Regret bounds for generalized Bayes updates

Pierre Alquier





Al seminar series - UCL Al Centre - May 19, 2021

Sequential prediction problem





 $\mathbf{0}$ x_1 given

- 1
- $\mathbf{0}$ x_1 given

- 0
- $\mathbf{0}$ x_1 given
- 2 predict $y_1: \hat{y}_1$
- $\mathbf{9}$ y_1 is revealed

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- $\mathbf{0}$ \mathbf{x}_2 given

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 - y_2 revealed
- 0 x_3 given

- $\mathbf{0}$ \mathbf{x}_1 given
 - **2** $predict <math>y_1 : \hat{y}_1$
 - $\mathbf{9}$ y_1 is revealed
- $\mathbf{0}$ \mathbf{x}_2 given
 - 2 predict $y_2: \hat{y}_2$
 - y₂ revealed
- 0 x_3 given
 - 2 predict $y_3: \hat{y}_3$

- $\mathbf{0}$ $\mathbf{0}$ x_1 given

 - $\mathbf{0}$ y_1 is revealed
- $\mathbf{0}$ \mathbf{x}_2 given
 - 2 predict $y_2: \hat{y}_2$
 - y₂ revealed
- 3 v₃ given
 - 2 predict $y_3: \hat{y}_3$
 - y_3 revealed
- 4

Sequential prediction problem

```
\mathbf{0} \mathbf{x}_1 given
```

2 predict $y_1 : \hat{y}_1$ **Objective**:

 $\mathbf{9}$ y_1 is revealed

 \mathbf{Q} \mathbf{Q} \mathbf{X}_2 given

2 predict $y_2 : \hat{y}_2$

y₂ revealed

2 predict $y_3: \hat{y}_3$

 y_3 revealed

4 . .

Sequential prediction problem

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 - $\mathbf{0}$ y_1 is revealed
- $\mathbf{0}$ \mathbf{x}_2 given
 - 2 predict $y_2: \hat{y}_2$
 - y_2 revealed
- - 2 predict $y_3: \hat{y}_3$
 - $\mathbf{0}$ y_3 revealed
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Objective: make sure that we learn to predict well as soon as possible.

Sequential prediction problem

- 0 x_1 given
 - 2 predict $y_1 : \hat{y}_1$
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 - y₂ revealed
- 3 u x3 given
 - 2 predict $y_3: \hat{y}_3$
 - $\mathbf{9}$ y_3 revealed

4 ...

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.

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

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Follow The Regularized Leader - FTRL

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Quadratic penalty + linearization :

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

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Differentiate:

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

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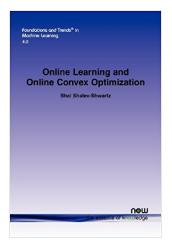
Follow The Regularized Leader - FTRL

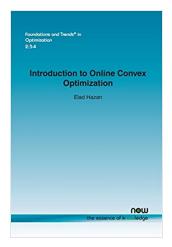
$$\theta^t := \arg\min_{\theta} \left\{ \sum_{\mathfrak{s}=1}^{t-1} \ell_{\mathfrak{s}}(\theta) + \frac{\mathrm{pen}(\theta)}{\eta} \right\}.$$

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

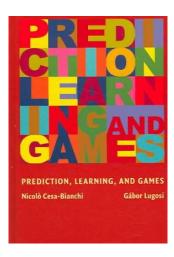
$$ho^t(heta) \propto \exp\left[-\eta \sum_{s=1}^{t-1} \ell_s(heta)
ight] \pi(heta)$$

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EWA

$$ho^t(heta) \propto \exp\left[-\eta \sum_{s=1}^{t-1} \ell_s(heta)
ight] \pi(heta)$$



EWA as FTRL

It is known that

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

That is, EWA is a special case of FTRL.

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

1st objective

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

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

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





Emtiyaz Khan





Approximate Bayesian Inference team

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

- Generalized Bayes update
 - Formula for the posterior : non-exponential weights
 - Regret bound

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 - The algorithms : SVA and SVB
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Reminder

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

Reminder

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

where

$$D_{\phi}(
ho||\pi) = \left\{ egin{array}{l} \mathbb{E}_{ heta \sim \pi} \left[\phi \left(rac{\mathrm{d}
ho}{\mathrm{d}\pi}(heta)
ight)
ight] & ext{if }
ho \ll \pi \ +\infty & ext{otherwise,} \end{array}
ight.$$

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

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

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

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

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

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

Formula for ρ^t

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

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

exists, and

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

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

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

•
$$\phi(x) = x^2 - 1$$
,

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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.

omparable 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.

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Theorem

$$\begin{split} \sum_{t=1}^{T} \mathbb{E}_{\theta \sim \rho^{t}}[\ell_{t}(\theta)] &\leq \inf_{\rho \in \mathcal{P}(\Theta)} \Biggl\{ \sum_{t=1}^{T} \mathbb{E}_{\theta \sim \rho}[\ell_{t}(\theta)] \\ &+ \frac{\eta L^{2} T}{\alpha} + \frac{D_{\phi}(\rho||\pi)}{\eta} \Biggr\}. \end{split}$$

Bound for EWA

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

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and the two conditions reduce to:

 $|\ell_t(\theta)| \leq L$ on the support of π .

Bound with χ^2

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but the two conditions reduce to:

$$\int \ell_t(\theta)^2 \pi(\mathrm{d}\theta) \le L^2.$$

- Generalized Bayes update
 - Formula for the posterior : non-exponential weights
 - Regret bound

- Online variational inference
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Motivation



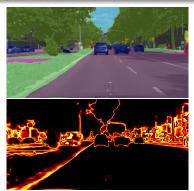
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- proposes a fast algorithm to approximate the posterior,
- applies it to train Deep Neural Networks on CIFAR-10, ImageNet ...
- observation : improved uncertainty quantification.



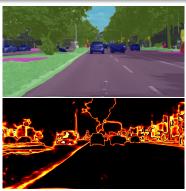
Picture · Roman Bachmann

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Picture: Roman Bachmann.

Objective: provide a theoretical analysis of this algorithm.

Sequential Variational Approximation (SVA)

We restrict ρ to belong to $\mathcal{F} = \{q_{\mu}, \mu \in M\}$ a parametric family. Example : Gaussian distributions.

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FTRL on this set:

$$\mu^t = \operatorname*{arg\,min}_{\mu \in M} \left\{ \sum_{s=1}^{t-1} \mathbb{E}_{\theta \sim q_\mu}[\ell_s(\theta)] + \frac{D_\phi(q_\mu, \pi)}{\eta} \right\}.$$

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Linearization gives :

SVA

$$\mu^t = \operatorname*{arg\,min}_{\mu \in \mathcal{M}} \left\{ \sum_{s=1}^{t-1} \left\langle \mu, \nabla \mathbb{E}_{\theta \sim q_{\mu^s}}[\ell_s(\theta)] \right\rangle + \frac{D_\phi(q_\mu, \pi)}{\eta} \right\}.$$

Streaming Variational Bayes (SVB)

(OGA) can actually be obtained via:

$$heta^t := rg \min_{ heta} \left\{ \sum_{s=1}^{t-1} \left\langle heta,
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OR

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

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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, $\mu = (m, \sigma)$.

SVA:
$$m_{t+1} \leftarrow m_t - \eta s^2 \bar{g}_{m_t}$$
, $g_{t+1} \leftarrow g_t + \bar{g}_{\sigma_t}$, $\sigma_{t+1} \leftarrow h(\eta s g_{t+1}) s$,
SVB: $m_{t+1} \leftarrow m_t - \eta \sigma_t^2 \bar{g}_{m_t}$, $\sigma_{t+1} \leftarrow \sigma_t h(\eta \sigma_t \bar{g}_{\sigma_t})$

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

$$ar{m{g}}_{m_t} = rac{\partial}{\partial m{m}} \mathbb{E}_{ heta \sim \pi_{m_t, \sigma_t}} [\ell_t(heta)], \ ar{m{g}}_{\sigma_t} = rac{\partial}{\partial \sigma} \mathbb{E}_{ heta \sim \pi_{m_t, \sigma_t}} [\ell_t(heta)].$$

Two assumptions :

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

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

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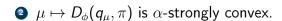
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 $\mathbf{Q} \quad \mu \mapsto D_{\phi}(q_{\mu}, \pi) \text{ is } \alpha\text{-strongly convex.}$

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

Theorem

Under the previous assumptions SVA leads to

$$\sum_{t=1}^T \mathbb{E}_{ heta \sim q_{\mu_t}}[\ell_t(heta)]$$

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

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Application to Gaussian approximation with KL:

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

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

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

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

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

Test on a simulated dataset

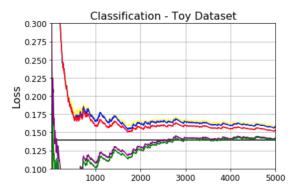


Figure – Average cumulative losses on different datasets for classification and regression tasks with OGA (yellow), OGA-EL (red), SVA (blue), SVB (purple) and NGVI (green).

Test on the Breast dataset

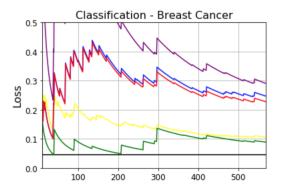


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Uses exponential family approximations $\{q_{\mu}, \mu \in M\}$ where m is the mean parameter. Denoting λ the natural parameter (with $\lambda = F(\mu)$),

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



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

The algorithms : SVA and SV Regret bounds

Thank you!