Refined Convergence Rates for Maximum Likelihood Estimation under Finite Mixture Models

Tudor Manole

Department of Statistics and Data Science Carnegie Mellon University

Joint work with: Nhat Ho (University of Texas, Austin)

International Conference on Machine Learning, July 2022

• Let $\mathcal{F} = \{f(\cdot; \theta) : \theta \in \Theta\}$ be a parameteric density family with parameter space Θ .

- Let $\mathcal{F} = \{f(\cdot; \theta) : \theta \in \Theta\}$ be a parameteric density family with parameter space Θ .
 - e.g. $f(\cdot; \theta)$ could be the $N(\mu, \Sigma)$ density with parameter $\theta = (\mu, \Sigma) \in \Theta \subseteq \mathbb{R}^d \times \mathbb{S}^d_{++}$.

▶ Let $\mathcal{F} = \{f(\cdot; \theta) : \theta \in \Theta\}$ be a parameteric density family with parameter space Θ .

• e.g. $f(\cdot; \theta)$ could be the $N(\mu, \Sigma)$ density with parameter $\theta = (\mu, \Sigma) \in \Theta \subseteq \mathbb{R}^d \times \mathbb{S}^d_{++}$.

• Given an integer $K \ge 1$, assume

$$X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} p_{G_0}(x) = \sum_{k=1}^K \pi_k^0 f(x; \theta_k^0)$$

- Let F = {f(·; θ) : θ ∈ Θ} be a parameteric density family with parameter space Θ.
 e.g. f(·; θ) could be the N(μ, Σ) density with parameter θ = (μ, Σ) ∈ Θ ⊆ ℝ^d × S^d_{±+}.
- Given an integer $K \ge 1$, assume

$$X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} p_{G_0}(x) = \sum_{k=1}^K \pi_k^0 f(x; \theta_k^0)$$

• Mixing Proportions:
$$0 < \pi_k^0 \le 1$$
, $\sum_{k=1}^K \pi_k^0 = 1$.

- Let F = {f(·; θ) : θ ∈ Θ} be a parameteric density family with parameter space Θ.
 e.g. f(·; θ) could be the N(μ, Σ) density with parameter θ = (μ, Σ) ∈ Θ ⊆ ℝ^d × S^d_{⊥⊥}.
- Given an integer $K \ge 1$, assume

$$X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} p_{G_0}(x) = \sum_{k=1}^K \pi_k^0 f(x; \theta_k^0)$$

• Mixing Proportions: $0 < \pi_k^0 \le 1$, $\sum_{k=1}^K \pi_k^0 = 1$.

• Atoms: $\theta_k^0 \in \Theta$, possibly overlapping.

- Let F = {f(·; θ) : θ ∈ Θ} be a parameteric density family with parameter space Θ.
 e.g. f(·; θ) could be the N(μ, Σ) density with parameter θ = (μ, Σ) ∈ Θ ⊆ ℝ^d × S^d_{⊥⊥}.
- Given an integer $K \ge 1$, assume

$$X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} p_{G_0}(x) = \sum_{k=1}^K \pi_k^0 f(x; \theta_k^0) = \int_{\Theta} f(x; \theta) dG_0(\theta)$$

• Mixing Proportions: $0 < \pi_k^0 \le 1$, $\sum_{k=1}^K \pi_k^0 = 1$.

• Atoms: $\theta_k^0 \in \Theta$, possibly overlapping.

Mixing Measure:

$$G_0 = \sum_{k=1}^K \pi_k^0 \delta_{\theta_k^0}$$

Maximum Likelihood Estimation (MLE) in Finite Mixtures

Let \mathcal{O}_K denote the set of mixing measures with at most K components, and define

$$\widehat{G}_n = \sum_{j=1}^K \widehat{\pi}_j \delta_{\widehat{\theta}_j} = \operatorname*{argmax}_{G \in \mathcal{O}_K} \sum_{i=1}^n \log p_G(X_i).$$

Maximum Likelihood Estimation (MLE) in Finite Mixtures

Let \mathcal{O}_K denote the set of mixing measures with at most K components, and define

$$\widehat{G}_n = \sum_{j=1}^K \widehat{\pi}_j \delta_{\widehat{\theta}_j} = \operatorname*{argmax}_{G \in \mathcal{O}_K} \sum_{i=1}^n \log p_G(X_i).$$

What is the risk of \widehat{G}_n ?

The Wasserstein Distances

• To quantify the risk of \widehat{G}_n , we require a loss function on \mathcal{O}_K .

The Wasserstein Distances

- To quantify the risk of \widehat{G}_n , we require a loss function on \mathcal{O}_K .
- Nguyen'13 proposed to use the *r*-Wasserstein distances ($r \ge 1$):

$$W_r^r(G,G') = \inf_{\substack{\theta,\theta'\\\theta\sim G\\\theta'\sim G'}} \mathbb{E}\Big[\|\theta-\theta'\|^r\Big], \quad G,G' \in \mathcal{O}_K,$$

• <u>Pointwise</u> convergence rate for "strongly identifiable" families \mathcal{F} :

$$\mathbb{E}\Big[W_2(\widehat{G}_n,G_0)\Big] \lesssim_{G_0} n^{-rac{1}{4}}$$
 (Chen'95, Ho & Nguyen'16)

• <u>Pointwise</u> convergence rate for "strongly identifiable" families \mathcal{F} :

$$\mathbb{E}\Big[W_2(\widehat{G}_n,G_0)\Big] \lesssim_{G_0} n^{-rac{1}{4}}$$
 (Chen'95, Ho & Nguyen'16)

Slower pointwise rates hold for location-scale Gaussian mixtures (Ho & Nguyen'16).

• <u>Pointwise</u> convergence rate for "strongly identifiable" families \mathcal{F} :

$$\mathbb{E}\Big[W_2(\widehat{G}_n,G_0)\Big] \lesssim_{G_0} n^{-rac{1}{4}}$$
 (Chen'95, Ho & Nguyen'16)

- Slower pointwise rates hold for location-scale Gaussian mixtures (Ho & Nguyen'16).
- <u>Uniform</u> rate for strongly identifiable families \mathcal{F} :

$$\sup_{G_0 \in \mathcal{O}_K} \mathbb{E}\Big[W_1(\widehat{G}_n, G_0) \Big] \lesssim n^{-\frac{1}{4K-2}}$$
 (Heinrich & Kahn'18)

• <u>Pointwise</u> convergence rate for "strongly identifiable" families \mathcal{F} :

$$\mathbb{E}\Big[W_2(\widehat{G}_n,G_0)\Big] \lesssim_{G_0} n^{-rac{1}{4}}$$
 (Chen'95, Ho & Nguyen'16)

- Slower pointwise rates hold for location-scale Gaussian mixtures (Ho & Nguyen'16).
- <u>Uniform</u> rate for strongly identifiable families \mathcal{F} :

$$\sup_{G_0 \in \mathcal{O}_K} \mathbb{E}\Big[W_1(\widehat{G}_n, G_0)\Big] \lesssim n^{-\frac{1}{4K-2}}$$
 (Heinrich & Kahn'18)

Our Contribution: In each of these settings, the Wasserstein distance can be replaced by a stronger loss function which implies faster convergence rates for the atoms of \hat{G}_n .

▶ <u>Pointwise</u> convergence rate for "strongly identifiable" families *F*:

 $\mathbb{E}\Big[W_2(\widehat{G}_n,G_0)\Big] \lesssim_{G_0} n^{-rac{1}{4}}$ (Chen'95, Ho & Nguyen'16)

- Slower pointwise rates hold for location-scale Gaussian mixtures (Ho & Nguyen'16).
- ▶ <u>Uniform</u> rate for strongly identifiable families *F*:

$$\sup_{G_0 \in \mathcal{O}_K} \mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim n^{-\frac{1}{4K-2}} \qquad (\text{Heinrich \& Kahn'18})$$

Our Contribution: In each of these settings, the Wasserstein distance can be replaced by a stronger loss function which implies faster convergence rates for the atoms of \hat{G}_n .

$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$



$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$





$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$



$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$

Voronoi Cells:

$$\hat{V}_{k} = \left\{ j : \left\| \hat{\theta}_{j} - \theta_{k}^{0} \right\| < \left\| \hat{\theta}_{j} - \theta_{l}^{0} \right\|, \forall l \neq k \right\}$$



$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$

Voronoi Cells:

$$\hat{V}_{k} = \left\{ j : \left\| \hat{\theta}_{j} - \theta_{k}^{0} \right\| < \left\| \hat{\theta}_{j} - \theta_{l}^{0} \right\|, \forall l \neq k \right\}$$

• Rate Interpretation: For all k, and $j \in \hat{V}_k$,

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim n^{-\frac{1}{4}}, \quad \text{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim n^{-\frac{1}{2}}.$$



$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$

Voronoi Cells:

$$\hat{V}_{k} = \left\{ j : \left\| \hat{\theta}_{j} - \theta_{k}^{0} \right\| < \left\| \hat{\theta}_{j} - \theta_{l}^{0} \right\|, \forall l \neq k \right\}$$

• Rate Interpretation: For all k, and $j \in \hat{V}_k$,

$$\mathbb{E}\|\hat{ heta}_j - heta_k^0\| \lesssim n^{-rac{1}{4}}, \quad ext{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim n^{-rac{1}{2}}.$$



$$\mathbb{E}\Big[W_2(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}$$

Voronoi Cells:

$$\hat{V}_{k} = \left\{ j : \left\| \hat{\theta}_{j} - \theta_{k}^{0} \right\| < \left\| \hat{\theta}_{j} - \theta_{l}^{0} \right\|, \forall l \neq k \right\}$$

• Rate Interpretation: For all k, and $j \in \hat{V}_k$,

$$\mathbb{E}\|\hat{ heta}_j - heta_k^0\| \lesssim n^{-rac{1}{4}}, \quad ext{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim n^{-rac{1}{2}}.$$

▶ Key Observation: This rate is loose for all k such that $|\hat{V}_k| = 1$.

Theorem (Informal). Assume strong identifiability and mild regularity conditions. (1) (Fast Rate) For all k such that $|\hat{V}_k| = 1$, and $j \in \hat{V}_k$, it holds that

 $\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{2}}.$

Theorem (Informal). Assume strong identifiability and mild regularity conditions. (1) (Fast Rate) For all k such that $|\hat{V}_k| = 1$, and $j \in \hat{V}_k$, it holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{2}}.$$

(2) (Slow Rate) For all k such that $|\hat{V}_k|>1$, and $j\in\hat{V}_k$, it either holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{4}}, \quad \text{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim_{G_0} n^{-\frac{1}{2}}.$$

Theorem (Informal). Assume strong identifiability and mild regularity conditions. (1) (Fast Rate) For all k such that $|\hat{V}_k| = 1$, and $j \in \hat{V}_k$, it holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{2}}.$$

(2) (Slow Rate) For all k such that $|\hat{V}_k|>1$, and $j\in\hat{V}_k$, it either holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{4}}, \quad \text{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim_{G_0} n^{-\frac{1}{2}}.$$

▶ In contrast, past work only implied option (2) for all k.

Theorem (Informal). Assume strong identifiability and mild regularity conditions. (1) (Fast Rate) For all k such that $|\hat{V}_k| = 1$, and $j \in \hat{V}_k$, it holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{2}}.$$

(2) (Slow Rate) For all k such that $|\hat{V}_k|>1$, and $j\in\hat{V}_k$, it either holds that

$$\mathbb{E}\|\hat{\theta}_j - \theta_k^0\| \lesssim_{G_0} n^{-\frac{1}{4}}, \quad \text{or} \quad \mathbb{E}[\hat{\pi}_j] \lesssim_{G_0} n^{-\frac{1}{2}}.$$

- ▶ In contrast, past work only implied option (2) for all k.
- We prove this by introducing a new loss function ${\cal D}$ which satisfies ${\cal D}\gtrsim W_2$ and

$$\mathbb{E}\Big[\mathcal{D}(\widehat{G}_n, G_0)\Big] \lesssim_{G_0} n^{-\frac{1}{4}}.$$

A Peak at our Refinements for Location-Scale Gaussian Mixtures



> Past work painted an overly pessimistic view of parameter estimation in mixtures.

- > Past work painted an **overly pessimistic** view of parameter estimation in mixtures.
- W_r is only able to quantify the **worst-case** convergence rate among the atoms of \widehat{G}_n .

- > Past work painted an **overly pessimistic** view of parameter estimation in mixtures.
- W_r is only able to quantify the **worst-case** convergence rate among the atoms of \widehat{G}_n .
- Our divergences reveal the **heterogeneity** of convergence rates among these atoms.

- > Past work painted an **overly pessimistic** view of parameter estimation in mixtures.
- W_r is only able to quantify the **worst-case** convergence rate among the atoms of \widehat{G}_n .
- Our divergences reveal the **heterogeneity** of convergence rates among these atoms.
- ▶ Many open questions (EM algorithm, method of moments, etc.).

Thank You