# Learning mixtures of spherical Gaussians: moment methods and spectral decompositions

Machine Learning Reading Group Fall 2020

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### What are the main contributions?

- Provide a computationally efficient and statistically consistent moment-based estimator for mixtures of spherical Gaussians
- Derive computational and information-theoretic barriers to efficient estimation in mixture models (for spherical Gaussians).
- Make connections to estimation problems related to independent component analysis (ICA).



### Just as a little refresher...

# **Problem Statement**



- K sub-populations
- Each modeled as multivariate Gaussian.
- Each label picked according to some mixture weight.



### In case you prefer the PGM...



Note that the "labels" are not observed.



### What do we want to do?

We want an efficient algorithm that approximately recovers parameters from samples.

### One example of such an algorithm...

This can be done with a local search for maximum likelihood parameters (EM algorithm).



### Well Separated Mixtures

Estimation is easier if there is a large minimum separation between component means.



This is not required in general but leads to exponential  $(\exp(\Omega(k)))$  where k is the number of clusters) running time / sample size.



### Result

We can create an efficient algorithms for "non-degenerate" models in high-dimensions  $(d \ge k)$  with spherical covariances.

### How is this done?

Using the Method of Moments, they approximate the first three moments of the GMM and then solve for the parameters of the true models (means, covariances, and labels) with respect to those estimated moments.





- Let  $w_i$  be the probability of choosing a component  $i \in [k] := \{1, 2, ..., k\}$
- Let  $\mu_1, \mu_2, ..., \mu_k \in \mathbb{R}^d$  be the component vectors
- Let  $\sigma_1^2, \sigma_2^2, ..., \sigma_k^2 \ge 0$  be component variances

We then define two matrices for convenience:

$$w := [w_1, w_2, ..., w_k]^\top \in \mathbb{R}^k, \quad A := [\mu_1 | \mu_2 | ... | \mu_k] \in \mathbb{R}^{d \times k}$$



### Assuming the following data distribution...

We assume that the data was generated following,  

$$x \sim \sum_{i=1}^{k} \mathcal{I}[c=i] z_i$$
 where  $z_i \sim \mathcal{N}(\mu_i^*, \sigma_i^{2*}I), c \sim Cat(w^*)$ 

### **Algorithm Idea**

Now we take these samples, compute empirical estimates of some of the moments, and then match our current set of parameters to those moments.

### Moments



### **Definition of Moment Generating function**

$$M_{\mathbf{X}}(\mathbf{t}) := \mathrm{E}\Big(e^{\mathbf{t}^{\mathrm{T}}\mathbf{X}}\Big).$$

#### Recall the Taylor series expansion

$$e^{t\,X} = 1 + t\,X + rac{t^2\,X^2}{2!} + rac{t^3\,X^3}{3!} + \dots + rac{t^n\,X^n}{n!} + \dots$$

### **Taylor Expansion of Moment Generating functions**

$$M_X(t) = \operatorname{E}(e^{t\,X}) = 1 + t\operatorname{E}(X) + rac{t^2\operatorname{E}(X^2)}{2!} + rac{t^3\operatorname{E}(X^3)}{3!} + \dots + rac{t^n\operatorname{E}(X^n)}{n!} + \dots = 1 + tm_1 + rac{t^2m_2}{2!} + rac{t^3m_3}{3!} + \dots + rac{t^nm_n}{n!} + \dots,$$



### Taylor Expansion of Moment Generating functions

$$egin{aligned} M_X(t) &= \mathrm{E}(e^{t\,X}) = 1 + t\,\mathrm{E}(X) + rac{t^2\,\mathrm{E}(X^2)}{2!} + rac{t^3\,\mathrm{E}(X^3)}{3!} + \cdots + rac{t^n\,\mathrm{E}(X^n)}{n!} + \cdots \ &= 1 + tm_1 + rac{t^2m_2}{2!} + rac{t^3m_3}{3!} + \cdots + rac{t^nm_n}{n!} + \cdots, \end{aligned}$$

### **Important Fact**

Recall from intro to probability, that a moment generating function uniquely identifies a given distribution.



### How do we apply the method of moments to GMMs?

- Define some subset of moments in terms of the parameters (means, variances, labels)
- Then solve for these parameters using empirical estimates of these moments.

### **Couple Questions**

- Which moments to use?
- How do we approximate them?



Low-Order Estimates			
moment order	reliable estimates?	unique solution?	
1 <sup>st</sup> , 2 <sup>nd</sup>	1	×	
<sup>st</sup> - and 2 <sup>nd</sup> -order	moments (e.a., mean.	covariance)	



# High-Order Estimates

moment order	reliable estimates?	unique solution?
1 <sup>st</sup> , 2 <sup>nd</sup>	✓	×
$\Omega(k)^{\text{th}}$	×	<ul> <li>Image: A set of the set of the</li></ul>

 $\Omega(k)^{\text{th}}$ -order moments (e.g.,  $\mathbb{E}_{\theta}$ [degree-k-poly( $\vec{x}$ )])

- Uniquely pins down the solution.
- Empirical estimates very unreliable.







### **Important Definitions**

Define  $M_{\theta} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$  and  $T_{\theta} : \mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$  as bi-linear and tri-linear functions.

### Variational Lemma

Lemma If  $\{\vec{\mu}_i\}$  are linearly independent and all  $w_i > 0$ , then each of the k distinct, isolated local maximizers  $\vec{u}^*$  of  $\max_{\vec{u} \in \mathbb{R}^d} T_{\theta}(\vec{u}, \vec{u}, \vec{u})$  s.t.  $M_{\theta}(\vec{u}, \vec{u}) \le 1$ satisfies, for some  $i \in [k]$ ,  $M_{\theta}(\cdot, \vec{u}^*) = \sqrt{w_i} \ \vec{\mu}_i, \qquad T_{\theta}(\vec{u}^*, \vec{u}^*, \vec{u}^*) = \frac{1}{\sqrt{w_i}}$ .

# **Proof Out-Line: Variational Lemma**





# How to Solve the Moment Equations



### Getting an Approximate Solution

Effectively want to solve

$$\min_{\theta} \| T_{\theta} - \widehat{T} \|^2 \quad \text{s.t.} \quad M_{\theta} = \widehat{M}. \tag{\dagger}$$

Not convex in parameters  $\theta = \{(\vec{\mu}_i, w_i)\}.$ 

What we do: find one component  $(\vec{\mu}_i, w_i)$  at a time, using local optimization of related (also non-convex) objective function.



New robust algorithm for "tensor eigen-decomposition" efficiently approximates *all* local optima, each corresponding to a component.  $\rightarrow$  Near-optimal solution to (†).

# Local Optimization and Approximate Solutions



### Initialization and Convergence

Want to find all local maximizers of

$$\max_{\vec{u}\in\mathbb{R}^d} \ \widehat{T}(\vec{u},\vec{u},\vec{u}) \quad \text{s.t.} \quad \widehat{M}(\vec{u},\vec{u}) \le 1.$$
(‡)

Must address initialization and convergence issues.

Crucially using special tensor structure of  $\hat{T} \approx T_{\theta^*}$ , together with non-linearity of  $\vec{u} \mapsto \hat{T}(\cdot, \vec{u}, \vec{u})$ :

- Random initialization is good with significant probability.
   ("Good" 
   ⇒ simple iteration will guickly converge to some local max.)
- Can check if initialization was good by checking objective value after a few steps.
  - If value large enough: initialization was good; improve by taking a few more steps.
  - Else: abandon and restart.



### Condition from Lemma 1 (Restated)

**Condition 1** (Non-degeneracy). The component means span a k-dimensional subspace (*i.e.*, the matrix A has column rank k), and the vector w has strictly positive entries.



#### **Computing Moments with Tensor Arithmetic**

**Theorem 1** (Observable moment structure). Assume Condition 1 holds. The average variance  $\bar{\sigma}^2 := \sum_{i=1}^k w_i \sigma_i^2$  is the smallest eigenvalue of the covariance matrix  $\mathbb{E}[(x - \mathbb{E}[x])(x - \mathbb{E}[x])^{\top}]$ . Let  $v \in \mathbb{R}^d$  be any unit norm eigenvector corresponding to the eigenvalue  $\bar{\sigma}^2$ . Define

$$\begin{split} M_1 &:= \mathbb{E}[x(v^{\top}(x - \mathbb{E}[x]))^2] \in \mathbb{R}^d, \\ M_2 &:= \mathbb{E}[x \otimes x] - \bar{\sigma}^2 I \in \mathbb{R}^{d \times d}, \\ M_3 &:= \mathbb{E}[x \otimes x \otimes x] - \sum_{i=1}^d (M_1 \otimes e_i \otimes e_i + e_i \otimes M_1 \otimes e_i + e_i \otimes e_i \otimes M_1) \in \mathbb{R}^{d \times d \times d} \end{split}$$

(where  $\otimes$  denotes tensor product, and  $\{e_1, e_2, \ldots, e_d\}$  is the coordinate basis for  $\mathbb{R}^d$ ). Then

$$M_1 = \sum_{i=1}^k w_i \ \sigma_i^2 \mu_i, \qquad M_2 = \sum_{i=1}^k w_i \ \mu_i \otimes \mu_i, \qquad M_3 = \sum_{i=1}^k w_i \ \mu_i \otimes \mu_i \otimes \mu_i.$$



#### Estimating parameters using moments

**Theorem 2** (Moment-based estimator). The following can be added to the results of Theorem 1. Suppose  $\eta^{\top}\mu_1, \eta^{\top}\mu_2, \ldots, \eta^{\top}\mu_k$  are distinct and non-zero (which is satisfied almost surely, for instance, if  $\eta$  is chosen uniformly at random from the unit sphere in  $\mathbb{R}^d$ ). Then the matrix

$$M_{
m GMM}(\eta) := M_2^{\dagger 1/2} M_3(\eta) M_2^{\dagger 1/2}$$

is diagonalizable (where <sup>†</sup> denotes the Moore-Penrose pseudoinverse); its non-zero eigenvalue / eigenvector pairs  $(\lambda_1, v_1), (\lambda_2, v_2), \ldots, (\lambda_k, v_k)$  satisfy  $\lambda_i = \eta^\top \mu_{\pi(i)}$  and  $M_2^{1/2} v_i = s_i \sqrt{w_{\pi(i)}} \mu_{\pi(i)}$  for some permutation  $\pi$  on [k] and signs  $s_1, s_2, \ldots, s_k \in \{\pm 1\}$ . The  $\mu_i, \sigma_i^2$ , and  $w_i$  are recovered (up to permutation) with

$$\mu_{\pi(i)} = \frac{\lambda_i}{\eta^\top M_2^{1/2} v_i} M_2^{1/2} v_i, \qquad \sigma_i^2 = \frac{1}{w_i} e_i^\top A^\dagger M_1, \qquad w_i = e_i^\top A^\dagger \mathbb{E}[x].$$

Here for a third order tensor  $T \in \mathbb{R}^{d \times d \times d}$   $T(\eta) = \sum_{i_1=1}^d \sum_{i_2=1}^d \sum_{i_3=1}^d T_{i_1,i_2,i_3} \eta_{i_3} e_{i_1} \otimes e_{i_2} \in \mathbb{R}^{d \times d}$  for any vector in  $\mathbb{R}^d$ 



### Where does this leave us?

Combining Theorem 1 and Theorem 2 basically gives us a plug in estimator that can be converted into an algorithm.



#### **Moment Estimates**

Let  $\{(x_i, h_i) : i \in [n]\}$  be n i.i.d. copies of (x,h), and S := $\{x_1, x_2, \dots, x_n\}$  with  $\overline{S}$  being some independent copy also of size n. Then we can define our empirical moment estimates:

$$\begin{split} \mu &:= \mathbb{E}[x], & \mathcal{M}_2 := \mathbb{E}[xx^\top], & \mathcal{M}_3 := \mathbb{E}[x \otimes x \otimes x], \\ \hat{\mu} &:= \frac{1}{|\mathcal{S}|} \sum_{x \in \mathcal{S}} x, & \widehat{\mathcal{M}}_2 := \frac{1}{|\mathcal{S}|} \sum_{x \in \mathcal{S}} xx^\top, & \underline{\widehat{\mathcal{M}}_3} := \frac{1}{|\underline{\mathcal{S}}|} \sum_{x \in \underline{\mathcal{S}}} x \otimes x \otimes x, & \underline{\hat{\mu}} := \frac{1}{|\underline{\mathcal{S}}|} \sum_{x \in \underline{\mathcal{S}}} x. \end{split}$$



### **Relationship of parameters and Moments**

If we restrict ourselves to the case where  $\sigma_1^2 = \sigma_2^2, ..., \sigma_k^2$ , then the relationships between each moment and our mixture parameters is defined under the following lemma:

Lemma 3 (Structure of moments).

$$\begin{split} \mu &= \sum_{i=1}^{k} w_{i} \mu_{i}, \\ \mathcal{M}_{2} &= \sum_{i=1}^{k} w_{i} \mu_{i} \mu_{i}^{\top} + \sigma^{2} I, \\ \mathcal{M}_{3} &= \sum_{i=1}^{k} w_{i} \mu_{i} \otimes \mu_{i} \otimes \mu_{i} + \sigma^{2} \sum_{j=1}^{d} \left( \mu \otimes e_{j} \otimes e_{j} + e_{j} \otimes \mu \otimes e_{j} + e_{j} \otimes e_{j} \otimes \mu \right). \end{split}$$



### Notational Aside

For a third-order tensor  $Y \in \mathbb{R}^{m \times m \times m}$  and  $U, V, W \in \mathbb{R}^{m \times n}$ , this paper lets  $Y[U, V, W] \in \mathbb{R}^{n \times n \times n}$  denote the third order tensor given by:

 $Y[U,V,W]_{j_1,j_2,j_3} = \sum_{1 \le i_1,i_2,i_3 \le m} U_{i_1,j_1} V_{i_2,j_2} W_{i_3,j_3} Y_{i_1,i_2,i_3}, \quad \forall j_1,j_2,j_3 \in [n].$ 



The algorithm can be broken up unto a couple of Key parts

- Split data set (of size 2n) into S and  $\overline{S}$  (each of size n)
- Use S to compute empirical moments μ̂, and M̂<sub>3</sub> which are used to construct σ<sup>2</sup>, M̂<sub>2</sub>, Ŵ, and B̂
- Do some magic with random projections....



#### Part 1

- 1. Using the first half of the sample, compute empirical mean  $\hat{\mu}$  and empirical second-order moments  $\widehat{\mathcal{M}}_2.$
- 2. Let  $\hat{\sigma}^2$  be the k-th largest eigenvalue of the empirical covariance matrix  $\widehat{\mathcal{M}}_2 \hat{\mu}\hat{\mu}^{\top}$ .
- 3. Let  $\widehat{M}_2$  be the best rank-k approximation to  $\widehat{\mathcal{M}}_2 \hat{\sigma}^2 I$

$$\widehat{M}_2 := \arg \min_{X \in \mathbb{R}^{d \times d}: \operatorname{rank}(X) \leq k} \| (\widehat{\mathcal{M}}_2 - \hat{\sigma}^2 I) - X\|_2$$

which can be obtained via the singular value decomposition.

- 4. Let  $\widehat{U} \in \mathbb{R}^{d \times k}$  be the matrix of left orthonormal singular vectors of  $\widehat{M}_2$ .
- 5. Let  $\widehat{W} := \widehat{U}(\widehat{U}^{\top}\widehat{M}_{2}\widehat{U})^{\dagger 1/2}$ , where  $X^{\dagger}$  denotes the Moore-Penrose pseudoinverse of a matrix X.

Also define  $\widehat{B} := \widehat{U}(\widehat{U}^{\top}\widehat{M}_2\widehat{U})^{1/2}$ .

# LearnGMM Algorithm: Technical Overview



#### Part 2

- 6. Using the second half of the sample, compute whitened empirical averages  $\widehat{W}^{\top}\underline{\hat{\mu}}$  and third-order moments  $\widehat{\mathcal{M}_3}[\widehat{W}, \widehat{W}, \widehat{W}]$ .
- 7. Let  $\widehat{M}_3[\widehat{W}, \widehat{W}, \widehat{W}] := \underline{\widehat{M}_3}[\widehat{W}, \widehat{W}, \widehat{W}] \hat{\sigma}^2 \sum_{i=1}^d ((\widehat{W}^\top \underline{\hat{\mu}}) \otimes (\widehat{W}^\top e_i) \otimes (\widehat{W}^\top e_i) + (\widehat{W}^\top e_i) \otimes (\widehat{W}^\top e_i) \otimes (\widehat{W}^\top \underline{\hat{\mu}})).$

#### Part 3

- 8. Repeat the following steps t times (where  $t := \lceil \log_2(1/\delta) \rceil$  for confidence  $1 \delta$ ):
  - (a) Choose  $\theta \in \mathbb{R}^k$  uniformly at random from the unit sphere in  $\mathbb{R}^k$ .
  - (b) Let  $\{(\hat{v}_i, \hat{\lambda}_i) : i \in [k]\}$  be the eigenvector/eigenvalue pairs of  $\widehat{M}_3[\widehat{W}, \widehat{W}, \widehat{W}\theta]$ .

Retain the results for which  $\min(\{|\hat{\lambda}_i - \hat{\lambda}_j| : i \neq j\} \cup \{|\hat{\lambda}_i| : i \in [k]\})$  is largest.

9. Return the parameter estimates  $\hat{\sigma}^2$ ,

$$\begin{split} \hat{\mu}_i &:= \frac{\hat{\lambda}_i}{\theta^{\top} \hat{v}_i} \widehat{B} \hat{v}_i, \quad i \in [k] \\ \hat{w} &:= [\hat{\mu}_1 | \hat{\mu}_2 | \cdots | \hat{\mu}_k]^{\dagger} \hat{\mu}. \end{split}$$

# LearnGMM Sample Complexity



### **Finite Sample Complexity**

**Theorem 3** (Finite sample bound). There exists a polynomial  $poly(\cdot)$  such that the following holds. Let  $M_2$  be the matrix defined in Theorem 2, and  $\varsigma_l[M_2]$  be its t-th largest singular value (for  $t \in [k]$ ). Let  $b_{\max} := \max_{i \in [k]} ||\mu_i||_2$  and  $w_{\min} := \min_{i \in [k]} w_i$ . Pick any  $\varepsilon, \delta \in (0, 1)$ . Suppose the sample size n satisfies

 $n \ge \operatorname{poly}\left(d, k, 1/\varepsilon, \log(1/\delta), 1/w_{\min}, \varsigma_1[M_2]/\varsigma_k[M_2], b_{\max}^2/\varsigma_k[M_2], \sigma^2/\varsigma_k[M_2], \right).$ 

Then with probability at least  $1 - \delta$  over the random sample and the internal randomness of the algorithm, there exists a permutation  $\pi$  on [k] such that the  $\{\hat{\mu}_i : i \in [k]\}$  returned by LEARNGMM satisfy

$$\|\hat{\mu}_{\pi(i)} - \mu_i\|_2 \le \left(\|\mu_i\|_2 + \sqrt{\varsigma_1[M_2]}\right)\varepsilon$$

for all  $i \in [k]$ .

Is this a nice result? I am not sure, but it relies on the empirical moments converging by CLT at rate of  $n^{-1/2}$ , which does not seem great.



### **Recommendation From Authors**

Alternatives to LearnGMM used to extract the parameters from estimates of M2 and M3 include:

- Simultaneous diagonalization techniques (Bunse-Gerstner et al., 1993)
- Orthogonal tensor decompositions (Anandkumar et al., 2012a)

These alternative methods are more robust to sampling error.



# **ICA** Overview

- *h* ∈ ℝ<sup>k</sup> be some random vector with independent entries (unobserved signal)
- $h \in \mathbb{R}^k$  be Multivariate Gaussian (noise)
- We observe x := Ah + z for some  $A \in \mathbb{R}^{k \times k}$  and h / z are independent
- Given a set of  $\{x_i, i = 1, 2, ...m\}$ , we want to recover h

# This means that we can use this third order moment matching scheme to solve ICA problems



### Formal Result

**Theorem 4.** In the ICA model described above, assume  $\mathbb{E}[h_i] = 0$ ,  $\mathbb{E}[h_i^2] = 1$ , and  $\kappa_i := \mathbb{E}[h_i^4] - 3 \neq 0$  (i.e., the excess kurtosis is non-zero), and that A is non-singular. Define  $f : \mathbb{R}^k \to \mathbb{R}$  by

$$f(\eta) := 12^{-1} (m_4(\eta) - 3m_2(\eta)^2)$$

where  $m_p(\eta) := \mathbb{E}[(\eta^\top x)^p]$ . Suppose  $\phi \in \mathbb{R}^k$  and  $\psi \in \mathbb{R}^k$  are such that  $\frac{(\phi^\top \mu_1)^2}{(\psi^\top \mu_1)^2}, \frac{(\phi^\top \mu_2)^2}{(\psi^\top \mu_2)^2}, \dots, \frac{(\phi^\top \mu_k)^2}{(\psi^\top \mu_k)^2} \in \mathbb{R}$  are distinct. Then the matrix

$$M_{\text{ICA}}(\phi,\psi) := \left(\nabla^2 f(\phi)\right) \left(\nabla^2 f(\psi)\right)^{-1}$$

is diagonalizable; the eigenvalues are  $\frac{(\phi^{\top}\mu_{1})^{2}}{(\phi^{\top}\mu_{2})^{2}}, \frac{(\phi^{\top}\mu_{2})^{2}}{(\psi^{\top}\mu_{3})^{2}}, \dots, \frac{(\phi^{\top}\mu_{k})^{2}}{(\psi^{\top}\mu_{k})^{2}}$  and each have geometric multiplicity one, and the corresponding eigenvectors are  $\mu_{1}, \mu_{2}, \dots, \mu_{k}$  (up to scaling and permutation).

Theorem 4 lets us estimate the columns of A up to scaling, which in turn lets us estimate h.



### What did we talk about today?

- Gaussian Mixture Models (GMM)
- Method of Moments Estimators
- How to use Method of Moments to estimate parameters in GMM
- Sample complexity of such an algorithm
- How it can be extended to ICA like algorithms

### for more recent work in this area see:

http://proceedings.mlr.press/v65/li17a/li17a.pdf



### **Recommended Reading**

- https://www.cs.ubc.ca/~jnutini/documents/ mlrg\_pca.pdf
- https://www.cs.columbia.edu/~djhsu/papers/ mog-slides.pdf
- https://arxiv.org/pdf/1206.5766.pdf
- https://www.cse.wustl.edu/~bjuba/cse519t/ f19/papers/Li17a.pdf