# Clustering Mixtures of Bounded Covariance Distributions Under Optimal Separation

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Joint work with Ilias Diakonikolas, Daniel Kane, Thanasis Pittas



**Mixture model**:

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**Mixture model**: **Data**:





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### **Setup:**

- $\epsilon$  -contaminated samples from  $k$ -mixture  $D =$
- $P_i$  has mean  $\mu_i$  and covariance  $\Sigma_i$ , both unknown
- $\mu_i$ ,  $\mu_j$  "well separated"

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\text{nixture } D = \sum_{i=1}^{k} w_i P_i
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## Robust Clustering Mixture Distributions

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**Goal:** Identify 95% of the samples correctly for **every** cluster

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## Robust Clustering Mixture Distributions

**What is the minimum separation?**



## Minimum Separation - Uniform Mixtures



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**Assume**: Uniform mixture (for now)

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### **arXiv:2312.11769** Minimum Separation - Uniform Mixtures

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#### **Jasper Lee Clustering Bounded Covariance Mixtures 3**

 $\sigma \sqrt{k}$ 



### **arXiv:2312.11769** Minimum Separation - Uniform Mixtures **Assume**: Uniform mixture (for now)  $D =$ *k* ∑ *i*=1 1 *k Pi*

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### **Natural Goal:** If all cluster covariances  $\leq \sigma^2 I$ , assume separation  $\gg \sigma \sqrt{k}$

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**Assume**: Uniform mixture (for now)

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**Pairwise** overlap fraction ≲ 1/*k*

### **Solved! [DKKLT22]**: Near-linear time algorithm, also for list-decodable mean estimation



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$$
\bigr|\, 2w
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**Clearly separable/clusterable**  $|2w|$ but [DKKLT22] fails

## **New Goal:** Between clusters  $i,j$ , assume separation  $\gg (\sigma_i + \sigma_j)\sqrt{k}$ **Fine-grained separation arXiv:2312.11769** Minimum Separation - Uniform Mixtures



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**Fine-grained separation**

### • [BKK22]:  $(\sigma_i + \sigma_j)$  poly $(k, \log n)$  separation + "No large sub-cluster" assumption



**Prior work**:

- [DKKLT22]:  $\max_i \sigma_i \sqrt{k}$  separation
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**Our work**:

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- [DKLP23]:  $(\sigma_i + \sigma_j) \sqrt{k}$  separation



## Theorem — Uniform Mixtures

**Theorem:** Given  $\tilde{O}((d + \log 1/\delta) k^2)$  samples from where  $P_i$  has mean  $\mu_i$  and covariance  $\Sigma_i \leq \sigma_i^2 I$  (all unknown) and  $\|\mu_i - \mu_j\| \gg (\sigma_i + \sigma_j) \sqrt{k}$  $\boldsymbol{A}$ lgorithm returns sets  $B_1, \dots, B_k$  such that up to index permutation: •  $B_i$  overlaps with 95% of cluster *i* samples  $S_i$ ) samples from  $D = \sum$ *i* 1 *k Pi* **Failure** probability  $\longrightarrow$  **Corrupted,**  $\epsilon \leq 1/(100k)$ 

• Mean of  $B_i$  is  $O(\sigma_i)$  close to  $\mu_i$ 



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### **Remarks**:

**•** Does not need to know *k* precisely, only need input *α* ∈ [0.6/*k*,1/*k*]



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**•** Does not need to know *k* precisely, only need input *α* ∈ [0.6/*k*,1/*k*] • Can work for almost-uniform mixtures, with each  $w_i \in [0.9/k, 1.1/k]$ 



### **Remarks**:

- 
- 



## Algorithm — Uniform Mixtures

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## Algorithm — Uniform Mixtures





## Algorithm Outline

### **Algorithm:**



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• Input:  $O((d + \log 1/\delta) k^2)$  samples, parameter  $\widetilde{O}((d+\log 1/\delta)k^2)$  samples, parameter  $k$


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- Input:  $O((d + \log 1/\delta) k^2)$  samples, parameter  $\widetilde{O}((d+\log 1/\delta)k^2)$  samples, parameter  $k$
- **1.** Generate many (but poly-sized many) candidate means



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**i.** Using list-decodable mean estimation

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- **2.** Pruning to get exactly 1 close-enough candidate mean per cluster





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- **1.** Generate many (but poly-sized many) candidate means
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- **2.** Pruning to get exactly 1 close-enough candidate mean per cluster
	- **i.** Ensure every candidate mean is close to a cluster mean



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- Input:  $O((d + \log 1/\delta) k^2)$  samples, parameter  $\widetilde{O}((d+\log 1/\delta)k^2)$  samples, parameter  $k$
- **1.** Generate many (but poly-sized many) candidate means
	- **i.** Using list-decodable mean estimation
- **2.** Pruning to get exactly 1 close-enough candidate mean per cluster
	- **i.** Ensure every candidate mean is close to a cluster mean
	- **ii.** Prune if too many means per cluster



### List-Decodable Mean Estimation

- **Problem:** Given  $\alpha n$  samples from a distribution  $P$  with covariance  $\leq \sigma^2 I$ ,
	- mixed with arbitrary  $(1 \alpha)n$  outliers, estimate the mean of  $P$ ?
		- **What can we do when**  $\alpha < 1/2$ ?



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- **Fact [DKKLT22]:** Near-linear time algorithm, outputs a *list* of  $O(1/\alpha)$  vectors
	- **One** of them is  $O(\sigma/\surd\alpha)$ -close to the true mean of  $P$



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#### **Caveat:** DKKLT22 requires knowing *σ* to constant factor.



## List-Decodable Mean Estimation

**Fact [DKKLT22]:** Near-linear time algorithm, outputs a *list* of  $O(1/\alpha)$  vectors



#### **Caveat:** DKKLT22 requires knowing *σ* to constant factor.

### **Solution:** First generate a  $poly(n)$ -sized list of candidate  $\sigma_i$ ,

then run DKKLT22 using all candidate standard deviations

# Algorithm Outline

### **Algorithm:**

- Input:  $O((d + \log 1/\delta) k^2)$  samples, parameter  $\widetilde{O}((d+\log 1/\delta)k^2)$  samples, parameter  $k$
- - **i.** Using list-decodable mean estimation
- -
	- **ii.** Prune if too many means per cluster

**1.** Generate many (but poly-sized many) candidate means + s.d. **2.** Pruning to get exactly 1 close-enough candidate mean per cluster **i.** Ensure every candidate mean is close to a cluster mean



# Pruning — Main Step

**Ingredient:** Check if candidate mean  $\hat{\mu}$  corresponds to cluster

of  $\approx n/k$  samples w/ standard deviation  $\hat{s}$ 

**Can be** *O*(*s* ̂ *k*) **from true cluster mean**





# Pruning — Main Step

**Ingredient:** Check if candidate mean  $\hat{\mu}$  corresponds to cluster

of  $\approx n/k$  samples w/ standard deviation  $\hat{s}$ 

Find:  $w_x \in [0,1]$  for all x in sample set

such that

$$
\left\| \sum_{x} w_x \left( x - \sum_{y} w_{y} y \right) \left( x - \sum_{y} w_{y} y \right)^{\top} \right\|_{op} \leq O(\hat{s}^2) \sum_{x} w_x
$$

$$
\sum_{x} w_x \geq 0.97 n/k \qquad \left\| \sum_{x} w_x x - \hat{\mu} \right\|_{2} \leq O(\hat{s} \sqrt{k})
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∑

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**Can be** *O*(*s* ̂ *k*) **from true cluster mean**

 $w_x \in [0,1]$  for all x in sample set



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# Pruning — Main Step

**Ingredient:** Check if candidate mean  $\hat{\mu}$  corresponds to cluster

∑ *x*  $w_x \geq 0.97n/k$ 

Find:

such that

∑ *x*





# Algorithm Outline

### **Algorithm:**

- **i.** Using list-decodable mean estimation **i.** Ensure every candidate mean is close to a cluster mean **ii.** Prune if too many means per cluster  $\widetilde{O}((d+\log 1/\delta)k^2)$  samples, parameter  $k$
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- Input:  $O((d + \log 1/\delta) k^2)$  samples, parameter **1.** Generate many (but poly-sized many) candidate means + s.d. **2.** Pruning to get exactly 1 close-enough candidate mean per cluster
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**Observation:** Multiple candidate means will *split* a cluster,

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# Pruning — By Mass

**Observation:** Multiple candidate means will *split* a cluster,

- 
- at least one with small size ( ≪ 1/*k* fraction)

- 
- and prune candidate means with cluster size  $\leq 0.96n/k$

**Solution:** Repeatedly cluster with nearest representative,



# Algorithm Outline

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**Goal:** Identify 95% of the samples correctly for **every** cluster

**arXiv:2312.11769**





## Robust Clustering Mixture Distributions



**Goal:** Identify 95% of **Impossible** very cluster



## Robust Clustering Mixture Distributions



### Non-identifiability



- $k = 3$
- **•** Min weight *α* = 1/4

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**Even if we know**:



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**Question:** What information *can* we compute about the clustering?





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# Non-identifiability

**Even if we know**:

**Even with infinite uncorrupted samples**

**Question:** What information *can* we compute about the clustering?

**Maybe:** Compute all sub-clusterings, except for the grouping





# Clustering Refinement

**Definition:** Given true cluster samples  $S_1, ..., S_k$ , totalling *n* samples,

the disjoint subsets  $B_1, ..., B_m$  form an *accurate refinement* if:

 $|B_j| \geq 0.95$ *αn* 

$$
\bullet \quad \|\mu_{B_j} - \mu_{B_j}\| \gg (\sigma_{B_j} + \sigma_{B_j})/\sqrt{\alpha}
$$

- They can be grouped into  $k$  sample sets  $S'_1, ..., S'_k$  such that
	- $S_i$  and  $S'_i$  have 92% overlap

**Theorem:** Given  $\tilde{O}((d + \log 1/\delta)/a^2)$  samples from





and 
$$
\|\mu_i - \mu_j\| \gg (\sigma_i + \sigma_j)/\sqrt{2}
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*Algorithm* returns sets  $B_1, \, ... , B_m$  that is an *accurate refinement* 

of true clustering  $S_1, \, ... , S_k$ 



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**Remarks**:

*•* One *single* algorithm for both theorems

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**Remarks**: **Previous alg (replace** *k* **with** 1/*α***) + distance-based pruning**
## Theorem — Arbitrary Mixtures

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**Remarks**:

- *•* One *single* algorithm for both theorems
- 

*•* **Corollary:** existence of a **common refinement** for all possible clusterings



**Previous alg (replace** *k* **with** 1/*α***) + distance-based pruning**



### Clustering Arbitrary Mixtures

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## Clustering Arbitrary Mixtures

### **Question:** What is a **sufficient** assumption to compute a clustering not just a refinement?

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## Clustering Arbitrary Mixtures



For every  $S_i$  and every subset  $S' \subseteq S_i$  of size  $\geq 0.8$ *αn*  $\longleftarrow$  Every large subset



# No Large Sub-Cluster Condition

**Definition:** The sample sets  $S_1, ..., S_k$  of total size  $n$  have "no large sub-clusters" if

We have  $\sigma_{\!S'} \geq 0.1 \sigma_{\!S_i}$ 

**Should not look like its own cluster**

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# No Large Sub-Cluster Condition

We have  $\sigma_{\!S'} \geq 0.1 \sigma_{\!S_i}$ 

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**Theorem:** If the (uncorrupted) input samples have no large sub-clusters,

then *Algorithm* returns a clustering with *k* sets instead of a refinement.

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# No Large Sub-Cluster Condition

We have  $\sigma_{\!S'} \geq 0.1 \sigma_{\!S_i}$ 

**Proposition:** For well-conditioned+high-d log-concave distributions, drawing  $\tilde{O}(d/\alpha^2)$ 

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 $O(d/\alpha^2)$  samples ensures no large sub-clusters, due to thin-shell behavior.



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≈ **isotropic covariance**

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**Proposition:** For well-conditioned+high-d log-concave distributions, drawing  $\approx$  **isotropic covariance**  $\sim$   $d \geq \text{polylog}(1/\alpha)$ 

 $O(d/\alpha^2)$  samples ensures no large sub-clusters, due to thin-shell behavior.  $\tilde{O}(d/\alpha^2)$ 

### **Should not look like its own cluster**





### Summary

 $M$ ean  $μ$ <sub>*i*</sub>, Covariance  $\Sigma$ <sub>*i*</sub>  $\leq \sigma_i^2 I$ 







*i*

- **Problem:** Cluster samples from  $\sum w_i P_i$  under fine-grained separation  $\|\mu_i \mu_j\| \gg (\sigma_i + \sigma_j)/\sqrt{\alpha}$ 
	- $M$ ean  $μ$ <sub>*i*</sub>, Covariance  $\Sigma$ <sub>*i*</sub>  $\leq \sigma_i^2 I$



### Summary

### **A single poly-time algorithm such that:**

**•** Near-uniform mixture: recovers clustering to 95% accuracy

- **•** Arbitrary mixtures: recovers *accurate refinement*
- **•** Arbitrary mixture + No Large Sub-Cluster condition: recovers clustering to 95% accuracy
- **•** Can tolerate corruption level *ϵ* ≤ *α*/100

*i*

- **Problem:** Cluster samples from  $\sum w_i P_i$  under fine-grained separation  $\|\mu_i \mu_j\| \gg (\sigma_i + \sigma_j)/\sqrt{\alpha}$ 
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### **A single poly-time algorithm such that:**

**•** Near-uniform mixture: recovers clustering to 95% accuracy

- **•** Arbitrary mixtures: recovers *accurate refinement*
- **•** Arbitrary mixture + No Large Sub-Cluster condition: recovers clustering to 95% accuracy
- **•** Can tolerate corruption level *ϵ* ≤ *α*/100

#### **Structural**:

**•** All ground truth clusterings of a mixture share a common refinement

*i*



### Open Problems



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**Goal:** Design the most *versatile* algorithm

- **Problem:** Cluster samples from  $\sum w_i P_i$  under fine-grained separation  $\|\mu_i \mu_j\| \gg (\sigma_i + \sigma_j)/\sqrt{\alpha}$ 
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