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## In this talk

Motivated by the Large scale Learning setting,

• Design a novel algorithm for the optimization problem:

find 
$$s_{\star} \in \mathbb{R}^q$$
 s.t.  $h(s_{\star}) = 0$ 

• Adapted to the finite sum setting (large number of examples n)

when 
$$h(s) = \frac{1}{n} \sum_{i=1}^{n} h_i(s)$$

- Stochastic optimization: it combines
  - the Stochastic Approximation method Robbins and Monro (1951); Benveniste et al. (1990)

$$\widehat{S}_{n+1} = \widehat{S}_n + \gamma_{n+1} H_{n+1} \qquad H_{n+1} \approx \mathsf{h}(\widehat{S}_n)$$

a variance reduction technique

I. Motivation: Expectation Maximization for inference in latent variable models (large scale learning)

Motivation: Expectation Maximization for inference in latent variable models

Reminder 1: Latent variable models

## Reminder 1: latent variable models

- The observations  $Y = (Y_1, \cdots, Y_n)$
- A parametric statistical model indexed by  $\theta\in\Theta$
- Some latent or hidden variables  $Z = (Z_1, \cdots, Z_n)$
- A complete data vector: (Y, Z), make easier or more general the definition of the observations

#### Example 1: Mixture models

$$Y_i \overset{i.i.d}{\sim} \sum_{g=1}^G \omega_g \, f_g(y_i; \theta_g) \mathsf{d} \mu_i \qquad \theta = (\theta_{1:G}, \omega_{1:G})$$

Or equivalently

$$Z_i \sim \omega_{\bullet}$$
  $Y_i | (Z_i = g) \sim f_g(y_i; \theta_g) \mathsf{d} \mu_i$ 

#### Example 2: Mixed Effect models

Random effects  $Z_{\bullet} \to$  non explicit expression of the likielihood of the observations

Motivation: Expectation Maximization for inference in latent variable models

Reminder 2: The (standard) EM algorithm

# Reminder 2: The (standard) EM algorithm to optimize the likelihood

- ► The objective function:
  - The likelihood, non explicit

$$\theta \mapsto \log p(Y_{1:n}; \theta) = \sum_{i=1}^{n} \log p(Y_i; \theta) = \sum_{i=1}^{n} \log \int \underbrace{\bar{p}(Y_i, z_i; \theta)}_{\text{complet date likel.}} \, \mathrm{d}\nu(z_i)$$

EM solves the optimization problem by iterating

• the Expectation-step:

$$Q(\theta, \theta^t) = \sum_{i=1}^{n} \mathbb{E}\left[\log \bar{p}(Y_i, \mathbf{Z}_i; \theta) | Y_{1:n}, \theta^t\right]$$

the latent variables are *imputed* with their best approximation at time #t• The Maximization step:

$$\boldsymbol{\theta}^{t+1} \in \operatorname{argmax}_{\boldsymbol{\theta} \in \boldsymbol{\theta}^{t}} Q(\boldsymbol{\theta}, \boldsymbol{\theta}^{t})$$

Motivation: Expectation Maximization for inference in latent variable models

Reminder 3: The curved exponential family

### Reminder 3: The curved exponential family

• Pbm: computation of the function

$$\theta \mapsto Q(\theta, \theta^t) = \sum_{i=1}^n \mathbb{E}\left[\log \bar{p}(Y_i, \mathbf{Z_i}; \theta) | Y_{1:n}, \theta^t\right]$$

Realistic when

$$\log \bar{p}(Y_i, \mathbf{Z}_i; \theta) = \psi(\theta) + \langle s_i(\mathbf{Z}_i), \phi(\theta) \rangle$$

In that case,

$$Q(\theta, \theta^{t}) = \psi(\theta) + \left\langle \sum_{i=1}^{n} \underbrace{\mathbb{E}\left[s_{i}(\mathbf{Z}_{i})|Y_{1:n}, \theta^{t}\right]}_{\bar{\mathbf{s}}_{i}(\theta^{t})}, \phi(\theta) \right\rangle$$

and the two steps of EM are

- E-step: compute  $\sum_{i=1}^{n} \bar{\mathsf{s}}_i(\theta^t)$
- M-step: update

$$\theta^{t+1} \in \operatorname{argmax} \psi(\theta) + \left\langle \sum_{i=1}^{n} \bar{\mathsf{s}}_{i}(\theta^{t}), \phi(\theta) \right\rangle$$

Motivation: Expectation Maximization for inference in latent variable models

L The optimization problem

# Optimization problem: finite sum setting, for curved exponential families

In this talk

• Solve on  $\Theta \subseteq \mathbb{R}^d$  the minimization problem

$$\operatorname{argmin}_{\theta \in \Theta} - \frac{1}{n} \sum_{i=1}^{n} \log \int_{\mathsf{Z}} p_i(z_i; \theta) \mathsf{d}\mu(z_i) + \tilde{\mathsf{R}}(\theta), \qquad p_i(z_i; \theta) > 0$$

• In the curved exponential family:

$$-\frac{1}{n}\sum_{i=1}^{n}\log\int_{\mathsf{Z}}h_{i}(z_{i})\,\exp\left(\langle s_{i}(z_{i}),\phi(\theta)\rangle-\psi(\theta)\right)\mathsf{d}\mu(z_{i})+\tilde{\mathsf{R}}(\theta)$$

• Via EM-based methods

Motivation: Expectation Maximization for inference in latent variable models

└─ EM in the finite-sum framework

#### Intractable EM Dempster, Laird, Rubin (1977)

Objective function:

$$-\sum_{i=1}^{n}\log\int_{\mathsf{Z}}p_{i}(z_{i};\boldsymbol{\theta})\mathsf{d}\boldsymbol{\mu}(z_{i})+\bar{\mathsf{R}}(\boldsymbol{\theta}), \qquad p_{i}(z_{i};\boldsymbol{\theta})=h_{i}(z_{i})\,\exp\left(\left\langle s_{i}(z_{i}),\boldsymbol{\phi}(\boldsymbol{\theta})\right\rangle-\psi(\boldsymbol{\theta})\right)$$

• EM algorithm: Repeat for t = 0, ...

E-step 
$$\bar{\mathbf{s}}(\theta_t) = \frac{1}{n} \sum_{i=1}^n \bar{\mathbf{s}}_i(\theta_t)$$
 where  $\bar{\mathbf{s}}_i(\theta) \stackrel{\text{def}}{=} \int_{\mathbf{Z}} \mathbf{s}_i(z_i) \frac{p_i(z_i;\theta)}{\int p_i(u;\theta) d\mu(u)} d\mu(z_i)$   
M-step  $\theta_{t+1} = \mathbf{T}(\bar{\mathbf{s}}(\theta_t))$ 

where

$$\mathsf{T}(s) \stackrel{\text{def}}{=} \operatorname{argmin}_{\theta \in \Theta} \quad (\mathsf{R}(\theta) - \langle s, \phi(\theta) \rangle)$$

#### E-step

 $\rightarrow$  sum over n expectations  $\rightarrow$  Large computational cost of each EM iteration, when n is large

#### $\rightarrow$ in some cases, the expectations $\bar{s}_i$ 's are intractable

We consider the case when the M-step (computation of T) is explicit

Motivation: Expectation Maximization for inference in latent variable models

EM in the finite-sum framework

#### EM in the expectation space

• EM: an algorithm in the expectation space

$$\theta_{t+1} = \mathsf{T} \circ \bar{\mathsf{s}}(\theta_t) = \mathsf{T} \circ \bar{\underline{\mathsf{s}}} \circ \mathsf{T} \circ \mathsf{T}$$

• EM designed to find the roots of

$$\mathbf{h}(s) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \overline{\mathbf{s}}_{i} \circ \mathbf{T}(s) - s$$
$$= \mathbb{E} \left[ \mathbf{h}_{I}(s) \right]$$
$$= \mathbb{E} \left[ \mathbf{h}_{I}(s) + V \right] \qquad \mathbb{E}[V] = 0$$

where  $I \sim U(\{1, ..., n\})$  and V is a *control variate* i.e. r.v. correlated with  $h_I$  and centered.

Motivation: Expectation Maximization for inference in latent variable models

L\_EM in the finite-sum framework

# A Lyapunov function

• EM designed to solve on  $\Theta \subseteq \mathbb{R}^d$ 

$$\operatorname{argmin}_{\theta \in \Theta} F(\theta), \qquad F(\theta) \stackrel{\text{def}}{=} \mathsf{R}(\theta) - \frac{1}{n} \sum_{i=1}^{n} \log \int_{\mathsf{Z}} p_i(z;\theta) \mathsf{d}\mu(z)$$

• For exact EM: F is a Lyapunov function

$$F(\theta_{t+1}) \le F(\theta_t)$$

• EM in the expectation space:

$$W \stackrel{\mathrm{def}}{=} F \circ \mathsf{T}$$

it holds (under regularity conditions)

$$\nabla W(s) = -B(s) h(s) \qquad h(s) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} (\bar{s}_i \circ T(s) - s)$$

 $\hookrightarrow$  An algorithm designed to find the roots of h is among the stochastic preconditioned gradient algorithms, with preconditioning matrix  $B^{-1}(s)$ .

II. Algorithm and Convergence analysis

A novel Variance Reduced incremental EM

Variance reduction within Stochastic Approximation scheme

Variance reduced incremental algorithms (in the EM context  $h_i = \bar{s}_i \circ T(s) - s$ )

solve on  $\mathbb{R}^q$ : h(s) = 0 with  $h(s) = n^{-1} \sum_{i=1}^n h_i(s) = \mathbb{E}[h_I(s)]$ 

$$\widehat{S}_{t+1} = \widehat{S}_t + \gamma_{t+1} \left( \frac{1}{\mathsf{b}} \sum_{i \in \mathcal{B}_{t+1}} \mathsf{h}_i(\widehat{S}_t) + V_{t+1} \right)$$

where  $\mathcal{B}_{t+1}$  is a mini-batch of examples of size b << n.

- Online-EM (Neal and Hinton, 1998; Cappé and Moulines, 2009). NO variance reduction  $(V_{t+1} = 0).$
- sEM-vr: Stochastic EM with Variance Reduction Chen et al, 2018
- FIEM: Fast Incremental EM Karimi et al, 2019; Fort et al, 2021
- SPIDER-EM Fort, Moulines, Wai NeurIPS 2020: Stochastic Path Integrated Differential EstimatoR EM

$$V_{t+1} = \sum_{\ell=0}^{t} \left\{ \frac{1}{\mathsf{b}} \sum_{i \in \mathcal{B}_{\ell}} \mathsf{h}_i(\widehat{S}_{\ell-1}) - \frac{1}{\mathsf{b}} \sum_{i \in \mathcal{B}_{\ell+1}} \mathsf{h}_i(\widehat{S}_{\ell-1}) \right\}$$

Nguyen et al. (2017), Fang et al. (2018), Wang et al. (2019)

#### SPIDER-EM (Stochastic Path Integrated Differential EstimatoR Expectation Maximization)

1: 
$$\widehat{S}_{1,0} = \widehat{S}_{1,-1} = \widehat{S}_{init}$$
  $V_{1,0} = 0$   $\mathcal{B}_{1,0} = \{1, \cdots, n\}$   
2: for  $t = 1, \cdots, k_{out}$  do  
3: for  $k = 0, \dots, \xi_t - 1$  do  
4: Sample a mini batch  $\mathcal{B}_{t,k+1}$  of size b from  $\{1, \cdots, n\}$   
5:  $V_{t,k+1} = V_{t,k} + \left(b^{-1}\sum_{i\in\mathcal{B}_{t,k}}h_i(\widehat{S}_{t,k-1}) - b^{-1}\sum_{i\in\mathcal{B}_{t,k+1}}h_i(\widehat{S}_{t,k-1})\right)$   
6:  $\widehat{S}_{t,k+1} = \widehat{S}_{t,k} + \gamma_{t,k+1}\left(b^{-1}\sum_{i\in\mathcal{B}_{t,k+1}}h_i(\widehat{S}_{t,k}) + V_{t,k+1}\right)$   
7: end for  
8:  $\widehat{S}_{t+1,-1} = \widehat{S}_{t,\xi_t}$   
9:  $V_{t+1,0} = 0$   $\mathcal{B}_{t+1,0} = \{1, \cdots, n\}$   
10:  $\widehat{S}_{t+1,0} = \widehat{S}_{t+1,-1} + \gamma_{t+1,0}\left(n^{-1}\sum_{i=1}^n h_i(\widehat{S}_{t+1,-1}) + V_{t+1,0}\right)$   
11: end for

- $k_{\mathrm{out}}$  outer loops, the outer #t is of length  $\xi_t$
- The control variate is refreshed at each outer loop #t (see Line 9)
- A full scan of the examples at each outer loop (see Line 9).

#### Extensions

- The length of the outer loop is a Geometric random variable with expectation  $\xi_t.$  Fort, Moulines, Wai ICASSP 2021
- Avoid the full scan of the examples when starting each outer loop  $\rightarrow$  reduction of the computational cost. Fort, Moulines, Wai ICASSP 2021
- An approximation of h<sub>i</sub> Fort, Moulines SSP 2021

$$\widehat{\mathbf{h}_i(\hat{S}_{t,k})} = \mathbf{h}_i(\hat{S}_{t,k}) + \eta_{t,k+1}$$

for example: in EM,  $h_i(s) = \bar{s}_i \circ T(s) - s$  and  $\bar{s}_i$  is an expectation w.r.t. the a posteriori distribution of the latent variables  $\rightarrow$  Monte Carlo approximation.

• A Proximal operator for constrained optimization Fort, Moulines - SSP 2021

$$\widehat{S}_{t,k+1} = \operatorname{Prox}_{B(\widehat{S}_k), \gamma_{t,k+1}} g\left(\widehat{S}_{t,k} + \gamma_{t,k+1} \left( \mathsf{b}^{-1} \sum_{i \in \mathcal{B}_{t,k+1}} \widehat{\mathsf{h}_i(\widehat{S}_{t,k})} + V_{t,k+1} \right) \right)$$

for example: find the roots of h in a compact set.

A novel Variance Reduced incremental EM

 $\Box$  Convergence analysis, explicit functions  $h_i$ 's

# Assumptions

**(**) There exists a continuously differentiable function  $W: \mathbb{R}^q \to \mathbb{R}$  such that

$$\nabla W(s) \stackrel{\text{def}}{=} -B(s) \mathsf{h}(s) \qquad \mathsf{h}(s) \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \mathsf{h}_i(s)$$

where B(s) is a  $q \times q$  positive definite matrix. In addition,  $\nabla W$  is globally Lipschitz with constant  $L_{\dot{W}}$ , and there exist  $0 < v_{\min} \leq v_{\max}$  such that the spectrum of B(s) is in  $[v_{\min}, v_{\max}]$ .

**②** For any  $i \in \{1, \dots, n\}$ , the function  $h_i$  is globally Lipschitz with constant  $L_i$ .

A novel Variance Reduced incremental EM

 $\Box$  Convergence analysis, explicit functions  $h_i$ 's

# Convergence in expectation, explicit $h_i$ 's

#### Under the previous assumptions:

(Fort, Moulines, Wai, NeurIPS 2020)

Set  $L^2 \stackrel{\text{def}}{=} n^{-1} \sum_{i=1}^n L_i^2$ . Fix  $k_{\text{out}}, k_{\text{in}}, \mathbf{b} \in \mathbb{N}_{\star}$ . Choose  $\alpha \in (0, v_{\min}/\mu_{\star}(k_{\text{in}}, \mathbf{b}))$  with

$$\mu_{\star}(k_{\mathrm{in}},\mathsf{b}) \stackrel{\mathrm{def}}{=} v_{\mathrm{max}} \frac{\sqrt{k_{\mathrm{in}}}}{\sqrt{\mathsf{b}}} + \frac{L_{\dot{W}}}{2L}.$$

Run the algorithm with  $\xi_t = k_{\rm in}$  and  $\gamma_{t,k} \stackrel{\rm def}{=} \alpha/L$ . Then

$$\mathbb{E}\left[\left\|\mathbf{h}\left(\widehat{S}_{\tau,\xi-1}\right)\right\|^{2}\right] \leq \left(\frac{1}{k_{\mathrm{in}}} + \frac{\alpha^{2}}{\mathbf{b}}\right) \frac{1}{k_{\mathrm{out}}} \frac{2L}{\alpha\{v_{\mathrm{min}} - \alpha\mu_{\star}(k_{\mathrm{in}}, \mathbf{b})\}} \left(\mathbb{E}\left[W(\widehat{S}_{\mathrm{init}})\right] - \min W\right)$$

where  $(\tau, \xi)$  is a uniform r.v. on  $\{1, \dots, k_{out}\} \times \{0, \dots, k_{in} - 1\}$  indep of  $\{\widehat{S}_{t,k}\}$ .

A novel Variance Reduced incremental EM

 $\Box$  Convergence analysis, explicit functions  $h_i$ 's

# Complexity for *c*-approximate stationarity

From this explicit expression of an upper bound for

$$\mathbb{E}\left[\left\|\mathsf{h}(\widehat{S}_{\tau,\xi-1})\right\|^2\right]$$

- in the non convex setting
- with a random stopping rule
- as a function of  $k_{\rm out},k_{\rm in},{\rm b},n$  and the learning rate  $\gamma$  (=  $\gamma_{t,k}$  for any t,k>0)

## To reach $\epsilon$ -stationarity, the complexity of SPIDER-EM

With: 
$$k_{in} = b = O(\sqrt{n}), \quad k_{out} = O(1/(\epsilon k_{in}))$$

Nbr of optimization steps:  $O(1/\epsilon)$ Nbr of  $\bar{s}_i$ 's evaluations:  $\mathcal{K} = O(\sqrt{n} \epsilon^{-1}) \rightarrow$  state of the art !

Algorithm	Complexity $\mathcal K$
Online-EM	$\epsilon^{-2}$
iEM	$n \epsilon^{-1}$
sEM-vr	$n^{2/3} \epsilon^{-1}$
FIEM	$n^{2/3} \epsilon^{-1} \wedge \sqrt{n} \epsilon^{-3/2}$

A novel Variance Reduced incremental EM

 $\Box$  Convergence analysis, explicit functions  $h_i$ 's

#### Sketch of proof

Inside an outer loop #t, then sum along the inner loops k = 0 to  $k = k_{in} - 1$ ; then sum along the outer loops t = 1 to  $t = k_{out}$ .

• W is Gradient-Lipschitz, and its gradient is a linear function of h

$$\begin{split} W(\hat{S}_{t,k+1}) - W(\hat{S}_{t,k}) &\leq \left\langle \nabla W(\hat{S}_{t,k}), \hat{S}_{t,k+1} - \hat{S}_{t,k} \right\rangle + \frac{L_{\dot{W}}}{2} \|\hat{S}_{t,k+1} - \hat{S}_{t,k}\|^2 \\ &\leq -\gamma_{t,k+1} v_{\min} \|H_{t,k+1}\|^2 + \gamma_{t,k+1} \left(\beta^2 v_{\max} + \gamma_{t,k+1} \frac{L_{\dot{W}}}{2}\right) \|H_{t,k+1}\|^2 \\ &+ \frac{\gamma_{t,k+1}}{\beta^2} v_{\max} \|H_{t,k+1} - \mathsf{h}(\hat{S}_{t,k})\|^2 \qquad \forall \beta > 0; \mathsf{choice:} \ \beta^2 \propto \gamma_{t,k+1} \end{split}$$

• Biased field; full scan when refreshing  $\rightarrow$  cancel the bias

$$\mathbb{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right] = h(\widehat{S}_{t,k}) + H_{t,k} - h(\widehat{S}_{t,k-1}) \qquad \qquad \mathbb{E}\left[H_{t,k+1}|\mathcal{F}_{t,0}\right] = 0.$$

•  $L^2$ -error of the field

$$\mathbb{E}\left[\left\|H_{t,k+1}-\mathsf{h}(\widehat{S}_{t,k})\right\|^{2}|\mathcal{F}_{t,0}\right] = \mathbb{E}\left[\left\|H_{t,k+1}-\mathbb{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right]\right\|^{2}|\mathcal{F}_{t,0}\right] + \mathbb{E}\left[\left\|\underbrace{\mathbb{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right]-\mathsf{h}(\widehat{S}_{t,k})}_{H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})}\right\|^{2}|\mathcal{F}_{t,0}\right] + \mathbb{E}\left[\left\|\underbrace{\mathbb{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right]-\mathsf{h}(\widehat{S}_{t,k-1})}_{H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})}\right\|^{2}|\mathcal{F}_{t,0}\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right\|^{2}|\mathcal{F}_{t,0}|\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k+1}|\mathcal{F}_{t,k}\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right\|^{2}|\mathcal{F}_{t,0}|\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})}{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]}\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})\right]\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})-\mathsf{h}(\widehat{S}_{t,k-1})\right]\right]\right] + \mathbb{E}\left[\left\|\frac{\mathsf{E}\left[H_{t,k}-\mathsf{h}(\widehat{S}_{t,k-1})\right]-\mathsf{h}(\widehat{S}_{t,k-1})-$$

• Variance: specific form of  $H_{t,k+1} \rightarrow \text{difference of } h_i$ 's

$$\begin{split} H_{t,k+1} &- \mathbb{E}\left[H_{t,k+1} | \mathcal{F}_{t,k}\right] = \frac{1}{\mathbf{b}} \sum_{i \in \mathcal{B}_{t,k+1}} \left\{ \mathbf{h}_i(\widehat{S}_{t,k}) - \mathbf{h}_i(\widehat{S}_{t,k-1}) \right\} - \frac{1}{n} \sum_{i=1}^n \left\{ \mathbf{h}_i(\widehat{S}_{t,k}) - \mathbf{h}_i(\widehat{S}_{t,k-1}) \right\} \\ & \text{use:} \|\mathbf{h}_i(\widehat{S}_{t,k}) - \mathbf{h}_i(\widehat{S}_{t,k-1})\|^2 \le L_i^2 \|\widehat{S}_{t,k} - \widehat{S}_{t,k-1}\|^2 = L_i^2 \gamma_{t,k}^2 \|H_{t,k}\|^2 \end{split}$$

A novel Variance Reduced incremental EM

 $\Box$  Convergence analysis, Monte Carlo approx of  $h_i$ 's

#### Assumptions (case: Monte Carlo approximation of $h_i$ 's)

In the case

$$\mathbf{h}_i(\widehat{S}_{t,k}) = \int \mathcal{H}(z) p_i(z; \widehat{S}_{t,k}) \mathrm{d}\mu(z) \approx \frac{1}{m_{t,k+1}} \sum_{r=1}^{m_{t,k+1}} \mathcal{H}(Z_r^{i,t,k})$$

error

$$\eta_{t,k+1} \stackrel{\text{def}}{=} \frac{1}{\mathsf{b}} \sum_{i \in \mathcal{B}_{\bullet}} \left( \frac{1}{m_{t,k+1}} \sum_{r=1}^{m_{t,k+1}} \mathcal{H}(Z_r^{i,t,k}) - \mathsf{h}_i(\widehat{S}_{t,k}) \right)$$

(bias) there exists  $C_b \ge 0$  s.t. for any t, k, with probability one

$$\left\|\mathbb{E}\left[\eta_{t,k+1}|\mathcal{F}_{t,k}\right]\right\| \leq \frac{C_b}{m_{t,k+1}}$$

• (variance) there exists  $C_v$  s.t. for any t, k with probability one

$$\mathbb{E}\left[\left\|\eta_{t,k+1} - \mathbb{E}\left[\eta_{t,k+1} | \mathcal{F}_{t,k}\right]\right\|^2 | \mathcal{F}_{t,k}\right] \le \frac{C_v}{M_{t,k+1}}$$

**Examples.** i.i.d. case:  $C_b = 0$ ; i.i.d. and MCMC cases:  $M_{t,k+1} = b m_{t,k+1}$ 

A novel Variance Reduced incremental EM

Convergence analysis, Monte Carlo approx of h<sub>i</sub>'s

## Convergence in expectation (i.i.d. case)

Fort, Moulines - SSP 2021; i.i.d. case and MCMC case

Choose  $\xi_t = k_{in}$  and  $\gamma_{t,k} = \gamma$  where

$$\gamma \stackrel{\text{def}}{=} \frac{v_{\min}}{L_{\dot{W}} + 2L v_{\max} \sqrt{k_{\text{in}}} / \sqrt{\mathsf{b}}}$$

Then

$$\begin{split} \gamma v_{\min} \mathbb{E}\left[\frac{\|\widehat{S}_{\tau,\xi} - \widehat{S}_{\tau,\xi-1}\|^2}{\gamma^2}\right] &\leq \frac{1}{k_{\text{out}}(1+k_{\text{in}})} \left(W(\widehat{S}_{\text{init}}) - \min W\right) \\ &+ C_1 \frac{v_{\max}}{L} \frac{1}{\sqrt{k_{\text{in}}\mathbf{b}}} \mathbb{E}\left[\frac{k_{\text{in}} - \xi}{m_{\tau,\xi+1}}\right] \end{split}$$

where  $(\tau, \xi)$  is a uniform r.v. on  $\{1, \dots, k_{out}\} \times \{0, \dots, k_{in}\}$  indep of  $\{\widehat{S}_{t,k}\}$ .

From

$$\widehat{S}_{t,k+1} - \widehat{S}_{t,k} = \gamma_{t,k+1} H_{t,k+1} \neq \gamma_{t,k+1} \operatorname{\mathsf{h}}(\widehat{S}_{t,k}),$$

a control is then obtained on  $\mathbb{E}\left[ \| \mathsf{h}(\widehat{S}_{ au,\xi}) \|^2 \right]$ 

A novel Variance Reduced incremental EM

Convergence analysis, Monte Carlo approx of h<sub>i</sub>'s

# Complexity for $\epsilon$ -approximate stationarity

From this explicit expression of an upper bound for

$$\mathbb{E}\left[\|\mathbf{h}(\widehat{S}_{\tau,\xi-1})\|^2\right]$$

- in the non convex setting
- with a random stopping rule
- ullet as a function of  $k_{\mathrm{out}},k_{\mathrm{in}},\mathsf{b},n$  and the learning rate  $\gamma$
- with a Monte Carlo approximation of the h<sub>i</sub>'s

#### To reach $\epsilon$ -stationarity, the complexity of Perturbed-SPIDER-EM

With:  $k_{\text{in}} = \mathbf{b} = O(\sqrt{n}), \quad k_{\text{out}} = O(1/(\epsilon k_{\text{in}})), \quad m_{t,k} = \epsilon^{-1}$ 

 $\begin{array}{ll} \textit{Nbr of optimization steps: } O(1/\epsilon) \\ \textit{Nbr of $\bar{s}_i$'s evaluations: } \mathcal{K} = O(\sqrt{n} \, \epsilon^{-1}) \rightarrow \textit{same as SPIDER-EM} \\ \textit{Nbr of Monte Carlo draws: } O(\sqrt{n}/\epsilon^2) \end{array}$ 

III. Numerical illustrations

- Numerical illustrations

Complexity of SPIDER-EM

## SPIDER-EM: state-of-the-art among the incremental EM algorithms

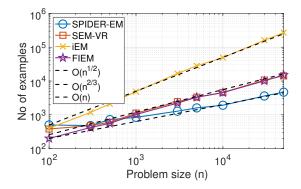


Figure: Nbr of processed examples required to reach convergence, as a function of the problem size n

-Numerical illustrations

Estimation of the parameters

# Estimation of the parameters (1/2)

Case: inference in a mixture of Gaussian distributions (from the MNIST data set). Gaussian mixture models in  $\mathbb{R}^{20}$ ; G = 12 components with the same cov matrix;  $n = 6 \, 10^4$  examples

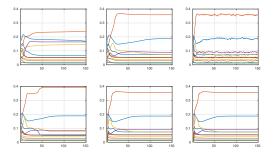


Figure: Evolution of the L = 12 iterates  $\alpha_k = (\alpha_{k,1}, \ldots, \alpha_{k,L})$  as a function of the number of epochs, for EM, iEM and Online EM on the top from left to right; FIEM, sEM-vr and SPIDER-EM on the bottom from left to right.

-Numerical illustrations

Estimation of the parameters

# Estimation of the parameters (2/2)

Case: inference in a mixture of Gaussian distributions (from the MNIST data set). Gaussian mixture models in  $\mathbb{R}^{20}$ ; G = 12 components with the same cov matrix;  $n = 6 \cdot 10^4$  examples

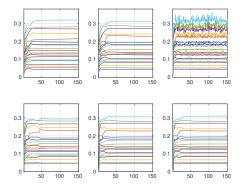


Figure: Evolution of the p=20 eigenvalues of the iterates  $\Sigma_k$  as a function of the number of epochs, for EM, iEM and Online EM on the top from left to right; FIEM, sEM-vr and SPIDER-EM on the bottom from left to right.

MaIAGE

- Numerical illustrations

- Objective function

## Evolution of the objective function

Case: inference in a mixture of Gaussian distributions (from the MNIST data set). Gaussian mixture models in  $\mathbb{R}^{20}$ ; G = 12 components with the same cov matrix;  $n = 6 \, 10^4$  examples

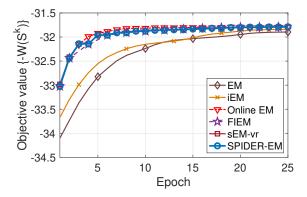


Figure: Evolution of the objective function  $-W(\widehat{S}_k)$  vs the number of epochs.

- Numerical illustrations

Choice of the design parameters

# Deterministic or geometric length of the outer loops? Full scan when refreshing ? (1/2)

Case: inference in a mixture of Gaussian distributions (from the MNIST data set). Gaussian mixture models in  $\mathbb{R}^{20}$ ; G=12 components with the same cov matrix;  $n=6\,10^4$  examples

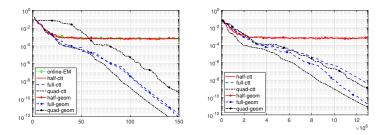


Figure: Quantile of order 0.5 of  $\|\mathbf{h}(\widehat{S}_{t,\xi_t})\|^2$  vs the number of epochs (left) and vs the number of  $\overline{s}_i$ 's evaluations (right)

Length of each outer loop: either constant (ctt)  $\xi_t=k_{\rm in},$  or a geometric r.v. (geom) with expectation  $k_{\rm in}$ 

When refreshing the control variate: use the full data set (full), or the half data set (half) or a quadratically increasing nbr of examples (quad).

- Numerical illustrations

Choice of the design parameters

# Deterministic or geometric length of the inner loops? Full scan when refreshing ? (2/2)

Case: inference in a mixture of Gaussian distributions (from the MNIST data set). Gaussian mixture models in  $\mathbb{R}^{20}$ ; G = 12 components with the same cov matrix;  $n = 6\,10^4$  examples

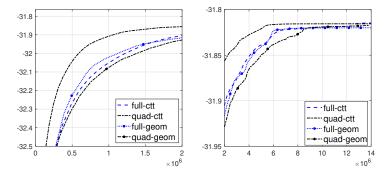


Figure: Evolution of the normalized log-likelihood vs the number of  $\bar{s}_i$ 's evaluations until 2*e*6 (left) and after (right).

- Numerical illustrations

Choice of the design parameters

### Monte Carlo approximations: benefit of variance reduction

**Case**: Ridge-penalized inference in a logistic regression model (from the MNIST data set). An individual regression vector  $Z_i \in \mathbb{R}^{1+50}$  assumed i.i.d.  $\mathcal{N}_{51}(\theta, 0.1 I)$ .  $n = 24\,989$ , 2 classes.

$$\Delta_{t,k+1} \stackrel{\text{def}}{=} \|\widehat{S}_{t,k+1} - \widehat{S}_{t,k}\|^2 / \gamma_{t,k+1}^2$$

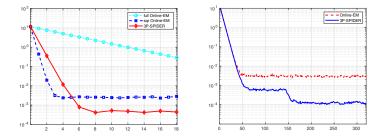


Figure: [left] Monte Carlo estimation of  $\mathbb{E}\left[\Delta_{t,k+1}\right]$  vs the number of epochs. Comparison of (Perturbed-Proximal-Preconditioned) 3P-SPIDER-EM and Online-EM when b = n (case full) and b =  $10\sqrt{n}$  (case sqr). Monte Carlo approximations with  $m_{t,k}=2\sqrt{n}$ . [right] Quantiles 0.75 of  $\Delta_{t,k}$  vs the number of epochs, for Online-EM and 3P-SPIDER-EM. For 3P-SPIDER-EM  $m_{t,k}=2\sqrt{n}$  for  $t\leq 9$  and  $m_{t,k}=10\sqrt{n}$  for  $t\geq 10$ .

- Numerical illustrations

Choice of the design parameters

#### Monte Carlo approximations: number of points in the Monte Carlo sum

**Case**: Ridge-penalized inference in a logistic regression model (from the MNIST data set). An individual predictor vector  $Z_i \in \mathbb{R}^{1+50}$  assumed i.i.d.  $\mathcal{N}_d(\theta, 0.1 I)$ .  $n = 24\,989$ , 2 classes.

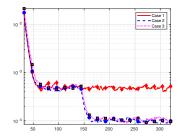


Figure: Monte Carlo estimation of  $\mathbb{E}\left[\Delta_{t,k+1}\right]$  vs the number of epochs. (Perturbed-Proximal-Preconditioned) SPIDER-EM applied with  $\gamma_{t,k}=0.1$  and  $m_{t,k}=2\sqrt{n}$  in Case 1; and with  $\gamma_{t,k}=0.1$  and  $m_{t,k}=2\sqrt{n}$  for  $t\leq 10$  and  $m_{t,k}=10\sqrt{n}$  for  $t\geq 11$  on Case 2 and Case 3. Case 2 and Case 3 differ in the choice of  $\gamma_{t,0}$ 

IV. Bibliography

## Results of this talk

Results of this talk

- G. Fort, E. Moulines, H.-T. Wai. A Stochastic Path Integrated Differential Estimator Expectation Maximization Algorithm. *In Conference Proceedings NeurIPS*, 2020.
- G. Fort, E. Moulines, H.-T. Wai. Geom-SPIDER-EM: Faster Variance Reduced Stochastic Expectation Maximization for Nonconvex Finite-Sum Optimization, *ICASSP 2021 – 2021 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP):3135–3139.*
- **G. Fort and E. Moulines.** The Perturbed Prox-Preconditioned SPIDER algorithm: non-asymptotic convergence bounds. *Accepted to IEEE Statistical Signal Processing Workshop (SSP 2021).*
- **G. Fort and E. Moulines.** The Perturbed Prox-Preconditioned SPIDER algorithm for EM-based large scale learning. *Accepted to IEEE Statistical Signal Processing Workshop (SSP 2021)*

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