

# Regret bounds for online variational inference

Pierre Alquier



Center for  
Advanced Intelligence Project

Mathematics of Online Decision Making  
Simons Institute for the Theory of Computing, Berkeley  
Oct. 29, 2020



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

Badr-Eddine  
Chérif-Abdellatif



Emtiyaz Khan

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



# Motivation



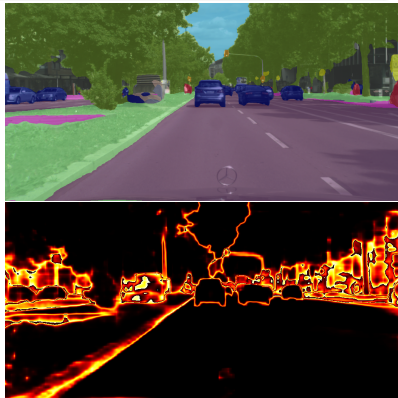
K. Osawa, S. Swaroop, A. Jain, R. Eschenhagen, R. E. Turner, R. Yokota, M. E. Khan (2019).  
*Practical Deep Learning with Bayesian Principles*. NeurIPS.

# Motivation



K. Osawa, S. Swaroop, A. Jain, R. Eschenhagen, R. E. Turner, R. Yokota, M. E. Khan (2019).  
*Practical Deep Learning with Bayesian Principles*. NeurIPS.

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



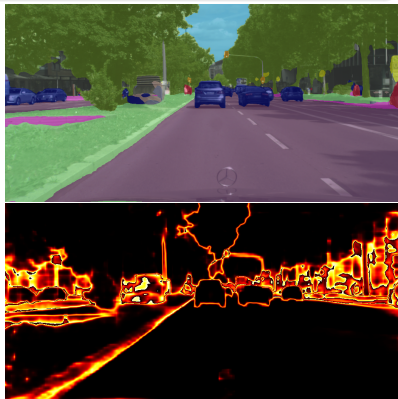
Picture : Roman Bachmann.

# Motivation



K. Osawa, S. Swaroop, A. Jain, R. Eschenhagen, R. E. Turner, R. Yokota, M. E. Khan (2019).  
*Practical Deep Learning with Bayesian Principles*. NeurIPS.

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



Picture : Roman Bachmann.

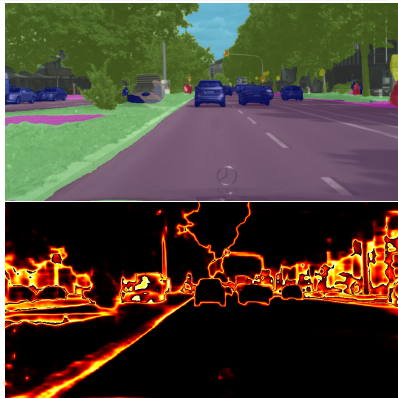
**Objective** : provide a theoretical analysis of this algorithm.

# Motivation



K. Osawa, S. Swaroop, A. Jain, R. Eschenhagen, R. E. Turner, R. Yokota, M. E. Khan (2019).  
*Practical Deep Learning with Bayesian Principles*. NeurIPS.

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



Picture : Roman Bachmann.

**Objective** : provide a theoretical analysis of this algorithm.

**First step** : simplified versions.

# Bayesian inference and variational approximations

## (Generalized) Bayesian inference

$$\pi(\theta|x_1, y_1, \dots, x_n, y_n) \propto \exp \left[ -\eta \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] \pi(\theta)$$

# Bayesian inference and variational approximations

## (Generalized) Bayesian inference

$$\pi(\theta | x_1, y_1, \dots, x_n, y_n) \propto \exp \left[ -\eta \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] \pi(\theta)$$

It is well known that

$$\begin{aligned} & \pi(\cdot | x_1, y_1, \dots, x_n, y_n) \\ &= \arg \min_p \left\{ \mathbb{E}_{\theta \sim p} \left[ \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] + \frac{KL(p, \pi)}{\eta} \right\}. \end{aligned}$$



# Bayesian inference and variational approximations

## (Generalized) Bayesian inference

$$\pi(\theta | x_1, y_1, \dots, x_n, y_n) \propto \exp \left[ -\eta \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] \pi(\theta)$$

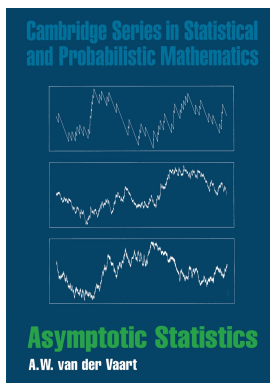
It is well known that

$$\begin{aligned} \pi(\cdot | x_1, y_1, \dots, x_n, y_n) \\ = \arg \min_p \left\{ \mathbb{E}_{\theta \sim p} \left[ \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] + \frac{KL(p, \pi)}{\eta} \right\}. \end{aligned}$$

## Variational approximation

$$\pi_n^{\text{approx}}(\theta) := \arg \min_{p \in \mathcal{F}} \left\{ \mathbb{E}_{\theta \sim p} \left[ \sum_{i=1}^n \ell(f_\theta(x_i), y_i) \right] + \frac{KL(p, \pi)}{\eta} \right\}.$$

# Consistency of Bayesian estimators



- in order to ensure consistency at rate  $r_n$ , many conditions including the prior mass condition :

$$\log \pi(B_{r_n}) \geq nr_n, \text{ where}$$

$$B_r = \left\{ \theta : \frac{\sum_{i=1}^n [\ell(f_\theta(x_i), y_i) - \ell(f_{\theta^*}(x_i), y_i)]}{n} \leq r \right\}$$

- note that this condition implies, for  $p = \pi$  restricted to  $B_{r_n}$ ,

$$\mathbb{E}_{\theta \sim p} \left[ \frac{\sum_{i=1}^n \ell(f_\theta(x_i), y_i)}{n} \right] + \frac{KL(p, \pi)}{n} \leq \frac{\sum_{i=1}^n \ell(f_{\theta^*}(x_i), y_i)}{n} + 2r_n.$$

# Consistency of variational approximations



P. Alquier, J. Ridgway, N. Chopin (2016). On the Properties of Variational Approximations of Gibbs Posteriors. *JMLR*.



P. Alquier & J. Ridgway (2020). Concentration of tempered posteriors and of their variational approximations. *The Annals of Statistics*.



Y. Yang, D. Pati & A. Bhattacharya (2020).  $\alpha$ -Variational Inference with Statistical Guarantees. *The Annals of Statistics*.



F. Zhang & C. Gao (2020). Convergence Rates of Variational Posterior Distributions. *The Annals of Statistics*.

These papers show that the variational approximation of the posterior in  $\mathcal{F}$  concentrates at the rate  $r_n$  if there is  $\rho \in \mathcal{F}$  such that

$$\mathbb{E}_{\theta \sim p} \left[ \frac{\sum_{i=1}^n \ell(f_{\theta}(x_i), y_i)}{n} \right] + \frac{KL(p, \pi)}{n} \leq \frac{\sum_{i=1}^n \ell(f_{\theta^*}^*(x_i), y_i)}{n} + 2r_n.$$

**Question** : can this be extended to the online setting?

# Bayesian learning and variational inference (VI)

$$\pi_{t+1}(\theta) := \pi(\theta|x_1, y_1, \dots, x_t, y_t) \propto \exp\left(-\eta \sum_{s=1}^t \ell_s(\theta)\right) \pi(\theta).$$

# Bayesian learning and variational inference (VI)

$$\pi_{t+1}(\theta) := \pi(\theta|x_1, y_1, \dots, x_t, y_t) \propto \exp\left(-\eta \sum_{s=1}^t \ell_s(\theta)\right) \pi(\theta).$$

Formula for the online update of  $\pi_{t+1}$  :

$$\pi_{t+1}(\theta) \propto \exp(-\eta \ell_t(\theta)) \pi_t(\theta).$$

# Bayesian learning and variational inference (VI)

$$\pi_{t+1}(\theta) := \pi(\theta|x_1, y_1, \dots, x_t, y_t) \propto \exp\left(-\eta \sum_{s=1}^t \ell_s(\theta)\right) \pi(\theta).$$

Formula for the online update of  $\pi_{t+1}$  :

$$\pi_{t+1}(\theta) \propto \exp(-\eta \ell_t(\theta)) \pi_t(\theta).$$

**Q1** : can we similarly define a sequential update for a variational approximation ?

# Regret bounds for Bayesian inference

Theorem (classical result) for bounded loss  $\ell \leq B$

Bayes update leads to

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim \pi_t} [\ell_t(\theta)]$$

$$\leq \inf_q \left\{ \sum_{t=1}^T \mathbb{E}_{\theta \sim q} [\ell_t(\theta)] + \frac{\eta B^2 T}{8} + \frac{KL(q, \pi)}{\eta} \right\}.$$

# Regret bounds for Bayesian inference

Theorem (classical result) for bounded loss  $\ell \leq B$

Bayes update leads to

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim \pi_t} [\ell_t(\theta)] \leq \inf_q \left\{ \sum_{t=1}^T \mathbb{E}_{\theta \sim q} [\ell_t(\theta)] + \frac{\eta B^2 T}{8} + \frac{KL(q, \pi)}{\eta} \right\}.$$

Under the prior mass condition with  $r_T = \sqrt{\frac{\log T}{T}}$  and  $\eta \sim r_T$ ,

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim \pi_t} [\ell_t(\theta)] \leq \inf_{\theta} \sum_{t=1}^T \ell_t(\theta) + \mathcal{O}(\sqrt{T \log(T)}).$$



# Regret bounds for Bayesian inference

Theorem (classical result) for bounded loss  $\ell \leq B$

Bayes update leads to

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim \pi_t} [\ell_t(\theta)] \leq \inf_q \left\{ \sum_{t=1}^T \mathbb{E}_{\theta \sim q} [\ell_t(\theta)] + \frac{\eta B^2 T}{8} + \frac{KL(q, \pi)}{\eta} \right\}.$$

Under the prior mass condition with  $r_T = \sqrt{\frac{\log T}{T}}$  and  $\eta \sim r_T$ ,

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim \pi_t} [\ell_t(\theta)] \leq \inf_{\theta} \sum_{t=1}^T \ell_t(\theta) + \mathcal{O}(\sqrt{T \log(T)}).$$

Q2 : can we derive similar results for online VI ?

# Online gradient algorithm (OGA)

Given

- a set of predictors  $\{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$ , e.g  $f_\theta(x) = \langle \theta, x \rangle$ ,
- an initial guess  $\theta_1$ ,

$$\hat{y}_t = f_{\theta_t}(x_t) \quad \text{and} \quad \theta_{t+1} = \theta_t - \eta \nabla_{\theta} \ell(f_{\theta_t}(x_t), y_t).$$

# Online gradient algorithm (OGA)

Given

- a set of predictors  $\{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$ , e.g  $f_\theta(x) = \langle \theta, x \rangle$ ,
- an initial guess  $\theta_1$ ,

$$\hat{y}_t = f_{\theta_t}(x_t) \quad \text{and} \quad \theta_{t+1} = \theta_t - \eta \nabla_{\theta} \ell_t(\theta_t).$$

# Online gradient algorithm (OGA)

Given

- a set of predictors  $\{f_\theta, \theta \in \Theta \subset \mathbb{R}^d\}$ , e.g  $f_\theta(x) = \langle \theta, x \rangle$ ,
- an initial guess  $\theta_1$ ,

$$\hat{y}_t = f_{\theta_t}(x_t) \quad \text{and} \quad \theta_{t+1} = \theta_t - \eta \nabla_{\theta} \ell_t(\theta_t).$$

Note that  $\theta_{t+1}$  can be obtained by :

- 1  $\min_{\theta} \left\{ \left\langle \theta, \sum_{s=1}^t \nabla_{\theta} \ell_s(\theta_s) \right\rangle + \frac{\|\theta - \theta_1\|^2}{2\eta} \right\},$
- 2  $\min_{\theta} \left\{ \left\langle \theta, \nabla_{\theta} \ell_t(\theta_t) \right\rangle + \frac{\|\theta - \theta_t\|^2}{2\eta} \right\}.$

# Two options for online VI

Parametric VI :  $\mathcal{F} = \{q_\mu, \mu \in M\}$ .

# Two options for online VI

Parametric VI :  $\mathcal{F} = \{q_\mu, \mu \in M\}$ .

- 1 Sequential Variational Approximation (SVA) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \sum_{s=1}^t \nabla_{\theta} \ell_s(\theta_s) \right\rangle + \frac{\|\theta - \theta_1\|^2}{2\eta} \right\},$$

- 2 Streaming Variational Bayes (SVB) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \nabla_{\theta} \ell_t(\theta_t) \right\rangle + \frac{\|\theta - \theta_t\|^2}{2\eta} \right\},$$

# Two options for online VI

Parametric VI :  $\mathcal{F} = \{q_\mu, \mu \in M\}$ .

- 1 Sequential Variational Approximation (SVA) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \sum_{s=1}^t \nabla_{\theta} \ell_s(\theta_s) \right\rangle + \frac{\|\theta - \theta_1\|^2}{2\eta} \right\},$$

$$\mu_{t+1} = \arg \min_{\mu} \left\{ \left\langle \mu, \sum_{s=1}^t \nabla_{\mu} \mathbb{E}_{\theta \sim q_{\mu_s}} [\ell_s(\theta)] \right\rangle + \frac{KL(q_{\mu}, \pi)}{\eta} \right\}.$$

- 2 Streaming Variational Bayes (SVB) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \nabla_{\theta} \ell_t(\theta_t) \right\rangle + \frac{\|\theta - \theta_t\|^2}{2\eta} \right\},$$

# Two options for online VI

Parametric VI :  $\mathcal{F} = \{q_\mu, \mu \in M\}$ .

- 1 Sequential Variational Approximation (SVA) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \sum_{s=1}^t \nabla_{\theta} \ell_s(\theta_s) \right\rangle + \frac{\|\theta - \theta_1\|^2}{2\eta} \right\},$$

$$\mu_{t+1} = \arg \min_{\mu} \left\{ \left\langle \mu, \sum_{s=1}^t \nabla_{\mu} \mathbb{E}_{\theta \sim q_{\mu_s}} [\ell_s(\theta)] \right\rangle + \frac{KL(q_{\mu}, \pi)}{\eta} \right\}.$$

- 2 Streaming Variational Bayes (SVB) :

$$\theta_{t+1} = \arg \min_{\theta} \left\{ \left\langle \theta, \nabla_{\theta} \ell_t(\theta_t) \right\rangle + \frac{\|\theta - \theta_t\|^2}{2\eta} \right\},$$

$$\mu_{t+1} = \arg \min_{\mu} \left\{ \left\langle \mu, \nabla_{\mu} \mathbb{E}_{\theta \sim q_{\mu_t}} [\ell_t(\theta)] \right\rangle + \frac{KL(q_{\mu}, q_{\mu_t})}{\eta} \right\}.$$



# SVA & SVB are tractable, and not equivalent

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

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

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

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

# Theoretical analysis of SVA

## Theorem 1

Under convexity and  $L$ -Lipschitz assumption on the loss, under  $\alpha$ -strong convexity assumption on the KL term, SVA leads to

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

# Theoretical analysis of SVA

## Theorem 1

Under convexity and  $L$ -Lipschitz assumption on the loss, under  $\alpha$ -strong convexity assumption on the KL term, SVA leads to

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

Application to Gaussian approximation leads to

$$\sum_{t=1}^T \mathbb{E}_{\theta \sim q_{\mu_t}} [\ell_t(\theta)] \leq \inf_{\theta} \sum_{t=1}^T \ell_t(\theta) + (1 + o(1)) \frac{2L}{\alpha} \sqrt{dT \log(T)}.$$

# Comments on the assumptions

The assumptions :

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

# Comments on the assumptions

The 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.

# Comments on the assumptions

The 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** : Lipschitz : in our paper ; convex :



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

# Comments on the assumptions

The 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** : Lipschitz : in our paper ; convex :



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

- 2  $\mu \mapsto KL(q_\mu, \pi)$  is  $\alpha$ -strongly convex ?

# Comments on the assumptions

The 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** : Lipschitz : in our paper ; convex :



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

- 2  $\mu \mapsto KL(q_\mu, \pi)$  is  $\alpha$ -strongly convex ?

→ True for many examples, for example when  $q_\mu$  and  $\pi$  are Gaussian (with upper-bounded variance).



# Theoretical analysis of SVB

## Theorem 2

Using **Gaussian approximations**, assuming the loss is convex,  $L$ -Lipschitz and the parameter space bounded (diameter =  $D$ ), SVB with adequate  $\eta$  leads to

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

# Theoretical analysis of SVB

## Theorem 2

Using **Gaussian approximations**, assuming the loss is convex,  $L$ -Lipschitz and the parameter space bounded (diameter =  $D$ ), SVB with adequate  $\eta$  leads to

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

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

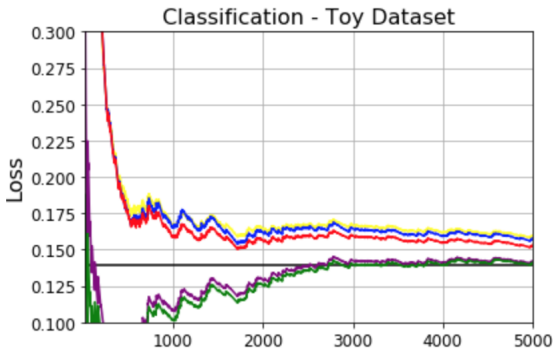


Figure – Average cumulative losses on different datasets for classification and regression tasks with OGA (yellow), OGA-EL (red), SVA (blue), SVB (purple) and NGVI (green).

# Test on the Breast dataset

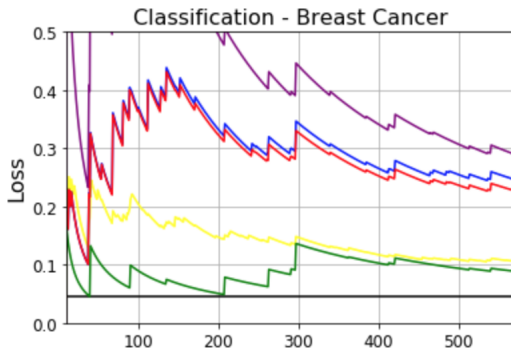


Figure – Average cumulative losses on different datasets for classification and regression tasks with OGA (yellow), OGA-EL (red), SVA (blue), SVB (purple) and NGVI (green).

# Open questions

# Open questions

- 1 Analysis of SVB in the general case.

# Open questions

- 1 Analysis of SVB in the general case.
- 2 Analysis of the uncertainty quantification.

# Open questions

- 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...



# Open questions

- 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  $\lambda$  the natural parameter (with  $\lambda = F(\mu)$ ),

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



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

Thank you !