

# Efficient Moment Methods and Mixture Models

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## Symmetric Moment Tensor

Given data  $\mathbf{x}_1, \dots, \mathbf{x}_p \in \mathbb{R}^n$ . It is often useful to form the moment

$$\mathbf{M}_d = \frac{1}{p} \sum_{i=1}^p \mathbf{x}_i^{\otimes d} \in S^d(\mathbb{R}^n)$$

where  $(\mathbf{x}^{\otimes d})_{i_1, \dots, i_d} = \mathbf{x}_{i_1} \dots \mathbf{x}_{i_d}$  for each  $(i_1, \dots, i_d) \in [n]^d$ .

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- ▶  $d = 1 \rightsquigarrow$  sample average
- ▶  $d = 2 \rightsquigarrow$  sample covariance matrix (uncentered)
- ▶  $d = 3 \rightsquigarrow n \times n \times n$  real symmetric tensor (sample third moment), etc.



# Moment Tensor Decompositions: A Mix of Algebra and Computation

When the data  $\mathbf{x}_1, \dots, \mathbf{x}_p$  follows a nice model, typically the moment tensors  $\mathbf{M}_d$  admit a nice algebraic decomposition. We'll see computing it helps to e.g. estimate model parameters.

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I will focus on two examples of (*model, decomposition*) pairs:

- I. Gaussian Mixture Models & CP Tensor Decompositions
- II. Mixture of Products & Coupled Incomplete CP Tensor Decompositions

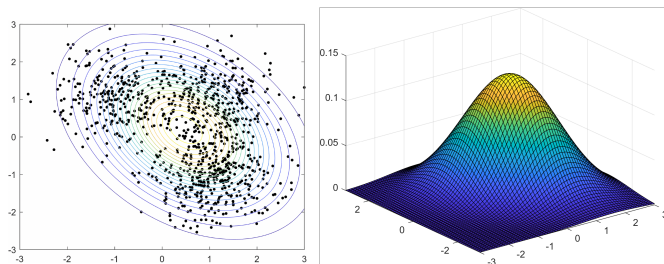
# **PART I:** *Gaussian Mixture Models & CP Tensor Decompositions*

# Gaussian Distribution

Gaussian vector:  $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

probability density function:  $\frac{\exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}))}{\sqrt{(2\pi)^n \det(\boldsymbol{\Sigma})}}$

parameters:  $\boldsymbol{\mu} = \mathbb{E}[\mathbf{x}] \in \mathbb{R}^n$ ,  $\boldsymbol{\Sigma} = \mathbb{E}[(\mathbf{x} - \boldsymbol{\mu}) \otimes^2] \in \mathcal{S}^2(\mathbb{R}^n)$

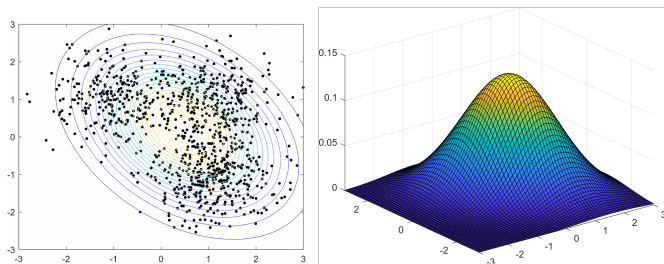


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- ▶ Limiting average of any (suff. integrable) i.i.d. random vectors
- ▶ Marginals are themselves lower-dimensional Gaussians

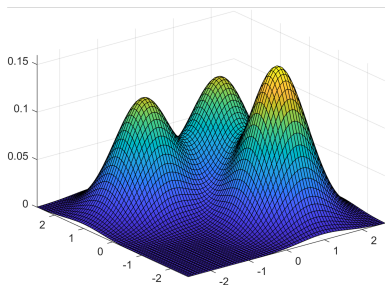
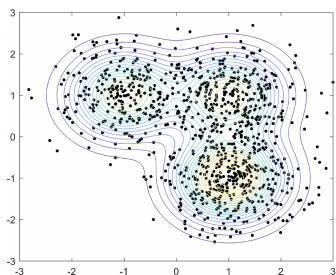


# Gaussian Mixture Models

$$\text{GMM: } \mathbf{x} \sim \sum_{j=1}^r \lambda_j \mathcal{N}(\mu_j, \Sigma_j)$$

$r$  is the number of components,  $\lambda_j$  are the mixing weights (convex combination)

parameters:  $\{(\lambda_j, \mu_j, \Sigma_j) : j = 1, \dots, r\}$

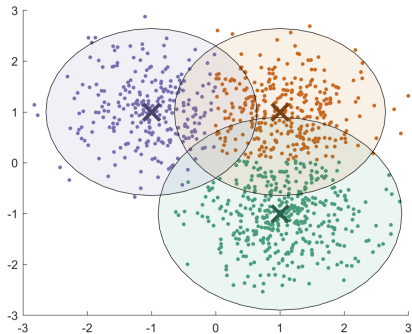


# The Many Applications of Gaussian Mixtures

**Density  
Estimation**

**Clustering**

**Anomaly  
Detection**

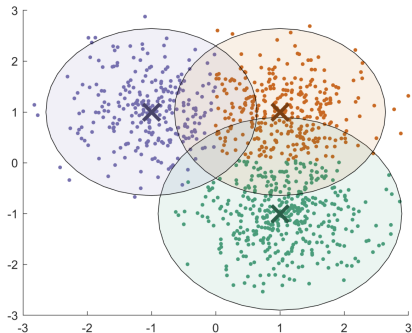


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**GMMs are one of the most prevalent tools in data analysis!**

# Neat Formula for Moment Tensors of GMM

Lemma (Wick '50, Pereira-K.-Kolda '22)

Let  $\mathbf{x}_1, \dots, \mathbf{x}_p$  be i.i.d. realizations of a GMM with parameters  $\{(\lambda_j, \mu_j, \Sigma_j)\}$ . Then

$$\mathbf{M}_d \longrightarrow \sum_{j=1}^r \lambda_j \sum_{k=0}^{\lfloor d/2 \rfloor} \binom{d}{2k} \frac{(2k)!}{k! 2^k} \text{sym}(\mu_j^{\otimes(d-2k)} \otimes \Sigma_j^{\otimes k}) \quad \text{as } p \rightarrow \infty.$$

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The proof is most easily done using the bijection  $\Phi$  from symmetric tensors to homogeneous forms, because  $\Phi(\text{sym}(S \otimes T)) = \Phi(S)\Phi(T)$ .

$$\text{sym} \left( \begin{array}{c} \text{Green} \\ \text{Red} \\ \text{Blue} \end{array} \right) = \frac{1}{6} \left( \begin{array}{c} \text{Green} \\ \text{Red} \\ \text{Blue} \end{array} + \begin{array}{c} \text{Blue} \\ \text{Red} \\ \text{Green} \end{array} + \begin{array}{c} \text{Green} \\ \text{Blue} \\ \text{Red} \end{array} + \begin{array}{c} \text{Blue} \\ \text{Green} \\ \text{Red} \end{array} + \begin{array}{c} \text{Red} \\ \text{Blue} \\ \text{Green} \end{array} + \begin{array}{c} \text{Red} \\ \text{Green} \\ \text{Blue} \end{array} \right)$$

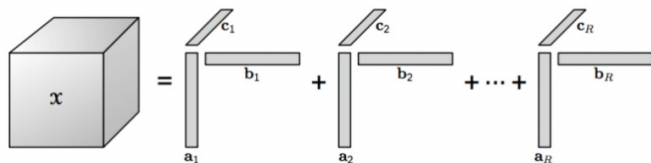
# Symmetric CP Tensor Decomposition

## Proposition (Pereira-Kileel-Kolda '22)

Let  $\mathbf{x}_1, \dots, \mathbf{x}_p$  be i.i.d. realizations of a GMM with parameters  $\{(\lambda_j, \mu_j, \Sigma)\}$ , i.e. there is a common covariance. Then as  $p \rightarrow \infty$ ,

$$\sum_{k=0}^{\lfloor d/2 \rfloor} (-1)^k \binom{d}{2k} \frac{(2k)!}{k!2^k} \text{sym}(\mathbf{M}_{d-2k} \otimes \Sigma^{\otimes k}) \longrightarrow \sum_{j=1}^r \lambda_j \mu_j^{\otimes d}.$$

The right-hand side is a real symmetric CP tensor decomposition.



# Computational Algebraic Geometry: GMM Identifiability

*What is the maximal number  $r$  of Gaussian components in  $\mathbb{R}^n$  that is uniquely determined by the first  $d$  moments?*

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Symmetric CP tensor decomposition is generically unique when

$$r \dim v_d(\mathbb{P}(\mathbb{R}^n)) + (r - 1) < \dim \mathbb{P}(S^d(\mathbb{R}^n)) \Leftrightarrow r < \frac{1}{n} \binom{n+d-1}{d}$$

if  $d \geq 3$ , with a few classified exceptions for  $(d, n, r)$  (see e.g. Chiantini-Ottaviani-Vannieuwenhoven '17 about secants of Veronese varieties). It implies that a GMM with a known common covariance and generic  $(\lambda_j, \mu_j)$  is determined by its moments of order  $\leq d$  up to such  $r$ .



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**To my knowledge, identifiability for the most general case of unknown, different and unconstrained  $\Sigma_j$  is currently unresolved.**

# Numerical Algorithm Beating the Curse of Dimensionality

To fit a GMM to data, consider minimizing the cost function

$$\operatorname{argmin}_{\lambda_j, \mu_j, \Sigma_j} \|\mathbf{M}_d - (\text{aforementioned formula in parameters})\|_F^2$$

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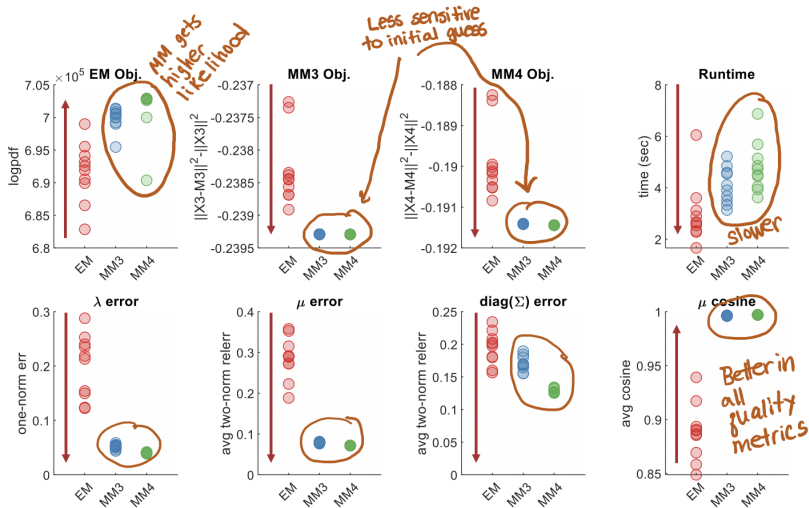
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## Theorem (Pereira-Kileel-Kolda '22)

*Given the parameters  $\lambda_j, \mu_j, \Sigma_j$  and data  $\mathbf{x}_i$ , there is an algorithm to evaluate the above cost and its gradient in  $\mathcal{O}(prn^2 + r^2n^3)$  flops and  $\mathcal{O}(rn^2 + pn)$  storage. If  $\Sigma_j$  are diagonal, these drop to  $\mathcal{O}(prn + r^2n)$  flops and  $\mathcal{O}(rn + pn)$  storage.*

# In Practice: Method of Moments Can Outperform EM



- ▶ Randomly-generated problems with overlapping Gaussians
- ▶  $n = 100$ ,  $r = 20$ ,  $p = 8000$ , common diagonal  $\Sigma$
- ▶ Compared EM, MM3 (moments  $d = 3$ ), MM4 (moments  $d = 4$ )

# Sketch: Expanding Out The Inner Products

Idea is to operate on moment tensors without forming them!

$$\min_{\theta} f(\theta) \equiv \left\| \frac{1}{p} \sum_{i=1}^p \mathbf{x}_i^{\otimes d} - \sum_{j=1}^m \lambda_j \mathcal{M}_j^{(d)} \right\|^2$$

$$f(\theta) = \left\| \frac{1}{p} \sum_{i=1}^p \mathbf{x}_i^{\otimes d} \right\|^2 + \left\| \sum_{j=1}^m \lambda_j \mathcal{M}_j^{(d)} \right\|^2 - 2 \left\langle \frac{1}{p} \sum_{i=1}^p \mathbf{x}_i^{\otimes d}, \sum_{j=1}^m \lambda_j \mathcal{M}_j^{(d)} \right\rangle$$

*constant*

$$f(\theta) = C + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \left\langle \mathcal{M}_i^{(d)}, \mathcal{M}_j^{(d)} \right\rangle - \frac{2}{p} \sum_{i=1}^p \sum_{j=1}^m \lambda_j \left\langle \mathbf{x}_i^{\otimes d}, \mathcal{M}_j^{(d)} \right\rangle$$

*dot product of 2 moments*

*dot product of moment + vector*

## Example Calculation: $d = 3$

$$f(\theta) = C + \sum_{i=1}^m \sum_{j=1}^m \lambda_i \lambda_j \langle \mathcal{M}_i^{(d)}, \mathcal{M}_j^{(d)} \rangle - \frac{2}{p} \sum_{i=1}^p \sum_{j=1}^m \lambda_j \langle \mathbf{x}_i^{\otimes d}, \mathcal{M}_j^{(d)} \rangle$$

$$\mathcal{M}_j^{(3)} = \boldsymbol{\mu}_j^{\otimes 3} + 3 \text{sym}(\boldsymbol{\mu}_j \otimes \boldsymbol{\Sigma}_j)$$

$$\begin{aligned} \langle \mathbf{x}_i^{\otimes 3}, \mathcal{M}_j^{(3)} \rangle &= \langle \mathbf{x}_i^{\otimes 3}, \boldsymbol{\mu}_j^{\otimes 3} \rangle + 3 \langle \mathbf{x}_i^{\otimes 3}, \text{sym}(\boldsymbol{\mu}_j \otimes \boldsymbol{\Sigma}_j) \rangle \\ &= (\mathbf{x}_i^{\top} \boldsymbol{\mu}_j)^3 + 3 \langle \mathbf{x}_i^{\otimes 3}, \boldsymbol{\mu}_j \otimes \boldsymbol{\Sigma}_j \rangle \\ &= (\mathbf{x}_i^{\top} \boldsymbol{\mu}_j)^3 + 3(\mathbf{x}_i^{\top} \boldsymbol{\mu}_j)(\mathbf{x}_i^{\top} \boldsymbol{\Sigma}_j \mathbf{x}_i) \end{aligned}$$

$$\langle \mathbf{a}^{\otimes 3}, \text{sym}(\mathbf{B}) \rangle = \langle \mathbf{a}^{\otimes 3}, \mathbf{B} \rangle$$

$$\langle \mathbf{a}^{\otimes 3}, \mathbf{b}^{\otimes 3} \rangle = (\mathbf{a}^{\top} \mathbf{b})^3$$

$$\langle \mathbf{a}^{\otimes 3}, \mathbf{b} \otimes \mathbf{C} \rangle = \mathbf{a}^{\top} \mathbf{b} \mathbf{a}^{\top} \mathbf{C} \mathbf{a}$$

Computing terms  $\langle \mathbf{M}_i^{(d)}, \mathbf{M}_j^{(d)} \rangle$  more involved (Bell polynomials).



# **PART II:** *Mixture of Products & Coupled Incomplete CP Decompositions*

## Other Noise Models

**Implicit moment tensor decomposition can be applied to mixtures with other noise models (e.g., Poisson noise).**

- ▶ Focus on conditionally-independent mixtures in  $\mathbb{R}^n$ :

$$\mathcal{D} = \sum_{j=1}^r w_j \mathcal{D}_j = \sum_{j=1}^r w_j \bigotimes_{i=1}^n \mathcal{D}_{ij}$$

for some distributions  $\mathcal{D}_{ij}$  on  $\mathbb{R}$ . That is, conditional on latent variable, standard coords in  $\mathbb{R}^n$  are indep. [e.g. Hall-Zhou '03]

- ▶ Make no parametric assumptions on  $\mathcal{D}_{ij}$ .

## Precise Formulation

$$\mathcal{D} = \sum_{j=1}^r w_j \mathcal{D}_j = \sum_{j=1}^r w_j \bigotimes_{i=1}^n \mathcal{D}_{ij}.$$

Denote  $d$ th joint moment and componentwise moments by

$$\mathbf{M}^d = \mathbb{E}_{X \sim \mathcal{D}}[X^{\otimes d}] \in \mathbb{R}^{n^d} \quad \text{and} \quad \mathbf{m}_j^d = \mathbb{E}_{X \sim \mathcal{D}_j}[X^{*d}] \in \mathbb{R}^n,$$

where  $*$  denotes entrywise power.

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where  $*$  denotes entrywise power.

### Problem

*Given data  $V \subset \mathbb{R}^n$  from a conditionally-independent mixture  $\mathcal{D}$  of  $r$  components. We want to estimate the mixing weights  $w$  and componentwise moments  $\{(\mathbf{m}_j^1, \mathbf{m}_j^2, \dots) : j = 1, \dots, r\}$  from the sample moment tensors  $\widehat{\mathbf{M}}^1, \widehat{\mathbf{M}}^2, \dots$  without parametrizing  $\mathcal{D}$ .*

# Incomplete Tensor Decomposition: Up To $d = 3$

Unknowns  $\{w_j, \mathbf{m}_j^1, \mathbf{m}_j^2, \mathbf{m}_j^3\}_{j \in [r]}$ .

$$\mathbf{M}^1 = \sum_{j=1}^r w_j \mathbf{m}_j^1 \in \mathbb{R}^n$$

$$P(\mathbf{M}^2) = P\left(\sum_{j=1}^r w_j (\mathbf{m}_j^1)^{\otimes 2}\right) \in \mathcal{S}^2(\mathbb{R}^n)$$

$$P_{(2)}(\mathbf{M}^2) = \sum_{j=1}^r w_j \mathbf{m}_j^2 \in \mathbb{R}^n$$

$$P(\mathbf{M}^3) = P\left(\sum_{j=1}^r w_j (\mathbf{m}_j^1)^{\otimes 3}\right) \in \mathcal{S}^3(\mathbb{R}^n)$$

$$P_{(2,1)}(\mathbf{M}^3) = P\left(\sum_{j=1}^r w_j \mathbf{m}_j^2 \otimes \mathbf{m}_j^1\right) \in \mathbb{R}^{n \times n}$$

$$P_{(3)}(\mathbf{M}^3) = \sum_{j=1}^r w_j \mathbf{m}_j^3 \in \mathbb{R}^n.$$

*For general  $d$ , this becomes a coupled system of partially symmetric incomplete CP tensor decomposition problems.*

# Identifiability Bound

## Theorem (Zhang-K. '23)

Let  $\mathcal{D}$  be a conditionally independent mixture with positive weights  $w \in \mathbb{R}^n$  and Zariski-generic means  $A \in \mathbb{R}^{n \times r}$ . Let  $d_1, d_2 \in \mathbb{N}$  be distinct such that  $2 < d_1 < n$ ,  $r \leq \binom{\lfloor (n-1)/2 \rfloor}{\lfloor d_1/2 \rfloor}$  and  $r \leq \binom{n}{d_2}$ . Then  $w$  and  $A$  are uniquely determined from the equations

$$P\left(\sum_{j=1}^r w_j m_j^{1 \otimes d_1}\right) = P(\mathbf{M}^{d_1}), \quad P\left(\sum_{j=1}^r w_j m_j^{1 \otimes d_2}\right) = P(\mathbf{M}^{d_2}),$$

up to possible sign flips on each  $m_j^1$  if  $d_1$  and  $d_2$  are both even.

# Numerical Optimization

Use least squares cost function:

$$f^{[d]}(w, A; V) = \sum_{i=1}^d \tau_i \left\| P \left( \underbrace{\frac{1}{p} \sum_{\ell=1}^p v_{\ell}^{\otimes i}}_{\widehat{M}^i} - \underbrace{\sum_{j=1}^r w_j a_j^{\otimes i}}_{M^i} \right) \right\|^2.$$

Residuals are **multilinear** in  $w$  (obvious) and each row of the mean matrix  $A$  (less obvious).

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**Algorithm 1** Baseline ALS algorithm for solving means and weights

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- 1: **function** SOLVEMEANANDWEIGHT(data  $V$ , initialization  $(w, A)$ , order  $d$ , hyperparameters  $\tau$ )
  - 2:     Compute  $\{G_s^{A,A}\}_{s=1}^d$  and  $\{G_s^{A,V}\}_{s=1}^d$
  - 3:     **while** not converged **do**
  - 4:          $A, \{G_s^{A,A}\}_{s=1}^d, \{G_s^{A,V}\}_{s=1}^d \leftarrow \text{UPDATEMEAN}(\{G_s^{A,A}\}_{s=1}^d, \{G_s^{A,V}\}_{s=1}^d, w, A, d, \tau)$
  - 5:          $w \leftarrow \text{UPDATEWEIGHT}(\{G_s^{A,A}\}_{s=1}^d, \{G_s^{A,V}\}_{s=1}^d, d, \tau)$
  - return**  $w, A$
-

# Implicit Tensor Computations

- ▶  $\widehat{\mathbf{M}}^d$  needs  $\mathcal{O}(n^d)$  to store and  $\mathcal{O}(pn^d)$  flops to compute.
- ▶ Implicit: compute the normal equations for the least square solves **without forming any higher-order tensors**. Flops:  $\mathcal{O}(npr + nr^3)$ . Storage:  $\mathcal{O}(n(r + p))$ .
- ▶ Main thing is to efficiently evaluate the **kernel**:

$$K_d(x, y) = \langle P(x^{\otimes d}), P(y^{\otimes d}) \rangle$$

at  $K_d(a_j, a_{j'})$  and  $K_d(a_j, v_\ell)$ .



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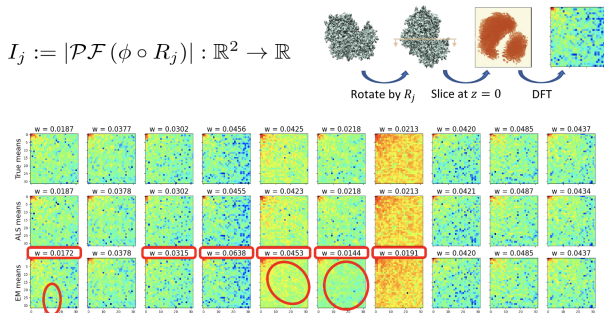
at  $K_d(a_j, a_{j'})$  and  $K_d(a_j, v_\ell)$ .

## Lemma

Let  $e_d$  be the elementary symmetric polynomial of degree  $d$ . Then  $K_d(x, y) = d! \cdot e_d(x * y)$ .

We evaluate  $e_d$  via *Newton-Gerard identities*, relating  $e_d$  to power sums.

# Example: Clustering X-Ray Free Electron Laser Images



- ▶ Here  $n = 1024$ ,  $r = 30$ ,  $p = 20000$ .
- ▶ Noise is pixelwise Poisson. Our algorithm doesn't know this, but EM does.
- ▶ We take  $\sim 40$  min to converge. Error 0.9% in weights, 0.5% in means.
- ▶ EM is initialized with best of 30  $k$ -means runs. We then run EM three times with different seeds. It takes  $\sim 50 - 70$  min. Error in means is  $> 13\%$ .

# CONCLUSIONS

## Summary

- ▶ Moment formulas for general Gaussian Mixture Models and a tensor-based algorithm avoiding exponential cost in order  $d$ .
- ▶ Variations for non-Gaussian mixtures, with product structure.
- ▶ Competitive with non-tensor approaches; in some cases better.

## References

Joao M. Pereira, Joe Kileel, Tamara G. Kolda, "Tensor moments of Gaussian mixture models: theory and applications", *preprint 2022*.

Yifan Zhang, Joe Kileel, "Moment estimation for nonparametric mixture models through implicit tensor decomposition", *SIAM Journal on Mathematics of Data Science 2023*.

Yulia Alexandr, Joe Kileel, Bernd Sturmfels, "Moment varieties for mixtures of products", *ACM International Symposium on Symbolic and Algebraic Computation 2023*.

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**THANK YOU!**