Theoretical study of variational inference

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RIKEN AIP Seminar
February 20, 2020

Notations

Assume that we observe $X_1, \ldots, X_n$ i.i.d from P_{θ_0} in a model $\{P_\theta, \theta \in \Theta\}$ dominated by Q : $\frac{\mathrm{d}P_\theta}{\mathrm{d}Q} = p_\theta$. Prior π on Θ.

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The tempered posterior - $0 < \alpha < 1$

$$\pi_{n,\alpha}(\mathrm{d}\theta) \propto [L_n(\theta)]^\alpha \pi(\mathrm{d}\theta).$$

Various reasons to use a tempered posterior

- Easier to sample from

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- Theoretical analysis easier

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For these reasons, in the past 20 years, many methods targeting an approximation of $\pi_{n,\alpha}$ became popular : **ABC**, **EP algorithm**, variational inference...

Variational approximations : definitions

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- parametric approximation

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- mean-field approximation, $\Theta = \Theta_1 \times \Theta_2$ and

$$\mathcal{F} = \left\{\rho : \rho(\mathrm{d}\theta) = \rho_1(\mathrm{d}\theta_1) \times \rho_2(\mathrm{d}\theta_2)\right\}.$$

Evidence Lower BOund (ELBO)

Note that :

$$\begin{aligned}\tilde{\pi}_{n,\alpha} &= \arg\min_{\rho\in\mathcal{F}} KL(\rho, \pi_{n,\alpha}) \\ &= \arg\min_{\rho\in\mathcal{F}} \underbrace{\left\{ -\alpha \int \frac{1}{n} \sum_{i=1}^{n} \log p_\theta(X_i)\rho(\mathrm{d}\theta) + KL(\rho, \pi) \right\}}_{-\mathrm{ELBO}(\rho)}.\end{aligned}$$

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So we have the equivalent definition :

$$\tilde{\pi}_{n,\alpha} := \arg\max_{\rho \in \mathcal{F}} \ \mathrm{ELBO}(\rho).$$

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Section 3 will address the following question :

Are there efficient algorithms to (provably) compute $\tilde{\pi}_{n,\alpha}$?

We will see that fast algorithms from online optimization can be used to compute variational approximations.

Tools for the consistency of VB

The α-Rényi divergence for $\alpha \in (0,1)$

$$D_\alpha(P,R) = \frac{1}{\alpha - 1} \log \int (\mathrm{d}P)^\alpha (\mathrm{d}R)^{1-\alpha}.$$

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All the properties derived in :

T. Van Erven & P. Harremos. Rényi divergence and Kullback-Leibler divergence. *IEEE Transactions on Information Theory*, 2014.

Among others, for $1/2 \leq \alpha$, link with Hellinger and Kullback :

$$\mathcal{H}^2(P,R) \leq D_\alpha(P,R) \xrightarrow[\alpha\nearrow 1]{} KL(P,R).$$

Notions of Concentration and Consistency

Concentration at rate r_n

$$\rho\left(\theta \in \Theta \;/\; D_\alpha(P_\theta, P_{\theta_0}) > M_n r_n\right) \xrightarrow[n\to+\infty]{} 0$$

in probability as $n \to +\infty$ for any $M_n \to +\infty$.

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Consistency implies concentration of the Bayesian distribution.

Technical condition for posterior concentration

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Prior mass condition for concentration of tempered posteriors

The rate (r_n) is such that

$$\pi[\mathcal{B}(r_n)] \geq e^{-nr_n}$$

where $\mathcal{B}(r) = \{\theta \in \Theta : KL(P_{\theta^0}, P_\theta) \leq r\}$.

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Prior mass condition for concentration of Variational Bayes

The rate (r_n) is such that there exists $\rho_n \in \mathcal{F}$ such that

$$\int KL(P_{\theta^0}, P_\theta)\rho_n(\mathrm{d}\theta) \leq r_n, \text{ and } KL(\rho_n, \pi) \leq nr_n.$$

What do we know about $\pi_{n,\alpha}$?

Theorem, variant of (Bhattacharya, Pati & Yang)

Under the prior mass condition, for any $\alpha \in (0,1)$,

$$\mathbb{E}\left[\int D_\alpha(P_\theta, P_{\theta_0})\pi_{n,\alpha}(\mathrm{d}\theta)\right] \leq \frac{1+\alpha}{1-\alpha} r_n.$$

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Extension of previous result to VB

Theorem (Alquier & Ridgway)

Under the extended prior mass condition, for any $\alpha \in (0,1)$,

$$\mathbb{E}\left[\int D_\alpha(P_\theta, P_{\theta_0})\tilde{\pi}_{n,\alpha}(\mathrm{d}\theta)\right] \leq \frac{1+\alpha}{1-\alpha} r_n.$$

P. Alquier & J. Ridgway. Concentration of tempered posteriors and of their variational approximations. *The Annals of Statistics*, 2019.

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Under a similar condition, for any $\alpha \in (0,1)$,

$$\mathbb{E}\left[\int D_\alpha(P_\theta, Q)\tilde{\pi}_{n,\alpha}(\mathrm{d}\theta)\right] \leq \frac{\alpha}{1-\alpha}\inf_\theta KL(Q, P_\theta) + \frac{1+\alpha}{1-\alpha} r_n.$$

Nonparametric regression & Deep Neural Networks

Nonparametric regression

- $X_i \sim \mathcal{U}([-1,1]^d)$,
- $Y_i = f_0(X_i) + \zeta_i$,
- $\zeta_i \sim \mathcal{N}(0, \sigma^2)$.

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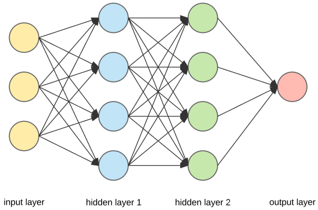

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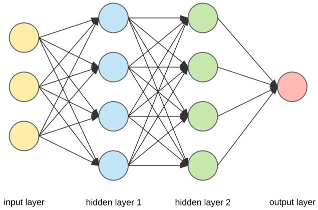

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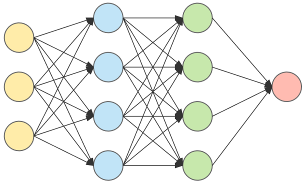

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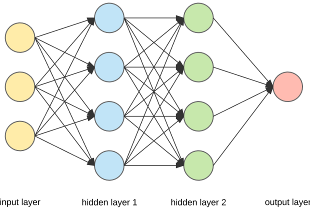

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- $f_\theta(x) = A_L \rho(A_{L-1} ... \rho(A_1 x + b_1) + ... + b_{L-1}) + b_L$.

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Theorem (C.-A.)

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$$\mathbb{E}\left[\int \|f_\theta - f_0\|_2^2 \tilde{\pi}_{n,\alpha}(d\theta)\right] \leq \frac{2}{1-\alpha} \inf_{\theta^*} \|f_{\theta^*} - f_0\|_2^2 + \frac{2}{1-\alpha}\left(1 + \frac{\sigma^2}{\alpha}\right) r_n^{S,L,D},$$

with $\quad r_n^{S,L,D} \sim \frac{S \log(nL/S)}{n} \vee \frac{LS \log D}{n}$.

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C.-A.. Convergence Rates of Variational Inference in Sparse Deep Learning. *Preprint Arxiv*, 2019.

More extensions

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3. approximation based on another distance, for example :

$$\tilde{\pi}_{n,\alpha} := \arg\min_{\rho \in \mathcal{F}} \mathcal{W}(\rho, \pi_{n,\alpha}) \text{ (Wasserstein distance)},$$

J. Huggins, T. Campbell, M. Kasprzak & T. Broderick. Practical bounds on the error of Bayesian posterior approximations : a nonasymptotic approach. *Preprint arXiv*, 2018.

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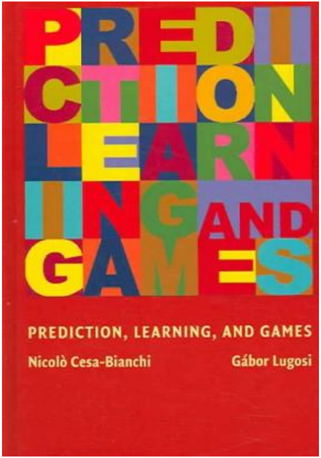
Objective : make sure that we learn to predict well **as fast as possible**. Keep

$$\sum_{t=1}^{T} \ell(x_t; \theta_t)$$

as small as possible for any T, **without stochastic assumptions on the data.**

Reference


PREDICTION LEARNING AND GAMES
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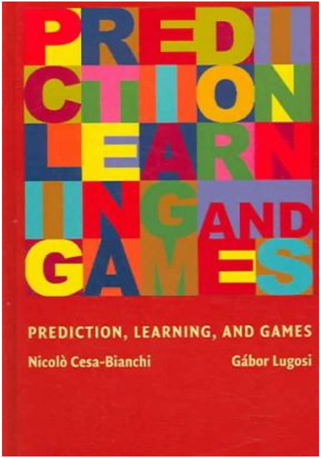

The regret :

$$\mathrm{R}(T) = \sum_{t=1}^{T} \ell(x_t;\theta_t) - \inf_{\theta\in\Theta} \sum_{t=1}^{T} \ell(x_t;\theta).$$

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Algorithm 2 Exponentially Weighted Aggregation

1: **for** $t = 1, 2, \dots$ **do**
2: $\quad \theta_t = \mathbb{E}_{\theta \sim p_t}[\theta]$,
3: $\quad x_t$ revealed, update $p_{t+1}(\mathrm{d}\theta) = \frac{[p_\theta(x_t)]^\alpha p_t(\mathrm{d}\theta)}{\int [p_\vartheta(x_t)]^\alpha p_t(\mathrm{d}\vartheta)}$.
4: **end for**

EWA strategy / multipicative update...

- learning rate $\alpha > 0$.
- initialize $p_1 = \pi$ (the prior).
- loss $\ell(x;\theta) = -\log p_\theta(x)$.

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2: $\theta_t = \mathbb{E}_{\theta \sim p_t}[\theta]$,
3: x_t revealed, update $p_{t+1}(\mathrm{d}\theta) = \frac{[p_\theta(x_t)]^\alpha p_t(\mathrm{d}\theta)}{\int [p_\vartheta(x_t)]^\alpha p_t(\mathrm{d}\vartheta)}$.
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- EWA algorithm has strong theoretical guarantees.
- We recover the tempered posterior $p_t = \pi_{t,\alpha}$.

A regret bound for EWA

From now, $\theta \mapsto [-\log p_\theta(x_t)]$ is convex + bounded : $|\cdot| \leq C$.

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Theorem

$$\sum_{t=1}^{T}[-\log p_{\theta_t}(x_t)] \leq \inf_p \left\{ \sum_{t=1}^{T} \mathbb{E}_{\theta\sim p}[-\log p_\theta(x_t)] + \frac{\alpha C^2 T}{2} + \frac{KL(p,\pi)}{\alpha} \right\}.$$

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Under similar assumptions than in the batch case, that is, the prior gives enough mass to relevant θ, and $\alpha \sim 1/\sqrt{T}$,

$$\sum_{t=1}^{T}[-\log p_{\theta_t}(x_t)] \leq \inf_{\theta\in\Theta} \sum_{t=1}^{T}[-\log p_\theta(x_t)] + \mathrm{cst.}\sqrt{T}$$

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$$\mathbb{E}\left[KL\left(Q, P_{\hat{\theta}_T}\right)\right] \leq \inf_{\theta\in\Theta} KL\left(Q, P_{\theta}\right) + \frac{\mathrm{cst}}{\sqrt{T}}.$$

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Drawback : θ_t is not tractable !

Variational approximations of EWA

B.-E. Chérief-Abdellatif, P. Alquier & M. E. Khan. A Generalization Bound for Online Variational Inference. *Proceedings of ACML*, 2019.

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Parametric variational approximation :

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

Objective : propose a way to update $\mu_t \to \mu_{t+1}$ so that q_{μ_t} leads to similar performances as p_t in EWA...

SVA and SVB strategies

Algorithm 3 SVA (Sequential Variational Approximation)

1: **for** $t = 1, 2, \ldots$ **do**
2: $\quad \theta_t = \mathbb{E}_{\theta \sim q_{\mu_t}}[\theta]$,
3: $\quad x_t$ revealed, update

$$\mu_{t+1} = \arg\min_{\mu \in M} \left\{ \sum_{i=1}^{t} \mathbb{E}_{\theta \sim q_\mu}[-\log p_\theta(x_i)] + \frac{KL(q_\mu, \pi)}{\alpha} \right\}.$$

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SVB (Streaming Variational Bayes) has update

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NGVI strategy

NGVI (Natural Gradient Variational Inference) : fix some $\beta > 0$,

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M. E. Khan & W. Lin. Conjugate-computation variational inference : Converting variational inference in non-conjugate models to inferences in conjugate models. *AISTAT*, 2017.

An example : SVB with Gaussian approximations

As an example, assume that $\theta \in \mathbb{R}^d$, the prior is $\pi = \mathcal{N}(0, s^2 I)$ and that we use the variational approximation family : $q_\mu = q_{m,\sigma} = \mathcal{N}\left(m, \begin{pmatrix} \sigma_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_d^2 \end{pmatrix}\right)$.

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In this case, the update in SVB is :

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\begin{aligned}
m_{t+1} &= m_t - \alpha\sigma_t^2 \odot \nabla_{m=m_t} \mathbb{E}_{\theta\sim q_{m,\sigma_t}}[-\log p_\theta(x_t)] \\
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where $\odot$ means "componentwise multiplication" and $h(x) = \sqrt{1+x^2} - x$ is also applied componentwise.

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where $\odot$ means "componentwise multiplication" and $h(x) = \sqrt{1+x^2} - x$ is also applied componentwise. We also have explicit formulas for SVA and NGVI (see the paper).

A regret bound for SVA

Theorem (C.A., Alquier & Khan)

Assume that $\mu \mapsto \mathbb{E}_{\theta \sim q_\mu}[-\log p_\theta(x_t)]$ is L-Lipschitz and convex.

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A regret bound for SVA

Theorem (C.A., Alquier & Khan)

Assume that $\mu \mapsto \mathbb{E}_{\theta\sim q_\mu}[-\log p_\theta(x_t)]$ is L-Lipschitz and convex. Assume that $\mu \mapsto KL(q_\mu, \pi)$ is γ-strongly convex. Then SVA satisfies :

$$\sum_{t=1}^{T}[-\log p_{\theta_t}(x_t)]$$

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For SVB : some results in the Gaussian case. For NGVI : we were not able to derive regret bounds until now.

Test on the Forest Cover Type dataset

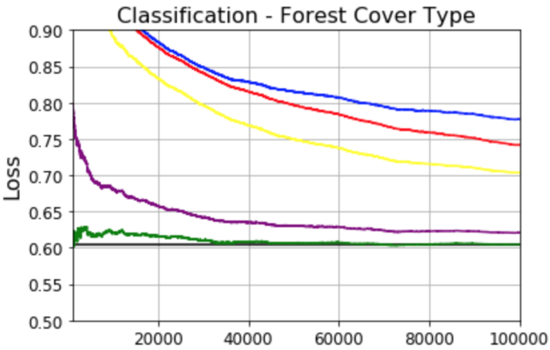
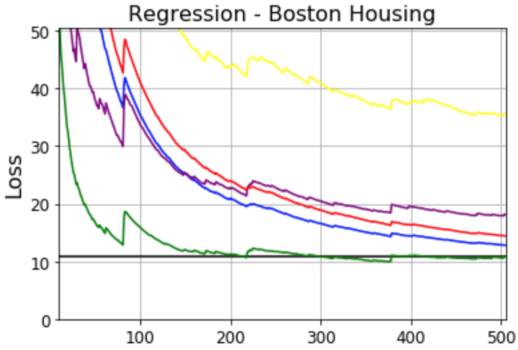


Figure – Average cumulative losses on different datasets for classification and regression tasks with OGA (yellow), OGA-EL (red), SVA (blue), SVB (purple) and NGVI (green).

Test on the Boston Housing dataset



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Conclusions

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1. Using online-to-batch conversion, we now have algorithms for variational inference with provable statistical properties after a finite number of steps.
2. SVA, SVB competitive with OGA (online gradient algorithm, "non-Bayesian").
3. NGVI is the best method on all datasets. Its theoretical analysis is thus an important open problem. Cannot be done with our current techniques (using natural parameters in exponential models lead to non-convex objectives).

Thank you !