

Séminaire de Calcul Scientifique du CERMICS



Variational Approximations in Machine Learning : Theory and Applications

Pierre Alquier (ENSAE)

25 juin 2018

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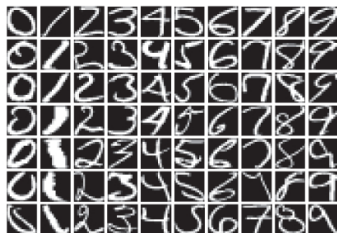
CERMICS - Monday, June 25, 2018

Learning vs. estimation

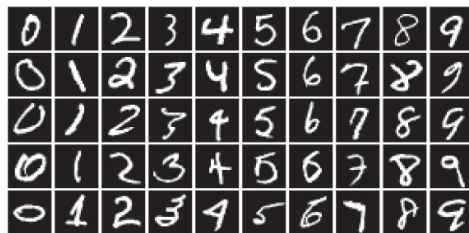
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(a) USPS



(b) MNIST

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$$\int R(\theta) \hat{\rho}_\lambda(d\theta) \leq \inf_{\rho} \left[\int R(\theta) \rho(d\theta) + \frac{1}{\lambda} \mathcal{K}(\rho, \pi) \right] + o(1).$$

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Usually $o(1)$ is explicit, λ is some tuning-parameter to be calibrated (constrained to some range by theory), and $\hat{\rho}_\lambda$ is the “Gibbs posterior”

$$\hat{\rho}_\lambda(d\theta) \propto \exp[-\lambda r(\theta)] \pi(d\theta).$$

Outline of the talk

- 1 Introduction : Learning with PAC-Bayes Bounds
 - A PAC-Bayesian Bound for Batch Learning
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- 2 Variational Approximation of the Posterior
 - Analysis of VB approximations of Gibbs posteriors
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Catoni's bound for batch learning

Theorem [Catoni 2007]

$$\begin{aligned} \forall \lambda > 0, \quad \mathbb{P} \left\{ \int R(\theta) \hat{\rho}_\lambda(d\theta) \right. \\ \left. \leq \inf_{\rho} \left[\int R(\theta) \rho(d\theta) + \frac{\lambda B^2}{n} + \frac{2}{\lambda} \left[\mathcal{K}(\rho, \pi) + \log \left(\frac{2}{\varepsilon} \right) \right] \right] \right\} \\ \geq 1 - \varepsilon. \end{aligned}$$

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improving on seminal work :

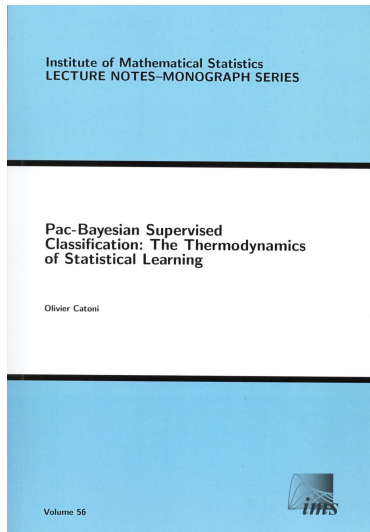


Shawe-Taylor, J. & Williamson, R. C. (1997). A PAC Analysis of a Bayesian Estimator. *COLT'97*.



McAllester, D. A. (1998). Some PAC-Bayesian Theorems. *COLT'98*.

Reference



Application : finite set of predictors $\theta_1, \dots, \theta_M$

With π the uniform distribution on $\{\theta_1, \dots, \theta_M\}$ we get

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$$\mathcal{R} = \sum_{t=1}^T \ell(Y_t, \hat{Y}_t) - \inf_{\theta} \sum_{t=1}^T \ell(Y_t, f_{\theta}(X_t)),$$

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PAC-Bayesian bound for online learning

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$$\hat{\rho}_{\lambda,t}(\mathrm{d}\theta) \propto \exp[-\lambda r_{t-1}(\theta)] \pi(\mathrm{d}\theta) \text{ and } \hat{Y}_t = \int f_{\theta}(X_t) \hat{\rho}_{\lambda,t}(\mathrm{d}\theta).$$

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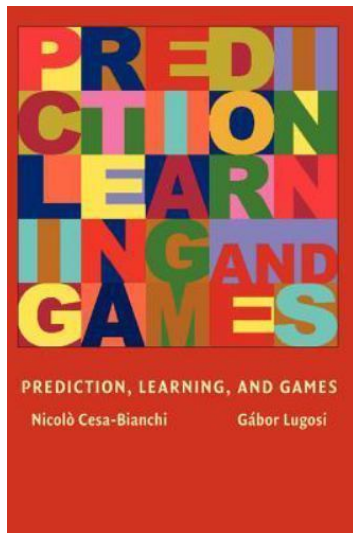
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Theorem [Consequence of Audibert, 2006]

$$\sum_{t=1}^T \ell(Y_t, \hat{Y}_t) \leq \inf_{\rho} \left\{ \int \sum_{t=1}^T \ell(Y_t, f_{\theta}(X_t)) \rho(\mathrm{d}\theta) + \frac{\lambda T B^2}{2} + \frac{\mathcal{K}(\rho, \pi)}{\lambda} \right\}.$$

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Posterior and variants

The posterior :

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Tempered posterior (or fractional posterior), for $0 < \alpha \leq 1$:

$$\begin{aligned}\pi_\alpha(\theta|X_1^n) &\propto \exp(-\alpha r_n(\theta))\pi(\theta) \\ &\propto L(\theta|X_1^n)^\alpha \pi(\theta).\end{aligned}$$

Various reasons to use a tempered posterior

- easier to sample from.



G. Behrens, N. Friel & M. Hurn. (2012). Tuning tempered transitions. *Statistics and Computing*.

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- theoretical analysis easier



A. Bhattacharya, D. Pati & Y. Yang (2016). Bayesian fractional posteriors. *Preprint arxiv :1611.01125*.

PAC-Bayesian inequality for the tempered posterior

(Based on [Bhattacharya, D. Pati & Y. Yang, 2016]).

Theorem [Alquier & Ridgway, 2017]

For any $\alpha \in (1/2, 1)$,

$$\begin{aligned} \mathbb{E} \left[\int h^2(P_\theta, P_{\theta_0}) \pi_\alpha(d\theta | X_1^n) \right] \\ \leq \inf_{\rho} \left\{ \frac{\alpha}{1-\alpha} \int \mathcal{K}(P_{\theta_0}, P_\theta) \rho(d\theta) + \frac{\mathcal{K}(\rho, \pi)}{n(1-\alpha)} \right\}. \end{aligned}$$

Concentration of the tempered posterior

$$\mathcal{B}(r) = \{\theta \in \Theta : \mathcal{K}(P_{\theta_0}, P_{\theta})\}.$$

Corollary

For any sequence (ε_n) such that

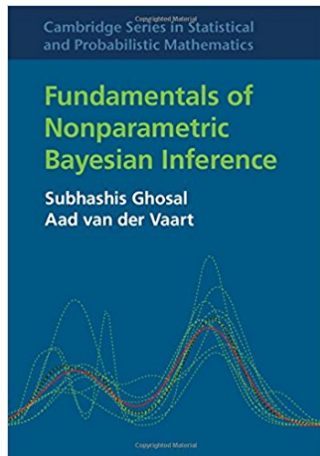
$$-\log \pi[B(r_n)] \leq n\varepsilon_n$$

we have

$$\mathbb{E} \left[\int h^2(P_{\theta}, P_{\theta_0}) \pi_{\alpha}(d\theta | X_1^n) \right] \leq \frac{1 + \alpha}{1 - \alpha} \varepsilon_n.$$

Reference

The (more classical) case $\alpha = 1$ is covered in depth in :



In Bayesian statistics :



Computations? A natural idea : MCMC methods

For the Gibbs posterior :

In Bayesian statistics :



1. Introduction

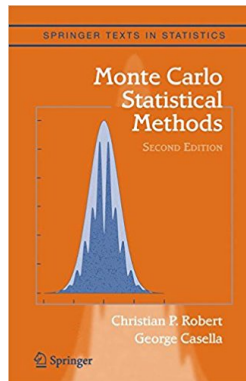
In recent years a great deal of attention has been devoted to learning in high-dimensional models under the sparsity scenario. This typically assumes that, in addition to the sample, we have a finite dictionary of very large cardinality such that a small set of its elements provides a nearly complete description of the underlying model. Here, the words "large" and "small" are understood in comparison with the sample size. Sparse learning methods have been successfully applied in bioinformatics, financial engineering, image processing, etc. [see, e.g., the survey in [1]].

A popular model in this context is linear regression. We observe a pair (X, Y) , where $X = (X_1, \dots, X_n)^T$, where each X_i is called the predictor, belongs to \mathbb{R}^d and Y is called the response, is scalar and satisfies $Y = \langle X, \theta \rangle + \epsilon$, with some noise level ϵ . The goal is to develop inference on the unknown vector $\theta \in \mathbb{R}^d$.

In such applications of linear regression the dimension of X_i is much larger than the sample size n , i.e., $d \gg n$. It is well known that in this case classical procedures, such as the least squares estimator, do not work. One of the most compelling ways for dealing with the situation where $d \gg n$ is to suppose that the sparse structure is helpful, i.e., that θ has only few non-zero entries different from 0. This assumption is helpful in that it has several theoretical advantages: it makes the problem tractable and the consistent estimation of θ becomes possible if the number of nonzero coefficients is small enough.

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doi:10.1016/j.jcss.2012.11.001



Problems : often slow, no guarantees on the quality...

Variational Bayes methods

Idea : approximate the posterior distribution $\pi(\theta|X_1^n)$. We fix a convenient family of probability distributions \mathcal{F} and approximate the posterior by $\tilde{\pi}(\theta)$:

$$\tilde{\pi} = \arg \min_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \pi(\cdot|X_1^n)).$$



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Theoretical guarantees on the approximation ?

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VB in the machine learning framework

$$\hat{\rho}_\lambda(d\theta) \propto \exp[-\lambda r(\theta)] \pi(d\theta).$$

Then :

$$\begin{aligned} \mathcal{K}(\rho_a, \hat{\rho}_\lambda) &= \int \log \left[\frac{d\rho_a}{d\pi} \frac{d\pi}{d\hat{\rho}_\lambda} \right] d\rho_a \\ &= \lambda \int r(\theta) \rho_a(d\theta) + \mathcal{K}(\rho_a, \pi) + \log \int \exp[-\lambda r] d\pi. \end{aligned}$$

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$$\hat{\rho}_\lambda(d\theta) \propto \exp[-\lambda r(\theta)] \pi(d\theta).$$

Then :

$$\begin{aligned} \mathcal{K}(\rho_a, \hat{\rho}_\lambda) &= \int \log \left[\frac{d\rho_a}{d\pi} \frac{d\pi}{d\hat{\rho}_\lambda} \right] d\rho_a \\ &= \lambda \int r(\theta) \rho_a(d\theta) + \mathcal{K}(\rho_a, \pi) + \log \int \exp[-\lambda r] d\pi. \end{aligned}$$

We put

$$\tilde{a}_\lambda = \arg \min_{a \in \mathcal{A}} \left[\lambda \int r(\theta) \rho_a(d\theta) + \mathcal{K}(\rho_a, \pi) \right] \text{ and } \tilde{\rho}_\lambda = \rho_{\tilde{a}_\lambda}.$$

A PAC-Bound for VB Approximation

Theorem



Alquier, P., Ridgway, J. & Chopin, N. (2015). On the Properties of Variational Approximations of Gibbs Posteriors. *JMLR*.

$$\begin{aligned} \forall \lambda > 0, \quad \mathbb{P} \left\{ \int R(\theta) \tilde{\rho}_\lambda(d\theta) \right. \\ \left. \leq \inf_{a \in \mathcal{A}} \left[\int R(\theta) \rho_a(d\theta) + \frac{\lambda}{n} + \frac{2}{\lambda} \left[\mathcal{K}(\rho_a, \pi) + \log \left(\frac{2}{\varepsilon} \right) \right] \right] \right\} \\ \geq 1 - \varepsilon. \end{aligned}$$

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--> if we can derive a tight oracle inequality from this bound, we know that the VB approximation is “at no cost”.

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Application to a linear classification problem

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Optimization criterion :

$$\frac{\lambda}{n} \sum_{i=1}^n \Phi \left(\frac{-Y_i \langle X_i, \mu \rangle}{\sqrt{\langle X_i, \Sigma X_i \rangle}} \right) + \frac{\|\mu\|^2}{2\vartheta} + \frac{1}{2} \left(\frac{1}{\vartheta} \text{tr}(\Sigma) - \log |\Sigma| \right)$$

using deterministic annealing and gradient descent.

Application of the main theorem

Corollary

Assume that, for $\|\theta\| = \|\theta'\| = 1$,
 $\mathbb{P}(\langle \theta, X \rangle \langle \theta', X \rangle) \leq c \|\theta - \theta'\|$ and take $\lambda = \sqrt{nd}$ and
 $\vartheta = 1/\sqrt{d}$. Then

$$\mathbb{P} \left\{ \int R(\theta) \tilde{\rho}_\lambda(d\theta) \leq \inf_{\theta} R(\theta) + \sqrt{\frac{d}{n}} \left[\log(4ne^2) + c \right] + \frac{2 \log \left(\frac{2}{\varepsilon} \right)}{\sqrt{nd}} \right\} \geq 1 - \varepsilon.$$

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N.B : under margin assumption, possible to obtain d/n rates...

Sketch of the proof

By the main theorem, with probability at least $1 - \varepsilon$,

$$\int R d\tilde{\rho}_\lambda \leq \inf_{\rho = \mathcal{N}(\theta, s^2 I)} \left[\int R d\rho + \frac{\lambda}{n} + \frac{2}{\lambda} \left[\mathcal{K}(\rho, \pi) + \log \left(\frac{2}{\varepsilon} \right) \right] \right].$$

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As $\pi = \mathcal{N}(0, \vartheta I)$ we have

$$\mathcal{K}(\rho, \pi) = \frac{1}{2} \left[M \left(\frac{s^2}{\vartheta} - 1 + \log \left(\frac{\vartheta}{s^2} \right) \right) + \frac{\|\theta_0\|^2}{\vartheta} \right].$$

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$$\int R d\rho \leq R(\theta) + \int 2c\|u - \theta\| \rho(du) \leq R(\theta) + 2c\sqrt{M}\sigma.$$

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Chose adequate values for λ , ϑ and s^2 to conclude.

Test on real data

Dataset	Covariates	VB	SMC	SVM
Pima	7	21.3	22.3	30.4
Credit	60	33.6	32.0	32.0
DNA	180	23.6	23.6	20.4
SPECTF	22	06.9	08.5	10.1
Glass	10	19.6	23.3	4.7
Indian	11	25.5	26.2	26.8
Breast	10	1.1	1.1	1.7

Table – Comparison of misclassification rates (%). Last column : kernel-SVM with radial kernel. The hyper-parameters λ and ϑ are chosen by cross-validation.

Convexification of the loss

Can replace the 0/1 loss by a convex surrogate at “no” cost :



Zhang, T. (2004). Statistical behavior and consistency of classification methods based on convex risk minimization. *Annals of Statistics*.

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--> the following criterion (which turns out to be convex!) :

$$\begin{aligned} & \frac{1}{n} \sum_{i=1}^n (1 - Y_i \langle \mu, X_i \rangle) \Phi \left(\frac{1 - Y_i \langle \mu, X_i \rangle}{\sigma \|X_i\|_2} \right) \\ & + \frac{1}{n} \sum_{i=1}^n \sigma \|X_i\| \varphi \left(\frac{1 - Y_i \langle \mu, X_i \rangle}{\sigma \|X_i\|_2} \right) + \frac{\|\mu\|_2^2}{2\vartheta} + \frac{d}{2} \left(\frac{\vartheta}{\sigma^2} - \log \sigma^2 \right). \end{aligned}$$

Application of the main theorem

Optimization with stochastic gradient descent on a ball of radius M . On this ball, the objective function is L -Lipschitz. After k step, we have the approximation $\tilde{\rho}_\lambda^{(k)}$ of the posterior.

Corollary

Assume $\|X\| \leq c_x$ a.s., take $\lambda = \sqrt{nd}$ and $\vartheta = 1/\sqrt{d}$. Then

$$\mathbb{P} \left\{ \int R(\theta) \tilde{\rho}_\lambda^{(k)}(d\theta) \leq \inf_{\theta} R(\theta) + \frac{LM}{\sqrt{1+k}} + \frac{c_x}{2} \sqrt{\frac{d}{n}} \log \left(\frac{n}{d} \right) + \frac{\frac{c_x^2+1}{2c_x} + 2c_x \log \left(\frac{2}{\varepsilon} \right)}{\sqrt{nd}} \right\} \geq 1 - \varepsilon.$$

The PACVB package (James Ridgway)



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PACVB: Variational Bayes (VB) Approximation of Gibbs Posteriors with Hinge Losses

Variational Bayesian approximations of Gibbs measures with hinge losses for classification and ranking.

Version: 1.1
Depends: [Rcpp](#), [MASS](#)
LinkingTo: [Rcpp](#), [RcppArmadillo](#), [BH](#)
Published: 2016-02-04
Author: James Ridgway
Maintainer: James Ridgway <james.ridgway@bristol.ac.uk>
License: [GPL-2](#) | [GPL-3](#) [expanded from: GPL (≥ 2)]
NeedsCompilation: yes
CRAN checks: [PACVB results](#)

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OS X Snow Leopard binaries: r-release: [PACVB_1.1.tgz](#), r-oldrel: not available
OS X Mavericks binaries: r-release: [PACVB_1.1.tgz](#)

Application to collaborative filtering

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Collaborative filtering as matrix completion

									
Stan									
Pierre									
Zoe									
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Collaborative filtering as matrix completion

									
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1-bit matrix completion

Object of interest : an $m_1 \times m_2$ matrix M , values in

$$\{\text{👎}, \text{👍}\} = \{-1, +1\}.$$

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Entries $X_1 = (i_1, j_1), \dots, (i_n, j_n)$ i.i.d from a distribution P , and $Y_\ell = M_{X_\ell}$.

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Usual assumption : $\text{rank}(M) = r \ll \min(m_1, m_2)$.

Prior specification

Prior π

$$\underbrace{M}_{m_1 \times m_2} = \underbrace{L}_{m_1 \times K} \underbrace{R^T}_{K \times m_2},$$

$$L_{i,k}, R_{j,k} | \gamma_k \sim \mathcal{N}(0, \gamma_k), \quad \frac{1}{\gamma_k} \sim \Gamma(a, b).$$

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Gibbs posterior : $\hat{\rho}_{\lambda}(L, R) = \exp[-\lambda r(L, R)] \pi(L, R).$

Variational approximation

Here, family of approximation : $\rho_a = \rho(\mathcal{L}, \mathcal{R}, S, \Sigma, \alpha, \beta)$

$L_{i,k}$ indep. $\mathcal{N}(\mathcal{L}_{i,k}, S_{i,k})$, $R_{i,k}$ indep. $\mathcal{N}(\mathcal{R}_{i,k}, \Sigma_{i,k})$,

$\frac{1}{\gamma_k}$ indep. $\Gamma(\alpha_k, \beta_k)$.

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$$\frac{1}{\gamma_k} \text{ indep. } \Gamma(\alpha_k, \beta_k).$$

In this case, the $\int r d\rho_a$ is not tractable but we prove that

$$\forall a \in \mathcal{A}, \quad \int r d\rho_a + \frac{\mathcal{K}(\rho_a, \pi)}{\lambda} \leq r(\mathcal{LR}^T) + \mathcal{B}_\lambda(a)$$

for some known and tractable $\mathcal{B}_\lambda(a)$.

Definition

$$\tilde{\rho} = \arg \min_{\rho_a} r(\mathcal{LR}^T) + \mathcal{B}_\lambda(a).$$

Application of the general result

Theorem



Cottet, V. & Alquier, P. (2018). 1-bit Matrix Completion : PAC-Bayesian Analysis of a Variational Approximation. *Machine Learning*.

With proba. at least $1 - \varepsilon$ on the sample,

$$\mathbb{P}_{(L,R) \sim \tilde{p}, (i,j) \sim P} [\text{sign}((LR^T)_{i,j}) \neq M_{i,j}] \leq C \frac{r(m_1 + m_2) \log(n)}{n}$$

for some (known) $C > 0$.

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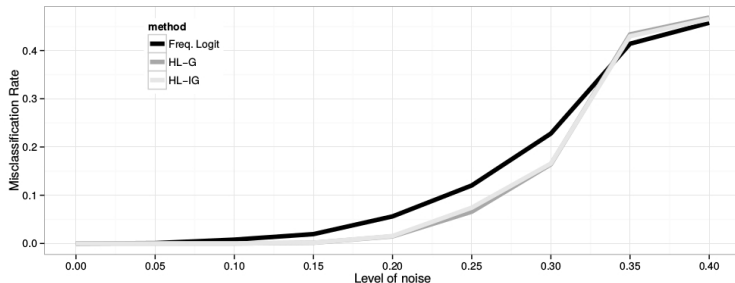
- in practice, blockwise coordinate optimization with gradient descent gives good results to compute $\tilde{\rho}$.
- in the paper, extention for noisy observations.

Simulation study

Comparison with the logistic regression approach with nuclear norm penalization from



J. Laffond, O. Klopp, E. Moulines & J. Salmon (2014). Probabilistic low-rank matrix completion on finite alphabets. *NIPS*.



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Reminder : concentration of the tempered posterior

$$\mathcal{B}(r) = \{\theta \in \Theta : \mathcal{K}(P_{\theta_0}, P_{\theta}) \leq r\}.$$

Theorem

For $1/2 \leq \alpha < 1$, for any sequence (ε_n) such that

$$-\log \pi[B(r_n)] \leq n\varepsilon_n$$

we have

$$\mathbb{E} \left[\int h^2(P_{\theta}, P_{\theta_0}) \pi_{\alpha}(d\theta | X_1^n) \right] \leq \frac{1 + \alpha}{1 - \alpha} \varepsilon_n.$$

Analysis of VB approx.

$$\text{VB. approx : } \tilde{\pi}_\alpha = \arg \min_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \pi_\alpha(\cdot | X_1^n)).$$

Theorem



Alquier, P. & Ridgway, J. (2017). Concentration of Tempered Posteriors and of their Variational Approximations. *Preprint arXiv*.

Fix $1/2 \leq \alpha < 1$. Assume that for the sequence (ε_n) there is $\rho_n \in \mathcal{F}$ such that

$$\int \mathcal{K}(P_{\theta_0}, P_\theta) \rho_n(d\theta) \leq \varepsilon_n \text{ and } \mathcal{K}(\rho_n, \pi) \leq \varepsilon_n.$$

$$\text{Then } \mathbb{E} \left[\int h^2(P_\theta, P_{\theta_0}) \tilde{\pi}_\alpha(d\theta | X_1^n) \right] \leq \frac{1 + \alpha}{1 - \alpha} \varepsilon_n.$$

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Further work (1/2)

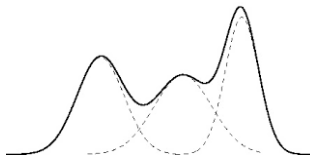
- our paper contains applications to various statistical models (logistic regression, nonparametric regression estimation).
- our paper also contains results for the misspecified case where the true distribution of the X_i does not belong to $(P_\theta, \theta \in \Theta)$.
- the case $\alpha = 1$ (“proper” Bayesian inference) is not covered by our paper. It was recently analyzed by



F. Zhang & C. Gao (2017). Convergence rates of variational posterior distributions. *Preprint arXiv*.

This requires additional assumptions and does not cover the misspecified case.

Further work (2/2)



- according to a recent survey (Blei *et al*), one of the most popular applications of VB is to mixture models. The upper bound is also used for model selection. Blei states that there is no justification to this. Badr-Eddine Chérif-Abdellatif since proved this is consistent.



D. Blei, A. Kucukelbir & J. D. McAuliffe (2017). Variational inference : A review for statisticians. *Journal of the American Statistical Association*.



B.-E. Chérif-Abdellatif & P. Alquier, (2018). Consistency of Variational Bayes Inference for Estimation and Model Selection in Mixtures. *Preprint arXiv*.

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Issue 1 : distortion of the posterior

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- we proved that the VB approx. concentrates at the optimal rate but what about the closeness of the approx. to the true posterior ?
- example : it is well known by practitioners that VB tends to reduce the variance of the posterior.
- is it possible to control the variance distortion ?
- controversial : it is also well known that Bayesian “credibility intervals” can be misleading.

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- in the case of classification with hinge loss, we obtain a convex minimization problem. This also happens for logistic regression.

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- in the case of classification with hinge loss, we obtain a convex minimization problem. This also happens for logistic regression.
- but in many other settings, the VB approximation is defined by a non-convex minimization problem. In this case, the convergence is an open issue in general. E.g : mixture models.

Issue 2 : convergence of the optimization algorithm

- in the case of classification with hinge loss, we obtain a convex minimization problem. This also happens for logistic regression.
- but in many other settings, the VB approximation is defined by a non-convex minimization problem. In this case, the convergence is an open issue in general. E.g : mixture models.
- the work on matrix completion relies on alternate optimisation of $d(M, UV)$ w.r.t U and V . The problem is convex in U , in V , but not in (U, V) . Still, recent work gives hope that this procedure might converge :



R. Ge, J. D. Lee & T. Ma (2016). Matrix Completion has No Spurious Local Minimum. *NIPS*.

Issue 3 : online variational approximations

- online algorithms (like OGA) are sometimes used to compute the variational approximation. This is called online variational inference by



C. Wang, J. Paisley & D. Blei (2011). Online variational inference for the hierarchical Dirichlet process. *AISTATS*.

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- but a more challenging question is to extend variational approximations to approximate EWA in the online setting (extend the result by [Audibert, 2016]) : it is well known that apart in the case of a finite number of predictors, EWA is not feasible in practice...

Issue 3 : reminder

Fix $\lambda > 0$ and define, at each time t ,

$$\hat{\rho}_{\lambda,t}(\mathrm{d}\theta) \propto \exp[-\lambda r_{t-1}(\theta)] \pi(\mathrm{d}\theta) \text{ and } \hat{Y}_t = \int f_{\theta}(X_t) \hat{\rho}_{\lambda,t}(\mathrm{d}\theta).$$

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Theorem [Consequence of Audibert, 2006]

$$\sum_{t=1}^T \ell(Y_t, \hat{Y}_t) \leq \inf_{\rho} \left\{ \int \sum_{t=1}^T \ell(Y_t, f_{\theta}(X_t)) \rho(\mathrm{d}\theta) + \frac{\lambda T B^2}{2} + \frac{\mathcal{K}(\rho, \pi)}{\lambda} \right\}.$$

Issue 3 : extension of VB

Many definitions are possible. For example :



C. V. Nguyen, T. D. Bui, Y. Li & R. E. Turner (2017). Online Variational Bayesian Inference : Algorithms for Sparse Gaussian Processes and Theoretical Bounds. *ICML*.

propose

$$\hat{\rho}_{\lambda,t}(\mathrm{d}\theta) \propto \exp[-\lambda r_{t-1}(\theta)] \pi(\mathrm{d}\theta) \text{ and } \tilde{\rho}_{\lambda,t} = \arg \min_{\rho \in \mathcal{F}} \mathcal{K}(\rho, \hat{\rho}_{\lambda,t}).$$

Interesting, but might be computationally expensive, and there is no accurate theoretical analysis.

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Interesting, but might be computationally expensive, and there is no accurate theoretical analysis.

We work currently on an alternative approach with Badr-Eddine.

Thank you !