Convergence of perturbed Proximal Gradient algorithms

Convergence of perturbed Proximal Gradient algorithms

Gersende Fort

Institut de Mathématiques de Toulouse CNRS and Univ. Paul Sabatier Toulouse, France

Based on joint works with

- Yves Atchadé (Univ. Michigan, USA)
- Eric Moulines (Ecole Polytechnique, France)
- \hookrightarrow On Perturbed Proximal-Gradient algorithms (JMLR, 2016)
 - Jean-François Aujol (IMB, Bordeaux, France)
 - Charles Dossal (IMB, Bordeaux, France).
- \hookrightarrow Acceleration for perturbed Proximal Gradient algorithms (work in progress)
 - Edouard Ollier (ENS Lyon, France)
 - Adeline Samson (Univ. Grenoble Alpes, France).
- \hookrightarrow Penalized inference in Mixed Models by Proximal Gradient methods (work in progress)

Motivation : Pharmacokinetic (1/2)

- N patients.
- At time 0: dose D of a drug.
- For patient i, observations $\{Y_{ij}, 1 \leq j \leq J_i\}$: evolution of the concentration at times $t_{ij}, 1 \leq j \leq J_i$.

Model:

$$Y_{ij} = \mathcal{F}(t_{ij}, X_i) + \epsilon_{ij} \qquad \epsilon_{ij} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

$$X_i = Z_i \beta + d_i \in \mathbb{R}^L \qquad d_i \overset{i.i.d.}{\sim} \mathcal{N}_L(0,\Omega) \text{ and independent of } \epsilon_{\bullet}$$

 Z_i known matrix s.t. each row of X_i has in intercept (fixed effect) and covariates

Motivation: Pharmacokinetic (1/2)

- N patients.
- At time 0: dose D of a drug.
- For patient i, observations $\{Y_{ij}, 1 \leq j \leq J_i\}$: evolution of the concentration at times $t_{ij}, 1 \leq j \leq J_i$.

Model:

$$Y_{ij} = \mathcal{F}(t_{ij}, X_i) + \epsilon_{ij} \qquad \epsilon_{ij} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

$$X_i = Z_i \beta + d_i \in \mathbb{R}^L$$
 $d_i \stackrel{i.i.d.}{\sim} \mathcal{N}_L(0,\Omega)$ and independent of ϵ_{\bullet}

 Z_i known matrix s.t. each row of X_i has in intercept (fixed effect) and covariates

Example of model \mathcal{F} : monocompartimental, oral administration

$$\mathcal{F}(t,[\ln\mathsf{CI},\ln\mathsf{V},\ln\mathsf{A}]) = \mathcal{C}(\mathsf{CI},\mathsf{V},\!\mathsf{A},\!\mathsf{D}) \ \left(\exp(-\frac{\mathsf{CI}}{\mathsf{V}}t) - \exp(-\mathsf{A}t)\right)$$

For each patient i,

$$\begin{bmatrix} \ln Cl \\ \ln V \\ \ln A \end{bmatrix}_i = \begin{bmatrix} \beta_{0,Cl} \\ \beta_{0,V} \\ \beta_{0,A} \end{bmatrix} + \begin{bmatrix} \beta_{1,Cl} Z_{1,Cl}^i + \dots + \beta_{K,Cl} Z_{K,Cl}^i \\ \text{idem, with covariates } Z_{k,V}^i \text{ and coefficients } \beta_{k,V} \\ \text{idem, with covariates } Z_{k,A}^i \text{ and coefficients } \beta_{k,A} \end{bmatrix} + \begin{bmatrix} d_{\text{Cl},i} \\ d_{\text{V},i} \\ d_{\text{A},i} \end{bmatrix}$$

Motivation : Pharmacokinetic (1/2)

- N patients.
- At time 0: dose D of a drug.
- For patient i, observations $\{Y_{ij}, 1 \leq j \leq J_i\}$: evolution of the concentration at times $t_{ij}, 1 \leq j \leq J_i$.

Model:

$$Y_{ij} = \mathcal{F}(t_{ij}, X_i) + \epsilon_{ij} \qquad \epsilon_{ij} \stackrel{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2)$$

$$X_i = Z_i \beta + d_i \in \mathbb{R}^L$$
 $d_i \overset{i.i.d.}{\sim} \mathcal{N}_L(0,\Omega)$ and independent of ϵ_{ullet}

 \mathcal{Z}_i known matrix s.t. each row of \mathcal{X}_i has in intercept (fixed effect) and covariates

Statistical analysis:

- estimation of $\theta = (\beta, \sigma^2, \Omega)$, under sparsity constraints on β
- selection of the covariates based on $\hat{\beta}$.

Motivation : Pharmacokinetic (2/2)

Model:

$$\begin{split} Y_{ij} &= f\left(t_{ij}, X_i\right) + \epsilon_{ij} & \qquad \epsilon_{ij} \overset{i.i.d.}{\sim} \mathcal{N}(0, \sigma^2) \\ X_i &= Z_i \beta + d_i \in \mathbb{R}^L & \qquad d_i \overset{i.i.d.}{\sim} \mathcal{N}_L(0, \Omega) \text{ and independent of } \epsilon_{\bullet} \\ Z_i \text{ known matrix s.t. each row of } X_i \text{ has in intercept (fixed effect) and covariates} \end{split}$$

Likelihoods:

- Likelihood: not explicit.
- Complete likelihood: the distribution of $\{Y_{ij}, X_i; 1 \le i \le N, 1 \le j \le J\}$ has an explicit expression.
- ML: here, the likelihood is not concave.

Outline

Penalized Maximum Likelihood inference in models with intractable likelihood

Example 1: Latent variable models

Example 2: Discrete graphical model (Markov random field)

Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms

Convergence analysis

Conclusion

- N observations : $\mathbf{Y} = (Y_1, \cdots, Y_N)$
- ullet A parametric statistical model $heta \in \Theta \subseteq \mathbb{R}^d$ the dependance upon Y is omitted

$$\theta \mapsto L(\theta)$$
 likelihood of the observations

• A penalty term on the parameter θ : $\theta \mapsto g(\theta) \geq 0$ for sparsity constraints on θ . Usually, g non-smooth and convex.

Goal: Computation of

$$\theta \mapsto \operatorname{argmax}_{\theta \in \Theta} \left(\frac{1}{N} \log L(\theta) - g(\theta) \right)$$

when the likelihood L has no closed form expression, and can not be evaluated.

Example 1: Latent variable model

• The log-likelihood of the observations Y is of the form

$$\theta \mapsto \log L(\theta)$$
 $L(\theta) = \int_{\mathsf{X}} p_{\theta}(x) \, \mu(\mathsf{d}x),$

where μ is a positive σ -finite measure on a set X.

• x collects the missing/latent data.

In these models.

- ullet the complete likelihood $p_{ heta}(x)$ can be evaluated explicitly,
- the likelihood has no closed form expression.
- The exact integral could be replaced by a Monte Carlo approximation;
 known to be inefficient

Numerical methods based on the a posteriori distribution of the missing data are preferred (see e.g. Expectation-Maximization approaches).

Gradient of the likelihood in a latent variable model

$$\log L(\theta) = \log \int_{\mathsf{X}} p_{\theta}(x) \, \mu(\mathsf{d}x)$$

Under regularity conditions, $\theta \mapsto \log L(\theta)$ is C^1 and

$$\begin{split} \nabla \log L(\theta) &= \frac{\int_{\mathsf{X}} \partial_{\theta} p_{\theta}(x) \, \mu(\mathsf{d}x)}{\int_{\mathsf{X}} p_{\theta}(z) \, \mu(\mathsf{d}z)} \\ &= \int_{\mathsf{X}} \partial_{\theta} \log p_{\theta}(x) \quad \underbrace{\frac{p_{\theta}(x) \, \mu(\mathsf{d}x)}{\int_{\mathsf{X}} p_{\theta}(z) \, \mu(\mathsf{d}z)}}_{\text{the a posteriori distribution}} \end{split}$$

Example 1: Latent variable models

Gradient of the likelihood in a latent variable model

$$\log L(\theta) = \log \int_{\mathsf{X}} p_{\theta}(x) \, \mu(\mathsf{d}x)$$

Under regularity conditions, $\theta \mapsto \log L(\theta)$ is C^1 and

$$\begin{split} \nabla \log L(\theta) &= \frac{\int_{\mathsf{X}} \partial_{\theta} p_{\theta}(x) \, \mu(\mathsf{d}x)}{\int_{\mathsf{X}} p_{\theta}(z) \, \mu(\mathsf{d}z)} \\ &= \int_{\mathsf{X}} \partial_{\theta} \log p_{\theta}(x) \quad \underbrace{\frac{p_{\theta}(x) \, \mu(\mathsf{d}x)}{\int_{\mathsf{X}} p_{\theta}(z) \, \mu(\mathsf{d}z)}}_{\text{the a posteriori distribution}} \end{split}$$

The gradient of the log-likelihood

$$\nabla_{\theta} \left\{ \log L(\theta) \right\} = \int_{X} \partial_{\theta} \log p_{\theta}(x) \ \pi_{\theta}(\mathsf{d}x)$$

is an intractable expectation w.r.t. the conditional distribution of the latent variable given the observations Y.

For all (x, θ) , $\partial_{\theta} \log p_{\theta}(x)$ can be evaluated.

Example 1: Latent variable models

Approximation of the gradient

$$\nabla_{\theta} \left\{ \log L(\theta) \right\} = \int_{\mathsf{X}} \partial_{\theta} \log p_{\theta}(x) \ \pi_{\theta}(\mathsf{d}x)$$

- Quadrature techniques: poor behavior w.r.t. the dimension of X
- ${\bf 9}$ use i.i.d. samples from π_θ to define a Monte Carlo approximation: not possible, in general.
- ① use m samples from a non stationary Markov chain $\{X_{j,\theta}, j \geq 0\}$ with unique stationary distribution π_{θ} , and define a Monte Carlo approximation. MCMC samplers provide such a chain.

Example 1: Latent variable models

Approximation of the gradient

$$\nabla_{\theta} \left\{ \log L(\theta) \right\} = \int_{\mathsf{X}} \partial_{\theta} \log p_{\theta}(x) \ \pi_{\theta}(\mathsf{d}x)$$

- Quadrature techniques: poor behavior w.r.t. the dimension of X
- @ use i.i.d. samples from π_{θ} to define a Monte Carlo approximation: not possible, in general.
- ullet use m samples from a non stationary Markov chain $\{X_{j,\theta}, j \geq 0\}$ with unique stationary distribution π_{θ} , and define a Monte Carlo approximation. MCMC samplers provide such a chain.

Stochastic approximation of the gradient

A biased approximation, since for MCMC samples $X_{j,\theta}$

$$\mathbb{E}\left[h(X_{j,\theta})\right] \neq \int h(x) \, \pi_{\theta}(\mathsf{d}x).$$

If the Markov chain is ergodic, the bias vanishes when $j \to \infty$.

Example 2: Discrete graphical model (Markov random field)

Example 2: Discrete graphical model (Markov random field)

N independent observations of an undirected graph with p nodes. Each node takes values in a finite alphabet ${\sf X}.$

ullet N i.i.d. observations Y_i in X^p with distribution

$$y = (y_1, \dots, y_p) \mapsto \pi_{\theta}(y) \stackrel{\text{def}}{=} \frac{1}{Z_{\theta}} \exp\left(\sum_{k=1}^{p} \theta_{kk} B(y_k, y_k) + \sum_{1 \le j < k \le p} \theta_{kj} B(y_k, y_j)\right)$$
$$= \frac{1}{Z_{\theta}} \exp\left(\langle \theta, \bar{B}(y) \rangle\right)$$

where B is a symmetric function.

- ullet θ is a symmetric $p \times p$ matrix.
- the normalizing constant (partition function) Z_{θ} can not be computed sum over $|\mathsf{X}|^p$ terms.

Example 2: Discrete graphical model (Markov random field)

Likelihood and its gradient in Markov random field

► Likelihood of the form (scalar product between matrices = Frobenius inner product)

$$\frac{1}{N}\log L(\theta) = \left\langle \theta, \frac{1}{N} \sum_{i=1}^{N} \bar{B}(Y_i) \right\rangle - \log Z_{\theta}$$

The likelihood is intractable.

Example 2: Discrete graphical model (Markov random field)

Likelihood and its gradient in Markov random field

▶ Likelihood of the form (scalar product between matrices = Frobenius inner product)

$$\frac{1}{N}\log L(\theta) = \left\langle \theta, \frac{1}{N} \sum_{i=1}^{N} \bar{B}(Y_i) \right\rangle - \log Z_{\theta}$$

The likelihood is intractable.

▶ Gradient of the form

$$\nabla_{\theta} \left(\frac{1}{N} \log L(\theta) \right) = \frac{1}{N} \sum_{i=1}^{N} \bar{B}(Y_i) - \int_{X^p} \bar{B}(y) \, \pi_{\theta}(y) \, \mu(\mathrm{d}y)$$

with

$$\pi_{\theta}(y) \stackrel{\text{def}}{=} \frac{1}{Z_{\theta}} \exp\left(\langle \theta, \bar{B}(y) \rangle\right).$$

The gradient of the (log)-likelihood is intractable.

Example 2: Discrete graphical model (Markov random field)

Approximation of the gradient

$$\nabla_{\theta} \left(\frac{1}{N} \log L(\theta) \right) = \frac{1}{N} \sum_{i=1}^{N} \bar{B}(Y_i) - \int_{X^p} \bar{B}(y) \, \pi_{\theta}(y) \, \mu(\mathsf{d}y).$$

The Gibbs measure

$$\pi_{\theta}(y) \stackrel{\text{def}}{=} \frac{1}{Z_{\theta}} \exp\left(\langle \theta, \bar{B}(y) \rangle\right)$$

is known up to the constant Z_{θ} .

Exact sampling from π_{θ} can be approximated by MCMC samplers (Gibbs-type samplers such as Swendsen-Wang, ...)

A biased approximation of the gradient is available.

Example 2: Discrete graphical model (Markov random field)

To summarize,

Problem:

$$\mathrm{argmin}_{\theta \in \Theta} F(\theta) \qquad \text{ with } F(\theta) = f(\theta) + g(\theta)$$

when

•
$$\theta \in \Theta \subseteq \mathbb{R}^d$$

ullet the function g convex non-smooth nonnegative function (explicit)

Example 2: Discrete graphical model (Markov random field)

To summarize,

Problem:

$$\mathrm{argmin}_{\theta \in \Theta} F(\theta) \qquad \text{ with } F(\theta) = f(\theta) + g(\theta)$$

when

- $\theta \in \Theta \subseteq \mathbb{R}^d$
- the function g convex non-smooth nonnegative function (explicit)
- ullet the function f is
 - not necessarily convex,
 - \cdot C^1 and ∇f is L-Lipschitz

$$\exists L > 0, \ \forall \theta, \theta' \qquad \|\nabla f(\theta) - \nabla f(\theta')\| \le L\|\theta - \theta'\|.$$

· with an intractable gradient of the form

$$\nabla f(\theta) = \int H_{\theta}(x) \, \pi_{\theta}(\mathsf{d}x);$$

which can be approximated by biased Monte Carlo techniques.

Outline

Penalized Maximum Likelihood inference in models with intractable likelihood

Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms
Algorithms
Numerical illustration

Convergence analysis

Conclusion

The Proximal-Gradient algorithm (1/2)

$$\operatorname{argmin}_{\theta \in \Theta} F(\theta) \qquad \text{with } F(\theta) = \underbrace{f(\theta)}_{\text{smooth}} + \underbrace{g(\theta)}_{\text{non smooth}}$$

The Proximal Gradient algorithm

Given a stepsize sequence $\{\gamma_n, n \geq 0\}$, iterative algorithm:

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \nabla f(\theta_n))$$

where

$$\operatorname{Prox}_{\gamma,g}(\tau) \stackrel{\text{def}}{=} \operatorname{argmin}_{\theta \in \Theta} \left(g(\theta) + \frac{1}{2\gamma} \|\theta - \tau\|^2 \right)$$

Proximal map: Moreau(1962)

 $Proximal\ Gradient\ algorithm:\ Beck-Teboulle (2010);\ Combettes-Pesquet (2011);\ Parikh-Boyd (2013)$

The Proximal-Gradient algorithm (1/2)

$$\operatorname{argmin}_{\theta \in \Theta} F(\theta) \qquad \text{with } F(\theta) = \underbrace{f(\theta)}_{\text{smooth}} + \underbrace{g(\theta)}_{\text{non smooth}}$$

The Proximal Gradient algorithm

Given a stepsize sequence $\{\gamma_n, n \geq 0\}$, iterative algorithm:

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \nabla f(\theta_n))$$

where

$$\operatorname{Prox}_{\gamma,g}(\tau) \stackrel{\text{def}}{=} \operatorname{argmin}_{\theta \in \Theta} \left(g(\theta) + \frac{1}{2\gamma} \|\theta - \tau\|^2 \right)$$

Proximal map: Moreau(1962)

Proximal Gradient algorithm: Beck-Teboulle(2010); Combettes-Pesquet(2011); Parikh-Boyd(2013)

- A generalization of the gradient algorithm to a composite objective function
- A MM/Majorize-Minimize algorithm from a quadratic majorization of f (since Lipschitz gradient) which produces a sequence $\{\theta_n, n \geq 0\}$ such that

$$F(\theta_{n+1}) < F(\theta_n).$$

The proximal-gradient algorithm (2/2)

$$\operatorname{argmin}_{\theta \in \Theta} F(\theta) \qquad \text{with } F(\theta) = \underbrace{f(\theta)}_{\text{smooth}} + \underbrace{g(\theta)}_{\text{non smooth}}$$

The Proximal Gradient algorithm

Given a stepsize sequence $\{\gamma_n, n \geq 0\}$, iterative algorithm:

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \nabla f(\theta_n))$$

where

$$\operatorname{Prox}_{\gamma,g}(\tau) \stackrel{\text{def}}{=} \operatorname{argmin}_{\theta \in \Theta} \left(g(\theta) + \frac{1}{2\gamma} \|\theta - \tau\|^2 \right)$$

About the Prox-step:

- when g = 0: $Prox(\tau) = \tau$
- when g is the $\{0, +\infty\}$ -valued indicator fct of a closed convex set: the algorithm is the projected gradient.
- in some cases, Prox is explicit (e.g. elastic net penalty). Otherwise, numerical approximation:

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \nabla f(\theta_n)) + \epsilon_{n+1}$$
 in this talk, $\epsilon_{n+1} = 0$

The perturbed proximal-gradient algorithm

Algorithms

The Perturbed Proximal Gradient algorithm

Given a stepsize sequence $\{\gamma_n, n \geq 0\}$, iterative algorithm:

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \mathbf{H}_{n+1})$$

where H_{n+1} is an approximation of $\nabla f(\theta_n)$.

Monte Carlo-Proximal Gradient algorithm

In the case:

$$\nabla f(\theta) = \int H_{\theta}(x) \, \pi_{\theta}(x) \mu(\mathsf{d}x),$$

The MC-Proximal Gradient algorithm

Choose a stepsize sequence $\{\gamma_n, n \geq 0\}$ and a batch size sequence $\{m_n, n \geq 0\}$. Given the current value θ_n .

- Sample a Markov chain $\{X_{j,n}, j \geq 0\}$ from a MCMC sampler with kernel $P_{\theta_n}(x, \mathrm{d} x')$, and unique invariant distribution $\pi_{\theta_n} \, \mathrm{d} \mu$.
- Set

$$H_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} H_{\theta_n}(X_{j,n}).$$

Update the value of the parameter

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1}, g} \left(\theta_n - \gamma_{n+1} H_{n+1} \right)$$

Stochastic Approximation-Proximal Gradient algorithm

In the case (ex. latent variable models with exponential complete likelihood;log-linear Markov random field)

$$\nabla f(\theta) = \int H_{\theta}(x) \, \pi_{\theta}(x) \mu(\mathsf{d}x), \qquad H_{\theta}(x) = \Phi(\theta) + \Psi(\theta) S(x)$$

which implies

$$\nabla f(\theta) = \Phi(\theta) + \Psi(\theta) \left(\int S(x) \, \pi_{\theta}(x) \mu(\mathrm{d}x) \right),$$

The SA-Proximal Gradient algorithm

Choose two stepsize sequences $\{\gamma_n, \delta_n, n \geq 0\}$ and a batch size sequence $\{m_n, n \geq 0\}$

Given the current value θ_n .

- **1** Sample a Markov chain $\{X_{j,n}, j \geq 0\}$ from a MCMC sampler with kernel $P_{\theta_n}(x, dx')$, and unique invariant distribution $\pi_{\theta_n} d\mu$.
- 2 Set $H_{n+1} = \Phi(\theta_n) + \Psi(\theta_n)S_{n+1}$ with

$$S_{n+1} = (1 - \delta_{n+1}) S_n + \delta_{n+1} \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} S(X_{j,n}).$$

Update the value of the parameter

(*) Penalized Expectation-Maximization (EM) vs Proximal-Gradient

- EM Dempster et al. (1977) is a Majorize-Minimize algorithm for the computation of the ML estimate in latent variable models.
- Penalized (Stochastic) EM algorithms

$$\tau_{n+1} = \operatorname{argmax}_{\theta} \int \log p_{\theta}(x) \ \pi_{\theta}(x) \, \mathrm{d}\mu(x) - g(\theta)$$
$$= \operatorname{argmax}_{\theta} \left\{ A(\theta) + \langle B(\theta), S_{n+1} \rangle - g(\theta) \right\}$$

with

$$S_{n+1} = \int S(x) \ \pi_{\tau_n}(x) \, \mathrm{d}\mu(x) \qquad \text{EM}$$

$$S_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} S(X_{j,n}) \qquad \text{Monte Carlo EM} \quad \text{\tiny Wei and Tanner (1990)}$$

$$S_{n+1} = (1-\delta_{n+1})S_n + rac{\delta_{n+1}}{m_{n+1}} \sum_{j=1}^{m_{n+1}} S(X_{j,n})$$
 Stoch. Approx. EM Delyon et al. (1999)

(*) Penalized Expectation-Maximization (EM) vs Proximal-Gradient

- EM Dempster et al. (1977) is a Majorize-Minimize algorithm for the computation of the ML estimate in latent variable models.
- Penalized (Stochastic) Generalized EM algorithms

$$\tau_{n+1} = \operatorname{argmax}_{\theta} \int \log p_{\theta}(x) \ \pi_{\theta}(x) \, d\mu(x) - g(\theta)$$
$$= \operatorname{argmax}_{\theta} \left\{ A(\theta) + \langle B(\theta), S_{n+1} \rangle - g(\theta) \right\}$$

or choose au_{n+1} s.t.

$$A(\tau_{n+1}) + \langle B(\tau_{n+1}), S_{n+1} \rangle - g(\tau_{n+1}) \ge A(\tau_n) + \langle B(\tau_n), S_{n+1} \rangle - g(\tau_n)$$

with

$$S_{n+1} = \int S(x) \ \pi_{\tau_n}(x) \, \mathrm{d}\mu(x) \qquad \mathsf{EM}$$

$$S_{n+1} = rac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} S(X_{j,n})$$
 Monte Carlo EM Wei and Tanner (1990)

$$S_{n+1} = (1 - \delta_{n+1})S_n + rac{\delta_{n+1}}{m_{n+1}} \sum_{i=1}^{m_{n+1}} S(X_{j,n})$$
 Stoch. Approx. EM Delyon et al. (1999)

(*) Penalized Expectation-Maximization (EM) vs Proximal-Gradient

- EM Dempster et al. (1977) is a Majorize-Minimize algorithm for the computation of the ML estimate in latent variable models.
- Penalized (Stochastic) Generalized EM algorithms

$$\tau_{n+1} = \operatorname{argmax}_{\theta} \int \log p_{\theta}(x) \ \pi_{\theta}(x) \, d\mu(x) - g(\theta)$$
$$= \operatorname{argmax}_{\theta} \left\{ A(\theta) + \langle B(\theta), S_{n+1} \rangle - g(\theta) \right\}$$

or choose τ_{n+1} s.t.

$$A(\tau_{n+1}) + \langle B(\tau_{n+1}), S_{n+1} \rangle - g(\tau_{n+1}) \ge A(\tau_n) + \langle B(\tau_n), S_{n+1} \rangle - g(\tau_n)$$

with

 MC-Prox Gdt and SA-Prox Gdt are Penalized Stochastic Generalized EM algorithms. Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms

Numerical illustration

Numerical illustration (1/3): pharmacokinetic

For the implementation of the algorithm

• Penalty term: $g(\theta) = \lambda ||\beta||_1$. How to choose λ ?

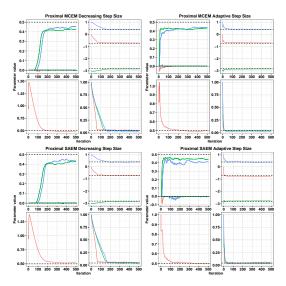
$$\hookrightarrow \lambda = \mathrm{argmin}_{\lambda_1, \cdots, \lambda_L} \mathsf{E}\text{-}\mathsf{BIC}(\hat{\beta}_\lambda)$$

- Stepsize sequences: constant or vanishing stepsize sequence $\{\gamma_n, n \geq 0\}$? (and δ_n for the SA-Prox Gdt algorithm)
- Monte Carlo approximation: fixed or increasing batch size ?

Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms

Numerical illustration

Numerical illustration (2/3): pharmacokinetic



└─ Numerical illustration

Numerical illustration (3/3): pharmacokinetic

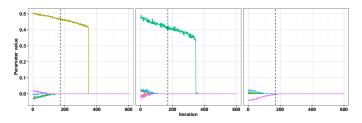


Figure: Regularization path of the covariate parameters for the clearance (left), absorption constant (middle) and volume of distribution (right) parameters. Black dashed line corresponds to the λ value selected by EBIC. Each colored curve corresponds to a covariate.

Outline

Penalized Maximum Likelihood inference in models with intractable likelihood

Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms

Convergence analysis

Conclusion

The assumptions

$$\operatorname{argmin}_{\theta \in \Theta} F(\theta)$$
 with $F(\theta) = f(\theta) + g(\theta)$

where

- the function $g\colon \mathbb{R}^d \to [0,\infty]$ is convex, non smooth, not identically equal to $+\infty$, and lower semi-continuous
- the function $f\colon \mathbb{R}^d \to \mathbb{R}$ is a smooth **convex** function i.e. f is continuously differentiable and there exists L>0 such that $\|\nabla f(\theta) \nabla f(\theta')\| < L \ \|\theta \theta'\| \qquad \forall \theta, \theta' \in \mathbb{R}^d$
- $\Theta \subseteq \mathbb{R}^d$ is the domain of g: $\Theta = \{\theta \in \mathbb{R}^d : g(\theta) < \infty\}$.
- The set $\operatorname{argmin}_{\Theta} F$ is a non-empty subset of Θ .

Existing results in the literature

There exist results under (some of) the assumptions

$$\mathbb{E}\left[H_{n+1}|\mathcal{F}_n\right] = \nabla f(\theta_n), \qquad \inf_n \gamma_n > 0, \qquad \sum_n \|H_{n+1} - \nabla f(\theta_n)\| < \infty,$$

i.e. results for

- unbiased sampling. Almost no conditions for the biased sampling, such as the MCMC one.
- non vanishing stepsize sequence $\{\gamma_n, n \geq 0\}$.
- increasing batch size: when H_{n+1} is a Monte Carlo sum i.e.

$$H_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} H_{\theta_n}(X_{j,n}),$$

the assumptions imply that $\lim_n m_n = +\infty$ at some rate.

Combettes (2001) Elsevier Science.

Combettes-Wajs (2005) Multiscale Modeling and Simulation.

Combettes-Pesquet (2015, 2016) SIAM J. Optim, arXiv

Lin-Rosasco-Villa-Zhou (2015) arXiv

Rosasco-Villa-Vu (2014,2015) arXiv

Schmidt-Leroux-Bach (2011) NIPS

Convergence of the perturbed proximal gradient algorithm (1/3)

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1},g} (\theta_n - \gamma_{n+1} \ H_{n+1})$$
 with $H_{n+1} \approx \nabla f(\theta_n)$

Set:
$$\mathcal{L} = \operatorname{argmin}_{\Theta}(f+g)$$
 $\eta_{n+1} = H_{n+1} - \nabla f(\theta_n)$

Theorem (Atchadé, F., Moulines (2015))

Assume

- g convex, lower semi-continuous; f convex, C^1 and its gradient is Lipschitz with constant L; \mathcal{L} is non empty.
- $\sum_n \gamma_n = +\infty$ and $\gamma_n \in (0, 1/L]$.
- Convergence of the series

$$\sum_{n} \gamma_{n+1}^{2} \|\eta_{n+1}\|^{2}, \qquad \sum_{n} \gamma_{n+1} \eta_{n+1}, \qquad \sum_{n} \gamma_{n+1} \langle \mathsf{T}_{n}, \eta_{n+1} \rangle$$

where
$$T_n = \text{Prox}_{\gamma_{n+1}, g}(\theta_n - \gamma_{n+1} \nabla f(\theta_n)).$$

Then there exists $\theta_{\star} \in \mathcal{L}$ such that $\lim_{n} \theta_{n} = \theta_{\star}$.

This convergence result

ullet for the convex case: f and g are convex.

This convergence result

- ullet for the convex case: f and g are convex.
- is a deterministic result.

Covered: deterministic and random approximations H_{n+1} of $\nabla f(\theta_n)$.

This convergence result

- ullet for the convex case: f and g are convex.
- is a deterministic result. Covered: deterministic and random approximations H_{n+1} of $\nabla f(\theta_n)$. Among random approximations:
- Applications in Computational Statistics

$$H_{n+1} = \Xi \left(X_{1,n}, \cdots, X_{m_{n+1},n}; \theta_n \right)$$

This convergence result

- ullet for the convex case: f and g are convex.
- is a deterministic result. Covered: deterministic and random approximations H_{n+1} of $\nabla f(\theta_n)$. Among random approximations:
- Applications in Computational Statistics
- 2 Applications in learning "finite sum context" :

(objective)
$$\operatorname{argmin}_{\theta} \left(\frac{1}{N} \sum_{i=1}^{N} f_i(\theta) + g(\theta) \right)$$
 (Approx. Gdt)
$$H_{n+1} = \frac{1}{|I_{n+1}|} \sum_{i \in I_{n+1}} \nabla f_i(\theta_n)$$
 (X_i 's) the indices $i \in I_{n+1}$

Its proof relies on

a deterministic Lyapunov inequality

$$\left\|\theta_{n+1} - \theta_{\star}\right\|^{2} \leq \left\|\theta_{n} - \theta_{\star}\right\|^{2} - \underbrace{2\gamma_{n+1}\left(F(\theta_{n+1}) - \min F\right)}_{\text{non-negative}} \underbrace{-2\gamma_{n+1}\left\langle\mathsf{T}_{n} - \theta_{\star}, \eta_{n+1}\right\rangle + 2\gamma_{n+1}^{2} \|\eta_{n+1}\|^{2}}_{\text{signed noise}}$$

2 (an extension of) the Robbins-Siegmund lemma

Let $\{v_n,n\geq 0\}$ and $\{\chi_n,n\geq 0\}$ be non-negative sequences and $\{\xi_n,n\geq 0\}$ be such that $\sum_n\xi_n$ exists. If for any $n\geq 0$,

$$v_{n+1} \le v_n - \chi_{n+1} + \xi_{n+1}$$

then $\sum_{n} \chi_n < \infty$ and $\lim_{n} v_n$ exists.

Its proof relies on

a deterministic Lyapunov inequality

$$\left\|\theta_{n+1} - \theta_{\star}\right\|^{2} \leq \left\|\theta_{n} - \theta_{\star}\right\|^{2} - \underbrace{2\gamma_{n+1}\left(F(\theta_{n+1}) - \min F\right)}_{\text{non-negative}} \underbrace{-2\gamma_{n+1}\left\langle\mathsf{T}_{n} - \theta_{\star}, \eta_{n+1}\right\rangle + 2\gamma_{n+1}^{2} \|\eta_{n+1}\|^{2}}_{\text{signed noise}}$$

2 (an extension of) the Robbins-Siegmund lemma

Let $\{v_n,n\geq 0\}$ and $\{\chi_n,n\geq 0\}$ be non-negative sequences and $\{\xi_n,n\geq 0\}$ be such that $\sum_n\xi_n$ exists. If for any $n\geq 0$,

$$v_{n+1} \le v_n - \chi_{n+1} + \xi_{n+1}$$

then $\sum_{n} \chi_n < \infty$ and $\lim_{n} v_n$ exists.

Note: deterministic lemma, signed noise.

Convergence: when H_{n+1} is a Monte-Carlo approximation (1/3) In the case

$$\begin{split} \nabla f(\theta_n) &\approx H_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} H_{\theta_n}(X_{j,n}), \\ X_{j+1,n} | \mathsf{past} &\sim P_{\theta_n}(X_{j,n}, \cdot) \qquad \pi_{\theta} P_{\theta} = \pi_{\theta}; \end{split}$$

Convergence: when H_{n+1} is a Monte-Carlo approximation (1/3) In the case

$$\begin{split} \nabla f(\theta_n) &\approx H_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} H_{\theta_n}(X_{j,n}), \\ X_{j+1,n} | \mathsf{past} &\sim P_{\theta_n}(X_{j,n}, \cdot) \qquad \pi_\theta P_\theta = \pi_\theta; \end{split}$$

let us check the condition " $\sum_n \gamma_n \eta_n < \infty$ w.p.1" under the condition $\sum_n \gamma_n = +\infty$:

$$\begin{split} \sum_{n} \gamma_{n+1} \eta_{n+1} &= \sum_{n} \gamma_{n+1} \left(H_{n+1} - \nabla f(\theta_{n}) \right) \\ &= \sum_{n} \gamma_{n+1} \left\{ H_{n+1} - \mathbb{E} \left[H_{n+1} | \mathcal{F}_{n} \right] \right\} + \sum_{n} \gamma_{n+1} \underbrace{\left\{ \mathbb{E} \left[H_{n+1} | \mathcal{F}_{n} \right] - \nabla f(\theta_{n}) \right\}}_{\text{if unbiased MC: } O(1/m_{n})} \end{split}$$

Convergence: when H_{n+1} is a Monte-Carlo approximation (1/3) In the case

$$\nabla f(\theta_n) \approx H_{n+1} = \frac{1}{m_{n+1}} \sum_{j=1}^{m_{n+1}} H_{\theta_n}(X_{j,n}),$$

$$X_{j+1,n} | \mathsf{past} \sim P_{\theta_n}(X_{j,n}, \cdot) \qquad \pi_{\theta} P_{\theta} = \pi_{\theta};$$

let us check the condition " $\sum_n \gamma_n \eta_n < \infty$ w.p.1" under the condition $\sum_n \gamma_n = +\infty$:

$$\begin{split} \sum_{n} \gamma_{n+1} \eta_{n+1} &= \sum_{n} \gamma_{n+1} \left(H_{n+1} - \nabla f(\theta_{n}) \right) \\ &= \sum_{n} \gamma_{n+1} \left\{ H_{n+1} - \mathbb{E} \left[H_{n+1} | \mathcal{F}_{n} \right] \right\} + \sum_{n} \gamma_{n+1} \underbrace{\left\{ \mathbb{E} \left[H_{n+1} | \mathcal{F}_{n} \right] - \nabla f(\theta_{n}) \right\}}_{\text{if unbiased MC: null if biased MC: } O(1/m_{n})} \end{split}$$

The most technical case: the biased case with constant batch size $m_n=m$

Solution \hat{H}_{θ} to the Poisson equation: $H_{\theta} - \pi_{\theta} H_{\theta} = \hat{H}_{\theta} - P_{\theta} \hat{H}_{\theta}$ $H_{n+1} - \nabla f(\theta_n) = \text{martingale increment} + \text{remainder}$

Regularity in θ of $\theta \mapsto \widehat{H}_{\theta}$ and $\theta \mapsto P_{\theta}\widehat{H}_{\theta}$.

Convergence: when H_{n+1} is a Monte-Carlo approximation (2/3)

Increasing batch size: $\lim_n m_n = +\infty$

Conditions on the step sizes and batch sizes

$$\sum_{n} \gamma_{n} = +\infty, \qquad \sum_{n} \frac{\gamma_{n}^{2}}{m_{n}} < \infty; \qquad \sum_{n} \frac{\gamma_{n}}{m_{n}} < \infty \text{ (biased case)}$$

Conditions on the Markov kernels: There exist $\lambda \in (0,1), b < \infty, p \geq 2$ and a measurable function $W: X \to [1,+\infty)$ such that

$$\sup_{\theta \in \Theta} |H_{\theta}|_{W} < \infty, \qquad \sup_{\theta \in \Theta} P_{\theta} W^{p} \le \lambda W^{p} + b.$$

In addition, for any $\ell \in (0,p]$, there exist $C < \infty$ and $\rho \in (0,1)$ such that for any $x \in X$,

$$\sup_{\theta \in \Theta} \|P_{\theta}^{n}(x, \cdot) - \pi_{\theta}\|_{W^{\ell}} \le C\rho^{n}W^{\ell}(x). \tag{1}$$

Condition on Θ : Θ is bounded.

Convergence: when H_{n+1} is a Monte-Carlo approximation (3/3)

Fixed batch size: $m_n = m$

Condition on the step size:

$$\sum_{n} \gamma_{n} = +\infty \qquad \sum_{n} \gamma_{n}^{2} < \infty \qquad \sum_{n} |\gamma_{n+1} - \gamma_{n}| < \infty$$

Condition on the Markov chain: same as in the case "increasing batch size" and there exists a constant C such that for any $\theta, \theta' \in \Theta$

$$|H_{\theta} - H_{\theta'}|_{W} + \sup_{x} \frac{||P_{\theta}(x, \cdot) - P_{\theta'}(x, \cdot)||_{W}}{W(x)} + ||\pi_{\theta} - \pi_{\theta'}||_{W} \le C ||\theta - \theta'||.$$

Condition on the Prox:

$$\sup_{\gamma \in (0,1/L]} \sup_{\theta \in \Theta} \gamma^{-1} \| \operatorname{Prox}_{\gamma,g}(\theta) - \theta \| < \infty.$$

Condition on Θ : Θ is bounded.

Rates of convergence (1/3): the problem

For non negative weights a_k , find an upper bound of

$$\sum_{k=1}^{n} \frac{a_k}{\sum_{\ell=1}^{n} a_\ell} F(\theta_k) - \min F$$

It provides

- an upper bound for the cumulative regret $(a_k = 1)$
- ullet an upper bound for an averaging strategy when F is convex since

$$F\left(\sum_{k=1}^{n} \frac{a_k}{\sum_{\ell=1}^{n} a_\ell} \theta_k\right) - \min F \le \sum_{k=1}^{n} \frac{a_k}{\sum_{\ell=1}^{n} a_\ell} F(\theta_k) - \min F.$$

Rates of convergence (2/3): a deterministic control

Theorem (Atchadé, F., Moulines (2016))

For any $\theta_{\star} \in \operatorname{argmin}_{\Theta} F$,

$$\begin{split} \sum_{k=1}^{n} \frac{a_{k}}{A_{n}} F(\theta_{k}) - \min F &\leq \frac{a_{0}}{2\gamma_{0}A_{n}} \|\theta_{0} - \theta_{\star}\|^{2} \\ &+ \frac{1}{2A_{n}} \sum_{k=1}^{n} \left(\frac{a_{k}}{\gamma_{k}} - \frac{a_{k-1}}{\gamma_{k-1}} \right) \|\theta_{k-1} - \theta_{\star}\|^{2} \\ &+ \frac{1}{A_{n}} \sum_{k=1}^{n} a_{k} \gamma_{k} \|\eta_{k}\|^{2} - \frac{1}{A_{n}} \sum_{k=1}^{n} a_{k} \left\langle \mathsf{T}_{k-1} - \theta_{\star}, \eta_{k} \right\rangle \end{split}$$

where

$$A_n = \sum_{k=1}^n a_\ell, \qquad \eta_k = H_k - \nabla f(\theta_{k-1}), \qquad \mathsf{T}_k = \mathrm{Prox}_{\gamma_k, g}(\theta_{k-1} - \gamma_k \nabla f(\theta_{k-1})).$$

Rates (3/3): when H_{n+1} is a Monte Carlo approximation, bound in L^q

$$\left\| F\left(\frac{1}{n}\sum_{k=1}^{n}\theta_{k}\right) - \min F \right\|_{L^{q}} \le \left\| \frac{1}{n}\sum_{k=1}^{n}F(\theta_{k}) - \min F \right\|_{L^{q}} \le u_{n}$$

$u_n = O(1/\sqrt{n})$

with fixed size of the batch and (slowly) decaying stepsize

$$\gamma_n = \frac{\gamma_{\star}}{n^a}, a \in [1/2, 1] \qquad m_n = m_{\star}.$$

With averaging: optimal rate, even with slowly decaying stepsize $\gamma_n \sim 1/\sqrt{n}$.

$u_n = O(\ln n/n)$

with increasing batch size and constant stepsize

$$\gamma_n = \gamma_\star \qquad \qquad m_n \propto n.$$

Rate with $O(n^2)$ Monte Carlo samples !

Acceleration (1)

Let $\{t_n, n \ge 0\}$ be a positive sequence s.t.

$$\gamma_{n+1}t_n(t_n-1) \le \gamma_n t_{n-1}^2$$

Nesterov acceleration of the Proximal Gradient algorithm

$$\theta_{n+1} = \operatorname{Prox}_{\gamma_{n+1}, g} (\tau_n - \gamma_{n+1} \nabla f(\tau_n))$$

$$\tau_{n+1} = \theta_{n+1} + \frac{t_n - 1}{t_{n+1}} (\theta_{n+1} - \theta_n)$$

Nesterov(2004), Tseng(2008), Beck-Teboulle(2009)

Zhu-Orecchia (2015); Attouch-Peypouquet(2015); Bubeck-Lee-Singh(2015); Su-Boyd-Candes(2015)

$$F(\theta_n) - \min F = O\left(\frac{1}{n}\right)$$

$$F(\theta_n) - \min F = O\left(\frac{1}{n^2}\right)$$

Acceleration (2) Aujol-Dossal-F.-Moulines, work in progress

Perturbed Nesterov acceleration: some convergence results

Choose γ_n, m_n, t_n s.t.

$$\gamma_n \in (0, 1/L], \quad \lim_n \gamma_n t_n^2 = +\infty, \quad \sum_n \gamma_n t_n (1 + \gamma_n t_n) \frac{1}{m_n} < \infty$$

Then there exists $\theta_* \in \operatorname{argmin}_{\Theta} F$ s.t $\lim_n \theta_n = \theta_*$. In addition

$$F(\theta_{n+1}) - \min F = O\left(\frac{1}{\gamma_{n+1}t_n^2}\right)$$

Schmidt-Le Roux-Bach (2011); Dossal-Chambolle(2014); Aujol-Dossal(2015)

γ_n	m_n	t_n	rate	NbrMC
γ	n^3	n	n^{-2}	n^4
γ/\sqrt{n}	n^2	n	$n^{-3/2}$	n^3

Table: Control of $F(\theta_n) - \min F$

Outline

Penalized Maximum Likelihood inference in models with intractable likelihood

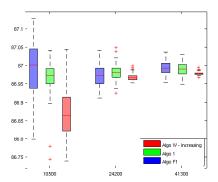
Numerical methods for Penalized ML in such models: Perturbed Proximal Gradient algorithms

Convergence analysis

Conclusion

Conclusion (1/2): acceleration ?

- with or without the acceleration: complexity $O(1/\sqrt{n})$.
- acceleration: longer Markov chains, few iterations.



Conclusion (2/2): weaken the assumptions

- $\bullet \ \theta \in \mathbb{R}^d \to \theta$ in a Hilbert space
- \bullet Θ bounded \to no boundedness condition on Θ
- $\bullet \ f \ \mathsf{convex} \to f \ \mathsf{non} \ \mathsf{convex} \\$