Accurately and efficiently solving structured nonconvex optimization problems

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These slides are publicly available at cs.cmu.edu/~alw1

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Accurately and efficiently solving structured nonconvex optimization problems

Convex optimization

Convex optimization is influential in many different fields

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Engineering

Controller stability, power allocation, truss design, +

Statistics

(Linear) Regression, parameter estimation, +



Finance Portfolio optimization, risk analysis, +

Convex optimization is accurate and efficient

Convex optimization, meet nonconvex problems

- Unfortunately, many practical optimization problems are nonconvex
- Example: Low-rank matrix completion (Netflix problem)

- Rank constraints, binary constraints, sparsity constraints generally hard
- But not always!

Some nonconvex problems can be solved using convex optimization

Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

• Completed work:

- Nonconvex problems: quadratically constrained quadratic programs (QCQPs)
- Convex relaxations: semidefinite programs (SDPs)

Today's questions

Understand **structures within QCQPs** that enable us to solve them exactly and efficiently using SDPs

• Preliminaries

QCQPs and their applications, the SDP relaxation

• Understand structures within QCQPs that enable us to solve them...

- exactly [IPCO 20], [Math. Prog. 21], [Math. Prog. *under review*] Objective value, convex hull exactness, applications
- efficiently [Math. Prog. 20], [SIAM J. Optim. *under review*], [Ongoing] The generalized trust-region subproblem and regular QCQPs

• Conclusion and future directions



2 Objective value exactness, convex hull exactness, applications

3 Efficient algorithms for regular QCQPs



Quadratically constrained quadratic programs (QCQPs)

• $q_{obj}, q_1, \dots, q_m : \mathbb{R}^n \to \mathbb{R}$ quadratic (possibly nonconvex!)

$$Opt := \inf_{x \in \mathbb{R}^n} \left\{ q_{\mathsf{obj}}(x) : q_i(x) \le 0, \, \forall i \in [m] \right\}$$

 $q_i(x) = x^{\mathsf{T}} A_i x + 2b_i^{\mathsf{T}} x + c_i$



- Highly expressive:
 - MAX-CUT, MAX-CLIQUE, pooling, truss design, facility location, production planning
 - binary programs $x_1(1-x_1) = 0$
 - polynomial optimization problems $x_1x_2 = z_{12}$
- NP-hard in general

The QCQP epigraph

• QCQP epigraph
$$\mathcal{D} := \begin{cases} (x,t) \in \mathbb{R}^{n+1} : & q_{\mathsf{obj}}(x) \leq t \\ & q_i(x) \leq 0, \, \forall i \in [m] \end{cases}$$



• How can we derive convex relaxations of \mathcal{D} ?

• If
$$\gamma \in \mathbb{R}^{m}_{+}$$
, then $\forall (x,t) \in \mathcal{D}, \qquad \underbrace{q_{\mathsf{obj}}(x) + \sum_{i=1}^{m} \gamma_{i}q_{i}(x)}_{=: q(\gamma, x)} \leq t$

m

The SDP relaxation

• SDP relaxation = impose all convex aggregated inequalities!

$$\mathcal{D}_{SDP} =$$

• Formally,

$$\begin{split} & \Gamma \coloneqq \left\{ \gamma \in \mathbb{R}^m_+ \colon q(\gamma, x) \text{ is convex in } x \right\} = \left\{ \gamma \in \mathbb{R}^m_+ \colon A_{\text{obj}} + \sum_{i=1}^m \gamma_i A_i \succeq 0 \right\} \\ & \mathcal{D}_{\text{SDP}} \coloneqq \bigcap_{\gamma \in \Gamma} \left\{ (x, t) \colon q(\gamma, x) \le t \right\} = \left\{ (x, t) \in \mathbb{R}^{n+1} \colon \sup_{\gamma \in \Gamma} q(\gamma, x) \le t \right\} \\ & \text{Opt}_{\text{SDP}} \coloneqq \inf_{x \in \mathbb{R}^n} \sup_{\gamma \in \Gamma} q(\gamma, x) \end{split}$$

The usual SDP relaxation

$$\begin{split} \inf_{x \in \mathbb{R}^n} \left\{ q_{\mathsf{obj}}(x) : q_i(x) \le 0, \, \forall i \in [m] \right\} \\ &= \inf_{x \in \mathbb{R}^n, Y \in \mathbb{S}^n} \left\{ \langle A_{\mathsf{obj}}, Y \rangle + 2b_{\mathsf{obj}}^\top x + c_{\mathsf{obj}} : \begin{array}{c} Y = xx^\top \\ \langle A_i, Y \rangle + 2b_i^\top x + c_i \le 0, \, \forall i \in [m] \end{array} \right\} \\ &\geq \inf_{x \in \mathbb{R}^n, Y \in \mathbb{S}^n} \left\{ \langle A_{\mathsf{obj}}, Y \rangle + 2b_{\mathsf{obj}}^\top x + c_{\mathsf{obj}} : \begin{array}{c} Y - xx^\top \ge 0 \\ \langle A_i, Y \rangle + 2b_i^\top x + c_i \le 0, \, \forall i \in [m] \end{array} \right\} \\ &= \inf_{x \in \mathbb{R}^n} \inf_{Y \in \mathbb{S}^n} \dots \\ &= \inf_{x \in \mathbb{R}^n} \inf_{\gamma \in \Gamma} q(\gamma, x) \end{split}$$

• Main objects of interest



• Γ = aggregation weights such that $q(\gamma, x)$ is convex

Preliminaries

2 Objective value exactness, convex hull exactness, applications

3 Efficient algorithms for regular QCQPs



Forms of exactness

- What does exactness mean?
 - Objective value exactness: $Opt = Opt_{SDP}$
 - Convex hull exactness: $conv(D) = D_{SDP} \leftarrow convexification of substructures$



Convex hull exactness



Based on: [IPCO 19], [Math. Prog. 21], [Math. Prog. under review]

Example: the trust-region subproblem

Convex hull exactness in the case of single ball constraint

$$Opt = \inf_{x \in \mathbb{R}^n} \left\{ q_{\mathsf{obj}}(x) : \|x\|^2 \le 1 \right\}$$





- Applications:
 - Nonlinear minimization (trust-region methods), combinatorial optimization, robust optimization

Related: Yakubovich [1971], Yıldıran [2009], Ho-Nguyen and Kılınç-Karzan [2017]

Based on: [IPCO 19], [Math. Prog. 20]

Example: QCQPs with symmetry

- Convex hull exactness in the case of "highly symmetric" QCQPs
- Suppose $A_{obj} = I_k \otimes \mathbb{A}_{obj}$, $A_i = I_k \otimes \mathbb{A}_i$ for all $i \in [m]$

$$A = I_k \otimes \mathbb{A} = \begin{pmatrix} \mathbb{A} & & \\ & \mathbb{A} & \\ & \ddots & \\ & & & \mathbb{A} \end{pmatrix}$$

and $k \ge m$

- Applications:
 - Robust least squares, sphere packing, QCQPs with spherical constraints, orthogonal Procrustes problem

Based on: [Math. Prog. under review] Related: Beck [2007], Beck et al. [2012]

Example: QCQPs with sign-definite linear terms

- Objective value exactness in the case of diagonal, sign-definite QCQPs
- Suppose A_{obj}, \ldots, A_m diagonal and

 $orall j \in [n], \left\{ (b_{\mathsf{obj}})_j, (b_1)_j, \dots, (b_m)_j
ight\}$ have the same sign

• Example:

$$\min_{x \in \mathbb{R}^n} \left\{ x^\top A_{\mathsf{obj}} x + 2b_{\mathsf{obj}}^\top x + c_{\mathsf{obj}} : \|x\|_2 \le 1, \|x\|_\infty \le \alpha \right\}$$

Related: Burer and Ye [2019], Sojoudi and Lavaei [2014]

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Based on: [Tut. Oper. Res. 21]

Summary of Part 1

- Sufficient conditions for convex hull exactness
- Necessary and sufficient if Γ is polyhedral (dual facially exposed)
- Sufficient conditions for objective value exactness
- Rank-one-generated (ROG) cones: QCQP-SDP analogue of integrality
- Applications:
 - Random, semi-random QCQPs, ratios of quadratic functions



Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

SDPs provide exact reformulations for broad classes of QCQPs!



1 Preliminaries

2 Objective value exactness, convex hull exactness, applications

3 Efficient algorithms for regular QCQPs



Revisiting the SDP relaxation

- SDPs polynomial time ← too expensive in modern machine learning regimes
- Usual SDP relaxation
 - Interior point method \longrightarrow iterations expensive $O(mn^3 + m^2n^2 + m^3)$ time

We can solve an SDP more efficiently if it is exact (regular)!

• Our view:
$$\operatorname{Opt}_{\mathsf{SDP}} \coloneqq \inf_{x \in \mathbb{R}^n} \left(\sup_{\gamma \in \Gamma} q(\gamma, x) \right)$$

is a minimization problem in the original space

Regularity will allow us to deal with max-type structure

Based on: [Math. Prog. 20], [SIAM J. Optim. under review], [Ongoing]

• Dual problem

$$Opt_{\mathsf{SDP}} \coloneqq \inf_{x \in \mathbb{R}^n} \sup_{\gamma \in \Gamma} q(\gamma, x) = \sup_{\gamma \in \Gamma} \inf_{x \in \mathbb{R}^n} q(\gamma, x)$$

Definition

Let
$$\gamma^*$$
 be dual optimizer. Define $\mu^* \coloneqq \lambda_{\min} \left(A_{\mathsf{obj}} + \sum_{i=1}^m \gamma_i^* A_i \right)$.
QCQP is regular if $\mu^* > 0$.

• Regularity \implies optimizer exactness

$$\mu^* > 0 \quad \Longrightarrow \quad \mathop{\arg\min}_{x \in \mathbb{R}^n} \left\{ q_{\mathsf{obj}}(x) : \, q_i(x) \le 0, \, \forall i \in [m] \right\} = \mathop{\arg\min}_{x \in \mathbb{R}^n} \, \sup_{\gamma \in \Gamma} q(\gamma, x)$$

Based on: [Ongoing]

The generalized trust-region subproblem (GTRS)

Special setting with single constraint (≤ or =)

$$Opt \coloneqq \inf_{x \in \mathbb{R}^n} \left\{ q_{\mathsf{obj}}(x) : q_1(x) \le 0 \right\}$$

- TRS applications:
 - nonlinear programming (trust-region methods), combinatorial optimization, robust optimization
- GTRS applications:
 - minimizing quartics of the form q(x, p(x))

$$\inf_{x \in \mathbb{R}^n, \alpha} \left\{ q(x, \alpha) : \, \alpha = p(x) \right\}$$

(source localization, constrained rank-one approximation), regression with adversarial data, iterative QCQP solvers

• Assume $\mu^* > 0 \longleftarrow \text{most GTRS}$



Based on: [Math. Prog. 20], [SIAM J. Optim. under review], [under review]

Efficient algorithms for regular GTRS: Intuition

Efficient algorithms for regular GTRS

• Key observation: If $\gamma^* \in [\gamma_-, \gamma_+] \subseteq \Gamma$, then

$$Opt_{\mathsf{SDP}} = \min_{x \in \mathbb{R}^n} \max_{\gamma \in \{\gamma_-, \gamma_+\}} q(\gamma, x)$$



- Algorithmic idea:
 - Solve for γ^* to low accuracy, $\gamma^* \in [\gamma_-, \gamma_+] \subseteq \operatorname{int}(\Gamma)$
 - Apply Accelerated Gradient Descent
 - for strongly convex nonsmooth function
- Putting pieces together:

$$\implies \tilde{O}\left(\frac{T}{\sqrt{\mu^*}}\log\left(\frac{1}{\epsilon}\right)\right)$$

where T is time for matrix vector product \leftarrow think O(n)

Related: Carmon and Duchi [2018], Jiang and Li [2019], Adachi and Nakatsukasa [2019]

Based on: [SIAM J. Optim. under review]

Numerical experiments, n = 1,000



Based on: [Math. Prog. 20], [SIAM J. Optim. *under review*] Related: Ben-Tal and den Hertog [2014], Jiang and Li [2019], Adachi and Nakatsukasa [2019]

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Numerical experiments, n = 1,000



Numerical experiments, n = 10,000



Numerical experiments, n = 100,000



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Efficient algorithms for regular QCQPs: Algorithm

- Regularity \implies optimizer exactness
- Regularity holds in a number of statistical recovery problems: phase-retrieval, clustering
- · Will leverage regularity to design efficient algorithms
- Key observation: If $\gamma^* \in \mathcal{U} \subseteq \Gamma$, then

 $Opt_{\mathsf{SDP}} = \min_{x \in \mathbb{R}^n} \max_{\gamma \in \mathcal{U}} q(\gamma, x)$

- Algorithm sketch:
 - Construct $\mathcal{U} \longrightarrow O(1)$ iterations, $O\left(\frac{mT}{\sqrt{\epsilon}}\right)$ / iter.
 - Solve min-max problem $\longrightarrow O\left(\frac{1}{\sqrt{\mu^*}}\log\left(\frac{1}{\epsilon}\right)\right)$ iterations, $O\left(\frac{mT}{\epsilon}\right)$ / iter.

Based on: [Ongoing]

Convergence behavior



Preliminary numerical experiments

- 10 synthetic instances: n = 5000, m = 50, density $= 0.001, \mu^* = 0.1$
- Primal-dual solver

Section	ncalls	avg time	%tot	avg error
Total	10	1740s	100%	
dual_solve	10	1691s	97.2%	1.15e-02
eigsolve	33.1k	506ms	96.0%	
primal_solve	10	48.7s	2.80%	<mark>3.61e-12</mark>

• Splitting Conic Solver (SCS): avg time 18150s

Summary of Part 2

- Efficient algorithms for the GTRS
 - \rightarrow nonlinear programming, iterative QCQP solvers, regression
- Efficient algorithms for regular QCQPs (low-rank SDPs)
 - \longrightarrow statistical recovery problems
- Algorithms for diagonalizing QCQPs

GTRS	Regular QCQPs	Diagonalizing QCQPs		
[Math. Prog. 20], [SIAM.] Optim under review]	[Ongoing]	[Math. Prog. under review]		
[under review]				

Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

Some nonconvex problems can be solved efficiently via first-order methods!



1 Preliminaries

2 Objective value exactness, convex hull exactness, applications

8 Efficient algorithms for regular QCQPs



Conclusion and future directions

Future work

Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

- Solving nonconvex problems accurately
 - Completed: SDPs provide exact reformulations for broad classes of QCQPs!
 - Future:
 - Can we understand approximation quality systematically within general framework?
 - Can we understand exactness/approximation for other convex relaxations?

Future work

Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

- Solving nonconvex problems efficiently
 - Completed: Some nonconvex problems can be solved efficiently via first-order methods!
 - Future:
 - Exactness \approx efficiency?
 - Can we develop efficient algorithms for semidefinite programs with low-rank solutions
 - Can we approximate "expensive" tools (e.g., SDPs) with cheap tools (e.g., linear programs, second-order cone programs)

Summary of my research



Long-term research goal

Understand **structures within nonconvex problems** that enable us to solve them "well" using **convex optimization**

Thank you! Questions?



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Definition

Cone
$$S \subseteq \mathbb{S}^n_+$$
 is rank-one-generated (ROG) if $S = \operatorname{conv} (S \cap \{xx^\top\})$.

Compare: $P \subseteq [0,1]^n$ is integral if $P = \operatorname{conv}(P \cap \{0,1\}^n)$

- Given QCQP, if constraints correspond to ROG cone, then objective value exactness and convex hull exactness regardless of objective function
- Suppose $\mathcal{S} = \left\{ X \in \mathbb{S}^n_+ : \langle M, X \rangle \le 0, \, \forall M \in \mathcal{M} \right\}$

Goal

What properties of $\mathcal{M} = \{M_1, \dots, M_k\}$ imply \mathcal{S} is ROG?

Based on: [Math. Oper. Res. 21], [Tut. Oper. Res. 21]

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Theorem (Sufficient conditions)

 ${\mathcal S}$ is ROG if

- for all $i \neq j$, there exists $(\alpha, \beta) \neq (0, 0)$ such that $\alpha M_i + \beta M_j \succeq 0$, or
- there exists $a \in \mathbb{R}^n$ such that $M_i = ab_i^\top + b_i a^\top$.

Theorem (Characterization of ROG for $|\mathcal{M}| = 2$)

Suppose $\mathcal{M} = \{M_1, M_2\}$. Then sufficient condition above is also necessary.

Based on: [Math. Oper. Res. 21], [Tut. Oper. Res. 21]

ROG and ratios of quadratic functions

$$\begin{split} \inf_{z \in \mathbb{R}^{n+1}} \left\{ \begin{aligned} z^\top M_{\mathsf{obj}} z &: z^\top M_i z \leq 0, \, \forall i \in [m] \\ z^\top B z &: z^\top B z > 0 \\ z_{n+1}^2 = 1 \end{aligned} \right\} \\ &= \inf_{\tilde{z} \in \mathbb{R}^{n+1}} \left\{ \begin{aligned} \tilde{z}^\top M_{\mathsf{obj}} \tilde{z} &: \tilde{z}^\top B \tilde{z} = 1 \\ \tilde{z}_{n+1}^2 > 0 \end{aligned} \right\} \\ &\geq \inf_{Z \in \mathbb{S}^{n+1}_+} \left\{ \langle M_{\mathsf{obj}}, Z \rangle : \begin{array}{c} \langle M_i, Z \rangle \leq 0, \, \forall i \in [m] \\ \langle B, Z \rangle = 1 \end{aligned} \right\} \end{split}$$

- Equality holds if $S(\{M_1, \ldots, M_m\})$ is ROG (+ minor assumptions)
- Example: Regularized total least squares

Based on: [Math. Oper. Res. 21], [Tut. Oper. Res. 21]

Stackelberg prediction games with least squares losses

- True data $(x_i, \alpha_i, \beta_i)_{i=1}^m$
- Leader (learner) chooses $w \in \mathbb{R}^n$
- Follower (data provider) modifies $x_i \to \tilde{x}_i$ so that $\langle w, \tilde{x}_i \rangle \approx \beta_i$

• Leader has loss
$$(\langle w, \tilde{x}_i \rangle - \alpha_i)^2$$

•
$$\min_{w \in \mathbb{R}^n} \left\{ \sum_{i=1}^m \left(\langle w, \tilde{x}_i \rangle - \alpha_i \right)^2 : \, \tilde{x}_i \in \operatorname*{arg\,min}_{x \in \mathbb{R}^n} \gamma \, \|x - x_i\|^2 + \left(\langle w, x \rangle - \beta_i \right)^2 \right\}$$

Based on: [under review]

Stackelberg prediction games with least squares losses

•
$$\min_{w \in \mathbb{R}^n} \left\{ \sum_{i=1}^m \left(\langle w, \tilde{x}_i \rangle - \alpha_i \right)^2 : \tilde{x}_i \in \operatorname*{arg\,min}_{x \in \mathbb{R}^n} \gamma \| x - x_i \|^2 + \left(\langle w, x \rangle - \beta_i \right)^2 \right\}$$
$$= \min_{w \in \mathbb{R}^n} \left\{ \left\| \tilde{X}^\top w - \alpha \right\|^2 : \tilde{X} = (\gamma I + w w^\top)^{-1} (\gamma X + w \beta^\top) \right\}$$
$$= \min_{w \in \mathbb{R}^n} \left\| \frac{\|w\|^2 \beta + \gamma X w}{\|w\|^2 + \gamma} - \alpha \right\|^2$$
$$= \min_{w \in \mathbb{R}^n, t \in \mathbb{R}} \left\{ \left\| \frac{t\beta + \gamma X w}{t + \gamma} - \alpha \right\|^2 : t = \|w\|^2 \right\}$$
$$= \min_{\tilde{w} \in \mathbb{R}^n, \tilde{t} \in \mathbb{R}} \left\{ \left\| \frac{\tilde{t}}{2} \beta + \frac{\sqrt{\gamma}}{2} X \tilde{w} - \left(\alpha - \frac{\beta}{2} \right) \right\|^2 : \|\tilde{w}\|^2 + \tilde{t}^2 = 1 \right\}$$

Based on: [under review]

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Definition

 $\{A_i\} \subseteq \mathbb{S}^n$ is simultaneously diagonalizable via congruence (SDC) if there exists invertible $P \in \mathbb{R}^{n \times n}$ such that $P^{\top}A_iP$ is diagonal $\forall i$.

• Nice property because: SDP relaxation of diagonal QCQP is SOCP (faster), Γ is polyhedral (better understanding of exactness)

Goal

Most sets of matrices are not SDC, can we find other computationally variants of SDC and understand such properties?

Based on: [Math. Prog. under review]

Definition

 $\{A_i\} \subseteq \mathbb{S}^n$ is almost SDC (ASDC) if for all $\epsilon > 0$, there exists $||A'_i - A_i|| \le \epsilon$ such that $\{A'_i\}$ is SDC.

• "Limit of SDC sets"

Definition

 $\{A_i\} \subseteq \mathbb{S}^n$ is <u>*d*-restricted SDC (*d*-RSDC)</u> if there exists $A'_i = \begin{pmatrix} A_i & * \\ * & * \end{pmatrix} \in \mathbb{S}^{n+d}$ such that $\{A'_i\}$ is SDC.

• "Restriction of SDC sets"

Based on: [Math. Prog. under review]

Theorem

Let $\{A, B\} \subseteq \mathbb{S}^n$ and suppose A invertible. Then $\{A, B\}$ is ASDC if and only if $A^{-1}B$ has real spectrum. (+ construction)

Theorem

Let $\{A, B\} \subseteq \mathbb{S}^n$. If $\{A, B\}$ is singular, then it is ASDC. (+ construction)

Theorem

Let $\{A, B, C\} \subseteq \mathbb{S}^n$ and suppose A invertible. Then $\{A, B, C\}$ is ASDC if and only if $\{A^{-1}B, A^{-1}C\}$ commute and have real spectrum. (+ construction)

Based on: [Math. Prog. under review]

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Theorem

Let $\{A, B\} \subseteq \mathbb{S}^n$. If A is invertible and $A^{-1}B$ has simple eigenvalues, then $\{A, B\}$ is 1-RSDC. (+ construction)

• Condition holds generically

Based on: [Math. Prog. under review]

"Fuzzy" spectral partitioning

- Connected graph G = (V, E)
- Vertex masses $\mu: V \to \mathbb{R}_{++}$ and edge weights $\kappa: E \to \mathbb{R}_{++}$
- Laplacian L = D A w.r.t. κ

Theorem (Cheeger's inequality)

If
$$\mu_v = d_v$$
, then $\frac{\Phi^2}{2} \le \lambda_2(L,M) \le 2\Phi$

- $\lambda_2(L, M)$ is first nontrivial generalized eigenvalue
- Φ is sparsest cut

"Fuzzy" spectral partitioning

• We define "Fuzzy cuts"

Definition

$$\Psi \approx \min_{A,B} \left\{ \frac{\kappa_{\text{eff}}(A,B)}{\min\left(\mu(A),\mu(B)\right)}, \, A, B \neq \varnothing, \, A \cap B = \varnothing \right\}$$

• Φ must partition, Ψ may leave out. $\Psi = \Phi$ if A, B is a partition.

Theorem

$$\frac{\Psi}{4} \le \lambda_2(L, M) \le \Psi$$

Based on: [APPROX 19]

- *k*-means clustering: $\{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d$
- Suppose there exist true clustering that is unique optimum even if for all *i*, $x_i \mapsto x'_i \in B(x_i, \epsilon)$

Theorem

Two clusters. There exists $c \ge 1$ such that for any fixed $\epsilon > 0$, we can recover true clustering in time $d \cdot n^{O(\epsilon^{-c})}$.

Additional results for ≥ 3 clusters given an additional "separation" assumption