots, n\}$, if the principal submatrix $D[\alpha]$ is fully specified, then $D[\alpha]$ is an EDM with $\operatorname{embdim}(D[\alpha]) \le r$

Problem: determine if there is a completion $\hat{D} \in \mathcal{E}^n$ with $\operatorname{embdim}(\hat{D}) = r$

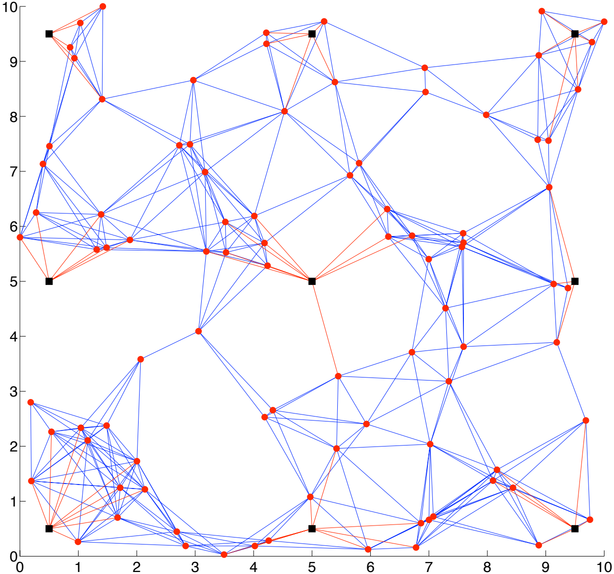
Graph of a Partial EDM

$G = (N, E, \omega)$ weighted graph with

- nodes $N := \{1, \dots, n\}$
- edges $E := \{ij : i \neq j, \text{and } D_{ij} \text{ is specified}\}$
- weights $\omega \in \mathbb{R}^E_+$ with $\omega_{ij} := \sqrt{D_{ij}}$

Problem: determine if there is a realization $p \colon N \to \mathbb{R}^r$ of G

Introduction



Outline

EDMs and Semidefinite Matrices

Linear Transformation $\mathcal{K}$

- Let $D \in \mathcal{E}^n$ be given by the points $p_1, \ldots, p_n \in \mathbb{R}^r$ (or $P \in \mathbb{R}^{n \times r}$)
- Let $Y := PP^T = (p_i^T p_j) \in \mathcal{S}_+^n$

$$\begin{aligned} D_{ij} &= \|p_i - p_j\|^2 \\ &= p_i^T p_i + p_j^T p_j - 2p_i^T p_j \\ &= Y_{ii} + Y_{jj} - 2Y_{ij} \end{aligned}$$

- Thus $D = \mathcal{K}(Y)$, where:

$$\boxed{\mathcal{K}(Y) := \mathrm{diag}(Y)e^T + e\,\mathrm{diag}(Y)^T - 2Y}$$

- $\mathcal{K}(\mathcal{S}_+^n) = \mathcal{E}^n$ (but not one-to-one)

EDMs and Semidefinite Matrices

Moore-Penrose Pseudoinverse of $\mathcal{K}$

$$\mathcal{K}^\dagger(D) = -\frac{1}{2} J \left[\mathrm{offDiag}(D)\right] J \qquad \text{where} \qquad J := I - \frac{1}{n} ee^T$$

Theorem: (Schoenberg, 1935)

A matrix D with $\mathrm{diag}(D) = 0$ is a Euclidean distance matrix if and only if

$\mathcal{K}^\dagger(D)$ is positive semidefinite.

EDMs and Semidefinite Matrices

Properties of $\mathcal{K}$ and $\mathcal{K}^\dagger$

$$\mathcal{S}^n_C := \{Y \in \mathcal{S}^n : Ye = 0\} \quad \text{and} \quad \mathcal{S}^n_H := \{D \in \mathcal{S}^n : \mathrm{diag}(D) = 0\}$$

$$\mathcal{K}(\mathcal{S}^n_C) = \mathcal{S}^n_H \quad \text{and} \quad \mathcal{K}^\dagger(\mathcal{S}^n_H) = \mathcal{S}^n_C$$

$$\mathcal{K}\left(\mathcal{S}^n_+ \cap \mathcal{S}^n_C\right) = \mathcal{E}^n \quad \text{and} \quad \mathcal{K}^\dagger(\mathcal{E}^n) = \mathcal{S}^n_+ \cap \mathcal{S}^n_C$$

$$\mathrm{embdim}(D) = \mathrm{rank}\left(\mathcal{K}^\dagger(D)\right), \quad \text{for all } D \in \mathcal{E}^n$$

EDMs and Semidefinite Matrices

Vector Formulation

Find $p_1, \ldots, p_n \in \mathbb{R}^r$ such that $\|p_i - p_j\|^2 = D_{ij}$, $\forall ij \in E$

Matrix Formulation using $\mathcal{K}$

Find $P \in \mathbb{R}^{n \times r}$ such that $H \circ \mathcal{K}(Y) = H \circ D$, $Y = PP^T$

Semidefinite Programming (SDP) Relaxation

Find $Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C$ such that $H \circ \mathcal{K}(Y) = H \circ D$

- Vector/Matrix Formulation is non-convex and NP-hard
- SDP Relaxation is tractable, but only problems of limited size can be directly handled by an SDP solver
- To solve this SDP, we use facial reduction to obtain a much smaller equivalent problem

Outline

An LP Example

$$\begin{array}{lcccccccccccc} \text{minimize} & 2x_1 & + & 6x_2 & - & x_3 & - & 2x_4 & + & 7x_5 & & \\ \text{subject to} & x_1 & + & x_2 & + & x_3 & + & x_4 & & & = & 1 \\ & x_1 & - & x_2 & - & x_3 & & & + & x_5 & = & -1 \\ & x_1 & , & x_2 & , & x_3 & , & x_4 & , & x_5 & \geq & 0 \end{array}$$

Summing the constraints:

$$2x_1 + x_4 + x_5 = 0 \quad \Rightarrow \quad x_1 = x_4 = x_5 = 0$$

Restrict LP to the face $\left\{x \in \mathbb{R}^5_+ \; : \; x_1 = x_4 = x_5 = 0\right\} \trianglelefteq \mathbb{R}^5_+$

$$\begin{array}{lccccc} \text{minimize} & 6x_2 & - & x_3 & & \\ \text{subject to} & x_2 & + & x_3 & = & 1 \\ & x_2 & , & x_3 & \geq & 0 \end{array}$$

Semidefinite Facial Reduction

The Minimal Face

If $K \subseteq \mathbb{E}$ is a convex cone and $S \subseteq K$, then

$$\mathrm{face}(S) := \bigcap_{S \subseteq F \trianglelefteq K} F$$

Proposition:

Let $K \subseteq \mathbb{E}$ be a convex cone and let $S \subseteq F \trianglelefteq K$.
If $S \neq \emptyset$ and convex, then:

- $\mathrm{face}(S) = F$ if and only if $S \cap \mathrm{relint}(F) \neq \emptyset$.

Representing Faces of $\mathcal{S}^n_+$

If $F \trianglelefteq \mathcal{S}^n_+$ and $X \in \operatorname{relint}(F)$ with $\operatorname{rank}(X) = t$, then

$$F = U\mathcal{S}^t_+ U^T \quad \text{and} \quad \operatorname{relint}(F) = U\mathcal{S}^t_{++} U^T,$$

where $U \in \mathbb{R}^{n \times t}$ has full column rank and $\operatorname{range}(U) = \operatorname{range}(X)$.

Semidefinite Facial Reduction

If:

$$\operatorname{face}\left(\left\{X \in \mathcal{S}^n_+ : \langle A_i, X\rangle = b_i,\ \forall i\right\}\right) = U\mathcal{S}^t_+ U^T$$

Then:

$$\begin{array}{ll} \text{minimize} & \langle C, X\rangle \\ \text{subject to} & \langle A_i, X\rangle = b_i,\ \forall i \\ & X \in \mathcal{S}^n_+ \end{array} \quad \Longrightarrow \quad \begin{array}{ll} \text{minimize} & \langle C, UZU^T\rangle \\ \text{subject to} & \langle A_i, UZU^T\rangle = b_i,\ \forall i \\ & Z \in \mathcal{S}^t_+ \end{array}$$

Outline

Facial Reduction Theory for EDM Completion

Theorem: Clique Facial Reduction

Let:

- $\bar{D} \in \mathcal{E}^k$
- $t := \operatorname{embdim}(\bar{D})$
- $\bar{\mathcal{F}} := \left\{ Y \in \mathcal{S}^k_+ : \mathcal{K}(Y) = \bar{D} \right\}$

Then:

$$\boxed{\operatorname{face}(\bar{\mathcal{F}}) = \bar{U} \mathcal{S}^{t+1}_+ \bar{U}^T}$$

where

- $\bar{U} := \begin{bmatrix} U_C & e \end{bmatrix}$
- $U_C \in \mathbb{R}^{k \times t}$ full column rank and

$$\operatorname{range}(U_C) = \operatorname{range}(\mathcal{K}^\dagger(\bar{D}))$$

Facial Reduction Theory for EDM Completion

Theorem: Extending the Facial Reduction

Let D be a partial EDM, $\alpha \subseteq \{1, \ldots, n\}$, and:

- $\mathcal{F} := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : H \circ \mathcal{K}(Y) = H \circ D \right\}$
- $\mathcal{F}_\alpha := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : H[\alpha] \circ \mathcal{K}(Y[\alpha]) = H[\alpha] \circ D[\alpha] \right\}$
- $\bar{\mathcal{F}}_\alpha := \left\{ Y \in \mathcal{S}^{|\alpha|}_+ : H[\alpha] \circ \mathcal{K}(Y) = H[\alpha] \circ D[\alpha] \right\}$

If:

$$\mathrm{face}(\bar{\mathcal{F}}_\alpha) \trianglelefteq \bar{U} \mathcal{S}^{t+1}_+ \bar{U}^T$$

Then:

$$\boxed{\mathrm{face}(\mathcal{F}_\alpha) \trianglelefteq \left(U \mathcal{S}^{n-|\alpha|+t+1}_+ U^T \right) \cap \mathcal{S}^n_C}$$

where $U := \begin{bmatrix} \bar{U} & 0 \\ 0 & I \end{bmatrix} \in \mathbb{R}^{n \times (n-|\alpha|+t+1)}$

Facial Reduction Theory for EDM Completion

Theorem: Distance Constraint Reduction

Let D be a partial EDM, $\alpha \subseteq \{1, \ldots, n\}$, and:

- $\mathcal{F}_\alpha := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : H[\alpha] \circ \mathcal{K}(Y[\alpha]) = H[\alpha] \circ D[\alpha] \right\}$
- $\bar{\mathcal{F}}_\alpha := \left\{ Y \in \mathcal{S}^{|\alpha|}_+ : H[\alpha] \circ \mathcal{K}(Y) = H[\alpha] \circ D[\alpha] \right\}$
- $\mathrm{face}(\bar{\mathcal{F}}_\alpha) \trianglelefteq \bar{U}\mathcal{S}^{t+1}_+ \bar{U}^T$

If $\exists \bar{Y} \in \bar{\mathcal{F}}_\alpha$ and $\beta \subseteq \alpha$ is a clique with $\mathrm{embdim}(D[\beta]) = t$, then:

$$\mathcal{F}_\alpha = \left\{ Y \in \left(U\mathcal{S}^{n-|\alpha|+t+1}_+ U^T \right) \cap \mathcal{S}^n_C : \mathcal{K}(Y[\beta]) = D[\beta] \right\}$$

where $U := \begin{bmatrix} \bar{U} & 0 \\ 0 & I \end{bmatrix} \in \mathbb{R}^{n \times (n-|\alpha|+t+1)}$

Facial Reduction Theory for EDM Completion

Theorem: Disjoint Subproblems

Let $\mathcal{F}$ be as above. Let $\{\alpha_i\}_{i=1}^{\ell}$ be disjoint subsets, $\alpha := \cup \alpha_i$, and :

- $\mathcal{F}_i := \left\{ Y \in \mathcal{S}_+^n \cap \mathcal{S}_C^n : H[\alpha_i] \circ \mathcal{K}(Y[\alpha_i]) = H[\alpha_i] \circ D[\alpha_i] \right\}$
- $\bar{\mathcal{F}}_i := \left\{ Y \in \mathcal{S}_+^{|\alpha_i|} : H[\alpha_i] \circ \mathcal{K}(Y) = H[\alpha_i] \circ D[\alpha_i] \right\}$

If $\operatorname{face}(\bar{\mathcal{F}}_i) \trianglelefteq \bar{U}_i \mathcal{S}_+^{t_i+1} \bar{U}_i^T$, then

$$\boxed{\operatorname{face}(\mathcal{F}) \trianglelefteq \left(U \mathcal{S}_+^{n-|\alpha|+t+1} U^T \right) \cap \mathcal{S}_C^n}$$

where $U := \begin{bmatrix} \bar{U}_1 & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & \bar{U}_\ell & 0 \\ 0 & \cdots & 0 & I \end{bmatrix} \in \mathbb{R}^{n \times (n-|\alpha|+t+1)}$

Facial Reduction Theory for EDM Completion

Facial Reduction Algorithm

- For each node $i = 1, \ldots, n$, find a clique C_i containing i
- Let C_{n+1} be the clique of anchors
- Let $F_i := \left(U_i \mathcal{S}_+^{n-|C_i|+t_i+1} U_i^T\right) \cap \mathcal{S}_C^n$ be the corresponding faces
- Compute $U \in \mathbb{R}^{n \times (t+1)}$ full column rank such that

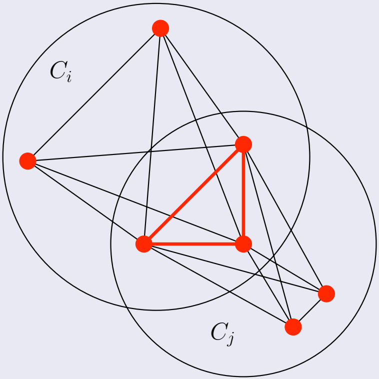
$$\mathrm{range}(U) = \bigcap_{i=1}^{n+1} \mathrm{range}(U_i)$$

- Then:

$$\mathrm{face}\left(\{Y \in \mathcal{S}_+^n \cap \mathcal{S}_C^n : H \circ \mathcal{K}(Y) = H \circ D\}\right) \trianglelefteq \left(U \mathcal{S}_+^{t+1} U^T\right) \cap \mathcal{S}_C^n$$

Facial Reduction Theory for EDM Completion

Rigid Intersection



Facial Reduction Theory for EDM Completion

Lemma: Rigid Face Intersection

Suppose:

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

and $U_1'', U_2'' \in \mathbb{R}^{k\times(t+1)}$ full column rank with $\mathrm{range}(U_1'') = \mathrm{range}(U_2'')$

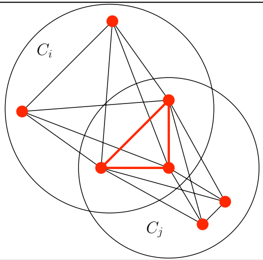
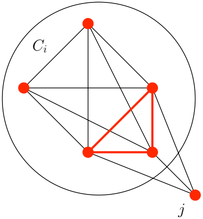
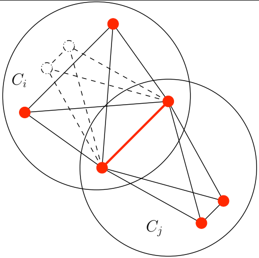
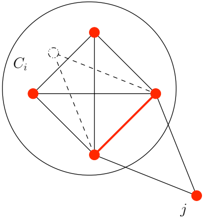
Then:

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

Satisfies:

$$\mathrm{range}(U) = \mathrm{range}(U_1) \cap \mathrm{range}(U_2)$$

Facial Reduction Theory for EDM Completion

	Clique Union	Node Absorption
Rigid		
Non-rigid		

Facial Reduction Theory for EDM Completion

Theorem: Euclidean Distance Matrix Completion

Let D be a partial EDM and :

- $\mathcal{F} := \left\{ Y \in \mathcal{S}^n_+ \cap \mathcal{S}^n_C : H \circ \mathcal{K}(Y) = H \circ D \right\}$
- $\operatorname{face}(\mathcal{F}) \trianglelefteq \left(U\mathcal{S}^{t+1}_+ U^T \right) \cap \mathcal{S}^n_C = (UV)\mathcal{S}^t_+(UV)^T$

If $\exists \bar{Y} \in \mathcal{F}$ and β is a clique with $\operatorname{embdim}(D[\beta]) = t$, then:

- $\bar{Y} = (UV)\bar{Z}(UV)^T$, where $\bar{Z}$ is the unique solution of

$$(JU[\beta,:]V)Z(JU[\beta,:]V)^T = \mathcal{K}^\dagger(D[\beta]) \qquad (1)$$

- $\mathcal{F} = \left\{ \bar{Y} \right\}$
- $\bar{D} := \mathcal{K}(\bar{P}\bar{P}^T) \in \mathcal{E}^n$ is the unique completion of D, where

$$\bar{P} := UV\bar{Z}^{1/2} \in \mathbb{R}^{n \times t}$$

Note: In this case, an SDP solver is not required.

Outline

Numerical Results

- Random *noiseless* problems
- Dimension $r = 2$
- Square region: $[0,1] \times [0,1]$
- $m = 4$ anchors
- R = radio range
- Using only Rigid Clique Union and Rigid Node Absorption
- Error measure: Root Mean Square Deviation

$$\text{RMSD} := \left(\frac{1}{\#\ \text{positioned}} \sum_{i \text{ positioned}} \|p_i - p_i^{\text{true}}\|^2 \right)^{\frac{1}{2}}.$$

- Results averaged over 10 instances
- Used MATLAB on a 2.16 GHz Intel Core 2 Duo with 2 GB of RAM
- Source code `SNLSDPclique` available on author's website, released under a GNU General Public License

Numerical Results

Face Representation Approach

# sensors	R	# Sensors Positioned	CPU Time	RMSD
2000	.07	2000.0	1 s	2e-13
2000	.06	1999.9	1 s	3e-13
2000	.05	1996.7	1 s	2e-13
2000	.04	1273.8	3 s	4e-12
6000	.07	6000.0	4 s	8e-14
6000	.06	6000.0	4 s	7e-14
6000	.05	6000.0	3 s	1e-13
6000	.04	5999.4	3 s	3e-13
10000	.07	10000.0	9 s	7e-14
10000	.06	10000.0	8 s	1e-13
10000	.05	10000.0	7 s	2e-13
10000	.04	10000.0	6 s	1e-13
20000	.030	20000.0	17 s	2e-13
60000	.015	60000.0	1 m 53 s	7e-13
100000	.011	100000.0	5 m 46 s	9e-11

Numerical Results

Point Representation Approach

# sensors	R	# Sensors Positioned	CPU Time	RMSD
2000	.07	2000.0	1 s	5e-16
2000	.06	1999.9	1 s	6e-16
2000	.05	1996.7	1 s	7e-16
2000	.04	1274.4	2 s	7e-16
6000	.07	6000.0	3 s	5e-16
6000	.06	6000.0	3 s	5e-16
6000	.05	6000.0	3 s	8e-16
6000	.04	5999.4	3 s	6e-16
10000	.07	10000.0	7 s	9e-16
10000	.06	10000.0	6 s	7e-16
10000	.05	10000.0	6 s	6e-16
10000	.04	10000.0	5 s	1e-15
20000	.030	20000.0	14 s	8e-16
60000	.015	60000.0	1 m 27 s	9e-16
100000	.011	100000.0	3 m 55 s	1e-15

Outline

Noisy Problems

Multiplicative Noise Model

$$d_{ij}^2 = \|p_i - p_j\|^2 (1 + \sigma \varepsilon_{ij})^2, \quad \text{for all } ij \in E$$

- ε_{ij} is normally distributed with mean 0 and standard deviation 1
- $\sigma \geq 0$ is the *noise factor*

Least Squares Problem

$$\begin{array}{ll} \text{minimize} & \displaystyle\sum_{ij \in E} v_{ij}^2 \\ \text{subject to} & \|p_i - p_j\|^2 (1 + v_{ij})^2 = d_{ij}^2, \quad \text{for all } ij \in E \\ & \sum_{i=1}^n p_i = 0 \\ & p_1, \ldots, p_n \in \mathbb{R}^r \end{array}$$

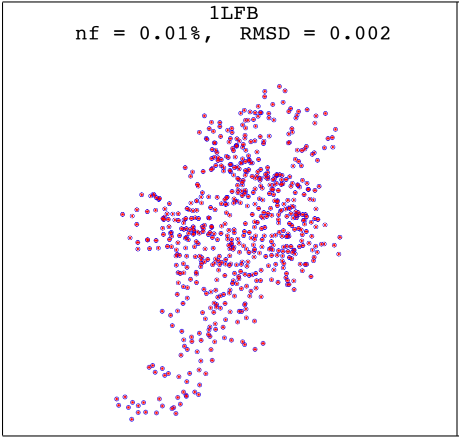
Noisy Problems

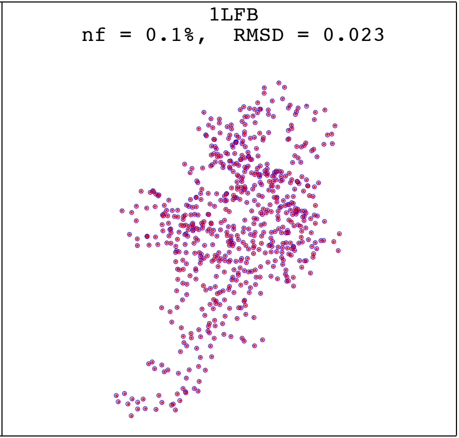
Point Representation Approach

σ	# sensors	R	CPU Time	RMSD
0	2000	.08	1 s	5e-16
1e-6	2000	.08	1 s	1e-06
1e-4	2000	.08	1 s	1e-04
1e-2	2000	.08	1 s	7e-02
0	6000	.06	3 s	5e-16
1e-6	6000	.06	3 s	1e-06
1e-4	6000	.06	3 s	1e-04
1e-2	6000	.06	3 s	2e-01
0	10000	.04	5 s	1e-15
1e-6	10000	.04	5 s	1e-06
1e-4	10000	.04	5 s	1e-04
1e-2	10000	.04	5 s	2e-01

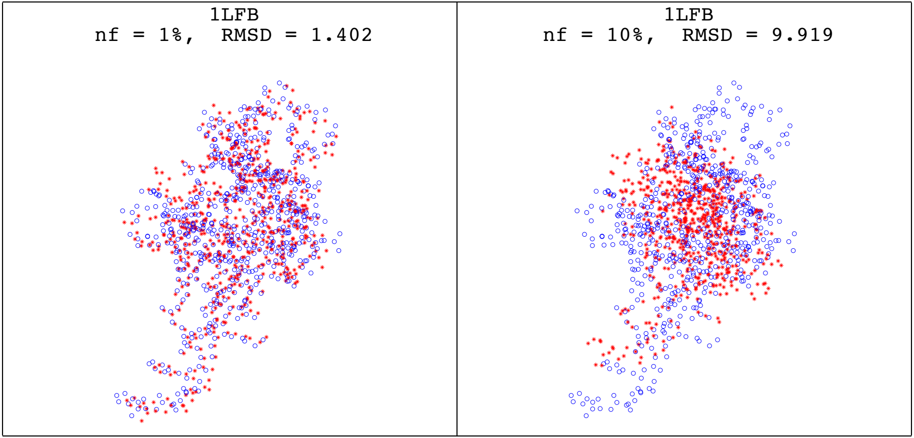
Note: No refinement technique is used in our numerical tests

Noisy Problems





Noisy Problems



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- Using this theory, we can transform the SDP relaxations into much smaller equivalent problems
- We developed a highly efficient algorithm for EDM completion:
  - SDP solver not required
  - can solve problems with up to 100,000 sensors in a few minutes on a laptop computer
  - obtained very high accuracy for noiseless problems
  - our running times are highly competitive with other SDP-based codes