Efficient Moment Methods and Mixture Models

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Symmetric Moment Tensor

Given data $\mathbf{x}_1, \ldots, \mathbf{x}_p \in \mathbb{R}^n$. 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 $(\mathbf{x} \otimes d)_{i_1, \ldots, i_d} = x_{i_1} \ldots x_{i_d}$ for each $(i_1, \ldots, i_d) \in [n]^d$. 

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- $d = 1 \rightarrow$ sample average
- $d = 2 \rightarrow$ sample covariance matrix (uncentered)
- $d = 3 \rightarrow n \times n \times n$ real symmetric tensor (sample third moment), etc.
Moment Tensor Decompositions: A Mix of Algebra and Computation

When the data \( x_1, \ldots, x_p \) follows a nice model, typically the moment tensors \( M_d \) 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:

1. Gaussian Mixture Models & CP Tensor Decompositions
2. Mixture of Products & Coupled Incomplete CP Tensor Decompositions
PART I: Gaussian Mixture Models & CP Tensor Decompositions
Gaussian Distribution

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

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

parameters: \( \mu = \mathbb{E}[\mathbf{x}] \in \mathbb{R}^n, \Sigma = \mathbb{E}[(\mathbf{x} - \mu)^\otimes 2] \in S^2(\mathbb{R}^n) \)
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- Limiting average of any (suff. integrable) i.i.d. random vectors
- Marginals are themselves lower-dimensional Gaussians
Gaussian Mixture Models

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

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

parameters: $\{(\lambda_j, \mu_j, \Sigma_j) : j = 1, \ldots, r\}$
The Many Applications of Gaussian Mixtures

- Density Estimation
- Clustering
- Anomaly Detection
The Many Applications of Gaussian Mixtures

Density Estimation
Clustering
Anomaly Detection

GMMs are one of the most prevalent tools in data analysis!
Lemma (Wick ’50, Pereira-K.-Kolda ’22)

Let $x_1, \ldots, x_p$ be i.i.d. realizations of a GMM with parameters $\{(\lambda_j, \mu_j, \Sigma_j)\}$. Then

$$M_d \xrightarrow{p \to \infty} \sum_{j=1}^{r} \lambda_j \sum_{k=0}^{\lfloor d/2 \rfloor} \binom{d}{2k} \frac{(2k)!}{k!2^k} \text{sym}(\mu_j^{\otimes(d-2k)} \otimes \Sigma_j^{\otimes k})$$

as $p \to \infty$. 

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

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M_d \rightarrow \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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\[
\text{sym} \left( \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right) = \frac{1}{6} \left( \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right) + \begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} + \begin{array}{ccc} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{array} + \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{array} + \begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{array} + \begin{array}{ccc} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{array} \right)
\]
Symmetric CP Tensor Decomposition

Proposition (Pereira-Kileel-Kolda '22)

Let $x_1, \ldots, x_p$ be i.i.d. realizations of a GMM with parameters $\{(\lambda_j, \mu_j, \Sigma)\}$, i.e. there is a common covariance. Then as $p \to \infty$,

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

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

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

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 $r$. 

[Others study identifiability of GMMs under different assumptions. Boils down to other secant varieties, e.g. Amãendola-Ranestad-Sturmfels ’17 about secants of Veronese varieties.] To my knowledge, identifiability for the most general case of unknown, different and unconstrained $\Sigma_j$ is currently unresolved.
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Computational Algebraic Geometry: GMM Identifiability

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Numerical Algorithm Beating the Curse of Dimensionality

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

$$\arg\min_{\lambda_j, \mu_j, \Sigma_j} \| M_d - (\text{aforementioned formula in parameters}) \|_F^2$$
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$$\arg\min_{\lambda_j, \mu_j, \Sigma_j} \| M_d - (\text{aforementioned formula in parameters}) \|^2_F$$

Naively forming the terms would take $O(pn^d)$ flops and $O(n^d)$ in storage!
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Naively forming the terms would take $O(pn^d)$ flops and $O(n^d)$ in storage!

Theorem (Pereira-Kileel-Kolda ’22)

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

\[
\min_\theta f(\theta) \equiv \left\| \frac{1}{p} \sum_{i=1}^{p} x_i^{\otimes d} - \sum_{j=1}^{m} \lambda_j M_j^{(d)} \right\|^2
\]

\[
f(\theta) = \left\| \frac{1}{p} \sum_{i=1}^{p} x_i^{\otimes d} \right\|^2 + \left\| \sum_{j=1}^{m} \lambda_j M_j^{(d)} \right\|^2 - 2 \left\langle \frac{1}{p} \sum_{i=1}^{p} x_i^{\otimes d}, \sum_{j=1}^{m} \lambda_j M_j^{(d)} \right\rangle
\]

\[
f(\theta) = C + \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_i \lambda_j \left\langle M_i^{(d)}, M_j^{(d)} \right\rangle - \frac{2}{p} \sum_{i=1}^{p} \sum_{j=1}^{m} \lambda_j \left\langle x_i^{\otimes d}, M_j^{(d)} \right\rangle
\]

Dot product of 2 moments

Dot product of moment + vector
Example Calculation: \( d = 3 \)

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

\[
\mathcal{M}^{(3)}_j = \mu_j^{\otimes 3} + 3 \text{ sym}(\mu_j \otimes \Sigma_j)
\]

\[
\left\langle x^{\otimes 3}_i, \mathcal{M}^{(3)}_j \right\rangle = \left\langle x^{\otimes 3}_i, \mu_j^{\otimes 3} \right\rangle + 3 \left\langle x^{\otimes 3}_i, \text{sym}(\mu_j \otimes \Sigma_j) \right\rangle = (x^T_i \mu_j)^3 + 3 \left\langle x^{\otimes 3}_i, \mu_j \otimes \Sigma_j \right\rangle \quad \left\langle a^{\otimes 3}, \text{sym}(B) \right\rangle = \left\langle a^{\otimes 3}, B \right\rangle
\]

\[
= (x^T_i \mu_j)^3 + 3(x^T_i \mu_j)(x^T_i \Sigma_j x_i) \quad \left\langle a^{\otimes 3}, b^{\otimes 3} \right\rangle = (a^T b)^3
\]

\[
\left\langle a^{\otimes 3}, b \otimes C \right\rangle = a^T b a^T C a
\]

Computing terms \( \left\langle \mathcal{M}^{(d)}_i, \mathcal{M}^{(d)}_j \right\rangle \) more involved (Bell polynomials).
PART II: Mixture of Products & Coupled Incomplete CP Decompositions
Implicit moment tensor decomposition can be applied to mixtures with other noise models (e.g., Poisson noise).

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

$$D = \sum_{j=1}^{r} w_j D_j = \sum_{j=1}^{r} w_j \bigotimes_{i=1}^{n} D_{ij}$$

for some distributions $D_{ij}$ 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 $D_{ij}$. 

Other Noise Models
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.
Precise Formulation

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where \( * \) denotes entrywisewise 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 \( \{(\mathbf{m}_j^1, \mathbf{m}_j^2, \ldots) : j = 1, \ldots, r\} \) from the sample moment tensors \( \mathbf{\hat{M}}^1, \mathbf{\hat{M}}^2, \ldots \) without parametrizing \( \mathcal{D} \).
Incomplete Tensor Decomposition: Up To $d = 3$

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

\[
M^1 = \sum_{j=1}^{r} w_j m_j^1 \in \mathbb{R}^n
\]

\[
P(M^2) = P(\sum_{j=1}^{r} w_j (m_j^1) \otimes^2) \in S^2(\mathbb{R}^n)
\]

\[
P(2)(M^2) = \sum_{j=1}^{r} w_j m_j^2 \in \mathbb{R}^n
\]

\[
P(M^3) = P(\sum_{j=1}^{r} w_j (m_j^1) \otimes^3) \in S^3(\mathbb{R}^n)
\]

\[
P(2,1)(M^3) = P(\sum_{j=1}^{r} w_j m_j^2 \otimes m_j^1) \in \mathbb{R}^{n \times n}
\]

\[
P(3)(M^3) = \sum_{j=1}^{r} w_j m_j^3 \in \mathbb{R}^n.
\]

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

[building on Guo-Nie-Yang '22]
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 $2 < d_1 < n$, $r \leq \binom{n-1}{\lfloor d_1/2 \rfloor}$ and $r \leq \binom{n}{d_2}$. Then $w$ and $A$ are uniquely determined from the equations

$$P\left(\sum_{j=1}^r w_j m_1^1 \otimes d_1\right) = P\left(M^{d_1}\right), \quad P\left(\sum_{j=1}^r w_j m_2^1 \otimes d_2\right) = P\left(M^{d_2}\right),$$

up to possible sign flips on each $m^1_j$ if $d_1$ and $d_2$ are both even.
Numerical Optimization

Use least squares cost function:

$$f[d](w, A; V) = \sum_{i=1}^{d} \tau_i \left\| P \left( \frac{1}{p} \sum_{\ell=1}^{p} v_\ell \otimes i - \sum_{j=1}^{r} w_j a_j \otimes i \right) \right\|_2^2.$$

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

1: function **SOLVE_MEAN_AND_WEIGHT**(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: $A, \{G_{s}^{A,A}\}_{s=1}^{d}, \{G_{s}^{A,V}\}_{s=1}^{d} \leftarrow \text{UPDATE\_MEAN}(\{G_{s}^{A,A}\}_{s=1}^{d}, \{G_{s}^{A,V}\}_{s=1}^{d}, w, A, d, \tau)$
5: $w \leftarrow \text{UPDATE\_WEIGHT}(\{G_{s}^{A,A}\}_{s=1}^{d}, \{G_{s}^{A,V}\}_{s=1}^{d}, d, \tau)$
6: return $w, A$
Implicit Tensor Computations

- \( \hat{\mathbf{M}}^d \) 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 \( K_d(a_j, v_\ell) \).
Implicit Tensor Computations

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- Implicit: compute the normal equations for the least square solves without forming any higher-order tensors. Flops: $O(npr + nr^3)$. Storage: $O(n(r + p))$.

- 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 $K_d(a_j, v_\ell)$.

Lemma

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

We evaluate $e_d$ via Newton-Gerard identities, relating $e_d$ to power sums.
Example: Clustering X-Ray Free Electron Laser Images

\[ I_j := |\mathcal{P}F(\phi \circ R_j)| : \mathbb{R}^2 \to \mathbb{R} \]

▶ 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


References


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


THANK YOU!