Statistical Guarantees for the EM Algorithm: From Population to Sample-Based Analysis

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Outline

1. Overview of Expectation–Maximization (EM) Algorithm
2. Population Analysis of First–Order EM Algorithm
3. Sample Analysis of First–Order EM Algorithm
4. Example: Gaussian Mixture Model
Overview of Expectation-Maximization Algorithm
Estimation of Linkage in Genetics

» 197 animals are distributed multinomially into 5 categories

» Observed data:

\[ \mathbf{x} = (x_1, x_2, x_3, x_4, x_5) = (x_1, x_2, 18, 20, 34) \]

with \( x_1 + x_2 = 125 \).

» Cell probabilities:

\[ \mathbf{p} = \left(\frac{1}{2}, \frac{1}{4}\pi, \frac{1}{4}(1 - \pi), \frac{1}{4}(1 - \pi), \frac{1}{4}\pi \right) \quad \text{for } \pi \in [0, 1]. \]
Example (continued)

» Likelihood function:

\[
L(p \mid x) = \frac{n!}{x_1!x_2!x_3!x_4!x_5!} \left( \frac{1}{2} \right)^{x_1} \left( \frac{\pi}{4} \right)^{x_2} \left( \frac{1 - \pi}{4} \right)^{x_3} \left( \frac{1 - \pi}{4} \right)^{x_4} \left( \frac{\pi}{4} \right)^{x_5}
\]

and

\[
\hat{\pi}_{MLE} = \frac{x_2 + x_5}{x_2 + x_3 + x_4 + x_5} = \frac{x_2 + 34}{x_2 + 18 + 20 + 34}
\]

» How to solve this type of incomplete data problem?
What is the EM Algorithm?

Expectation–Maximization (EM) Algorithm is an iterative method that attempts to find the maximum likelihood estimator of a parameter $\theta$ of a parametric probability distribution in incomplete data problems.

Incompleteness:
- Missing data
- Censored or grouped data
- Latent class and latent data structures
- ...
Basic Setup

» Let \((Y, Z) \in \mathcal{Y} \times \mathcal{Z}\) with the joint density function \(f_{\theta^*}\), where

› \(f_{\theta^*} \in \{f_\theta : \theta \in \Omega\}\)

› \(\Omega\) is non-empty, compact convex set

» Observe \(n\) i.i.d. copies of \(Y\), \(\{Y_1, \ldots, Y_n\}\)

› \(Z_1, \ldots, Z_n\) are missing or latent

» Goal: Estimate \(\theta^*\) by maximizing log-likelihood:

\[
\ell_n(\theta) := \frac{1}{n} \sum_{i=1}^{n} \log \left( \int_{\mathcal{Z}} f_\theta(Y_i, z) \, dz \right)
\]
EM Idea

Unfortunately, maximizing $\ell_n$ directly can be hard! But often the complete data log-likelihood

$$\frac{1}{n} \sum_{i=1}^{n} \log f_{\theta}(Y_i, Z_i)$$

is easier to maximize. So we replace the complete data log-likelihood by its conditional expectation:

$$Q_n(\theta \mid \theta^t) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\theta^t} \{ \log f_{\theta}(Y_i, Z_i) \mid Y_i \}$$

where expectation is computed with respect to current iterate $\theta^t$. 
EM Algorithm

Starting with initial iterate $\theta^0 \in \Omega$, iterate the following steps for $t = 1, 2, \cdots$.

$\triangleright$ **Expectation Step:** Compute EM surrogate $Q_n : \Omega \times \Omega \rightarrow \mathbb{R}$:

$$Q_n(\theta \mid \theta^t) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{\theta^t} \{ \log f_\theta(Y_i, Z_i) \mid Y_i \}$$

$\triangleright$ **Maximization Step:** Maximize EM surrogate:

$$\theta^{t+1} = \arg \max_{\theta \in \Omega} Q_n(\theta \mid \theta^t)$$
Source: people.duke.edu/~ccc14/sta-663/EMAlgorithm.html
Advantages 😊

» Easy to implement
» Requires small storage space
» Low cost per iteration

» If $\ell(\theta)$ is bounded, $\ell(\theta^t)$ converges monotonically to $\ell(\tilde{\theta})$, where $\tilde{\theta}$ is a stationary point

» …
Drawbacks 😞

» Finding the exact maximizer in the M step can be hard
As for the First Drawback...

**Generalized EM Algorithm:** Just choose $\theta^{t+1} \in \Omega$ so that

$$Q_n (\theta^{t+1} \mid \theta^t) \geq Q_n (\theta^t \mid \theta^t).$$

**First-Order EM Algorithm:** Assume $Q_n (\theta \mid \theta^t)$ is differentiable in the first argument at each iteration $t$. Given a step size $\alpha > 0$, the updates are

$$\theta^{t+1} = \theta^t + \alpha \cdot \nabla Q_n (\theta \mid \theta^t) \big|_{\theta=\theta^t} \quad \text{for } t = 0, 1, 2, \cdots,$$

where the gradient is taken in the first argument of $Q_n$. 
Drawbacks 😞

» Finding the exact maximizer in the M step can be hard
» No guarantees to converge to the global maximum of $\ell_n$ (depending on the choice of starting point)
An Example (Murray, 1977; Wu, 1983)

Twelve observations are collected from a bivariate normal distribution with mean 0, correlation coefficient $\rho$ and variances $\sigma_1^2$, $\sigma_2^2$

| Variable 1 | 1 | 1 | -1 | -1 | 2 | 2 | -2 | -2 | * * | * | * |
| Variable 2 | 1 | -1 | 1 | -1 | * | * | * | * | 2 | 2 | -2 | -2 |

The likelihood function has
- two global maxima: $\rho = \pm \frac{1}{2}, \sigma_1^2 = \sigma_2^2 = \frac{8}{3}$; and
- a saddle point: $\rho = 0, \sigma_1^2 = \sigma_2^2 = \frac{5}{2}$.

The EM algorithm starting at $\rho = 0$ will return the saddle point.
Drawbacks 😞

» Finding the exact maximizer in the M step can be hard

» No guarantees to converge to the global maximum of $\ell_n$
  (depending on the choice of starting point)

» $\ell (\theta^t) \rightarrow \ell (\theta)$, where $\theta$ is a stationary point, does NOT imply
  $\theta^t \rightarrow \theta^*$ and Wu (1983) only established the conditions of
  convergence of $\{\theta^t\}_{t=1}^{\infty}$ to a stationary point
Contributions of Balakrishnan et al. (2017)

- Quantitative characterization of a basin of attraction around $\theta^*$
- Where to choose the initialization to ensure $\theta^t \rightarrow \theta^*$
- Establishment of the convergence rate and the corresponding conditions
- Establishment of connections between population and sample analysis
Population Version of EM Algorithm

**E Step:** Compute the following population version surrogate function

$$Q (\theta | \theta^t) = E_{\theta^t} \{ E_{\theta^t} (\log f_{\theta}(Y, Z) | Y) \}$$

**M Step:**

- **Standard EM:**

  $$\theta^{t+1} = \arg \max_{\theta \in \Omega} Q (\theta | \theta^t)$$

- **First-Order EM:**

  $$\theta^{t+1} = \theta^t + \alpha \cdot \nabla Q (\theta | \theta^t) \big|_{\theta = \theta^t}$$
Oracle Surrogate Function and Iterates

Oracle Surrogate Function

$$q(\theta) := Q(\theta \mid \theta^*) = E_{\theta^*} \left\{ E_{\theta^*} \left( \log f_{\theta} (Y, Z) \mid Y \right) \right\}$$

Oracle Iterates

$$\tilde{\theta}^{t+1} = \tilde{\theta}^t + \alpha \cdot \nabla q \left( \tilde{\theta}^t \right)$$
Oracle Surrogate Function and Iterates

Why do we need them?

» If $q(\theta)$ satisfies strong concavity and smoothness, then the gradient ascent updates achieve geometric convergence rate to $\theta^*$

» The population version first-order EM updates can be viewed as a perturbation of the oracle updates

» Therefore, in the population level analysis of EM algorithm, we need to control the quantity

$$\nabla q(\theta) - \nabla Q(\theta \mid \theta)$$
Population Analysis of First-Order EM Algorithm
Recall the population first-order updates are

\[ \theta^{t+1} = \theta^t + \alpha \cdot \nabla Q(\theta \mid \theta^t) \big|_{\theta=\theta^t} , \]

and the oracle updates are

\[ \theta^{t+1} = \theta^t + \alpha \cdot \nabla q(\theta^t) . \]

**Condition 1: Gradient Smoothness**

For an appropriately small parameter \( \gamma \geq 0 \),

\[ \| \nabla q(\theta) - \nabla Q(\theta \mid \theta) \|_2 \leq \gamma \| \theta - \theta^* \|_2 \]

for all \( \theta \in \mathbb{B}(r; \theta^*) \).
Condition 2: $\lambda$-Strong Concavity

There is some $\lambda > 0$ such that

$$q(\theta_1) - q(\theta_2) - \langle \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \leq -\frac{\lambda}{2} \| \theta_1 - \theta_2 \|_2^2$$

or, equivalently,

$$\langle \nabla q(\theta_1) - \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \leq -\lambda \| \theta_1 - \theta_2 \|_2^2$$

for all pairs $\theta_1, \theta_2 \in B(r; \theta^*)$. 
Condition 3: $\mu$-Smoothness

There is some $\mu > 0$ such that

$$q(\theta_1) - q(\theta_2) - \langle \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \geq -\frac{\mu}{2} \|\theta_1 - \theta_2\|^2_2$$

or, equivalently,

$$\langle \nabla q(\theta_1) - \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \geq -\mu \|\theta_1 - \theta_2\|^2_2$$

for all pairs $\theta_1, \theta_2 \in \mathbb{B}(r; \theta^*)$. 
\[ \theta_2 \]

\[ -\frac{\lambda}{2} \| \theta - \theta_2 \|^2 \]

\[ -\frac{\mu}{2} \| \theta - \theta_2 \|^2 \]

\[ q(\theta) \]
Theorem 1
(General Population-Level Guarantee)

For some radius $r > 0$ and a triplet $(\gamma, \lambda, \mu)$ with $0 \leq \gamma < \lambda \leq \mu$ such that $\gamma$-gradient smoothness, $\lambda$-strong concavity and $\mu$-smoothness conditions hold;

Choose the step size $\alpha = \frac{2}{\mu + \lambda}$.

Then, given any $\theta^0 \in \mathbb{B}(r; \theta^*)$, the population first-order EM iterates satisfy the bound

$$\|\theta^t - \theta^*\|_2 \leq \left(1 - \frac{2\lambda - 2\gamma}{\mu + \lambda}\right)^t \|\theta^0 - \theta^*\|_2 \quad \text{for all } t = 1, 2, \cdots.$$
Sample Analysis of First-Order EM Algorithm
Recall that the sample first-order EM updates are

\[ \theta^{t+1} = \theta^t + \alpha \cdot \nabla Q_n (\theta \mid \theta^t) \big|_{\theta=\theta^t}. \]

The analysis of the finite sample first-order EM algorithm depends on the empirical process

\[ \{ \nabla Q_n (\theta \mid \theta) - \nabla Q (\theta \mid \theta), \theta \in \mathbb{B} (r; \theta^*) \}. \]
For a given sample size $n$ and tolerance parameter $\delta \in (0, 1)$, let $\epsilon_Q^{\text{unif}}(n, \delta)$ be the smallest scalar such that

$$\sup_{\theta \in \mathbb{B}(r; \theta^*)} \| \nabla Q_n(\theta | \theta) - \nabla Q(\theta | \theta) \|_2 \leq \epsilon_Q^{\text{unif}}(n, \delta)$$

with probability at least $1 - \delta$. 
Theorem 2
(General Sample-Level Guarantee)

» For some radius $r > 0$ and a triplet $(\gamma, \lambda, \mu)$ with $0 \leq \gamma < \lambda \leq \mu$ such that the $\gamma$-gradient smoothness, $\lambda$-strong concavity and $\mu$-smoothness conditions hold;

» Choose the step size $\alpha = \frac{2}{\mu + \lambda}$;

» Suppose the sample size $n$ is large enough to ensure

$$\varepsilon_Q^{\text{unif}}(n, \delta) \leq (\lambda - \gamma) \cdot r.$$
Theorem 2

(General Sample-Level Guarantee) (continued)

Then, with probability at least $1 - \delta$, given any initialization $\theta^0 \in \mathbb{B}(r; \theta^*)$, the finite-sample first-order EM iterates $\{\theta^t\}_{t=0}^{\infty}$ satisfy the bound

$$
\|\theta^t - \theta^*\|_2 \leq \left(1 - \frac{2\lambda - 2\gamma}{\mu + \lambda}\right)^t \|\theta^0 - \theta^*\|_2 + \frac{\epsilon^\text{unif}_Q (n, \delta)}{\lambda - \gamma}
$$

for all $t = 1, 2, \ldots$.  


Example: Gaussian Mixture Model
Consider the following two-component Gaussian mixture model

\[ Y = \psi \cdot \theta^* + \epsilon, \]

where

\[ \psi = \begin{cases} +1, & \text{w.p. } \frac{1}{2} \\ -1, & \text{w.p. } \frac{1}{2} \end{cases}, \quad \epsilon \sim \mathcal{N}_d \left(0, \sigma^2 I\right), \]

and \( \psi \) and \( \epsilon \) are independent.

Key Quantity:

\[ \text{SNR} = \frac{\| \theta^* \|_2}{\sigma}. \]
To analyze the EM algorithm at the population level, i.e., apply Theorem 1, one needs to establish the gradient smoothness, $\lambda$-strong concavity and $\mu$-smoothness.

Oracle Function:

$$q(\theta) = -\frac{1}{2} \cdot \mathbb{E}_{\theta^*} \left\{ (1 - w_{\theta^*}(Y)) \cdot \|Y + \theta\|^2_2 + w_{\theta^*}(Y) \cdot \|Y - \theta\|^2_2 \right\},$$

where the weighting function $w_{\theta^*}(y)$ is a smooth function.

It is easy to verify that $q$ is strongly-concave and smooth with parameters 1, i.e., $\lambda = \mu = 1$. 
What about *gradient smoothness*?

**Lemma 2**

\[\text{Let } \frac{\|\theta^*\|_2}{\sigma} \geq \eta \text{ for a sufficiently large } \eta > 0;\]

\[\text{Let the radius be } r = \frac{\|\theta^*\|_2}{4}.\]

Then, there is a constant \(\gamma \in (0, 1)\) with \(\gamma \leq \exp(-c_2 \eta^2)\) such that

\[\|E \{2 \cdot (w_\theta(Y) - w_{\theta^*}(Y)) \cdot Y\}\|_2 \leq \gamma \cdot \|\theta - \theta^*\|_2.\]
Corollary 1

(Population result for the first-order EM algorithm for GMM)

» Let $\text{SNR} = \frac{\|\theta^*\|_2}{\sigma} \geq \eta$ for a sufficiently large $\eta > 0$;

» Let the radius $r = \frac{\|\theta^*\|_2}{4}$;

» Choose the step size $\alpha = 1$. 
Corollary 1

(Population result for the first-order EM algorithm for GMM) (continued)

Then, there is a contraction coefficient \( \kappa(\eta) \leq \exp(-c\eta^2) \), where \( c \) is a universal constant, such that for any initialization \( \theta^0 \in B\left(\frac{\|\theta^*\|_2^2}{4}; \theta^*\right) \), the population first-order EM iterates satisfy the bound

\[
\|\theta^t - \theta^*\|_2 \leq \kappa^t \|\theta^0 - \theta^*\|_2
\]

for all \( t = 1, 2, \ldots \).
Now, we go from the population to the sample-based analysis of this particular model.

At the *sample* level, we study the random variable

\[
\left\| \alpha \cdot \nabla Q_n (\theta | \theta) - \alpha \cdot \nabla Q (\theta | \theta) \right\|_2
\]

\[
= \left\| \frac{1}{n} \sum_{i=1}^{n} (2w_\theta (Y_i) - 1) Y_i - E (2 \cdot w_\theta (Y) Y - Y) \right\|_2
\]

over the ball \( \mathbb{B} \left( \frac{\| \theta^* \|_2}{4}; \theta^* \right) \).
Corollary 4
(Sample-based result for first-order EM guarantees for GMM)

» Let $\text{SNR} = \frac{\|\theta^*\|_2}{\sigma} \geq \eta$ for a sufficiently large $\eta > 0$;

» Choose the radius $r = \frac{\|\theta^*\|_2}{4}$;

» Choose the step size $\alpha = 1$;

» Suppose the sample size $n$ is lower bounded by $n \geq c_1 d \log(1/\delta)$. 
Corollary 4

(Sample-based result for first-order EM guarantees for GMM)(continued)

Then, there is a contraction coefficient \( \kappa(\eta) \leq \exp(-c\eta^2) \), where \( c \) is a universal constant, such that, for any initialization \( \theta^0 \in \mathbb{B} \left( \frac{||\theta^*||_2}{4}; \theta^* \right) \), the first-order EM iterates \( \{\theta_t\}_{t=0}^{\infty} \) satisfy the bound

\[
||\theta^t - \theta^*||_2 \leq \kappa^t ||\theta^0 - \theta^*||_2 + \frac{c_2}{1 - \kappa} ||\theta^*||_2 \left( 1 + \frac{||\theta^*||_2^2}{\sigma^2} \right) \sqrt{\frac{d}{n} \log \left( \frac{1}{\delta} \right)},
\]

with probability at least \( 1 - \delta \).
Summary

- This paper advances our *theoretical* understanding of EM algorithm.
- This paper concentrates on how to obtain a *near-optimal* estimate of $\theta^*$ using EM algorithm.
- With the help of *optimization theory*, this paper establishes the *size* of the region of attraction where the initialization should be chosen and the *rate of convergence* of the EM algorithm.
- This paper also develops techniques to analyze other algorithms for solving non-convex problems.
- What's next...