Regret bounds for generalized Bayes updates

Pierre Alquier

RIKEN

AIP
Center for
Advanced Intelligence Project

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The sequential prediction problem

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Objective :

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Objective : make sure that we learn to predict well **as soon as possible**. Keep

$$\sum_{t=1}^{T} \ell(\hat{y}_t, y_t)$$

as small as possible.

1st approach : "follow the regularized leader"

- set of predictors : $\{f_\theta, \theta \in \Theta\}$.
- $\ell_t(\theta) := \ell(f_\theta(x_t), y_t))$.

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Follow The Regularized Leader – FTRL

$$\theta^t := \arg\min_{\theta} \left\{ \sum_{s=1}^{t-1} \ell_s(\theta) + \frac{\mathrm{pen}(\theta)}{\eta} \right\}.$$

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Quadratic penalty + linearization :

$$\theta^t := \arg\min_\theta \left\{ \sum_{s=1}^{t-1} \langle \theta, \nabla \ell_s(\theta^s) \rangle + \frac{\|\theta\|^2}{2\eta} \right\}.$$

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Differentiate :

$$0 = \sum_{s=1}^{t-1} \nabla \ell_s(\theta^s) + \frac{\theta^t}{\eta}.$$

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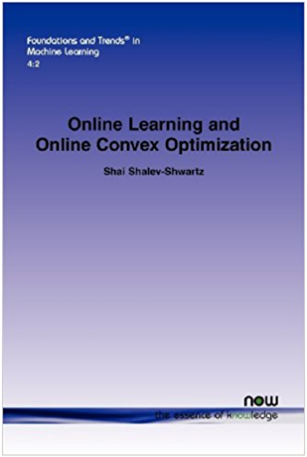
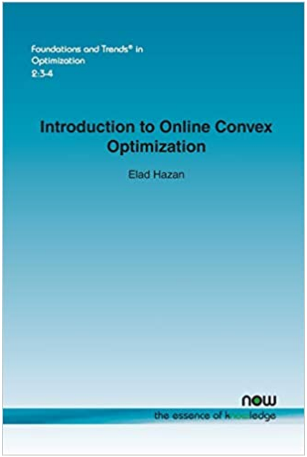
Online Gradient Algorithm – OGA

$$\theta^t := \theta^{t-1} - \eta \nabla \ell_{t-1}(\theta^{t-1}).$$

Theoretical properties of FTRL & OGA





2nd approach : (generalized) Bayes

Generalized Bayes, multiplicative weights, Exponential Weight Aggregation (EWA)...

EWA

$$\rho^t(\theta) \propto \exp\left[-\eta \sum_{s=1}^{t-1} \ell_s(\theta)\right] \pi(\theta)$$

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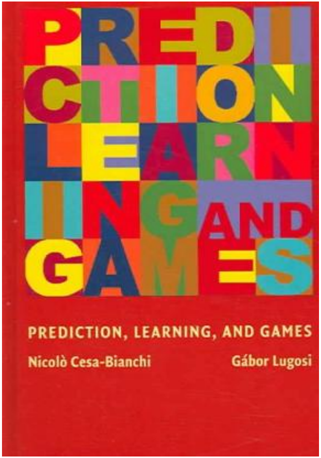


EWA as FTRL

It is known that

$$\rho^t = \operatorname*{arg\,min}_{\rho \in \mathcal{P}(\Theta)} \left\{ \sum_{s=1}^{t-1} \underbrace{\mathbb{E}_{\theta\sim\rho}[\ell_s(\theta)]}_{=: L_s(\rho)} + \underbrace{\frac{\mathrm{KL}(\rho\|\pi)}{\eta}}_{=: \frac{\mathrm{pen}(\rho)}{\eta}} \right\}.$$

That is, EWA is a special case of FTRL.

$$\mathrm{KL}(\rho\|\pi) = \begin{cases} \mathbb{E}_{\theta\sim\rho}\left[\log\left(\frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta)\right)\right] & \text{if } \rho \ll \pi \\ +\infty & \text{otherwise.} \end{cases}$$

1st objective

We will study a more general version of FTRL on ρ :

$$\rho^t = \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \sum_{s=1}^{t-1} \mathbb{E}_{\theta \sim \rho}[\ell_s(\theta)] + \frac{D(\rho \| \pi)}{\eta} \right\},$$

for more general divergences D.

P. Alquier. *Non-exponentially Weighted Aggregation : Regret Bounds for Unbounded Loss Functions*. Accepted for ICML 2021.

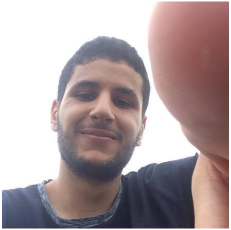
2nd objective

EWA is often non feasible in practice. We will thus modify it : we will constrain ρ^t to belong to a feasible set of probability distributions (e.g. : Gaussian).

B.-E. Chérief-Abdellatif, P. Alquier, M. E. Khan (2019). *A regret bound for online variational inference*. 11th Asian Conference on Machine Learning (ACML).

Co-authors

Badr-Eddine Chérief-Abdellatif



UNIVERSITY OF OXFORD

Emtiyaz Khan

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Approximate Bayesian Inference team

https : //team − approx − bayes.github.io/

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   - Regret bound
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Reminder

$$\rho^t = \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \sum_{s=1}^{t-1} \mathbb{E}_{\theta\sim\rho}[\ell_s(\theta)] + \frac{D_\phi(\rho\|\pi)}{\eta} \right\},$$

Reminder

$$\rho^t = \arg\min_{\rho \in \mathcal{P}(\Theta)} \left\{ \sum_{s=1}^{t-1} \mathbb{E}_{\theta\sim\rho}[\ell_s(\theta)] + \frac{D_\phi(\rho\|\pi)}{\eta} \right\},$$

where

$$D_\phi(\rho\|\pi) = \begin{cases} \mathbb{E}_{\theta\sim\pi}\left[\phi\left(\frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta)\right)\right] & \text{if } \rho \ll \pi \\ +\infty & \text{otherwise,} \end{cases}$$

and $\phi : \mathbb{R}_+ \to \mathbb{R} \cup \{+\infty\}$ with :

- ϕ convex,
- $\phi(1) = 0$,
- $\inf_{x\geq 0} \phi(x) > -\infty$.

Differential of the convex conjugate

Assume that ϕ is differentiable, strictly convex. Put

$$\tilde{\phi}(x) = \begin{cases} \phi(x) \text{ if } x \geq 0, \\ +\infty \text{ if } x < 0. \end{cases}$$

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Then

$$\tilde{\phi}^* = \sup_{x \in \mathbb{R}} [xy - \tilde{\phi}(x)] = \sup_{x \geq 0} [xy - \phi(x)]$$

is differentiable and for any $y \in \mathbb{R}$,

$$\nabla \tilde{\phi}^*(y) = \arg\max_{x \geq 0} \left\{ xy - \phi(x) \right\}.$$

Formula for ρ^t

Assume moreover that $\tilde{\phi}^*(\lambda - a) - \lambda \to \infty$ when $\lambda \to \infty$, for any $a \geq 0$. Then :

$$\lambda_t = \arg\min_{\lambda \in \mathbb{R}} \left\{ \int \tilde{\phi}^* \left(\lambda - \eta \sum_{s=1}^{t-1} \ell_s(\theta) \right) \pi(\mathrm{d}\theta) - \lambda \right\}$$

exists, and

$$\rho^t(\mathrm{d}\theta) = \nabla \tilde{\phi}^* \left(\lambda_t - \eta \sum_{s=1}^{t-1} \ell_s(\theta) \right) \pi(\mathrm{d}\theta).$$

The classical example : KL and exponential weights

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$$\rho^t(\mathrm{d}\theta) = \frac{\exp\left[-\eta\sum_{s=1}^{t-1}\ell_s(\theta)\right]\pi(\mathrm{d}\theta)}{\int\exp\left[-\eta\sum_{s=1}^{t-1}\ell_s(\vartheta)\right]\pi(\mathrm{d}\vartheta)}.$$

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$$\rho^t(\mathrm{d}\theta) = \left[\frac{\lambda_t - \eta\sum_{s=1}^{t-1}\ell_s(\theta)}{2}\right]_+ \pi(\mathrm{d}\theta).$$

Some references

- the formula was known for a finite Θ :

M. D. Reid, R. M. Frongillo, R. C. Williamson, N. Mehta (2015). *Generalized mixability via entropic duality*. COLT.

- the proof for the general case relies on :

R. Agrawal, T. Horel (2020). *Optimal bounds between f-divergences and integral probability metrics*. ICML.

- comparable PAC-Bayes bounds (no online update) :

P. Alquier and B. Guedj (2018). *Simpler PAC-Bayesian bounds for hostile data*. Machine Learning.

- defense of the generalized Bayes update :

J. Knoblauch, J. Jewson, T. Damoulas (2019). *Generalized variational inference : Three arguments for deriving new posteriors.*. Preprint arXiv.

- more : see the paper.

General regret bound

Assume there is a norm $\|\cdot\|$ such that

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Theorem

$$\sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho^t}[\ell_t(\theta)] \leq \inf_{\rho\in\mathcal{P}(\Theta)} \left\{ \sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho}[\ell_t(\theta)] + \frac{\eta L^2 T}{\alpha} + \frac{D_\phi(\rho\|\pi)}{\eta} \right\}.$$

Bound for EWA : the conditions

- known result : $KL(\rho\|\pi)$ is 1-strongly convex with respect to $\|\cdot\|_{\mathrm{TV}}$;

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- we have :

$$\left|\int \ell_t(\theta)\rho(\mathrm{d}\theta) - \int \ell_t \rho'(\mathrm{d}\theta)\right| \leq \int \ell_t(\theta) \left|\frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta) - \frac{\mathrm{d}\rho'}{\mathrm{d}\pi}(\theta)\right| \pi(\mathrm{d}\theta)$$

$$\leq L \underbrace{\int \left|\frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta) - \frac{\mathrm{d}\rho'}{\mathrm{d}\pi}(\theta)\right| \pi(\mathrm{d}\theta)}_{=2\|\rho-\rho'\|_{\mathrm{TV}}}$$

on the condition that $0 \leq \ell_t(\theta) \leq L$ for any θ.

Bound for EWA

Assume $0 \leq \ell_t(\theta) \leq L$ for any θ, t, then

$$\sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho^t}[\ell_t(\theta)] \leq \inf_{\rho\in\mathcal{P}(\Theta)} \left\{ \sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho}[\ell_t(\theta)] + \eta L^2 T + \frac{\mathrm{KL}(\rho\|\pi)}{\eta} \right\}.$$

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(This is a well-known result).

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$$\left| \int \ell_t(\theta)\rho(\mathrm{d}\theta) - \int \ell_t \rho'(\mathrm{d}\theta) \right| \leq \int \ell_t(\theta) \left| \frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta) - \frac{\mathrm{d}\rho'}{\mathrm{d}\pi}(\theta) \right| \pi(\mathrm{d}\theta)$$

$$\leq L \left(\int \left(\frac{\mathrm{d}\rho}{\mathrm{d}\pi}(\theta) - \frac{\mathrm{d}\rho'}{\mathrm{d}\pi}(\theta) \right)^2 \pi(\mathrm{d}\theta) \right)^{1/2}$$

on the condition that $\left(\int \ell_t(\theta)^2 \pi(\mathrm{d}\theta)\right)^{1/2} \leq L$.

Bound with χ^2

Assume $\int \ell_t(\theta)^2 \pi(\mathrm{d}\theta) \leq L^2$ for any t, then

$$\sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho^t}[\ell_t(\theta)] \leq \inf_{\rho\in\mathcal{P}(\Theta)} \left\{ \sum_{t=1}^{T} \mathbb{E}_{\theta\sim\rho}[\ell_t(\theta)] + \frac{\eta L^2 T}{2} + \frac{\chi^2(\rho\|\pi)}{\eta} \right\}.$$

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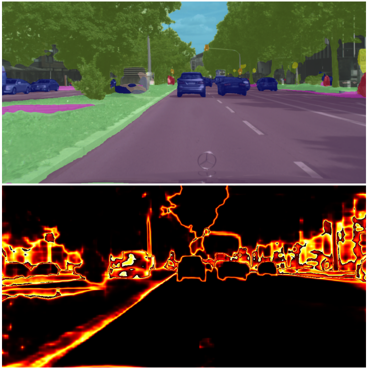

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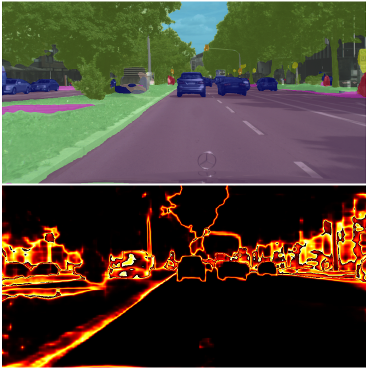

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Objective : provide a theoretical analysis of this algorithm.

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Linearization gives :

SVA

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Streaming Variational Bayes (SVB)

(OGA) can actually be obtained via :

$$\theta^t := \arg\min_{\theta} \left\{ \sum_{s=1}^{t-1} \langle \theta, \nabla \ell_s(\theta^s) \rangle + \frac{\|\theta\|^2}{2\eta} \right\}$$

OR

$$\theta^t := \arg\min_{\theta} \left\{ \langle \theta, \nabla \ell_{t-1}(\theta^{t-1}) \rangle + \frac{\|\theta - \theta^{t-1}\|^2}{2\eta} \right\}$$

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SVA & SVB are tractable, and not equivalent

Example : Gaussian prior $\theta \sim \pi = \mathcal{N}(0, s^2 I)$, $D_\phi = \mathrm{KL}$ and mean-field Gaussian approximation, $\mu = (m, \sigma)$.

$$\begin{aligned} \mathrm{SVA} : m_{t+1} &\leftarrow m_t - \eta s^2 \bar{g}_{m_t}, \qquad g_{t+1} \leftarrow g_t + \bar{g}_{\sigma_t}, \\ \sigma_{t+1} &\leftarrow h\left(\eta s g_{t+1}\right) s, \\ \mathrm{SVB} : m_{t+1} &\leftarrow m_t - \eta \sigma_t^2 \bar{g}_{m_t}, \\ \sigma_{t+1} &\leftarrow \sigma_t h\left(\eta \sigma_t \bar{g}_{\sigma_t}\right) \end{aligned}$$

where $h(x) := \sqrt{1 + x^2} - x$ is applied componentwise, as well as the multiplication of two vectors, and

$$\bar{g}_{m_t} = \frac{\partial}{\partial m} \mathbb{E}_{\theta \sim \pi_{m_t, \sigma_t}}[\ell_t(\theta)],$$
$$\bar{g}_{\sigma_t} = \frac{\partial}{\partial \sigma} \mathbb{E}_{\theta \sim \pi_{m_t, \sigma_t}}[\ell_t(\theta)].$$

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Two assumptions :

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Proof :

J. Domke (2019). *Provable smoothness guarantees for black-box variational inference.* NeurIPS.

Theoretical analysis of SVA

Two assumptions :

1. $\mu \mapsto \mathbb{E}_{\theta \sim q_\mu}[\ell_t(\theta)]$ is L-Lipschitz and convex.

Proposition

Assume $\theta \mapsto \ell_t(\theta)$ is $L/2$-Lipschitz and convex, and $\mu = (m, \Sigma)$ is a location scale parameter, then : satisfied.

Proof :

J. Domke (2019). *Provable smoothness guarantees for black-box variational inference.* NeurIPS.

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   For example true when q_μ is Gaussian with $\mu = (m, \Sigma)$ and $D_\phi = \mathrm{KL}$.

Theoretical analysis of SVA

Theorem

Under the previous assumptions SVA leads to

$$\sum_{t=1}^{T} \mathbb{E}_{\theta\sim q_{\mu_t}}[\ell_t(\theta)] \leq \inf_{\mu\in M}\left\{ \sum_{t=1}^{T} \mathbb{E}_{\theta\sim q_{\mu}}[\ell_t(\theta)] + \frac{\eta L^2 T}{\alpha} + \frac{D_\phi(q_\mu,\pi)}{\eta} \right\}.$$

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Application to Gaussian approximation with KL :

$$\sum_{t=1}^{T} \mathbb{E}_{\theta\sim q_{\mu_t}}[\ell_t(\theta)] \leq \inf_{\theta} \sum_{t=1}^{T} \ell_t(\theta) + (1+o(1)) L\sqrt{dT\log(T)}.$$

Theoretical analysis of SVB

Theorem 2

Using Gaussian approximations and $D_\phi = \mathrm{KL}$, assuming the loss is convex, L-Lipschitz and the parameter space bounded (diameter $= D$), SVB with adequate η leads to

$$\sum_{t=1}^{T} \ell_t\left(\mathbb{E}_{\theta\sim q_{\mu_t}}(\theta)\right) \leq \inf_{\theta} \sum_{t=1}^{T} \ell_t(\theta) + DL\sqrt{2T}.$$

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If, moreover, the loss is H-strongly convex,

$$\sum_{t=1}^{T} \ell_t\left(\mathbb{E}_{\theta\sim q_{\mu_t}}(\theta)\right) \leq \inf_\theta \sum_{t=1}^{T} \ell_t(\theta) + \frac{L^2(1+\log(T))}{H}.$$

Test on a simulated dataset

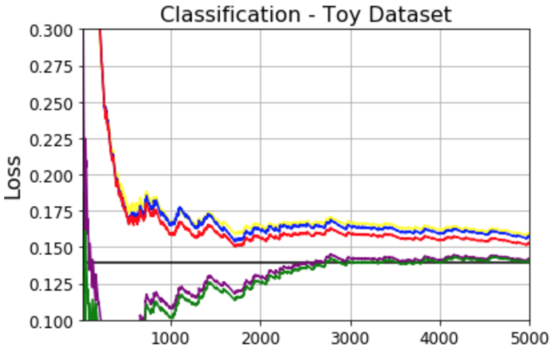
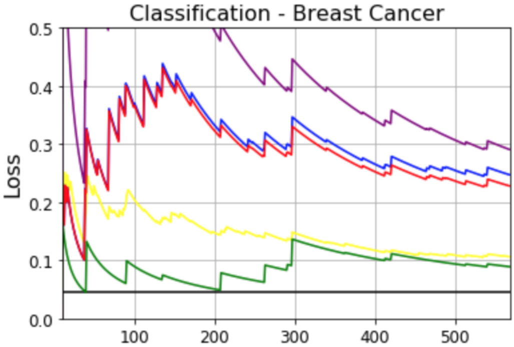


Figure – Average cumulative losses on different datasets for classification and regression tasks with OGA (yellow), OGA-EL (red), SVA (blue), SVB (purple) and NGVI (green).

Test on the Breast dataset



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1. Analysis of SVB in the general case.
2. Analysis of the uncertainty quantification.
3. NGVI is the next step in going closer to algorithms used to train Neural Networks with Bayesian principles. But being based on a different parametrization, it does not satisfy our convexity assumption...

   Uses exponential family approximations $\{q_\mu, \mu \in M\}$ where m is the mean parameter. Denoting λ the natural parameter (with $\lambda = F(\mu)$),

$$\lambda^t = (1-\rho)\lambda^{t-1} + \rho \nabla_\mu \mathbb{E}_{\theta \sim q_{\mu^{t-1}}} [\ell_t(\theta)] ,$$

M. E. Khan, D. Nielsen (2018). *Fast yet Simple Natural-Gradient Descent for Variational Inference in Complex Models.* ISITA.

Thank you !