Estimating Mixture Models via Mixtures of Polynomials

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Motivation: estimate mixture models

- Mixture models are important in ML with many applications
- We have no general and tractable methods for parameter estimation in mixture models
  - EM is generally applicable, but prone to local optima
  - method of moments can sometimes provide global guarantees, but difficult to use
- We want to generalize the class of mixture models solvable by the method of moments.

Method	Model	Result
maximum-likelihood	any	intractable for most mixture models
expectation-maximization	latent variables	convergence to local min.
solving moment equations	case by case	moment matching
tensor factorization	tensor structured models	moment matching
polymom (this work)	**polynomial structure**	moment matching

Contributions: more general, unifying, and turnkey

- **More general**: we can estimate any mixture model with **polynomial moments**
  - More general than tensor structured models
  - Includes mixtures of Gaussians, Poissons, and linear regressions. Also multiview mixtures.
- **Unifying**: the same algorithm can be used in both Pearson's mixture of 2 Gaussians (need high order moments) in 1D and high dimensional mixtures (low order moments).
- Naturally supports parameter sharing, like EM
- **Turnkey**: the user just needs to provide coefficients of some polynomials
- Connecting estimating mixture models to polynomial optimization and computer algebra

Problem setup: the model class we want to mix (user specified)

- $p(x;\theta)$ is a distribution parameterized by θ.
- Moments $\mathbb{E}_{x\sim p(x;\theta)}[\phi(x)]$ of $p(x;\theta)$ can be expressed in terms of parameters θ.
  - For example $\phi(x) = x_1$, or $x_1^2 x_3$, $\log(x_1)$, $\sin(x_1)$
- The scope of this work is when these moments are polynomials

$$f(\theta) \triangleq \mathbb{E}_{x\sim p(x;\theta)}[\phi(x)] = \sum_\alpha a_\alpha \theta^\alpha, \text{ where } \theta^\alpha = \prod_{p=1}^{P} \theta_p^{\alpha_p}. \tag{1}$$

- The choice of $\phi(x)$ and the coefficients of $f(\theta)$ are both model dependent and **user specified**. Choosing a suitable set of $\phi(x)$ and findings the corresponding coefficients is what Polymom needs as inputs.

Example

For the Gaussian distribution in 1d with mean ξ and variance σ^2. The observation functions $\phi(x) = [x^1, \dots, x^6, x^7]$ corresponds to polynomials $f(\theta) = [\xi, \xi^2+\sigma^2, \xi^3+3\xi\sigma^2, \dots]$. Note that this is for a single component to be mixed.

Problem setup: the mixture model

Given the component model $p(x;\theta)$, we can defined the corresponding mixture model, where each data point $x \in \mathbb{R}^D$ is associated with a latent component $z \in [K]$:

$$z \sim \text{Multinomial}(\pi), \quad x \mid z \sim p(x;\theta_z), \tag{2}$$

where $\pi = (\pi_1, \dots, \pi_K)$ are the mixing coefficients, $\theta_k^* \in \mathbb{R}^P$ are the true model parameters for the k^{th} *mixture component*, and $x \in \mathbb{R}^D$ is the data.

From a component to its mixture

For each **component**, we have polynomials expressions for observation functions $\phi(x)$.

$$f(\theta) \triangleq \mathbb{E}_{x\sim p(x;\theta)}[\phi(x)] = \sum_\alpha a_\alpha \theta^\alpha \tag{3}$$

The moments for the entire **mixture** is

$$\mathbb{E}[\phi(x)] = \sum_{k=1}^{K} \pi_k \mathbb{E}[\phi(x) \mid z=k] = \sum_{k=1}^{K} \pi_k f(\theta_k). \tag{4}$$

- Solving this system of polynomial equations is the task of parameter estimation using method of moments.
- Unfortunately, partially due to its symmetries ($K!$ solutions), this is a hard polynomial system to solve even when it is easy to solve the single component case.

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1. Write down a mixture model

$$z \sim \text{Multinomial}(\pi_1, \pi_2)$$
$$x \mid z \sim \mathcal{N}(\xi_z, \sigma_z) \in \mathbb{R}$$
$$\theta_k = (\xi_k, \sigma_k) \in \mathbb{R}^2$$

2. Derive single mixture moment equations

$\phi(x)$	$f(\theta)$
x	ξ
x^2	$\xi^2+\sigma^2$
x^3	$\xi^3+3\xi\sigma^2$
$\vdots$	$\vdots$

3. Add data

$$x_1 \sim p(x;\theta^*)$$
$$\vdots$$
$$x_T \sim p(x;\theta^*)$$

user specified | framework specified

4. Recover parameter moments (y)

$$M_r(y) = \begin{array}{c|cccc} & 1 & \xi & \xi^2 & \sigma^2 \\ \hline 1 & y_{0,0} & y_{1,0} & y_{2,0} & y_{0,1} \\ \xi & y_{1,0} & y_{2,0} & y_{3,0} & y_{1,1} \\ \xi^2 & y_{2,0} & y_{3,0} & y_{4,0} & y_{2,1} \\ \sigma^2 & y_{0,1} & y_{1,1} & y_{2,1} & y_{0,2} \end{array}$$

$$\begin{aligned} \underset{y}{\text{minimize}} \quad & \operatorname{tr}(M_r(y)) \\ \text{s.t.} \quad & M_r(y) \succeq 0, \; y_{0,0} = 1 \\ & y_{1,0} = \tfrac{1}{T}\textstyle\sum_t^T x_t \\ & y_{2,0} + y_{0,1} = \tfrac{1}{T}\textstyle\sum_t^T x_t^2 \\ & y_{3,0} + 3y_{1,1} = \tfrac{1}{T}\textstyle\sum_t^T x_t^3 \\ & \dots \end{aligned}$$

5. Solve for parameters

$$M_r(y) = VPV^\top$$
$$\downarrow \text{sim. diag.}$$
$$P = \operatorname{diag}([\pi_1, \pi_2])$$

$$V = \begin{array}{c|cc} & v(\theta_1) & v(\theta_2) \\ \hline 1 & 1 & 1 \\ \xi & 2 & -2 \\ \sigma^2 & 3 & 5 \\ \xi^2 & 4 & 4 \\ \xi\sigma^2 & 6 & -10 \\ \sigma^4 & 9 & 25 \\ \xi^2\sigma^2 & 12 & 20 \end{array}$$

Conceptual idea: get rid of symmetries by working with moments of parameters

The key idea of Polymom is to exploit the mixture structure of the moment equations (4). Specifically, let μ^* be a particular "mixture" over the component parameters $\theta_1^*, \dots, \theta_k^*$ (i.e. μ^* is a probability measure). Then we can express the moment conditions (4) in terms of μ^*

$$\mathbb{E}[\phi_n(x)] = \int f_n(\theta)\, \mu^*(d\theta), \text{ where } \mu^*(\theta) = \sum_{k=1}^{K} \pi_k \delta(\theta - \theta_k^*). \tag{5}$$

The following feasibility problem is equivalent to the moment conditions in (4):

$$\begin{aligned} \text{find} \quad & \mu \in \mathcal{M}_+(\mathbb{R}^P), \text{ the set of probability measures over } \mathbb{R}^P \\ \text{s.t.} \quad & \textstyle\int f_n(\theta)\, \mu(d\theta) = \mathbb{E}[\phi_n(x)], \quad n = 1, \dots, N \\ & \mu \text{ is } K\text{-atomic (i.e. sum of } K \text{ deltas)}, \end{aligned} \tag{6}$$

where we deliberately "forget" the permutation of the components by using μ to represent the problem instead of $[\theta_1, \dots, \theta_K]$.

Moment Completion: making things tractable

The **Generalized Moment Problem** framework allows us to work with measures by working with their moments using semidefinite programming. Let $\mathscr{L}_y(\theta^\alpha) \triangleq y_\alpha$, and we will work with the moment sequence $y = (y_\alpha)_{\alpha \in \mathbb{N}^P}$. Note that these moments y are moments in the **parameter space** (like $y_\alpha = \mathbb{E}_\mu[\theta^\alpha]$), and not of the data as before (like $\mathbb{E}_{p(x;\theta^*)}[\phi_n(x)]$).

$$\begin{aligned} \text{find} \quad & y \in \mathbb{R}^{\mathbb{N}} \quad (\text{or equivalently, find } M(y)) \\ \text{s.t.} \quad & \textstyle\sum_\alpha a_{n\alpha} y_\alpha = \mathbb{E}[\phi_n(x)], \quad n = 1, \dots, N \\ & M_r(y) \succeq 0, \; y_0 = 1 \\ & \operatorname{rank}(M_r(y)) = K \text{ and } \operatorname{rank}(M_{r-1}(y)) = K. \end{aligned} \tag{7}$$

Unfortunately, we still cannot deal with rank constraints, but the following relaxation (a semidefinite program) is tractable:

$$\begin{aligned} \underset{y}{\text{minimize}} \quad & \operatorname{tr}(CM_r(y)) \\ \text{s.t.} \quad & \textstyle\sum_\alpha a_{n\alpha} y_\alpha = \mathbb{E}[\phi_n(x)], \quad n = 1, \dots, N \\ & M_r(y) \succeq 0, \; y_0 = 1 \end{aligned} \tag{8}$$

- For some models like multiview mixture and mixture of linear regressions, the linear constraints might fully determines y and we do not need to solve an SDP. In such cases, Polymom provides an unifying view and some guarantees.
- After obtaining y, there are several generic ways to extract θ based on solving some kind of eigenvalue problem.

Experimental results

	Methd.	EM	TF	Poly	EM	TF	Poly	EM	TF	Poly
Gaussians	K, D	$T = 10^3$			$T = 10^4$			$T = 10^5$		
spherical	**2, 2**	**0.37**	2.05	0.58	**0.24**	0.73	0.29	0.19	0.36	**0.14**
diagonal	**2, 2**	**0.44**	~~2.15~~	0.48	0.48	~~4.03~~	**0.40**	0.38	~~2.46~~	**0.35**
constrained	**2, 2**	0.49	~~7.52~~	**0.38**	0.47	~~2.56~~	**0.30**	0.34	~~3.02~~	**0.29**
Others	K, D	$T = 10^4$			$T = 10^5$			$T = 10^6$		
3-view	**3, 3**	**0.38**	0.51	0.57	0.31	0.33	**0.26**	0.36	0.16	**0.12**
lin. reg.	**2, 2**	-	-	**3.51**	-	-	**2.60**	-	-	**2.52**

Table : T is the number of samples. **Methods:** EM: sklearn initialized with k-means using 5 random restarts; TF: tensor power method implemented in Python; Poly: Polymom by solving Problem 8. **Models:** for mixture of Gaussians, we have $\sigma \approx 2\|\mu_1 - \mu_2\|_2$; 'spherical' and 'diagonal' describes the type of covariance matrix. The mean parameters of constrained Gaussians satisfies $\mu_1 + \mu_2 = 1$. The best result is **bolded**. TF only handles spherical variance, but it was of interest to see what TF does if the data is drawn from mixture of Gaussians with diagonal covariance, these results are in ~~strikeout~~.

Examples: what the user needs to provide Polymom

Table : Applications of the Polymom framework.

Mixture of linear regressions

Model

$x = [x, v]$ is observed where $x \in \mathbb{R}^D$ is drawn from an unspecified distribution and $v \sim \mathcal{N}(w \cdot x, \sigma^2 I)$, and σ^2 is known. The parameters are $\theta_k^* = (w_k) \in \mathbb{R}^D$.

Observation functions

$\phi_{\alpha,b}(x) = x^\alpha v^b$ for $0 \le |\alpha| \le 3$, $b \in [2]$.

Moment polynomials

$f_{\alpha,1}(\theta) = \sum_{p=1}^P \mathbb{E}[x^{\alpha+\gamma_p}] w_p$

$f_{\alpha,2}(\theta) = \mathbb{E}[x^\alpha]\sigma^2 + \sum_{p,q=1}^P \mathbb{E}[x^\alpha x_p x_q] w_p w_q$, where the $\gamma_p \in \mathbb{N}^P$ is 1 in position p and 0 elsewhere.

Mixture of Gaussians

Model

$x \in \mathbb{R}^D$ is observed where x is drawn from a Gaussian with diagonal covariance: $x \sim \mathcal{N}(\xi, \operatorname{diag}(c))$. The parameters are $\theta_k^* = (\xi_k, c_k) \in \mathbb{R}^{D+D}$.

Observation functions

$\phi_\alpha(x) = x^\alpha$ for $0 \le |\alpha| \le 4$.

Moment polynomials

$f_\alpha(\theta) = \prod_{d=1}^D h_{\alpha_d}(\xi_d, c_d)$.

Multiview mixtures

Model

With 3 views, $x = [x^{(1)}, x^{(2)}, x^{(3)}]$ is observed where $x^{(1)}, x^{(2)}, x^{(3)} \in \mathbb{R}^D$ and $x^{(\ell)}$ is drawn from an unspecified distribution with mean $\xi^{(\ell)}$ for $\ell \in [3]$. The parameters are $\theta_k^* = (\xi_k^{(1)}, \xi_k^{(2)}, \xi_k^{(3)}) \in \mathbb{R}^{D+D+D}$.

Observation functions

$\phi_{ijk}(x) = x_i^{(1)} x_j^{(2)} x_k^{(3)}$ where $1 \le i, j, k \le D$.

Moment polynomials

$f_{ijk}(\theta) = \xi_i^{(1)} \xi_j^{(2)} \xi_k^{(3)}$.

Discussions, future work, and limitations

- Compared to previous literature on this topic, we do not need a 1-to-1 correspondence between the data dimensions and the parameter dimensions. The structure of the model class is encoded in these polynomials that can be derived systematically.
- Constraints on parameters like $\xi_1 = \xi_2$, or $\xi_1^2 \ge 3\sigma^2$ translates to tractable linear or semidefinite constraints.
- More statistically efficient formulations? For example, the generalized method of moments allows us to model variances in data moments using a weighting matrix W:

$$\begin{aligned} \underset{g,y}{\text{minimize}} \quad & g^T W g \\ \text{s.t.} \quad & g_n = \textstyle\sum_\alpha a_{n\alpha} y_\alpha - \mathbb{E}[\phi_n(x)], \quad n = 1, \dots, N \\ & M(y) \succeq 0 \end{aligned} \tag{9}$$

Limitations and wishlist

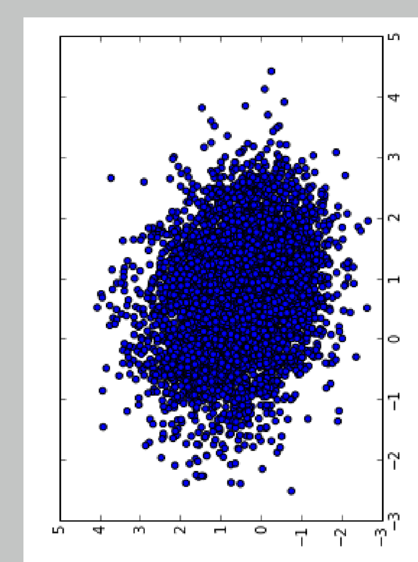
- Price for generality: Polymom only gives us moment matching solutions, we do not have formal guarantees on consistent parameter estimations except for specific models
- Solving big SDPs is still an issue: fragile and scales badly
- Does this optimization viewpoint give us insight on identifiability?
- More than just the mixture structure?

We hope that the Polymom point of view can be a step towards making method of moments more systematic, and more statistically efficient.

Software

https://github.com/sidaw/polymom
https://github.com/sidaw/mompy: a Generalized Moment Problem package

Mixture of 2 Gaussians and constraints



$$\begin{aligned} \xi_1 - 0.7567\xi_2 - 0.5174 \\ c_1 + \xi_1^2 - 1.4955 \\ 3c_2\xi_2 + \xi_2^3 - 2.0393 \\ 3c_1^2 + 6c_1\xi_1^2 + \xi_1^4 - 5.7752 \\ 3c_1\xi_1\xi_2 + \xi_1^3\xi_2 - 0.3837 \\ c_1c_2 + c_1\xi_2^2 + c_2\xi_1^2 + \xi_1^2\xi_2^2 - 1.6215 \\ 3c_2\xi_1\xi_2 + \xi_1\xi_2^3 - 0.5527 \\ 3c_2^2 + 6c_2\xi_2^2 + \xi_2^4 - 5.8174 \end{aligned}$$