Gersende Fort (CNRS, Institut de Mathématiques de Toulouse, France)

Joint work with Eric Moulines (CMAP, Ecole Polytechnique, France) and Hoi-To Wai (Chinese Univ. of Hong Kong, Hong-Kong)

and on going discussions with Florence Forbes (INRIA, France) and Hien Duy Nguyen (Univ. Queensland, Australia)

SMOR Seminar, Univ. of Queensland







In this talk

Motivated by the Large scale Learning setting,

 $\operatorname{argmin}_{\theta} \mathbb{E}_{\pi} \left[\ell(X, \theta) \right] \text{ from } (X_i)_i \sim \pi$

$$\operatorname{argmin}_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(X_i, \theta)$$

solved by a Majorize-Minimization (MM) algorithm

- Part 1. Is it tractable ? no.
- Part 2. Identify the limiting points of MM.
- Part 3. Design a stochastic optimization algorithm with the same limiting points: it combines
 - the Stochastic Approximation method Robbins and Monro (1951); book by Benveniste et al. (1990)

$$\widehat{S}_{n+1} = \widehat{S}_n + \gamma_{n+1}H_{n+1} \qquad H_{n+1}$$

- a variance reduction technique for the random approximation H_{n+1} .
- Part 4. Explicit bounds of convergence for the SPIDER MM.
- Part 5. Numerical illustrations.

I. The Majorize Minimization algorithm in the large scale learning setting

└─ The MM algorithm

L The large scale learning setting

The large scale learning setting

$$\operatorname{argmin}_{\theta \in \mathbb{R}^d} \ (F(\theta) + g(\theta)) \qquad \qquad g(\theta): \text{ exact}$$

• "Large batch" learning

$$F(heta) \stackrel{ ext{def}}{=} rac{1}{n} \sum_{i=1}^n \ell(X_i, heta)$$
 size n , prohibitive

• Online learning

 $F(\theta) \stackrel{\text{def}}{=} \mathbb{E}_{\pi} \left[\ell(X, \theta) \right]$ from a stream of observations $X_i \stackrel{i.i.d.}{\sim} \pi$

- The MM algorithm
 - L The algorithm and its possible intractability

The MM algorithm book by K. Lange (2016)

- An iterative algorithm
- Repeat:
- $\theta_t \rightarrow \text{majorizing fct} \rightarrow \theta_{t+1} \rightarrow \text{majorizing fct} \rightarrow \cdots$
- Given θ_t , the majorizing function satisfies majorize $F(\cdot) \leq G(\cdot; \theta_t)$ $F(\cdot) + g(\cdot) \leq G(\cdot; \theta_t) + g(\cdot)$ tangent $F(\theta_t) = G(\theta_t; \theta_t)$
- From the majorizing function,

$$\theta_{t+1} \stackrel{\text{def}}{=} \operatorname{argmin}_{\theta} \left(G(\theta; \theta_t) + g(\theta) \right)$$

• A descent property:

 $F(\theta_{t+1}) + g(\theta_{t+1}) \leq G(\theta_{t+1}; \theta_t) + g(\theta_{t+1}) \leq G(\theta_t; \theta_t) + g(\theta_t) = F(\theta_t) + g(\theta_t)$

The MM algorithm

L The algorithm and its possible intractability

Intractability ?

$\operatorname{argmin}_{\theta} \operatorname{MajorizingFct}(\theta; \theta_t)$

• [Considered here] The explicit expression of the majorizing function

$$F(\theta) + g(\theta) = n^{-1} \sum_{i=1}^{n} \ell(X_i; \theta) + g(\theta) \Longrightarrow \theta \mapsto n^{-1} \sum_{i=1}^{n} (\quad) + g(\theta)$$
$$F(\theta) + g(\theta) = \mathbb{E}_{\pi} \left[\ell(X; \theta) \right] + g(\theta) \Longrightarrow \theta \mapsto \mathbb{E}_{\pi} \left[\quad] + g(\theta)$$

• [assumed explicit, here] The optimization step

 $\operatorname{argmin}_{\theta} \mathsf{MajorizingFct}(\theta; \theta_t)$

The MM algorithm

An example of MM algorithm: Expectation Maximization (EM)

Example of MM: EM Dempster et al (1977); book by G. McLachlan and T. Krishnan (2007)

• Inference in latent variable models

$$\ell(X; \theta) \stackrel{\text{def}}{=} -\log \int_{\mathcal{H}} p(X, h; \theta) \, \mathrm{d}\mu(h)$$

• The construction of the majorizing function at the point θ_t :

- The MM algorithm

An example of MM algorithm: Expectation Maximization (EM)

Example of MM: EM Dempster et al (1977); book by G. McLachlan and T. Krishnan (2007)

Inference in latent variable models

$$\ell(X;\theta) \stackrel{\text{def}}{=} -\log \int_{\mathcal{H}} p(X,h;\theta) \,\mathrm{d}\mu(h)$$

• The construction of the majorizing function at the point θ_t :

$$\begin{split} \ell(X;\theta) - \ell(X;\theta_t) &= -\log\left(\frac{\int_{\mathcal{H}} p(X,h;\theta) \, \mathrm{d}\mu(h)}{\int_{\mathcal{H}} p(X,h';\theta_t) \, \mathrm{d}\mu(h')}\right) \\ &= -\log\left(\int_{\mathcal{H}} \frac{p(X,h;\theta)}{\int_{\mathcal{H}} p(X,h';\theta_t) \, \mathrm{d}\mu(h')} \, \mathrm{d}\mu(h)\right) \\ &= -\log\left(\int_{\mathcal{H}} \frac{p(X,h;\theta)}{p(X,h;\theta_t)} \, \frac{p(X,h;\theta_t)}{\int_{\mathcal{H}} p(X,h';\theta_t) \, \mathrm{d}\mu(h')} \, \mathrm{d}\mu(h)\right) \\ &\leq -\int_{\mathcal{H}} \log p(X,h;\theta) \, \pi_{\theta_t}(h|X) \, \mathrm{d}\mu(h) + C_t \end{split}$$

- The MM algorithm

An example of MM algorithm: Expectation Maximization (EM)

Example of MM: EM Dempster et al (1977); book by G. McLachlan and T. Krishnan (2007)

• Inference in latent variable models

$$\ell(X;\theta) \stackrel{\text{def}}{=} -\log \int_{\mathcal{H}} p(X,h;\theta) \,\mathrm{d}\mu(h)$$

• The construction of the majorizing function at the point θ_t :

large batch

$$\theta \mapsto -\frac{1}{n} \sum_{i=1}^{n} \int_{\mathcal{H}} \log p(X_i, h; \theta) \ \pi_{\theta_t}(h|X_i) \, \mathrm{d}\mu(h) + g(\theta) + C_t$$

online learning

$$\theta \mapsto \mathbb{E}_{\pi} \left[-\int_{\mathcal{H}} \log p(X,h;\theta) \ \pi_{\theta_t}(h|X) \, \mathrm{d}\mu(h) \right] + g(\theta) + C_t$$

• Intractability: outer sum, inner sum

The MM algorithm

An example of MM algorithm: Expectation Maximization (EM)

Example of MM: EM for curved exponential family

• A frequent assumption:

$$\log p(X,h;\theta) = \langle S(X,h), \phi(\theta) \rangle - \psi(\theta)$$

• The majorizing function under this assumption

$$\boldsymbol{\theta} \mapsto \boldsymbol{g}(\boldsymbol{\theta}) + \boldsymbol{\psi}(\boldsymbol{\theta}) - \left\langle \mathbb{E}_{\pi} \left[\int_{\mathcal{H}} S(\boldsymbol{X}, h) \ \pi_{\boldsymbol{\theta}_{t}}(h | \boldsymbol{X}) \, \mathrm{d}\boldsymbol{\mu}(h) \right], \boldsymbol{\phi}(\boldsymbol{\theta}) \right\rangle + C_{t}$$

in the parametric functional family

$$\theta \mapsto R(\theta) - \langle s, \phi(\theta) \rangle$$

• Under this assumption, the E-step \equiv compute the parameter "s", defined as expectations (outer, inner).

EM, seen in the **surrogate**-space (*s*-space): iterative construction of fcts through iterative construction of a parameter "*s*"

The MM algorithm

└─ Other examples of MM

Other examples of MM algorithms

• F is L-smooth \rightarrow quadratic surrogate of $F \rightarrow$ gradient-type algorithm.

$$\operatorname{argmin}_{\theta} a + \langle \nabla \xi(\theta_t), \theta - \theta_t \rangle + \frac{1}{2\gamma} \| \theta - \theta_t \|^2 = \theta_t - \gamma \nabla \xi(\theta_t)$$

- $\bullet\,$ Difference of convex functions $\rightarrow\,$ linear surrogate of a concave function
- $\ell(X, \theta) = \inf_h \ell(X, h; \theta) \rightarrow$ variational surrogates

In many examples, and assumed HEREAFTER

(large batch) MajorizingFct(
$$\theta; \theta_t$$
) = $C_t + R(\theta) - \left\langle \frac{1}{n} \sum_{i=1}^n \bar{S}(X_i; \theta_t), \phi(\theta) \right\rangle$
(online) MajorizingFct($\theta; \theta_t$) = $C_t + R(\theta) - \left\langle \mathbb{E}_{\pi} \left[\bar{S}(X; \theta_t) \right], \phi(\theta) \right\rangle$

Conclusion of Part I.

 $\bullet~$ MM defines a sequence of surrogate functions $\rightarrow~$ MM defines a sequence of parameters "s"

$$\theta \mapsto R(\theta) - \langle s, \phi(\theta) \rangle$$

• In large scale learning: the exact value of "s" is intractable.

Solution ?

- Identify the limiting points of the (exact) MM
- Design a stochastic algorithm having the same limiting points.

└─ The MM algorithm

Conclusion of Part I.

II. The limiting points of MM

Assumptions

We consider MM algorithms having

• a surrogate function in the family indexed by s:

$$\theta \mapsto R(\theta) - \langle s, \phi(\theta) \rangle$$

At iteration #t let us write it in the "online learning setting"

$$\theta \mapsto R(\theta) - \left\langle \mathbb{E}_{\pi} \left[\bar{S}(X, \theta_t) \right], \phi(\theta) \right\rangle$$

• an explicit optimization of this surrogate

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

Case of EM

Hyp 1: OK when the complete data likelihood is from *the curved exponential family*.

Hyp 2: for convenience.

Fixed points in the surrogate space

 $s_{\star}: \qquad s_{\star} = \mathbb{E}_{\pi} \left[\bar{S}(X, \mathsf{T}(s_{\star})) \right]$

MM finds the roots of

$$s \mapsto \mathsf{h}(s) \stackrel{\text{def}}{=} \mathbb{E}_{\pi} \left[\bar{S}(X, \mathsf{T}(s)) - s \right].$$

The outer expectation is intractable.

Conclusion of Part II.

- Forget the MM scheme
- Keep in mind: algorithm to find the roots of

$$s \mapsto \mathsf{h}(s) \stackrel{\text{def}}{=} \mathbb{E}_{\pi} \left[\overline{S}(X, \mathsf{T}(s)) - s \right].$$

• Replace exact MM with: a **Stochastic Approximation** algorithm designed to find the roots of the *mean field* h.

Limiting points of MM

Conclusion of Part II.

III. Variance reduction within Stochastic Approximation

Variance reduction within Stochastic Approximation scheme

Stochastic Approximation

UQ April22

Stochastic Approximation algorithms

• Mean field:

$$\mathsf{h}(s) \stackrel{\text{def}}{=} \mathbb{E}_{\pi} \left[\bar{S}(X, \mathsf{T}(s)) - s \right]$$

• Iterative scheme:

$$\widehat{S}_{t+1} = \widehat{S}_t + \gamma_{t+1} \left(\frac{1}{\mathbf{b}} \sum_{i \in \mathcal{B}_{t+1}} \overline{S}(X_i, \mathsf{T}(\widehat{S}_t)) - \widehat{S}_t \right)$$

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

- (large batch) sampled with replacement; b << n
- (online) from the data stream

Examples of MM designed for large scale learning

Review of MM for large scale learning / EM context (1/2)

• Online-EM.

Neal and Hinton, 1998; Cappé and Moulines, 2009); Nguyen et al (2020); Karimi et al (2019a, 2019b).

• (large batch) iEM. Incremental EM

Case $\gamma_t=1$. Neal and Hinton (1998); Ng and McLachlan (2003); Gunawardana and Byrne (2005); Karimi et al (2019c)

Based on an incremental approximation of

$$\mathsf{h}(\widehat{S}_t) = n^{-1} \sum_{i=1}^n S(X_i, \mathsf{T}(\widehat{S}_t)) - \widehat{S}_t.$$

* Init: store for all i, $\sigma_i \stackrel{\text{def}}{=} S(X_i, \mathsf{T}(\widehat{S}_0))$ and compute $\mathsf{h}(\widehat{S}_0)$. * At iter #(t+1):

sample an index I; update $\sigma_I \leftarrow S(X_I, \mathsf{T}(\widehat{S}_t))$; update the term #I in the approximation of $h(\widehat{S}_t)$.

Variance reduction within Stochastic Approximation scheme

Examples of MM designed for large scale learning

UQ April22

Stochastic Approximation algorithms with Variance Reduction

Variance reduction through control variates

$$\widehat{S}_{t+1} = \widehat{S}_t + \gamma_{t+1} \left(\frac{1}{\mathsf{b}} \sum_{i \in \mathcal{B}_{t+1}} \overline{S}(X_i, \mathsf{T}(\widehat{S}_t)) - \widehat{S}_t + V_{t+1} \right)$$

- V_{t+1} is centered \rightarrow the mean field is not modified.
- V_{t+1} and $\frac{1}{b} \sum_{i \in \mathcal{B}_{t+1}} \overline{S}(X_i, \mathsf{T}(\widehat{S}_t)) \widehat{S}_t$ are correlated.

Examples of MM designed for large scale learning

Review of MM for large scale learning / EM context (2/2)

• (large batch) sEM-vr. Stochastic EM with Variance Reduction

```
Chen et al, 2018. Parallel with "SVRG" by Johnson and Zhang (2013)
```

• (large batch) FIEM. Fast Incremental EM

```
Karimi et al, 2019; Fort et al, 2021. Parallel with "SAGA" by Defazio et al (2014).

The control variate V_{t+1} is defined as in iEM:

* Init: store the \sigma_i's

* At iter \#(t+1)

sample two indices I, J.

Update \sigma_I and the sum n^{-1} \sum_{i=1} \sigma_i by modifying the term \#I

Correlate V_{t+1} to the natural field S(X_J, T(\widehat{S}_t)) - \widehat{S}_t:
```

$$V_{t+1} \stackrel{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \sigma_i - \sigma_J.$$

A novel Variance-reduced MM: SPIDER-MM

UQ April22

(large batch) A novel variance-reduction: SPIDER MM Fort, Moulines, Wai - NeurIPS 2020

Stochastic Path Integrated Differential EstimatoR MM

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

$$V_{t+1} = V_t + \frac{1}{b} \sum_{i \in \mathcal{B}_t} \bar{S}(X_i, \mathsf{T}(\widehat{S}_{t-1})) - \frac{1}{b} \sum_{i \in \mathcal{B}_{t+1}} \bar{S}(X_i, \mathsf{T}(\widehat{S}_{t-1}))$$

- learn zero through an approximation of " $h(\widehat{S}_{t-1}) h(\widehat{S}_{t-1})$ ".
- correlated to the natural field through \mathcal{B}_{t+1} .
- biased ! refresh the control variates regularly.

SPIDER-MM

UQ April22

SPIDER-MM (Stochastic Path Integrated Differential EstimatoR MM)

1:
$$\hat{S}_{1,0} = \hat{S}_{1,-1} = \hat{S}_{init}$$
 $V_{1,0} = 0$ $\mathcal{B}_{1,0} = \{1, \cdots, n\}$
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: $V_{t,k+1} = V_{t,k} + b^{-1} \left(\sum_{i \in \mathcal{B}_{t,k}} \bar{S}(X_i, T(\hat{S}_{t,k-1})) - \sum_{i \in \mathcal{B}_{t,k+1}} \bar{S}(X_i, T(\hat{S}_{t,k-1})) \right)$
6: $\hat{S}_{t,k+1} = \hat{S}_{t,k} + \gamma_{t,k+1} \left(b^{-1} \sum_{i \in \mathcal{B}_{t,k+1}} \bar{S}(X_i, T(\hat{S}_{t,k})) - \hat{S}_{t,k} + V_{t,k+1} \right)$
7: end for
8: $\hat{S}_{t+1,-1} = \hat{S}_{t,\xi_t}$
9: $V_{t+1,0} = 0$ $\mathcal{B}_{t+1,0} = \{1, \cdots, n\}$
10: $\hat{S}_{t+1,0} = \hat{S}_{t+1,-1} + \gamma_{t+1,0} \left(h(\hat{S}_{t+1,-1}) + V_{t+1,0} \right)$
11: end for

- k_{out} outer loops, the outer #t is of length ξ_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 ξ_t . Fort, Moulines, Wai ICASSP 2021
- \bullet Avoid the full scan of the examples when starting each outer loop \to reduction of the computational cost. Fort, Moulines, Wai ICASSP 2021
- An approximation of $\bar{S}(X_i, \theta)$ Fort, Moulines SSP 2021

for example: in EM, $\bar{S}(X_i, \theta)$ 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

$$\widehat{S}_{t,k+1} = \operatorname{Prox}_{\gamma_{t,k+1} g} \left(\widehat{S}_{t,k} + \gamma_{t,k+1} H_{t,k+1} \right)$$

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

└─ SPIDER-MM

IV. Convergence analysis of SPIDER MM

Assumptions

Assumptions

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

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

where B(s) is a $q \times q$ positive definite matrix. In addition, ∇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 $[v_{\min}, v_{\max}]$.

Ø For any *i* ∈ {1, · · · , *n*}, the function *s* → $\bar{S}(X_i, T(s)) - s$ is globally Lipschitz with constant *L_i*.

What kind of convergence results ?

- The objective fct: non necessarily convex but T(s) exists, unique.
- Explicit control of *errors* given a fixed nbr of observations (given a "budget").
- What is "errors"

$$\mathbb{E}\left[\| \mathsf{h}(\widehat{S}_t) \|^2 \right]$$

- At time t ? no \cdots at some random time τ ! non convex optim.
- What do we learn from an explicit control ? how design parameters scale with n, in order to reach an accuracy ϵ

$$\mathbb{E}\left[\left\|\mathbf{h}(\widehat{S}_{\tau})\right\|^{2}\right] \leq \epsilon$$

Convergence analysis

Assumptions

UQ April22

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

Convergence analysis

Assumptions

UQ April22

Complexity for ϵ -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 γ (= $\gamma_{t,k}$ for any t,k>0)

To reach ϵ -stationarity, the complexity of SPIDER-MM

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

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

Algorithm	Complexity \mathcal{K}
Online-MM	ϵ^{-2}
iMM	$n \epsilon^{-1}$
sMM-vr	$n^{2/3} \epsilon^{-1}$
FIMM	$n^{2/3} \epsilon^{-1} \wedge \sqrt{n} \epsilon^{-3/2}$

Convergence analysis

L_Assumptions

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 $t = k_{out}$.

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

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

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

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

 \bullet L^2 -error of the field

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

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

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

Convergence analysis

 \square Convergence analysis, Monte Carlo approx of $\bar{S}(X_i, \theta)$'s

Assumptions (case: Monte Carlo approximation of $\overline{S}(X_i, \theta)$'s)

In the case

$$\bar{S}(X_i,\mathsf{T}(\widehat{S}_{t,k})) = \int \mathcal{H}(h) \, \pi_{t,k}(h|X_i) \mathsf{d}\mu(h) \approx \frac{1}{m_{t,k+1}} \sum_{r=1}^{m_{t,k+1}} \mathcal{H}(Z_r^{i,t,k})$$

error

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

(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

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

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

Convergence analysis

 \Box Convergence analysis, Monte Carlo approx of $\bar{S}(X_i, \theta)$'s

UQ April22

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 (τ, ξ) 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 $\mathbb{E}\left[\| \mathsf{h}(\widehat{S}_{ au,\xi}) \|^2
ight]$

Convergence analysis

Convergence analysis, Monte Carlo approx of $\bar{S}(X_i, \theta)$'s

Complexity for ϵ -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 γ
- with a Monte Carlo approximation of the $\bar{S}(X_i, \theta)$'s

To reach ϵ -stationarity, the complexity of Perturbed-SPIDER-MM

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

Nbr of optimization steps: $O(1/\epsilon)$ Nbr of $\overline{S}(X_i, \cdot)$'s evaluations: $\mathcal{K} = O(\sqrt{n} \epsilon^{-1}) \rightarrow$ same as SPIDER-MM Nbr of Monte Carlo draws: $O(\sqrt{n}/\epsilon^2)$ V. Numerical illustrations Herafter, MM means EM - 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

UQ April22

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; $n = 6 \cdot 10^4$ 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

UQ April22

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; $n = 6 \, 10^4$ examples



Figure: Evolution of the p = 20 eigenvalues of the iterates Σ_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.

- 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 $\gamma_{t,0}$

VI. Bibliography

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)

Bibliography

└─ Other references

Other references

- Benveniste, A. and Métivier, M. and Priouret P. Adaptive Algorithms and Stochastic Approxima-tions. Springer Verlag, 1990.
- Cappé, O. and Moulines, E. On-line expectation-maximization algorithm for latent data models. J. R. Stat. Soc. Ser. B Stat. Methodol., 71(3):593–613, 2009.
- Chen, J. Zhu, Y. Teh, and T. Zhang. Stochastic Expectation Maximization with variance reduction. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Gar-nett, editors, Advances in Neural Information Processing Systems 31, pages 7967–7977. 2018.
- Dempster, A.P. and Laird, N.M. and Rubin, D.B. Maximum Likelihood from Incomplete Data Via the EM Algorithm Journal of the Royal Statistical Society: Series B (Methodological), 1977.
- Fang, C. and Li, C. and Lin, Z. and Zhang, T. SPIDER: Near-Optimal Non-Convex Optimization viaStochastic Path-Integrated Differential Estimator. In S.Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 689–699. Curran Associates, Inc., 2018.
- Fort, G. and Gach, P. and Moulines, E. The Fast Incremental Expectation Maximization for finite-sum optimization: asymptotic convergence, Statistics and Computing, 2021.
- Karimi, B. and Wai, H.-T., and Moulines, E. and Lavielle, M. On the Global Convergence of (Fast) In-cremental Expectation Maximization Methods. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information ProcessingSystems 32, pages 2837–2847. Curran Associates, Inc., 2019.
- Neal, R.M. and Hinton, G.E. A View of the EM Algorithm that Justifies Incremental, Sparse, and other Variants. In M. I. Jordan, editor, Learning in Graphical Models, pages 355–368. Springer Netherlands, Dordrecht, 1998.
- Nguyen, L.M. and Liu, K. and Scheinberg, K. and Takác M. SARAH: A novel method for machine learning problems using stochastic recursive gradient. In Proceedings of the 34th International Conference on Machine Learning - Volume 70, ICML'17, page 2613–2621. 2017
- Robbins, H. and Monro, S.. A Stochastic Approximation Method. The Annals of Mathematical Statistics. 22 (3): 400, 1951.
- Wang, Z. and Ji, K. and Zhou, Y. and Liang, Y. and and Tarokh, V. SpiderBoost and Momentum: Faster Stochastic Variance Reduction Algorithms. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d' Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 2406–2416. 2019.