Paper review: Statistical guarantees for the EM: From population to sample-based analysis

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Contribution

Resolve the gap between the global minimizer and the local optima

$$\|M_n(\theta^{t-1}) - \theta^*\|_2 \le \kappa^t \|\theta^0 - \theta^*\|_2 + \frac{1}{1-\kappa} \varepsilon_M^{unif}(n,\delta)$$
 (1)

- Provide non-asymptotic guarantees for EM algorithms
- Apply their general theory for three specific models

 Gaussian mixture model

 Mixture of regression model

 Linear regression with missing covariates

Outline

- Review for EM and Gradient EM Algorithm
- General convergence result for EM
- Guarantees for population-version EM
- Guarantees for sample-based EM
- Some related works

Expectation-maximization algorithm

- ▶ The pair (Y, Z) has a joint density function f_{θ^*} , where Y is observed and Z is missing.
- ▶ Compute some $\hat{\theta} \in \Omega$ maximizing $g_{\theta}(y)$, where

$$g_{\theta}(y) = \int_{\mathcal{Z}} f_{\theta}(y, z) dz \tag{2}$$

 $k_{\theta}(z|y)$ denotes the conditional density of z given y. We have a lower bound:

$$\underbrace{L(\theta')}_{\log(g_{\theta'}(y))} \ge \underbrace{\int_{\mathcal{Z}} k_{\theta}(z|y) \log f_{\theta'}(y,z) dz}_{Q(\theta'|\theta)} - \int_{\mathcal{Z}} k_{\theta}(z|y) \log k_{\theta'}(z|y) dz \quad (3)$$

Expectation-maximization algorithm

Standard EM updates:

E-step: Calculate $Q(\theta'|\theta)$

M-step: Compute the maximizer $\theta_{t+1} = \operatorname{argmax}_{\theta' \in \Omega} Q(\theta' | \theta_t)$

We let $\theta_{t+1} = M(\theta_t)$, which is a mapping $M : \Omega \to \Omega$

Generalized EM updates:

M-step: Choose θ_{t+1} such that $Q(\theta_{t+1}|\theta_t) \geq Q(\theta_t|\theta_t)$

Gradient EM updates:

M-step: Update $\theta_{t+1} = \theta_t + \alpha \nabla Q(\theta_t | \theta_t)$

We let $G(\theta) = \theta + \alpha \nabla Q(\theta|\theta)$

Population version versus sample version

Population version:

$$Q(\theta'|\theta) = \int_{\mathcal{Y}} (\int_{\mathcal{Z}} k_{\theta}(z|y) log f_{\theta'}(y,z) dz) g_{\theta^*}(y) dy \tag{4}$$

Sample-based version:

$$Q_n(\theta'|\theta) = \frac{1}{n} \sum_{i=1}^n \left(\int_{\mathcal{Z}} k_{\theta}(z|y) log f_{\theta'}(y, z) dz \right)$$
 (5)

General convergence results for EM

Wu(1983) established some of the most general convergence results for the EM algorithm.

- Suppose $Q(\theta'|\theta)$ is continuous in both θ' and θ . Then all the limit points of any θ_t of an EM algorithm are stationary points of L.
- Additionally, suppose $\sup_{\Phi' \in \Omega} Q(\Phi'|\Phi) > Q(\Phi|\Phi)$. Then all the limit points are local maxima.
- Suppose that $L(\theta')$ is *unimodal* in Ω with θ^* being the only stationary point. Then θ_t converges to the unique maximizer θ^* .

Guarantees for population-level EM

Definition (Self-consistency)

$$\theta^* = argmax_{\theta \in \Omega} Q(\theta | \theta^*)$$

Definition (Contractive Mapping)

A contractive mapping on a metric space(\mathcal{M} , d) is a function f from \mathcal{M} to itself, such that for all x and y in \mathcal{M}

$$d(f(x), f(y)) \le k \cdot d(x, y), 0 \le k < 1$$

- lacktriangle Add some convexity and smoothness conditions on $q(\cdot) = Q(\cdot| heta^*)$
- ► Then, the population operators are contractive on a ball containing the fixed point θ^* , where $B_2(r; \theta^*) = \{\theta \in \Omega | \|\theta \theta^*\|_2 \le r\}$

Two key conditions

Condition $(\lambda - strongly concave)$

$$q(\theta_1) - q(\theta_2) - \langle \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \le -\frac{\lambda}{2} \|\theta_1 - \theta_2\|_2^2 \tag{6}$$

for all pairs (θ_1, θ_2) in a neighborhood of θ^* .

Condition (First-order Stability(FOS))

The function $Q(\cdot|\theta), \theta \in \Omega$ satisfy condition $FOS(\gamma)$ over $B_2(r; \theta^*)$ if

$$\|\nabla Q(M(\theta)|\theta^*) - \nabla Q(M(\theta)|\theta)\|_2 \le \gamma \|\theta - \theta^*\|_2$$

$$B_2(r; \theta^*) := \{ \theta \in \Omega | \|\theta - \theta^*\|_2 \le r \}$$

Actually, FOS is the Lipschitz condition for $\nabla Q(M(\theta)|\cdot)$.

Characterizations condition

Proposition (First order optimality condition(Bubeck 2014))

Let f be convex and X a closed convex set on which f is differentiable. Then

$$x^* \in \operatorname{argmin}_{x \in X} f(x) \tag{7}$$

if and only if one has

$$\nabla f(x^*)^T (x^* - y) \le 0, \forall y \in X$$
 (8)

Condition (First-order optimality)

$$\langle \nabla Q(\theta^*|\theta^*), \theta' - \theta^* \rangle \le 0$$
 (9)

$$\langle \nabla Q(M(\theta)|\theta), \theta' - M(\theta) \rangle \le 0$$
 (10)

$$\theta^* = \operatorname{argmax}_{\theta \in \Omega} Q(\theta | \theta^*) \ M(\theta) = \operatorname{argmax}_{\theta' \in \Omega} Q(\theta' | \theta)$$

Population version EM theorem

Theorem

For some radius r>0 and pair (γ,λ) such that $0\leq \gamma<\lambda$, suppose that the function $Q(\cdot|\theta^*)$ is λ -strongly concave, and that the FOS (λ) condition holds on the ball $B_2(r;\theta^*)$. Then the population EM operator M is contractive over $B_2(r;\theta^*)$, in particular with

$$\|M(\theta) - \theta^*\|_2 \le \frac{\gamma}{\lambda} \|\theta - \theta^*\|_2, \forall \theta \in B_2(r; \theta^*)$$
 (11)

$$\|\theta^t - \theta^*\|_2 \le (\frac{\gamma}{\lambda})^t \|\theta^0 - \theta^*\|_2$$
 (12)

Guarantees for sample-based EM

- ▶ Recall $M_n(\theta) := argmax_{\theta' \in R^d} Q_n(\theta'|\theta)$
- ► For a given sample size n, tolerance parameter $\delta \in (0,1)$ and any fixed $\theta \in B_2(r; \theta^*)$, we have

$$||M_n(\theta) - M(\theta)||_2 \le \varepsilon_M(n, \delta)$$
(13)

with probability at least 1- δ

A stronger condition: uniform upper bound

$$sup_{\theta \in B_2(r;\theta^*)} \| M_n(\theta) - M(\theta) \|_2 \le \varepsilon_M^{unif}(n,\delta)$$
 (14)

with probability at least 1- δ

For specific models, we have a close form for $\varepsilon_M^{unif}(n,\delta)$

Main Result

Theorem

Suppose that the population EM operator $M: \Omega \to \Omega$ is contractive with parameter $\kappa \in (0,1)$ on the ball $B_2(r;\theta^*)$, and the initial vector θ^0 belongs to $B_2(r;\theta^*)$.

If the sample size n is large enough to ensure that

$$\varepsilon_M^{unif}(n,\delta) \le (1-\kappa)r$$
 (15)

then the EM iterates $\{\theta^t\}_{t=0}^{\infty}$ satisfy the bound

$$\|\theta^{t} - M(\theta^{t-1}) + M(\theta^{t-1}) - \theta^{*}\|_{2} \leq \underbrace{\kappa^{t} \|\theta^{0} - \theta^{*}\|_{2}}_{Optimization \ Error} + \underbrace{\frac{1}{1 - \kappa} \varepsilon_{M}^{unif}(n, \delta)}_{Statistical \ Error}$$
(16)

with probability at least 1- δ

Decomposition of the error!

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A similar idea for Bayes risk (Martin Wainwright's lecture)

- ▶ $R(\hat{g_n}) = P[Y \neq sign(\hat{g_n}(X) \frac{1}{2})]$, corresponding to the true error probability of our classifier.
- $ightharpoonup R^* = inf_{g \in F} P[Y \neq sign(g(X) \frac{1}{2})]$, corresponding to the best rule.
- ► Decomposition:

$$R(\hat{g_n}) - R^* = \underbrace{\{R(\hat{g_n}) - inf_{g \in \mathcal{F}_{\epsilon_n}} R(g)\}}_{\textit{Estimation error}} + \underbrace{\{inf_{g \in \mathcal{F}_{\epsilon_n}} R(g) - inf_{g \in \mathcal{F}} R(g)\}}_{\textit{Approximation error}}$$

where \mathcal{F}_{ϵ_n} is an ϵ_n – covering of \mathcal{F} .

Stopping Rule

Consider any positive integer T such that

$$T \ge \log_{\frac{1}{\kappa}} \frac{(1-\kappa)\|\theta^0 - \theta^*\|_2}{\varepsilon_M^{unif}(n,\delta)}$$
 (17)

Then the *Optimization Error* is dominated by *Statistical Error*.

However, this T is not computable based only on data. It just provides a iteration complexity growth ratio.

Graph illustration

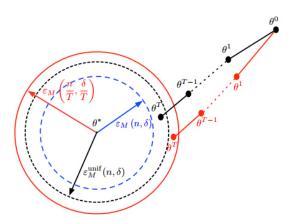


Figure: An illustration of Main Theorem

Sample-splitting version of the EM algorithm

- ▶ Divide the full data set into T subsets of size [n/T]
- ▶ Perform the updates $\theta^{t+1} = M_{T/n}(\theta^t)$
- ▶ Use a fresh subset of samples at each iteration
- ▶ Do we need to consider the divide and conquer procedure?

Gradient EM algorithm(Population version)

Definition 1 (μ – smooth)

$$q(\theta_1) - q(\theta_2) - \langle \nabla q(\theta_2), \theta_1 - \theta_2 \rangle \ge -\frac{\mu}{2} \|\theta_1 - \theta_2\|_2^2$$
 (18)

Definition 2 (Gradient Stability(GS))

$$\|\nabla Q(\theta|\theta^*) - \nabla Q(\theta|\theta)\|_2 \le \gamma \|\theta - \theta^*\|_2 \tag{19}$$

for all $\theta \in B_2(r; \theta^*)$

Gradient Decent v.s Gradient EM

Gradient Decent
$$T(\theta) := \theta + \alpha \nabla Q(\theta|\theta^*)$$

Gradient EM $G(\theta) := \theta + \alpha \nabla Q(\theta|\theta)$

In the standard optimization theory, the gradient operator $T: \Omega \to \Omega$ with step size $\alpha = \frac{2}{\mu + \lambda}$ is contractive over $B_2(r; \theta^*)$,

$$\|T(\theta) - \theta^*\|_2 \le (\frac{\mu - \lambda}{\mu + \lambda}) \|\theta - \theta^*\|_2$$
 (20)

We use the condition $\lambda - strong$ concavity and $\mu - smooth$.

The population gradient EM operator G with step size $\alpha = \frac{2}{\mu + \lambda}$ is contractive over $B_2(r; \theta^*)$,

$$\|G(\theta) - \theta^*\|_2 \le (1 - \frac{2\lambda - 2\gamma}{\mu + \lambda}) \|\theta - \theta^*\|_2$$
 (21)

We use the condition $\lambda-strong$ concavity, $\mu-smooth$ and GS.

Main result for Gradient EM algorithm

Theorem

Suppose that the population gradient EM operator $G: \Omega \to \Omega$ is contractive with parameter $\kappa \in (0,1)$ on the ball $B_2(r;\theta^*)$, and the initial vector θ^0 belongs to $B_2(r;\theta^*)$.

If the sample size n is large enough to ensure that

$$\varepsilon_G^{unif}(n,\delta) \le (1-\kappa)r$$
 (22)

then the EM iterates $\{\theta^t\}_{t=0}^{\infty}$ satisfy the bound

$$\|\theta^{t} - \theta^{*}\|_{2} \leq \underbrace{\kappa^{t} \|\theta^{0} - \theta^{*}\|_{2}}_{Optimization \ Error} + \underbrace{\frac{1}{1 - \kappa} \varepsilon_{G}^{unif}(n, \delta)}_{Statistical \ Error}, \tag{23}$$

with probability at least $1-\delta$

Some related works

- ► Two-stage alternating minimization(Yi, Caramanis, Sanghavi(2014))
- ► High dimensional EM (Wang, Gu, Ning, Liu(2014))

Two-stage alternating minimization

Only consider the mixed linear regression model

$$y_i = \langle x_i, \beta_1^* \rangle z_i + \langle x_i, \beta_2^* \rangle (1 - z_i) + w_i$$
 (24)

- SVD a algorithm for initialization step
- Using $O(klog^2k)$ samples, with high probability their initialization procedure returns $\beta_1^{(0)}$, $\beta_2^{(0)}$ which are within a constant distance of the true β_1^* , β_2^* .

$$\max\{\|\beta_1^{(t)} - \beta_1^*\|_2, \|\beta_2^{(t)} - \beta_2^*\|_2\} \le \tilde{c}\min\{p_1, p_2\}\|\beta_1^* - \beta_2^*\|_2 \quad (25)$$

High dimensional EM

- ► Attach a truncation step to the expectation step and maximization step
- ▶ The iterative solution sequence $\{\beta^{(t)}\}_{t=0}^{T}$ satisfies

$$\|\beta^{(t)} - \beta^*\|_2 \le \underbrace{\Delta_1 \rho^{t/2}}_{Optimization \ Error} + \underbrace{\Delta_2 \sqrt{\frac{s^* logd}{n}}}_{Statistical \ Error}$$
(26)

with high probability

Add some high-dimensional inferences

References

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Thank you!