Infinite-dimensional α-divergence minimisation for Variational Inference

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OxCSML seminar
19/11/2021

Joint work with Randal Douc and François Portier

Outline

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Bayesian statistics

- Compute / sample from the posterior density of the latent variables y given the data $\mathscr{D}$

$$p(y|\mathscr{D}) = \frac{p(\mathscr{D}, y)}{p(\mathscr{D})} \ .$$

- Problem : for many important models, we can only evaluate $p(y|\mathscr{D})$ up to the constant $p(\mathscr{D})$.

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Variational Inference in a nutshell

→ Variational Inference : inference is seen as an optimisation problem.

1. Posit a *simpler* variational family $\mathcal{Q}$, where $q \in \mathcal{Q}$.
2. Fit q to obtain the best approximation to the posterior density

$$\inf_{q \in \mathcal{Q}} D(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) ,$$

where D is a measure of dissimilarity between the variational distribution $\mathbb{Q}$ and the posterior distribution $\mathbb{P}_{|\mathscr{D}}$

→ Typically, D : exclusive Kullback-Leibler (KL) divergence and $\mathcal{Q}$: parametric family (e.g. Mean-field)

$$\begin{cases} D_{KL}(\mathbb{Q}||\mathbb{P}) = \int_{\mathsf{Y}} \log\left(\frac{q(y)}{p(y)}\right) q(y)\nu(\mathrm{d}y) \\ \mathcal{Q} = \{q : y \mapsto k(\theta, y) \ : \ \theta \in \mathsf{T}\} \end{cases}$$

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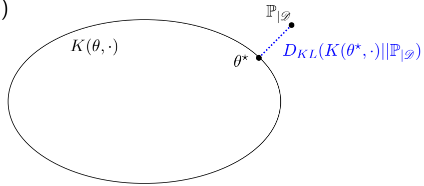

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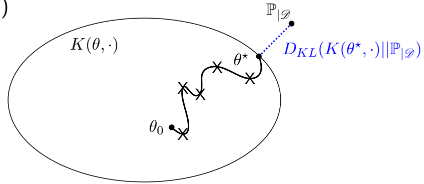

Core question in Variational Inference

$$\inf_{q \in \mathcal{Q}} D(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}})$$

Question : How to choose D and $\mathcal{Q}$?

$\rightarrow D$: exclusive Kullback-Leibler (KL) divergence and $\mathcal{Q}$: Mean-field family

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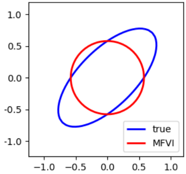

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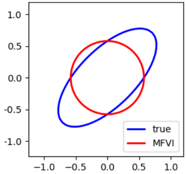

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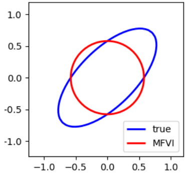

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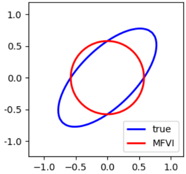

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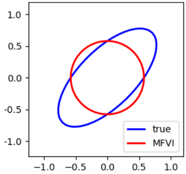

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- Can we design more expressive variational families $\mathcal{Q}$ beyond traditional parametric families?
  $\rightarrow$ Put a prior on the variational parameter θ

Variational Inference with the α-divergence family

$(\mathsf{Y}, \mathcal{Y}, \nu)$: measured space, ν is a σ-finite measure on $(\mathsf{Y}, \mathcal{Y})$.
$\mathbb{Q}$ and $\mathbb{P}$: $\mathbb{Q} \preceq \nu$, $\mathbb{P} \preceq \nu$ with $\frac{\mathrm{d}\mathbb{Q}}{\mathrm{d}\nu} = q$, $\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}\nu} = p$.

α-divergence between $\mathbb{Q}$ and $\mathbb{P}$

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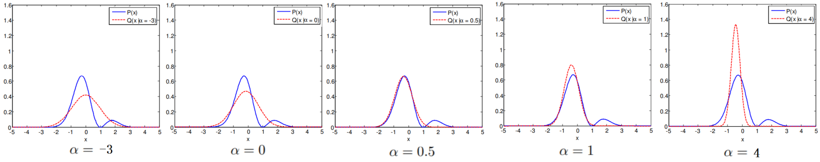
❶ A flexible family of divergences...

Figure: In red, the Gaussian which minimises $D_\alpha(\mathbb{Q}||\mathbb{P})$ for a varying α



Adapted from V. Cevher's lecture notes (2008) https://www.ece.rice.edu/~vc3/elec633/AlphaDivergence.pdf

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Black-box alpha divergence minimization. J. Hernandez-Lobato et al. (2016). ICML
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K. Daudel, R. Douc and F. Portier. Ann. Statist. 49 (4) 2250 - 2270, August 2021.
https://doi.org/10.1214/20-AOS2035.

Idea : Extend the traditional variational parametric family

$$\mathcal{Q} = \{y \mapsto k(\theta, y) \ : \ \theta \in \mathsf{T}\}$$

by putting a prior on the variational parameter θ

$$\mathcal{Q} = \left\{q : y \mapsto \mu k(y) := \int_{\mathsf{T}} \mu(\mathrm{d}\theta) k(\theta, y) \ : \ \mu \in \mathsf{M}\right\}$$

and propose an update formula for μ that ensures a systematic decrease in the α-divergence at each step

$\rightarrow$ Finite Mixture Models : $\mu = \sum_{j=1}^{J} \lambda_j \delta_{\theta_j}$

NB: The mapping $\mu \mapsto \Psi_\alpha(\mu k; p)$ is convex!

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The (α, Γ)-descent algorithm

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- $K : (\theta, A) \mapsto \int_A k(\theta, y) \nu(\mathrm{d}y)$ is a Markov transition kernel defined on $\mathsf{T} \times \mathcal{Y}$ with density k

Algorithm

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$$\mu_{n+1} = \mathcal{I}_\alpha(\mu_n) \, , \qquad n \geqslant 1$$

where for all $\mu \in \mathrm{M}_1(\mathsf{T})$ and all $\theta \in \mathsf{T}$,

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Let $\mu_1 \in \mathrm{M}_1(\mathsf{T})$ be such that $\Psi_\alpha(\mu_1 k) < \infty$. The sequence of probability measures $(\mu_n)_{n \geqslant 1}$ is defined iteratively by

$$\mu_{n+1} = \mathcal{I}_\alpha(\mu_n) , \qquad n \geqslant 1$$

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The (α, Γ)-descent algorithm

Optimisation problem

$$\inf_{\mu \in \mathsf{M}} \Psi_\alpha(\mu k; p) \quad \text{with} \quad \Psi_\alpha(\mu k; p) := \int_{\mathsf{Y}} f_\alpha\left(\frac{\mu k(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$$

- p is a nonnegative measurable function defined on $(\mathsf{Y}, \mathcal{Y})$
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Conditions for a monotonic decrease

(A1) For all $(\theta, y) \in \mathsf{T} \times \mathsf{Y}$, $k(\theta, y) > 0$, $p(y) \geqslant 0$ and $\int_{\mathsf{Y}} p(y)\nu(\mathrm{d}y) < \infty$.

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$$[(\alpha - 1)(v - \kappa) + 1] (\log \Gamma)'(v) + 1 \geqslant 0 \, .$$

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Assume (A1) and (A2). Let $\mu \in \mathrm{M}_1(\mathsf{T})$ be such that $\Psi_\alpha(\mu k) < \infty$ and $\mu(\Gamma(b_{\mu,\alpha} + \kappa)) < \infty$. Then,

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Convergence results

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Entropic Mirror Descent $\eta \in (0, \frac{1}{\lvert\alpha-1\rvert\lvert b\rvert_{\infty,\alpha}+1})$, $\kappa \in \mathbb{R}$	
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The special case of finite mixture models

$$S_J = \left\{ \boldsymbol{\lambda} = (\lambda_1, ..., \lambda_J) \in \mathbb{R}^J \ : \ \forall j \in \{1, ..., J\} \,, \ \lambda_j \geqslant 0 \text{ and } \sum_{j=1}^J \lambda_j = 1 \right\}$$

Let $\theta_1, ..., \theta_J \in \mathsf{T}$ be fixed and denote

$$\mu_{\boldsymbol{\lambda}} = \sum_{j=1}^J \lambda_j \delta_{\theta_j} \quad \text{where} \quad \boldsymbol{\lambda} \in \mathcal{S}_J \ .$$

Then, $\mu_n = \underbrace{\mathcal{I}_\alpha \circ \cdots \circ \mathcal{I}_\alpha}_{n \text{ times}}(\mu_{\boldsymbol{\lambda}})$ is of the form $\mu_n = \sum_{j=1}^J \lambda_{j,n} \delta_{\theta_j}$ with

$$\begin{cases} \boldsymbol{\lambda}_1 = \boldsymbol{\lambda} \\ \lambda_{j,n+1} = \frac{\lambda_{j,n} \Gamma(b_{\mu_n,\alpha}(\theta_j) + \kappa)}{\sum_{i=1}^J \lambda_{i,n} \Gamma(b_{\mu_n,\alpha}(\theta_i) + \kappa)} \end{cases} .$$

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Outline

Numerical experiments

- Gaussian kernel with density k_h and bandwidth h, $\mathsf{T} = \mathbb{R}^d$

$$\left\{ y \mapsto \mu_{\boldsymbol{\lambda},\Theta} k_h(y) = \sum_{j=1}^{J} \lambda_j k_h(y - \theta_j) \ : \ \boldsymbol{\lambda} \in \mathcal{S}_J, \Theta \in \mathsf{T}^J \right\} .$$

Full algorithm

1. Exploitation step : optimise $\boldsymbol{\lambda}$ using the (α, Γ)-descent.
2. Exploration step : update Θ (e.g. by sampling under $\mu_{\boldsymbol{\lambda},\Theta} k_h$, $h \propto J^{-1/(4+d)}$)

- Toy example
  $p(y) = Z \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$, $Z = 2$

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- Bayesian Logistic Regression Covertype dataset ($581,012$ data points and 54 features)

Toy example : Entropic Mirror Descent vs Power Descent

Comparison between

- 0.5-Mirror descent : $\Gamma(v) = e^{-\eta v}$ and $\alpha = 0.5$,
- 0.5-Power descent : $\Gamma(v) = [(\alpha - 1)\, v + 1]^{\eta/(1-\alpha)}$ and $\alpha = 0.5$.

$J = M = 100$, initial mixture weights : $[1/J, ..., 1/J]$, $N = 10$, $T = 20$
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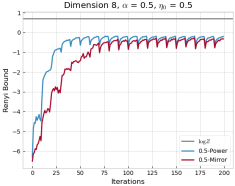

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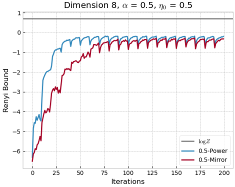

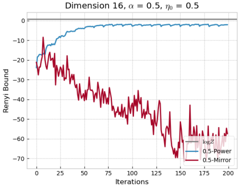

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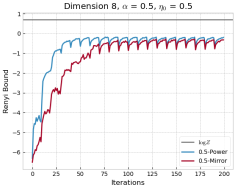

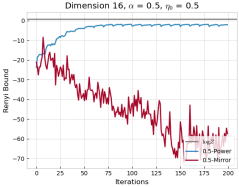

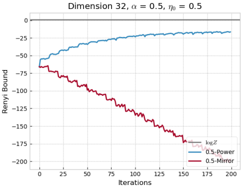

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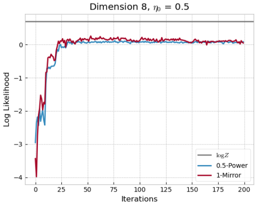

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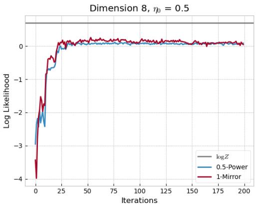

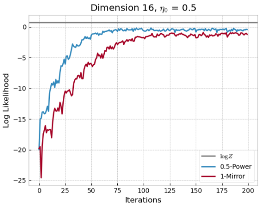

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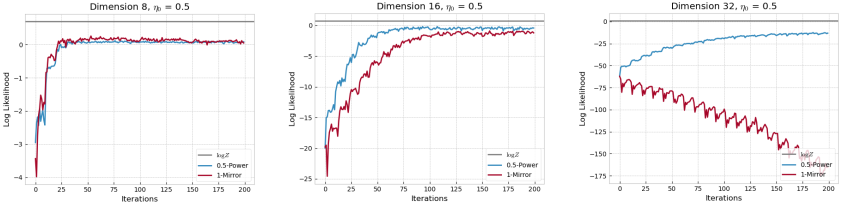

Bayesian Logistic Regression

$\rightarrow$ $\mathscr{D} = \{\boldsymbol{c}, \boldsymbol{x}\}$: I binary class labels, $c_i \in \{-1, 1\}$, L covariates for each datapoint, $\boldsymbol{x}_i \in \mathbb{R}^L$

$\rightarrow$ Model : L regression coefficients $w_l \in \mathbb{R}$, precision parameter $\beta \in \mathbb{R}^+$

$$p_0(\beta) = \mathrm{Gamma}(\beta; a, b) \; ,$$
$$p_0(w_l|\beta) = \mathcal{N}(w_l; 0, \beta^{-1}) \; , \quad 1 \leqslant l \leqslant L$$
$$p(c_i = 1|\boldsymbol{x}_i, \boldsymbol{w}) = \frac{1}{1 + e^{-\boldsymbol{w}^T \boldsymbol{x}_i}} \; , \quad 1 \leqslant i \leqslant I$$

where $a = 1$ and $b = 0.01$

Nonparametric variational inference S. Gershman, M. Hoffman, and D. Blei (2012). ICML

$\rightarrow$ Quantity of interest : $p(y|\mathscr{D})$ with $y = [\boldsymbol{w}, \log \beta]$

Comparison between

- 0.5-Power descent
- Typical AIS

$N = 1$, $T = 500$, $J_0 = M_0 = 20$, $J_{t+1} = M_{t+1} = J_t + 1$
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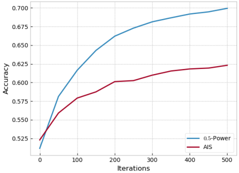

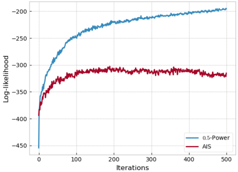

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Outline

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General framework for infinite-dimensional α-divergence minimisation over

$$\mathcal{Q} = \left\{ q : y \mapsto \int_{\mathsf{T}} \mu(\mathrm{d}\theta) k(\theta, y) \;:\; \mu \in \mathsf{M} \right\}$$

- recovers the Entropic Mirror Descent algorithm
- novel Power Descent algorithm
- conditions for a systematic decrease + convergence results
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$$\mathcal{Q} = \left\{ q : y \mapsto \sum_{j=1}^{J} \lambda_j k(\theta_j, y) \;:\; \boldsymbol{\lambda} \in \mathcal{S}_J, \Theta \in \mathsf{T}^J \right\}$$

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1. Update for Θ not specified (e.g. your favorite update for Θ)
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Thank you for your attention!

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