

CLUSTERING MIXTURE MODELS :

BEYOND GAUSSIANS

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MIT

## Central Open Question

Can we efficiently cluster mixtures of  
non-spherical log-concave distributions?

## Plan:

- ① Problem Setup
- ② Bottlenecks
- ③ Recent Progress

Setup :

Let  $D$  be the uniform distribution over a convex body

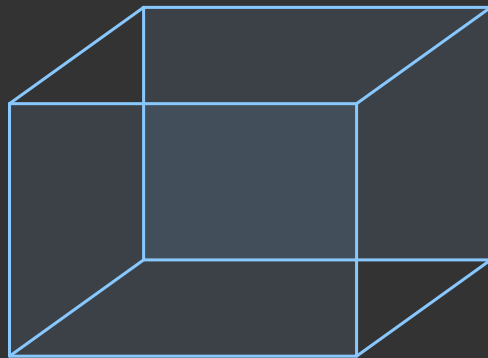
$K \in \mathbb{R}^d$  with mean  $\mu$  and Covariance  $\Sigma$ .

(log-concave)

Ex. ① Unit sphere

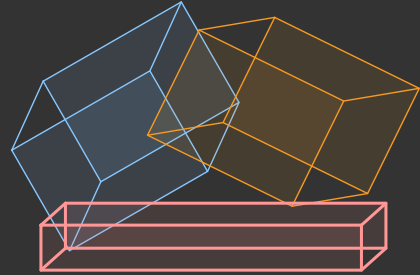
② Unit cube

③ Simplex



Setup :

Let  $M = \sum_{i \in [k]} w_i \mathcal{D}(\mu_i, \Sigma_i)$  be a mixture of log-concave distributions.

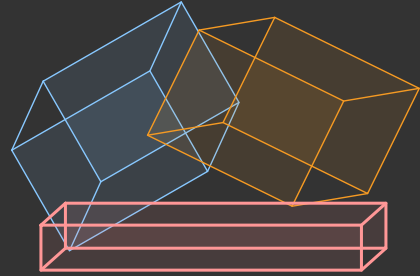


Setup :

Let  $M = \sum_{i \in [k]} w_i D(\mu_i, \Sigma_i)$  be a mixture of log-concave distributions.

Definition:  $M$  is "clusterable" if  $\forall i, j \in [k]$   
 $D(\mu_i, \Sigma_i)$  and  $D(\mu_j, \Sigma_j)$  are either

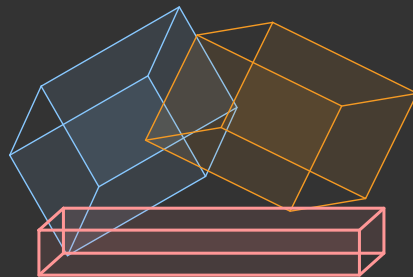
- ① Mean-separated
- ② Spectrally-separated
- ③ Shell / Frobenius-separated



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- ③ Shell / Frobenius-separated



- For Gaussians, this captures separation in total-variation distance

[B-kothari'20, Diakonikolas-Hopkins-Kane-Karmalkar'20]

- Implies all known\* notions of parameter separation

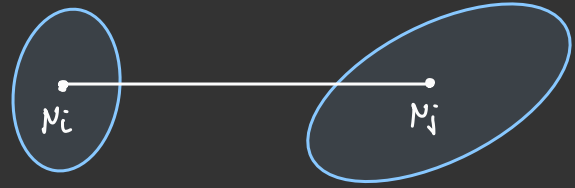
- Generalizes clustering spherical mixtures

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① Mean-separated:  $\exists v$  s.t.

$$\langle \mu_i - \mu_j, v \rangle^2 \gg v^T (\Sigma_i + \Sigma_j) v.$$





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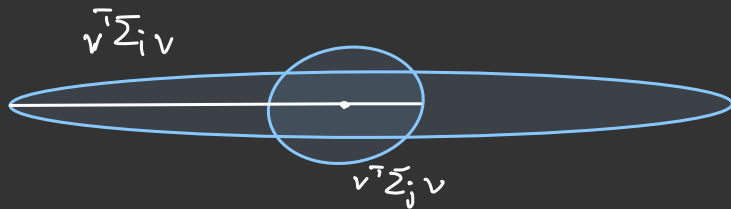
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$$v^T \Sigma_1 v \gg v^T \Sigma_2 v.$$

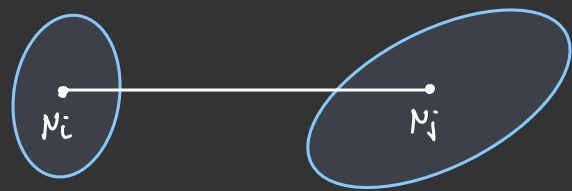


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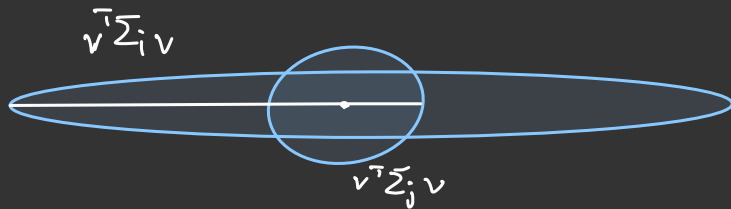
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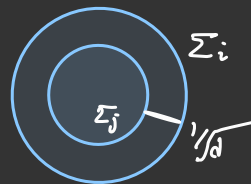
② Spectrally-separated:  $\exists v$  s.t.

$$v^T \Sigma_i v \gg v^T \Sigma_j v.$$



③ Shell / Frobenius-separated:

$$\left\| \Sigma_i^{-1/2} \Sigma_j \Sigma_i^{-1/2} - \mathbf{I} \right\|_F^2 \gg \left\| \Sigma_i^{-1/2} \cdot \Sigma_j^{1/2} \right\|_{op}^2$$



## Recap : Gaussian Mixtures

① Hyper-contractivity of linear forms  $\Rightarrow$  Mean-Separated Clustering

[Kothari-Steinhardt'18, Hopkins-Li'18]

② Hyper-contractivity of deg-2 polynomials  $\Rightarrow$  Shell / Frobenius-Sep Clustering

[B.-Kothari'20, Diaconikolas-Hopkins-Kane-Karmalkar'20]

③ Anti-Concentration  $\Rightarrow$  Spectral-Sep Clustering

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[B.-Kothari'20, Diaconikolas-Hopkins-Kane-Karmalkar'20]

\* SoS certifiable versions of these conditions imply efficient algorithms

## Beyond Gaussians:

Claim: Any log-concave distribution satisfies:

- ① Hyper-contractivity of linear forms
- ② Hyper-contractivity of deg-2 polynomials
- ③ Anti-Concentration

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Proof Sketch:

$\forall v \in \mathbb{R}^d$ , the PDF is pointwise bounded by  $\exp(-\langle x, v \rangle / c)$ .

How do we get efficient algorithms?

# Analytic Certificates

Def [Certifiable Hycontractivity of linear forms]:

$$\forall v \in \mathbb{R}^d, \quad c_k \cdot \underbrace{\left( \mathbb{E} \langle x, v \rangle^2 \right)^k}_{\text{variance}} - \underbrace{\mathbb{E} \langle x, v \rangle^{2k}}_{\text{linear form}} = \text{sos}(v).$$

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↳ a priori, a statement with infinite constraints

↳ admits a polynomial size representation



# Analytic Certificates imply Efficient Algorithms

Mean Separation

Shell separation

Spectral Separation

Clustering



# Analytic Certificates imply Efficient Algorithms

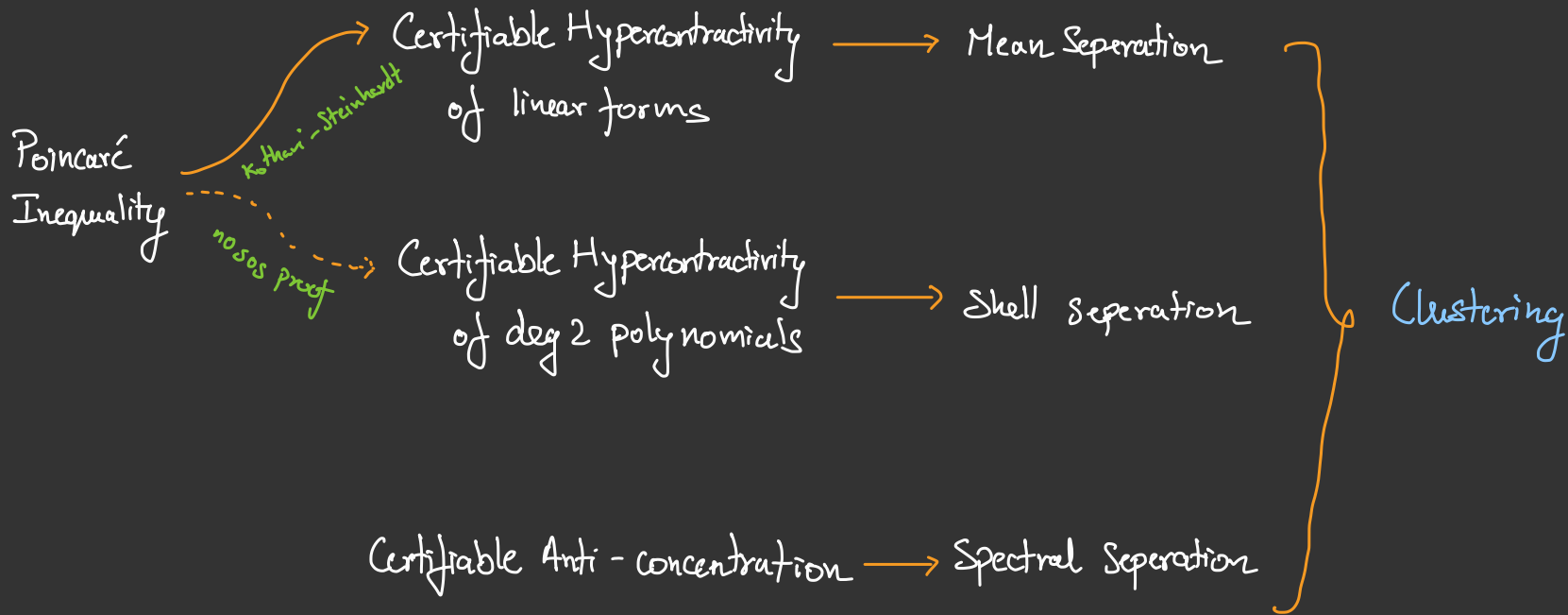
Certifiable Hypercontractivity  
of linear forms  $\longrightarrow$  Mean Separation

Certifiable Hypercontractivity  
of deg 2 polynomials  $\longrightarrow$  Shell separation

Certifiable Anti-concentration  $\longrightarrow$  Spectral Separation

Clustering

# Analytic Certificates imply Efficient Algorithms



# Analytic Certificates imply Efficient Algorithms

KLS Conjecture



Poincaré  
Inequality

→ Certifiable Hypercontractivity  
of linear forms

*Kothari-Steinhardt*

→ Certifiable Hypercontractivity  
of deg 2 polynomials

*no sos proof*

→ Mean Separation

→ Shell separation

Certifiable Anti-concentration → Spectral Separation

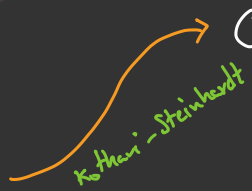
Clustering

# Analytic Certificates imply Efficient Algorithms

KLS Conjecture



Poincaré Inequality



Certifiable Hypercontractivity of linear forms

Mean Separation

Certifiable Hypercontractivity of deg 2 polynomials

Shell separation

Clustering

Rotational Invariance



Karmalkar-Klivans-Kothari

B. - Kothari

Certifiable Anti-concentration

Spectral Separation

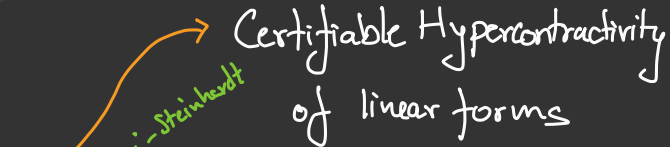


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KLS Conjecture



Poincaré Inequality



Certifiable Hypercontractivity of linear forms



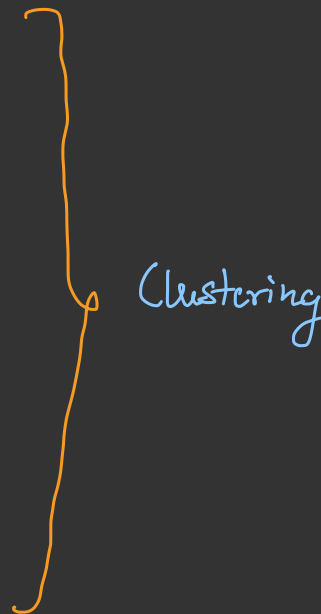
Mean Separation



Certifiable Hypercontractivity of deg 2 polynomials



Shell separation



Relaxing Rotational Invariance

This Talk



Certifiable Anti-concentration



Spectral Separation



List-Decodable Regression

# Certifiable Anti-Concentration: Beyond Gaussians

joint w/ Praveen Kothari, Goutham Rajendran, Madhur Tulsiani & Aravindan Vijayaraghavan



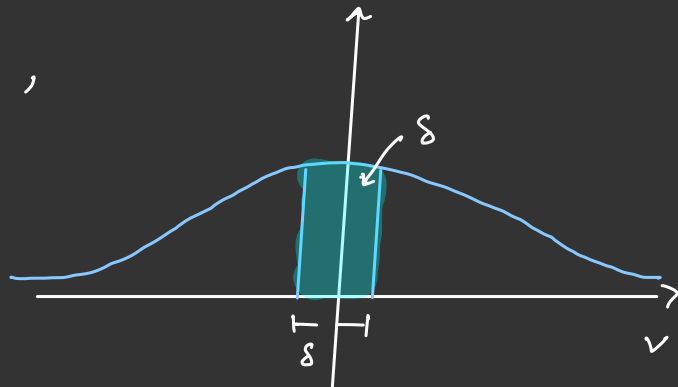
## Certifiable Anti-Concentration: Beyond Gaussians

joint w/ Praveen Kothari, Goutham Rajendran, Madhur Tulsiani & Aravindan Vijayaraghavan

Def [Anti-concentration]: Given a distribution  $D$  over  $\mathbb{R}^d$ ,  $\forall$  directions  $v$  and all intervals  $I$  of length  $\delta \sqrt{v^T \Sigma v}$ , if

$$\Pr_{x \sim D} [\langle x, v \rangle \in I] \leq \delta,$$

then  $D$  is  $\delta$ -anti-concentrated.



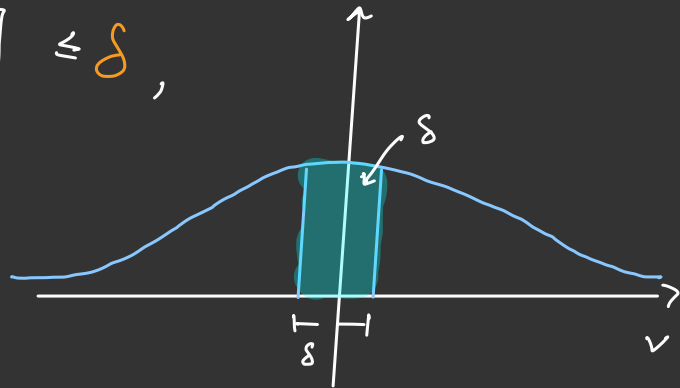


## Certifiable Anti-Concentration: Beyond Gaussians

Def [Anti-concentration]: Given  $n$  iid samples  $\{x_i\}_{i \in [n]}$  from a distribution  $\mathcal{D}$ ,  
for all directions  $v$  in  $\mathbb{R}^d$ , if

$$\Pr_{x_i \sim \{x_i\}_{i \in [n]}} \left[ \langle x_i, v \rangle^2 \leq \delta \cdot v^T \Sigma v \right] \leq \delta,$$

then  $\mathcal{D}$  is  $\delta$ -anti-concentrated.



Can we formulate this as an integer program?

## Certifiable Anti-Concentration: Integer Program

Given  $\{x_i\}_{i \in [n]}$ ,

Def [Anti-concentration]: Given samples  $\{x_i\}_{i \in [n]}$  from a distribution  $\mathcal{D}$ ,

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$$\Pr [|\langle x_i, v \rangle| \leq \delta \cdot \sqrt{v^T \Sigma v}] \leq \delta$$

$$\max_{v \in \mathbb{R}^d} \frac{1}{n} \sum_{i \in [n]} \mathbb{1} \left[ \langle x_i, v \rangle^2 \leq \delta v^T \Sigma v \right]$$

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Claim: If  $\text{OPT} \leq \delta$ , then the uniform distribution over  $\{x_i\}_{i \in [n]}$  is  $\delta$ -anti-concentrated.

# Certifiable Anti-Concentration: Integer Program

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$$\max_{v, w} \quad \frac{1}{n} \sum_{i \in [n]} w_i \quad \text{s.t.}$$

$$\forall i \in [n] \quad w_i^2 = w_i$$

[Indicator variables]

$$\forall i \in [n] \quad w_i \langle x_i, v \rangle^2 \leq w_i \delta \cdot v^T \Sigma v \quad [\text{Counting concentrated points}]$$

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How do we certify upper bounds on the objective value of this program?

# Certifiable Anti-Concentration: Efficient Certificates

**Key Idea:** Derive an upper bound on the objective  
in the sum-of-squares proof system

$\Rightarrow$  Efficiently representable certificate

$$\mathcal{A} := \left\{ \begin{array}{ll} \forall i \in [n] & w_i^2 = w_i \\ \forall i \in [n] & w_i \langle x_i, v \rangle^2 \leq \delta \cdot v^T \Sigma v \end{array} \right\}$$

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OR

$$\delta - \frac{1}{n} \sum_{i \in [n]} w_i = \underbrace{\text{sos}(v, w)}_{\text{non-negative}} + \underbrace{\sum_{i \in [n]} q_i^2 w_i (\delta v^T \Sigma v - \langle x_i, v \rangle^2)}_{\text{non-negative whenever constraints are satisfied}}$$



# Certifiable Anti-Concentration: Efficient Certificates

$$\mathcal{A} := \left\{ \begin{array}{ll} \forall i \in [n] & w_i = \omega_i \\ \forall i \in [n] & \omega_i \langle x_i, v \rangle^2 \leq \delta \cdot v^T \Sigma v \end{array} \right\}$$

**Main Theorem:** Given  $n$  samples from a 'reasonably anti-concentrated' distribution

there is a degree- $O_\delta(\log d)$  certificate of anti-concentration, i.e.

$$\mathcal{A} \vdash_{O_\delta(\log d)} \left\{ \delta - \frac{1}{n} \sum_{i \in [n]} \omega_i \geq 0 \right\}.$$

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- ① Running Time:  $n^{O_s(\log d)}$  (Quasi-polynomial)
- ②  $\delta$ -Dependence:  $\exp(1/\delta)^{\exp(1/\delta)}$  (Doubly-exponential)
- ③ No direct sum-of-squares proof

## Certifiable Anti-Concentration: Efficient Certificates

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④ Certificate works for affine transformations of uniform distributions over  $L_p$  balls, anti-concentrated product distributions etc.

⑤ All prior certificates required rotational invariance.

## Certifiable Anti-Concentration: Efficient Certificates

**Main Theorem:** Given  $n$  samples from a "reasonably anti-concentrated" distribution there is a degree- $O(\log d)$  certificate of anti-concentration, i.e.

### Applications:

1. Clustering: A  $n^{\frac{O(\log d)}{d}}$  time (robust) algorithm for clustering spectrally-separated components.  
↳ A  $n^{\Theta_{k,t}(\log^2 d)}$  time (robust) algorithm for clustering mixtures.

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↳ A  $n^{O_{\epsilon, \alpha}(\log^2 d)}$  time (robust) algorithm for clustering mixtures.
2. List-Decodable Regression: A  $n^{O_{\epsilon, \alpha}(\log d)}$  time algorithm for outputting a list of size  $O(1/d)$  s.t.  $\|\hat{\Theta} - \Theta\|_2 \leq \epsilon$ .

## Certifiable Anti-Concentration: Overview

**Starting Point:** For uniform distributions over  $L_p$  balls, the marginals along random directions are Gaussian-like.

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**Lemma:**  $\{ \mathbb{H} \ \|\cdot\|_4^4 \leq \lambda \cdot \|\cdot\|_2^4 \}$  analytic density

then

$$\underbrace{\mathbb{E}_{x \sim D} \langle x, v \rangle^{2k}}_{2k\text{-th moment along } v} = \underbrace{\frac{(2k)!}{2^k k!}}_{\text{Gaussian } 2k\text{-th moment}} \|\cdot\|_2^{2k} \pm \underbrace{\lambda \cdot k^k}_{\text{dim-independent deviation}} \|\cdot\|_2^{2k}$$

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$\hookrightarrow$  We provide an explicit sum-of-squares proof of this (in the indeterminate  $v$ ).



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then 
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How do we handle the remaining directions?

↳ Do not admit a small cover ex:  $v = \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2\sqrt{d}}, \dots, \frac{1}{2\sqrt{d}} \right)$

## Certifiable Anti-Concentration: Overview

Lemma: If  $\|v\|_4^4 \leq \lambda \|v\|_2^4$

then 
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How do we handle the remaining directions?

Lemma: Any direction  $v$  can be decomposed in  $v_L + v_H$  s.t.  $v_L$  has  $1/\lambda$  non-zero coordinates and  $v_H$  is analytically dense i.e.

$$\|v_H\|_4^4 \leq \lambda \|v_H\|_2^4.$$

Does not seem to help if  $v$  is an indeterminate.

# Certifiable Anti-Concentration: Overview

**Lemma:** Any direction  $v$  can be decomposed in  $v_L + v_H$  s.t.  $v_L$  has  $\forall \lambda$  non-zero coordinates and  $v_H$  is analytically dense i.e.

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① Switch to dual:

**Fact:** If  $\forall$  deg  $t$  pseudo-distributions  $\mu \in \tilde{\mathcal{E}}_\mu$   $p(x) \geq 0$ ,  $\exists$  a sos proof of  $p(x) \geq 0$ .

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② Assume for contradiction there is such  $\mu$  pseudo-distribution

③ Condition on "large" coordinates of  $v$  by "re-weighting" the pseudo-distribution

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 $\|v_H\|_4 \leq \lambda \|v_H\|_2$ .

① Switch to dual:

**Fact:** If  $\forall \deg t$  pseudo-distributions  $\mu \sum_{\mu} p(x) \geq 0$ ,  $\exists$  a sos proof of  $p(x) \geq 0$ .

② Assume for contradiction there is no such pseudo-distribution

③ Condition on "large" coordinates of  $v$  by "re-weighting" the pseudo-distribution

④ The resulting vector is analytically dense and we can invoke the explicit proof for analytically dense directions

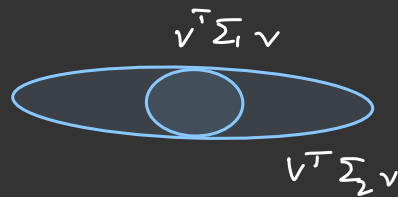
# Certifiable Anti-Concentration: Toy Application

$\{x_i\}_{i \in [n]}$  samples from  $M = \frac{1}{2} \mathcal{D}(0, \Sigma_1) + \frac{1}{2} \mathcal{D}(0, \Sigma_2)$  s.t.

1.  $\forall v \quad v^T \Sigma_1 v \leq v^T \Sigma_2 v$

2.  $\exists v$  s.t.  $v^T \Sigma_1 v < \delta^2 v^T \Sigma_2 v$

(w.l.o.g. assume  $M$  is isotropic)



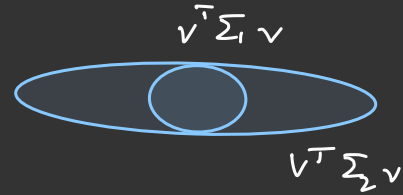
# Certifiable Anti-Concentration: Toy Application

$\{x_i\}_{i \in [n]}$  samples from  $M = \frac{1}{2} \mathcal{D}(0, \Sigma_1) + \frac{1}{2} \mathcal{D}(0, \Sigma_2)$  s.t.

1.  $\forall v \quad v^T \Sigma_1 v \leq v^T \Sigma_2 v$

2.  $\exists v$  s.t.  $v^T \Sigma_1 v < \delta^2 v^T \Sigma_2 v$

(w.l.o.g. assume  $M$  is isotropic)



$$A := \begin{cases} \forall i \in [n] & \omega_i = \omega_i \\ \forall i \in [n] & \omega_i \langle x_i, v \rangle^2 \leq \omega_i \delta^2 \|v\|^2 \\ \sum \omega_i = n/2 \end{cases}$$

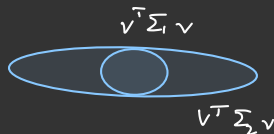
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## Algorithm:

1. Compute a deg  $O_\delta(\log d)$  pseudo-distribution
2. Sample  $g \sim N(0, \mathbb{E} v v^T)$
3. Output  $g / \|g\|$ .



# Certifiable Anti-Concentration: Toy Application

$\{x_i\}_{i \in [n]}$  samples from  $M = \frac{1}{2} \mathcal{D}(0, \Sigma_1) + \frac{1}{2} \mathcal{D}(0, \Sigma_2)$  s.t.

1.  $\forall v \quad v^T \Sigma_1 v \leq v^T \Sigma_2 v$

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$$A := \begin{cases} \forall i \in [n] & \omega_i^2 = \omega_i \\ \forall i \in [n] & \omega_i \langle x_i, v \rangle^2 \leq \omega_i \delta \|v\|^2 \\ \sum \omega_i = n/2 \end{cases}$$

Key SoS Lemma:

$$A \vdash \left\{ \langle \Sigma_1, w^T \rangle^2 \leq O(\delta) \|v\|^4 \right\}$$

Finishing the Proof:

$$\langle \Sigma_1, \tilde{\mathbb{E}} w^T \rangle^2 \leq \tilde{\mathbb{E}} \langle \Sigma_1, v^T \rangle^2 \leq O(\delta)$$

Observe  $\mathbb{E} g g^T = \tilde{\mathbb{E}} w^T$  and the claim follows from Markov's.

# Take aways:

KLS Conjecture



Poincaré  
Inequality

→ Certifiable Hypercontractivity  
of linear forms

*Kothari - Steinfeldt*

→ Certifiable Hypercontractivity  
of deg 2 polynomials

*no sos proof*

→ Mean Separation

→ Shell separation

Clustering

Uniform over  
 $L_p$  balls

*This  
Talk*

→ Certifiable Anti-concentration → Spectral Separation

→ List-Decodable  
Regression