2) Statistical Analysis of Variational Approximations

Pierre Alquier





Heilbronn Institute - University of Bristol - Nov. 27, 2019

Pierre Alquier, RIKEN AIP Lectures on Variational Inference - 2

Reminder on the notations Theorems on the concentration of the posterior

Lecture 2

Concentration of the posterior

- Reminder on the notations
- Theorems on the concentration of the posterior

2 Concentration of variational approximations

- Theorem for variational approximation
- Proof
- Applications

3 Further results

- Further results in statistical estimation
- Further results in machine learning

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The likelihood

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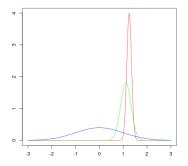
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The tempered posterior - 0 $< \alpha < 1$

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

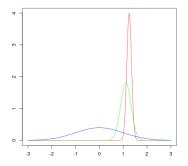
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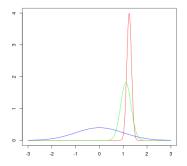


Do we have for some d, $\forall t > 0$

$$\mathbb{P}_{\theta \sim \pi_{n,\alpha}} \Big[d(\theta, \theta_0) \geq t \Big] \xrightarrow[n \to \infty]{} 0 ?$$

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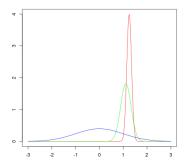


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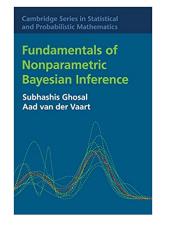
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Reminder on the notations Theorems on the concentration of the posterior

A simpler result

We will state a simpler results than the concentration theorems in this book, by following ideas from

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Definition - Rényi divergence

Assume that P and Q have respective densities p and q with respect to a measure μ , define, for $0 < \alpha < 1$,

$$D_{lpha}(P,R) = rac{1}{lpha-1}\log\int q(x)^{1-lpha}p(x)^{lpha}\mu(\mathrm{d} x).$$

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We use $d(\theta, \theta_0) = D_{\alpha}(P_{\theta}, P_{\theta_0})$ to measure the concentration.

Reminder on the notations Theorems on the concentration of the posterior

Properties of the Rényi divergence

It is important to note that $D_{\alpha}(P, Q)$ does not depend on the choice of μ as can be "seen" from

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

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

Reminder on the notations Theorems on the concentration of the posterior

A theorem in expectation

Define

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

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Theorem (BPY 19, simplified version)

For any sequence (r_n) such that $r_n \ge 0$ and

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

we have

$$\mathbb{E}_{X_1,\ldots,X_n}\left\{\mathbb{E}_{\theta\sim\pi_{n,\alpha}}\left[D_{\alpha}(P_{\theta},P_{\theta_0})\right]\right\}\leq \frac{1+\alpha}{1-\alpha}r_n.$$

Reminder on the notations Theorems on the concentration of the posterior

From expectation to concentration

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$$\mathbb{P}_{ heta \sim \pi_{n,lpha}} \Big[D_lpha(P_ heta, P_{ heta_0}) \geq t \Big] \leq rac{\mathbb{E}_{ heta \sim \pi_{n,lpha}} \Big[D_lpha(P_ heta, P_{ heta_0}) \Big]}{t},$$

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 $\mathbb{E}_{X_1, \dots, X_n} \Bigg\{ \mathbb{P}_{ heta \sim \pi_{n,lpha}} \Big[D_{lpha}(P_{ heta}, P_{ heta_0}) \ge t \Big] \Bigg\} \le rac{(1+lpha)}{(1-lpha)t} r_n \xrightarrow[n o \infty]{} 0,$

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$$\mathbb{E}_{X_1,...,X_n} \left\{ \mathbb{P}_{ heta \sim \pi_{n,lpha}} \Big[D_lpha(P_ heta, P_{ heta_0}) \ge t \Big]
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Theorem for variational approximation Proof Applications

Generalization to variational approximations

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Generalization to variational approximations

In the following paper, we extended BPY's approach to variational approximations.

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Reminder :

$$ilde{\pi}_{n,lpha} = rgmin_{
ho\in\mathcal{F}}\mathcal{K}(
ho,\pi_{n,lpha}).$$

Theorem for variational approximation Proof Applications

Concentration of VB

Theorem - AR 17

Assume that there is (r_n) and $\rho_n \in \mathcal{F}$ such that

$$\mathbb{E}_{ heta \sim
ho_n} \Big[\mathcal{K}(P_{ heta_0}, P_{ heta}) \Big] \leq r_n$$

and

$$\mathcal{K}(\rho_n,\pi) \leq nr_n.$$

Then, for any $\alpha \in (0, 1)$,

$$\mathbb{E}_{X_1,\ldots,X_n}\left\{\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\left[D_{\alpha}(P_{\theta},P_{\theta_0})\right]\right\}\leq \frac{1+\alpha}{1-\alpha}r_n.$$

Theorem for variational approximation **Proof** Applications

Proof (1/2)

Define the log-likelihood ratio : $r_n(\theta, \theta_0) = \sum_{i=1}^n \log \frac{p_{\theta_0}(X_i)}{p_{\theta}(X_i)}.$

Theorem for variational approximation **Proof** Applications

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Its expectation :

$$\mathbb{E}_{X_1,\ldots,X_n}[r_n(\theta,\theta_0)]=n\mathcal{K}(P_{\theta_0},P_{\theta}).$$

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Its exponential moment :

$$\mathbb{E}_{X_1,\dots,X_n} \left\{ \exp\left[-\alpha r_n(\theta,\theta_0)\right] \right\} = \prod_{i=1}^n \int \left(\frac{p_\theta(x_i)}{p_{\theta_0}(x_i)}\right)^\alpha p_{\theta_0}(x_i) \mathrm{d}x_i$$
$$= \prod_{i=1}^n \exp\left[\log \int p_\theta(x_i)^\alpha p_{\theta_0}(x_i)^{1-\alpha} \mathrm{d}x_i\right]$$
$$= \exp\left[-n(1-\alpha)D_\alpha(P_\theta,P_{\theta_0})\right].$$

Proof (2/2)

Theorem for variational approximation **Proof** Applications

Start from the exponential moment :

$$\mathbb{E}_{X_1,\dots,X_n}\left\{\exp\left[-\alpha r_n(\theta,\theta_0)+n(1-\alpha)D_\alpha(P_\theta,P_{\theta_0})\right]\right\}=1.$$

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Expectation w.r.t $\theta \sim \pi$ and Fubini :

 $\mathbb{E}_{X_1,\ldots,X_n}\mathbb{E}_{\theta \sim \pi}\left\{\exp\left[-\alpha r_n(\theta,\theta_0) + n(1-\alpha)D_\alpha(P_\theta,P_{\theta_0})\right]\right\} = 1.$

Theorem for variational approximation **Proof** Applications

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Expectation w.r.t $\theta \sim \pi$ and Fubini :

$$\mathbb{E}_{X_1,\dots,X_n} \mathbb{E}_{\theta \sim \pi} \left\{ \exp \left[-\alpha r_n(\theta, \theta_0) + n(1 - \alpha) D_\alpha(P_\theta, P_{\theta_0}) \right] \right\} = 1.$$

Then :

$$\mathbb{E}_{X_1,...,X_n} \mathbb{E}_{\theta \sim \tilde{\pi}_{n,lpha}} \left\{ \exp \left[-lpha r_n(heta, heta_0) + n(1-lpha) D_lpha(P_ heta, P_{ heta_0}) + \log \left(rac{\pi(heta)}{\tilde{\pi}_{n,lpha}(heta)}
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Theorem for variational approximation **Proof** Applications

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Jensen's inequality :

$$\begin{split} \exp & \left\{ \mathbb{E}_{X_1,...,X_n} \mathbb{E}_{\theta \sim \tilde{\pi}_{n,\alpha}} \Big[-\alpha r_n(\theta, \theta_0) + n(1-\alpha) D_\alpha(P_\theta, P_{\theta_0}) \\ & + \log \Big(\frac{\pi(\theta)}{\tilde{\pi}_{n,\alpha}(\theta)} \Big) \Big] \right\} \leq 1. \end{split}$$

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Rearranging :

$$\mathbb{E}_{X_{1},...,X_{n}}\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\left[D_{\alpha}(P_{\theta},P_{\theta_{0}})\right]$$

$$\leq \frac{1}{n(1-\alpha)}\mathbb{E}_{X_{1},...,X_{n}}\left\{\underbrace{\alpha\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\left[r_{n}(\theta,\theta_{0})\right]+\mathcal{K}(\tilde{\pi}_{n,\alpha},\pi)}_{\bullet}\right\}$$

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Theorem for variational approximation **Proof** Applications

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As $\pi_{n,\alpha}$ minimizes the ELBO :

$$\begin{split} \mathbb{E}_{X_{1},...,X_{n}} \mathbb{E}_{\theta \sim \tilde{\pi}_{n,\alpha}} \left[D_{\alpha}(P_{\theta}, P_{\theta_{0}}) \right] \\ & \leq \frac{1}{n(1-\alpha)} \mathbb{E}_{X_{1},...,X_{n}} \left\{ \inf_{\rho \in \mathcal{F}} \left[\alpha \mathbb{E}_{\theta \sim \rho} \left[r_{n}(\theta, \theta_{0}) \right] + \mathcal{K}(\rho, \pi) \right] \right\} \\ & \leq \frac{1}{n(1-\alpha)} \inf_{\rho \in \mathcal{F}} \left\{ n \alpha \mathbb{E}_{\theta \sim \rho} \left[\mathcal{K}(P_{\theta_{0}}, P_{\theta}) \right] + \mathcal{K}(\rho, \pi) \right\}. \end{split}$$

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We end the proof by using the assumption that there is a $\rho \in \mathcal{F}$ such that $\mathbb{E}_{\theta \sim \rho}[\mathcal{K}(P_{\theta_0}, P_{\theta})] \leq r_n$ and $\mathcal{K}(\rho, \pi) \leq nr_n$:

$$\mathbb{E}_{X_1,\ldots,X_n}\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\Big[D_{\alpha}(P_{\theta},P_{\theta_0})\Big]\leq \frac{1}{n(1-\alpha)}\left[\alpha nr_n+nr_n\right]=\frac{1+\alpha}{1-\alpha}r_n.$$

Theorem for variational approximation Proof Applications

A toy example : Gaussian variables

Toy example : assume that X_1, \ldots, X_n are i.i.d from $P_{\theta_0} = \mathcal{N}(\theta_0, 1)$.

Theorem for variational approximation Proof Applications

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Toy example : assume that X_1, \ldots, X_n are i.i.d from $P_{\theta_0} = \mathcal{N}(\theta_0, 1)$. Cauchy prior $\theta \sim \pi = \mathcal{C}(0, 1)$. Gaussian approximation of the posterior :

$$\mathcal{F} = \left\{ \mathcal{N}(m, \sigma^2), m \in \mathbb{R}, \sigma^2 > 0 \right\}.$$

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Note that $\mathcal{K}(P_{ heta_0},P_{ heta})=| heta- heta_0|^2/2$ and so

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Moreover, rough upper bounds lead to

$$\mathcal{K}(\mathcal{N}(m,\sigma^2),\pi) \leq \log\left(\sqrt{rac{\pi}{2\sigma^2}}
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Theorem for variational approximation Proof Applications

Gaussian example (continued)

$$\frac{|m-\theta_0|^2+\sigma^2}{2} \leq r_n$$

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Theorem for variational approximation Proof Applications

Gaussian example (continued)

$$\frac{|m - \theta_0|^2 + \sigma^2}{2} \le r_n$$

$$\log\left(\sqrt{\frac{\pi}{2\sigma^2}}\right) + \log(1 + 2m^2) + \sqrt{\frac{2\sigma^2}{\pi}} \le nr_n$$
For example satisfied by $m = \theta_0$, $\sigma^2 = 1/n$ and
$$r_n = \frac{\frac{1}{2}\log\left(\frac{n\pi}{2}\right) + \log(1 + 2\theta_0^2) + \sqrt{\frac{\pi}{2}}}{n}.$$

Theorem for variational approximation Proof Applications

Gaussian example (continued)

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For example satisfied by $m = \theta_0$, $\sigma^2 = 1/n$ and
$$r_n = \frac{\frac{1}{2}\log\left(\frac{n\pi}{2}\right) + \log(1+2\theta_0^2) + \sqrt{\frac{\pi}{2}}}{n}.$$

We can apply our theorem :

$$\mathbb{E}_{X_1,\ldots,X_n}\left\{\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\left[D_{\alpha}(P_{\theta},P_{\theta_0})\right]\right\}\leq\frac{1+\alpha}{1-\alpha}r_n.$$

Theorem for variational approximation Proof Applications

Gaussian example (continued)

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Here, we have actually

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Theorem for variational approximation Proof Applications

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$$\begin{split} \mathbb{E}_{X_{1},...,X_{n}} &\left\{ \mathbb{E}_{\theta \sim \tilde{\pi}_{n,\alpha}} \Big[|\theta - \theta_{0}|^{2} \Big] \right\} \\ &\leq \left(\frac{\alpha(1 + \alpha)}{1 - \alpha} \right) \frac{\frac{1}{2} \log \left(\frac{n\pi}{2} \right) + \log(1 + 2\theta_{0}^{2}) + \sqrt{\frac{\pi}{2}}}{n}. \end{split}$$

Theorem for variational approximation Proof Applications

Second example : matrix completion

	WARS		ACIN VOISIN TOTORO	
Claire	4	?	3	
Nial	?	4	?	
Brendon	?	5	4	
Andrew	?	4	?	
Adrian	1	?	?	
Damien	?	1	?	
:	:	-	-	·

Theorem for variational approximation Proof Applications

Matrix completion (continued)

Reminder on matrix completion :

$$M = \sum_{\ell=1}^{k} U_{\cdot,\ell} (V_{\cdot,\ell})^{\mathsf{T}}$$
 is $p imes m$

with prior π given by

• $U_{\cdot,\ell}, V_{\cdot,\ell} \sim \mathcal{N}(0, \gamma_{\ell}I),$ • $\frac{1}{\gamma_{\ell}} \sim \text{Gamma}(a, b).$ Mean-field variational approximation with Gaussian and inverse gamma disitributions on U, V and γ_{ℓ} respectively.

Theorem for variational approximation Proof Applications

Matrix completion : rate of convergence

$$\mathbb{E}_{X_1,...,X_n} \left\{ \mathbb{E}_{\theta \sim \tilde{\pi}_{n,\alpha}} \Big[D_{\alpha}(P_M, P_{M_0}) \Big]
ight\}$$

= $\mathcal{O}\left(\frac{\operatorname{rank}(M_0)(m+p) + \log(nmp)}{n} \right).$

Further results in statistical estimation Further results in machine learning

Generalization to variational approximations

1 Concentration of the posterior

- Reminder on the notations
- Theorems on the concentration of the posterior
- 2 Concentration of variational approximations
 - Theorem for variational approximation
 - Proof
 - Applications

3 Further results

- Further results in statistical estimation
- Further results in machine learning

Further results in statistical estimation Further results in machine learning

Misspecified case

Further results in statistical estimation Further results in machine learning

Misspecified case

Assume we observe X_1, \ldots, X_n i.i.d from P^0 and use a model $\mathcal{M} = \{P_{\theta}, \theta \in \Theta\}$, but it is possible that $P^0 \notin \mathcal{M}$.

Further results in statistical estimation Further results in machine learning

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Theorem - AR 17

Assume that there is (r_n) and $\rho_n \in \mathcal{F}$ such that

$$\mathbb{E}_{\theta \sim \rho} \left\{ \mathbb{E}_{X \sim P^0} \left[\log \left(\frac{p_{\theta^*}(x)}{p_{\theta}(x)} \right) \right] \right\} \leq r_n$$

and $\mathcal{K}(\rho_n, \pi) \leq nr_n$. Then

$$\mathbb{E}_{X_{1},\ldots,X_{n}}\left\{\mathbb{E}_{\theta\sim\tilde{\pi}_{n,\alpha}}\left[D_{\alpha}(P_{\theta},P^{0})\right]\right\}\leq\frac{\alpha}{1-\alpha}\mathcal{K}(P_{\theta^{*}},P^{0})+\frac{1+\alpha}{1-\alpha}r_{n}.$$

Model selection

Assume that we have K models, define $\tilde{\pi}_{n,\alpha}^k$ a variational approximation of the tempered posterior in model k, and $r_n^{(k)}$ its convergence rate if model k is correct. Put :

$$\hat{k} = rg\max_k \mathrm{ELBO}(ilde{\pi}^{(k)}_{n,lpha}).$$

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If the true model is actually k_0 ,

$$\mathbb{E}\bigg[\int D_{\alpha}(P_{\theta}, P^{0})\tilde{\pi}_{n,\alpha}^{\hat{k}}(d\theta)\bigg] \leq \frac{1+\alpha}{1-\alpha}r_{n}^{(k_{0})} + \frac{\log(K)}{n(1-\alpha)}.$$

Further results in statistical estimation Further results in machine learning

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This result is actually due to my PhD student :





Further results in statistical estimation Further results in machine learning

Models with hidden variables (1/2)

The results presented so far do not include approximations in models with hidden variables.

Further results in statistical estimation Further results in machine learning

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B.-E. Chérief-Abdellatif, P. Alquier (2018). Consistency of Variational Bayes Inference for Estimation and Model Selection in Mixtures. *Electronic Journal of Statistics*.

Further results in statistical estimation Further results in machine learning

Models with hidden variables (2/2)

For a general approach for models with hidden variables, including

- mixture models,
- hidden Markov chains,
- 3 . . .

see :

Y. Yang, D. Pati & A. Bhattacharya (2017). α -Variational Inference with Statistical Guarantees. The Annals of Statistics (to appear), preprint arXiv :1712.08983.

Further results in statistical estimation Further results in machine learning

The case
$$lpha=1$$

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Case $\alpha = 1$

$$\left[L_n(\theta)\right]^{\alpha} \pi(\mathrm{d}\theta) = L_n(\theta)\pi(\mathrm{d}\theta)$$

Further results in statistical estimation Further results in machine learning

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Covered in the following paper – note that this case requires **much stronger** assumptions :

F. Zhang & C. Gao (2017). Convergence Rates of Variational Posterior Distributions. Preprint arxiv :1712.02519.

Further results in statistical estimation Further results in machine learning

More general machine learning problem

Reminder of the context of machine learning :

- X_1, \ldots, X_n i.i.d from P^0 ,
- $\ \mathbf{R}(\theta) = \mathbb{E}_{X \sim P^0}[\ell(\theta, X)].$

3
$$R_n(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(\theta, X_i).$$

Further results in statistical estimation Further results in machine learning

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Further results in statistical estimation Further results in machine learning

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We define a variational approximation of the Gibbs posterior :

$$\tilde{\pi}_{n,\alpha}(\theta) = \operatorname*{arg\,min}_{\rho\in\mathcal{F}}\mathcal{K}(
ho,\pi_{n,\alpha}).$$

Further results in statistical estimation Further results in machine learning

Variational approximation of Gibbs posteriors

Bounds on the generalization error of the variational approximation of the Gibbs posterior

 $\mathbb{E}_{\theta \sim \tilde{\pi}_{n, \alpha}} \left[R(\theta) \right]$

provided in the paper :

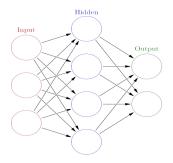
P. Alquier, J. Ridgway , N. Chopin (2016). On the Properties of Variational Approximations of Gibbs Posteriors. *JMLR*.





Further results in statistical estimation Further results in machine learning

Neural networks



Source : Wikipedia.

 $\mathsf{Prior}\ \pi:\mathsf{independent}$

$$\theta_{i,j}^{(\ell)} \sim \mathcal{N}(0, \sigma_{\ell}^2).$$

Variational approximation : independent

$$\theta_{i,j}^{(\ell)} \sim \mathcal{N}(m_{i,j}^{(\ell)}, (\sigma_{i,j}^{(\ell)})^2).$$

Neural networks for non parametric regression

Badr-Eddine Chérief-Abdellatif proved that, in regression with quadratic loss, suitable neural networks estimate β -Hölder functions at rate :

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B.-E. Chérief-Abdellatif (2018). Convergence Rates of Variational Inference in Sparse Deep Learning. Preprint arXiv :1908 :04847.

Further results in statistical estimation Further results in machine learning

Thank you!