Variational Inference
Foundations and recent advances
(Part 1)

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University of Bristol – 09/03/2022

Outline

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Bayesian inference

- Goal : model a phenomenon given some observed data while taking into account prior knowledge on the model parameters.

- Core quantity in Bayesian Inference : posterior density of the latent variables y given the data $\mathscr{D}$

$$p(y|\mathscr{D}) = \frac{p(\mathscr{D}, y)}{p(\mathscr{D})} = \frac{p(\mathscr{D}|y)p_0(y)}{p(\mathscr{D})}$$

  $p(\mathscr{D})$: normalisation constant 'marginal likelihood'

- What we would like : compute / sample from the posterior density (posterior mean, posterior predictive distribution...)

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

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Approximate Bayesian Inference

Two broad categories of methods :

1. Monte Carlo methods → sampling methods
   - Importance Sampling (IS)
   - Markov Chain Monte Carlo (MCMC)
   - Sequential Monte Carlo (SMC) ...
2. **Variational Inference methods** → optimisation-based methods
   - Mean-field Variational Inference (MFVI)
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Variational Inference in a nutshell

Variational Inference methodology

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

$$\inf_{q \in \mathcal{Q}} D(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \tag{1}$$

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

$\rightarrow$ D and $\mathcal{Q}$ are key elements in the optimisation problem (1) !

What we want :

- $\mathcal{Q}$ is easy to sample from / optimise over, yet can capture the complexity inside $p(y|\mathscr{D})$ (e.g. well-chosen parametric family $\mathcal{Q} = \{q : y \mapsto k(\theta, y) \ : \ \theta \in \mathsf{T}\}$)
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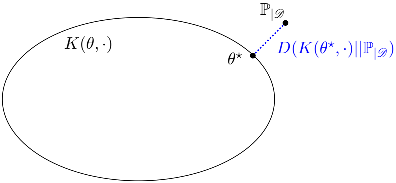

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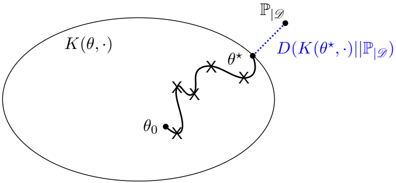

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Mean-field Variational Inference (MFVI)

$\rightarrow D$: Kullback-Leibler (KL) divergence

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

$$D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) = \int_{\mathsf{Y}} \log\left(\frac{q(y)}{p(y|\mathscr{D})}\right) q(y)\nu(\mathrm{d}y) \ .$$

$D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \geqslant 0$ and $D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) = 0$ iif $\mathbb{Q} = \mathbb{P}_{|\mathscr{D}}$

$\rightarrow \mathcal{Q}$: Mean-field family

The latent variable y is made of L **independent** latent variables $(y_1, \ldots, y_L) \in \mathsf{Y}_1 \times \ldots \times \mathsf{Y}_L$ and

$$\mathcal{Q} = \left\{ q : y \mapsto \prod_{\ell=1}^{L} q_\ell(y_\ell) \right\}$$

i.e each latent variable y_ℓ is governed by its own variational probability density q_ℓ with $\nu(\mathrm{d}y) = \bigotimes_{\ell=1}^{L} \nu_\ell(\mathrm{d}y_\ell)$.

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Why this choice of D?

$$D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) = \int_{\mathsf{Y}} \log\left(\frac{q(y)}{p(y|\mathscr{D})}\right) q(y)\nu(\mathrm{d}y)$$

$$= \int_{\mathsf{Y}} q(y)\log\left(\frac{q(y)}{p(y,\mathscr{D})}\right)\nu(\mathrm{d}y) + \log p(\mathscr{D})$$

$$:= -\mathsf{ELBO}(q;\mathscr{D}) + \log p(\mathscr{D})$$

Evidence Lower BOund (ELBO)

$$\mathsf{ELBO}(q;\mathscr{D}) := \int_{\mathsf{Y}} q(y)\log\left(\frac{p(y,\mathscr{D})}{q(y)}\right)\nu(\mathrm{d}y)\ .$$

$\rightarrow$ We deduce :

1. $\inf_{q\in\mathcal{Q}} D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \Leftrightarrow \sup_{q\in\mathcal{Q}}\ \mathsf{ELBO}(q;\mathscr{D})$
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$$\mathsf{ELBO}(q;\mathscr{D}) := \int_{\mathsf{Y}} q(y) \log\left(\frac{p(y,\mathscr{D})}{q(y)}\right) \nu(\mathrm{d}y) \, .$$

$\rightarrow$ We deduce :

1. $\inf_{q\in\mathcal{Q}} D_{KL}(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \Leftrightarrow \sup_{q\in\mathcal{Q}}$ $\mathsf{ELBO}(q;\mathscr{D})$
2. $\mathsf{ELBO}(q;\mathscr{D}) \leqslant \log p(\mathscr{D})$ with equality iif $\mathbb{Q} = \mathbb{P}_{|\mathscr{D}}$

Why this choice of $\mathcal{Q}$?

Recall that

Mean-field assumption

The latent variable y is made of L **independent** latent variables $(y_1, \dots, y_L) \in \mathsf{Y}_1 \times \dots \times \mathsf{Y}_L$ and

$$\mathcal{Q} = \left\{ q : y \mapsto \prod_{\ell=1}^{L} q_\ell(y_\ell) \right\}$$

i.e each latent variable y_ℓ is governed by its own variational probability density q_ℓ with $\nu(\mathrm{d}y) = \bigotimes_{\ell=1}^{L} \nu_\ell(\mathrm{d}y_\ell)$.

$\to$ Plugging this into the ELBO and keeping all factors but ℓ fixed :

$$q_\ell^*(y_\ell) \propto \exp\left(\mathbb{E}_{-\ell}[\log p(y, \mathscr{D})]\right) \quad \text{(optimal rule)}$$

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Input: $(q_\ell)_{1 \leqslant \ell \leqslant L}$: initial variational factors.
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for all $y \in \mathsf{Y}$, $q(y) = \prod_{\ell=1}^{L} q_\ell(y_\ell)$.

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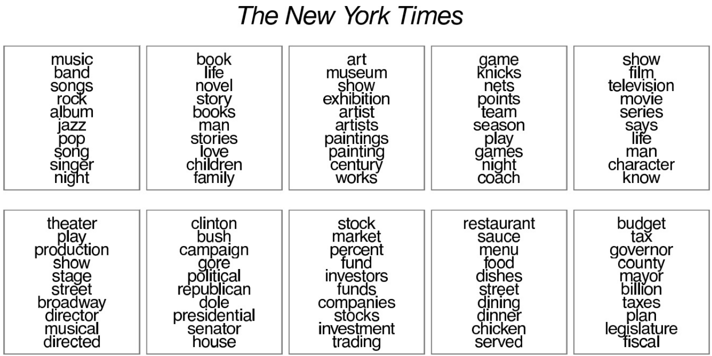
Variational Inference: A Review for Statisticians. D. Blei et al. (2017). JASA



Data : 1.8M articles from the New York Times

Model : hierarchical Dirichlet process topic model

Taken from **Stochastic Variational Inference.** M. D. Hoffman et al. (2013). JMRL.

Toy example : Bayesian Linear Regression (BLR) - 1

- $\mathscr{D} = \{\boldsymbol{c}, \boldsymbol{x}\}$: I 1-D class labels $(c_i)_{1 \leqslant i \leqslant I}$, I 2-D covariates $(\boldsymbol{x}_i)_{1 \leqslant i \leqslant I}$
- $y = \{y_1, y_2\} \in \mathbb{R}^2$: regression coefficients
- Model :

$$
\begin{aligned}
p(c_i|\boldsymbol{x}_i, y) &= \mathcal{N}(c_i; y^T \boldsymbol{x}_i, \sigma^2) \; , \quad 1 \leqslant i \leqslant I \\
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μ_0, Λ_0, σ : fixed hyperparameters

In that case,

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$$q_1(y_1) \propto \exp\left(-\frac{1}{2}\left\{(y_1 - \mu_1)^2\Lambda_{1,1} + 2(y_1 - \mu_1)(\mathbb{E}_{y_2 \sim q_2}\left[y_2\right] - \mu_2)\Lambda_{1,2}\right\}\right)$$
$$\propto \exp\left(-\frac{1}{2}\left\{y_1^2\Lambda_{1,1} - 2y_1\left[\mu_1\Lambda_{1,1} - (\mathbb{E}_{y_2 \sim q_2}[y_2] - \mu_2)\Lambda_{1,2}\right]\right\}\right)$$

so that : $q_1(y_1) = \mathcal{N}(y_1; \mu_1 - \Lambda_{1,1}^{-1}(\mathbb{E}_{y_2 \sim q_2}[y_2] - \mu_2)\Lambda_{1,2}, \Lambda_{1,1}^{-1})$

Toy example : Bayesian Linear Regression (BLR) - 3

$$p(y|\mathscr{D}) = \mathcal{N}(y; \mu, \Lambda^{-1})$$

Optimal updates :

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Setting $m_1 = \mathbb{E}_{y_1 \sim q_1}[y_1]$ and $m_2 = \mathbb{E}_{y_2 \sim q_2}[y_2]$, the CAVI algorithm alternates between :

$$m_1 \leftarrow \mu_1 - \Lambda_{1,1}^{-1}(m_2 - \mu_2)\Lambda_{1,2}$$
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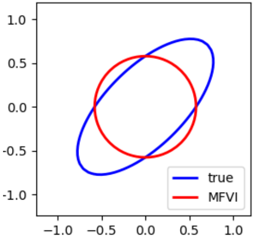
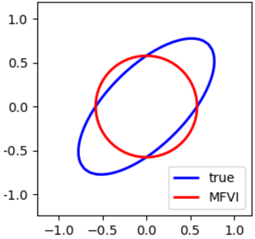


Limitations of MFVI



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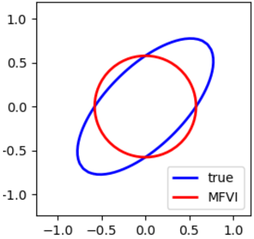

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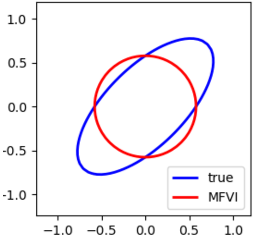

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→ Black-box Variational Inference

Black Box Variational Inference. R. Ranganath et al. (2014). PMLR.

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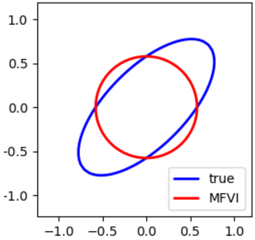

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$\rightarrow$ Alpha-divergence Variational Inference

Black-box alpha divergence minimization. J. Hernandez-Lobato et al. (2016). ICML

Rényi divergence variational inference. Y. Li and R. E Turner. (2016). NeurIPS

Variational inference via χ-upper bound minimization A. Dieng et al. (2017). NeurIPS

Outline

Black-box Variational Inference (BBVI) - 1

Idea of BBVI : Consider a **parametric** family

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

and perform Gradient Ascent on the ELBO with a learning policy $(r_n)_{n\geqslant 1}$

$$\theta_{n+1} = \theta_n + r_n \nabla_\theta \mathrm{ELBO}(k(\theta,\cdot);\mathscr{D})|_{\theta=\theta_n}$$

We have that :

$$\begin{aligned}
\nabla_\theta \mathrm{ELBO}(k(\theta,\cdot);\mathscr{D})|_{\theta=\theta_n} &= \nabla_\theta \left(\int_{\mathsf{Y}} k(\theta,y) \log\left(\frac{p(y,\mathscr{D})}{k(\theta,y)}\right) \nu(\mathrm{d}y) \right) \Big|_{\theta=\theta_n} \\
&= -\int_{\mathsf{Y}} \frac{\partial}{\partial\theta} \left(\frac{k(\theta,y)}{p(y,\mathscr{D})} \log\left(\frac{k(\theta,y)}{p(y,\mathscr{D})}\right)\right) \Big|_{(\theta,y)=(\theta_n,y)} p(y,\mathscr{D})\nu(\mathrm{d}y) \\
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In practice...

1. **Stochastic** Gradient Ascent using the **unbiased** estimate

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2. Large-scale learning using **mini-batching**

$\rightarrow$ convergence towards a **local** optimum of the ELBO ($(r_n)_{n \geqslant 1}$ follows Robbins-Monro)

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$$\nabla_\theta \mathsf{ELBO}(k(\theta, \cdot); \mathscr{D})|_{\theta=\theta_n} = \int_{\mathsf{Y}} k(\theta_n, y) \log\left(\frac{p(y, \mathscr{D})}{k(\theta_n, y)}\right) \frac{\partial \log k(\theta, y)}{\partial \theta}\bigg|_{(\theta,y)=(\theta_n,y)} \nu(\mathrm{d}y)$$

In practice...

1. **Stochastic** Gradient Ascent using the **unbiased** estimate

$$\hat{\nabla}_\theta \mathsf{ELBO}(k(\theta, \cdot); \mathscr{D})|_{\theta=\theta_n} = \frac{1}{M} \sum_{m=1}^{M} \log\left(\frac{p(Y_m, \mathscr{D})}{k(\theta_n, Y_m)}\right) \frac{\partial \log k(\theta, y)}{\partial \theta}\bigg|_{(\theta,y)=(\theta_n,Y_m)}$$

   where $Y_1, \ldots, Y_M$: M i.i.d. samples generated from $k(\theta_n, \cdot)$

2. Large-scale learning using **mini-batching**

$\rightarrow$ convergence towards a **local** optimum of the ELBO ($(r_n)_{n \geqslant 1}$ follows Robbins-Monro)

Remarks on BBVI

In short, BBVI resorts to Stochastic Gradient Ascent on the ELBO

- The updates are not model-specific ("Black-box")
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$$\mathcal{Q} = \{y \mapsto k(\theta, y) \ : \ \theta \in \mathsf{T}\}$$

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   - Rao-blackwellisation
   - Reparameterisation (used in VAEs)
   - Control variates
   - Quasi-Monte Carlo methods
   - ... This is an active area of research!

2. $Y_1 \sim k(\theta_n, \cdot)$ with $p(Y_1, \mathscr{D}) = 0$ makes the gradient blow up...
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Outline

The alpha-divergence family

$(\mathsf{Y}, \mathcal{Y}, \nu)$: measured space, ν is a σ-finite measure on $(\mathsf{Y}, \mathcal{Y})$.

$\mathbb{Q}$ and $\mathbb{P}_{|\mathscr{D}}$: $\mathbb{Q} \preceq \nu$, $\mathbb{P}_{|\mathscr{D}} \preceq \nu$ with $\frac{\mathrm{d}\mathbb{Q}}{\mathrm{d}\nu} = q$, $\frac{\mathrm{d}\mathbb{P}_{|\mathscr{D}}}{\mathrm{d}\nu} = p(\cdot|\mathscr{D})$

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$$D_\alpha(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y|\mathscr{D})}\right) p(y|\mathscr{D})\nu(\mathrm{d}y) \ ,$$

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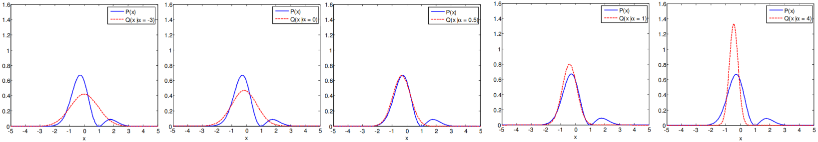
1. A flexible family of divergences...

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



$\alpha = -3$ $\alpha = 0$ $\alpha = 0.5$ $\alpha = 1$ $\alpha = 4$

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

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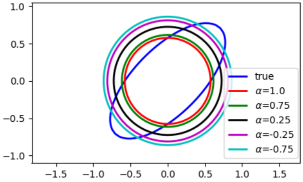
Figure: Optimal mean-field approximation for a varying α (BLR revisited)



Adapted from **Rényi divergence variational inference.** Y. Li and R. E Turner. (2016). NeurIPS

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1. A flexible family of divergences...
2. ...suitable for Variational Inference purposes...

$$\inf_{q \in \mathcal{Q}} D_\alpha(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \Leftrightarrow \inf_{q \in \mathcal{Q}} \Psi_\alpha(q; p)$$

with $\Psi_\alpha(q;p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$ and $p = p(\cdot, \mathscr{D})$

3. ...with good convexity properties : f_α is convex!

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$$f_\alpha(u) = \begin{cases} \frac{1}{\alpha(\alpha-1)}\left[u^\alpha - 1 - \alpha(u-1)\right], & \text{if } \alpha \in \mathbb{R} \setminus \{0,1\}, \\ u\log(u) + 1 - u, & \text{if } \alpha = 1 \text{ (Exclusive KL)}, \\ -\log(u) + u - 1, & \text{if } \alpha = 0 \text{ (Inclusive KL)}. \end{cases}$$

1. A flexible family of divergences...
2. ...suitable for Variational Inference purposes...

$$\inf_{q \in \mathcal{Q}} D_\alpha(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) \Leftrightarrow \inf_{q \in \mathcal{Q}} \Psi_\alpha(q; p)$$

with $\Psi_\alpha(q;p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$ and $p = p(\cdot, \mathscr{D})$

3. ...with good convexity properties : f_α is convex!

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Consider a **parametric** family

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

and perform **Gradient Descent** on $\Psi_\alpha(k(\theta,\cdot);p)$

We have that : for all $\alpha \in \mathbb{R} \setminus \{1\}$, $f'_\alpha(u) = \frac{1}{\alpha-1}\left[u^{\alpha-1} - 1\right]$ and

$$\begin{aligned}\nabla_\theta \Psi_\alpha(k(\theta,\cdot);p)|_{\theta=\theta_n} &= \nabla_\theta \left(\int_{\mathsf{Y}} f_\alpha\left(\frac{k(\theta,y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)\right)\Big|_{\theta=\theta_n} \\ &= \dots \\ &= \int_{\mathsf{Y}} \frac{k(\theta_n,y)^\alpha p(y)^{1-\alpha}}{\alpha-1} \left.\frac{\partial \log k(\theta,y)}{\partial\theta}\right|_{(\theta,y)=(\theta_n,y)} \nu(\mathrm{d}y) \\ &\approx \frac{1}{M}\sum_{m=1}^{M} \frac{k(\theta_n,Y_m)^{\alpha-1}p(Y_m)^{1-\alpha}}{\alpha-1} \left.\frac{\partial \log k(\theta,y)}{\partial\theta}\right|_{(\theta,y)=(\theta_n,Y_m)}\end{aligned}$$

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$\rightarrow$ derived from Rényi's α-divergence, linked to the α-divergence.

$$\begin{aligned} \nabla_\theta \mathcal{L}_\alpha(k(\theta,\cdot);p)|_{\theta=\theta_n} &= \frac{\alpha}{1-\alpha} \int_{\mathsf{Y}} \frac{k(\theta_n,y)^\alpha p(y)^{1-\alpha}}{\int_{\mathsf{Y}} k(\theta_n,y')^\alpha p(y')^{1-\alpha} \nu(\mathrm{d}y')} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right|_{(\theta,y)=(\theta_n,y)} \nu(\mathrm{d}y) \\ &\approx \frac{\alpha}{1-\alpha} \sum_{m=1}^{M} \frac{w_{n,m}}{\sum_{m'=1}^{M} w_{n,m'}} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right|_{(\theta,y)=(\theta_n,Y_m)} \end{aligned}$$

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Alpha-divergence Variational Inference : summary

Alpha-Divergence approach	Rényi's Alpha-Divergence approach
$\inf_{\theta \in \mathsf{T}} \Psi_\alpha(k(\theta, \cdot); p)$	$\sup_{\theta \in \mathsf{T}} \mathcal{L}_\alpha(k(\theta, \cdot); p)$
$\frac{1}{\alpha-1} \frac{1}{M} \sum_{m=1}^M w_{n,m} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right\|_{(\theta,y)=(\theta_n,Y_m)}$	$\frac{\alpha}{1-\alpha} \sum_{m=1}^M \frac{w_{n,m}}{\sum_{m'=1}^M w_{n,m'}} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right\|_{(\theta,y)=(\theta_n,Y_m)}$

Alpha : $\quad \theta_{n+1} = \theta_n + \frac{r_n}{1-\alpha} \frac{1}{M} \sum_{m=1}^M w_{n,m} \left. \frac{\partial \log k(\theta, y)}{\partial \theta} \right|_{(\theta,y)=(\theta_n,Y_m)}$

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Alpha-divergence Variational Inference : summary

Alpha-Divergence approach	Rényi's Alpha-Divergence approach
$\inf_{\theta \in \mathsf{T}} \Psi_\alpha(k(\theta, \cdot); p)$	$\inf_{\theta \in \mathsf{T}} -\alpha^{-1} \mathcal{L}_\alpha(k(\theta, \cdot); p)$
$\frac{1}{\alpha-1} \frac{1}{M} \sum_{m=1}^M w_{n,m} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right\rvert_{(\theta,y)=(\theta_n,Y_m)}$	$\frac{1}{\alpha-1} \sum_{m=1}^M \frac{w_{n,m}}{\sum_{m'=1}^M w_{n,m'}} \left. \frac{\partial \log k(\theta,y)}{\partial \theta} \right\rvert_{(\theta,y)=(\theta_n,Y_m)}$

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Outline

Conclusion of Part 1

Variational Inference : optimisation-based methods for Bayesian Inference

Core questions in Variational Inference :
- choice of the **variational family** $\mathcal{Q}$
- choice of the **measure of dissimilarity** D

1. MFVI : mean-field family, model-specific updates using the ELBO
2. SVI : scales MFVI to large datasets
3. BBVI : parametric family, Stochastic Gradient Ascent on the ELBO
4. **Alpha-divergence Variational Inference** : parametric family, extends BBVI to more general objective functions derived from the Alpha-divergence

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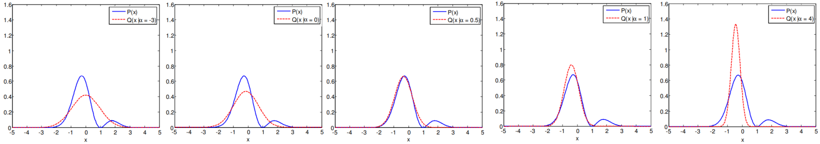
Food for thoughts



$\alpha = -3$ $\alpha = 0$ $\alpha = 0.5$ $\alpha = 1$ $\alpha = 4$

Question : Can we further extend the approximating family $\mathcal{Q}$ in the context of Alpha-divergence Variational Inference?

Some answers in Part 2 and 3!

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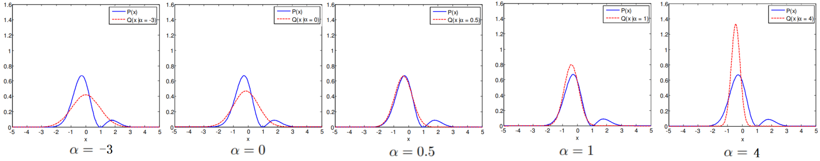

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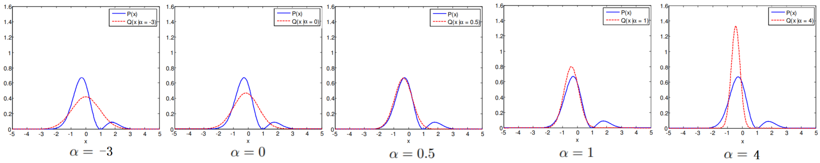

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Proof of the optimal rule $q_\ell^*(y_\ell) \propto \exp\left(\mathbb{E}_{-\ell}[\log p(y, \mathscr{D})]\right)$

For notational convenience : $\mathsf{Y} = \mathsf{Y}_\ell \times \mathsf{Y}_{-\ell}$, $q(y) = q_\ell(y_\ell) q_{-\ell}(y_{-\ell})$ and $\nu(\mathrm{d}y) = \nu_\ell(\mathrm{d}y_\ell)\nu_{-\ell}(\mathrm{d}y_{-\ell})$.

$$\mathsf{ELBO}(q; \mathscr{D}) = \int_{\mathsf{Y}} q(y) \log\left(\frac{p(y, \mathscr{D})}{q(y)}\right) \nu(\mathrm{d}y)$$

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\begin{aligned}
\mathsf{ELBO}(q;\mathscr{D}) &= \int_{\mathsf{Y}} q(y) \log\left(\frac{p(y,\mathscr{D})}{q(y)}\right)\nu(\mathrm{d}y) \\
&= \int_{\mathsf{Y}_\ell}\int_{\mathsf{Y}_{-\ell}} q_\ell(y_\ell)q_{-\ell}(y_{-\ell}) \log\left(\frac{p(y,\mathscr{D})}{q_\ell(y_\ell)q_{-\ell}(y_{-\ell})}\right)\nu_{-\ell}(\mathrm{d}y_{-\ell})\nu_\ell(\mathrm{d}y_\ell) \\
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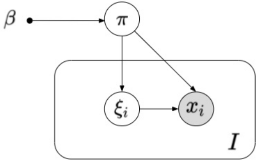
CAVI for large datasets : Stochastic Variational Inference



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- $y = \{\pi, \xi_1, \dots, \xi_I\}$, π : global latent variable, $\xi_1, \dots, \xi_I$: local latent variables (β : hyperparameter)

In that case, $p(y, \mathscr{D}) = p(\pi|\beta) \prod_{i=1}^{I} p(\xi_i|\pi) p(x_i|\xi_i, \pi)$

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$$q(y) = q(\pi|\gamma) \prod_{i=1}^{I} q(\xi_i|\phi_i)$$

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Problem : I is often very large (e.g. 1.8M articles from the New York Times)

$\rightarrow$ The use of **stochastic** optimisation enabled large scale learning

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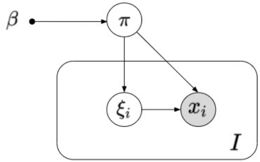

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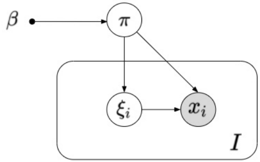

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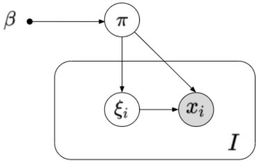

- $\mathscr{D} = \{x_1, \ldots x_I\}$, $x_1, \ldots, x_I$: i.i.d. observations
- $y = \{\pi, \xi_1, \ldots, \xi_I\}$, π : global latent variable, $\xi_1, \ldots, \xi_I$: local latent variables (β : hyperparameter)

In that case, $p(y, \mathscr{D}) = p(\pi|\beta) \prod_{i=1}^{I} p(\xi_i|\pi) p(x_i|\xi_i, \pi)$

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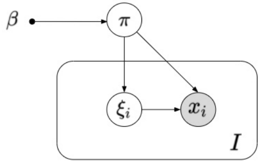

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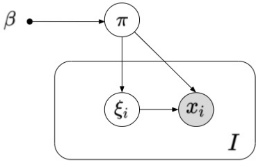

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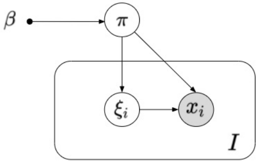

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Variational Inference
Foundations and recent advances
(Part 2)

Kamélia Daudel

UNIVERSITY OF OXFORD

University of Bristol – 09/03/2022

Reminder - 1

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

- Variational Inference optimisation problem :

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

where $\mathcal{Q}$ is the variational family and D is the measure of dissimilarity

- **Alpha-Divergence Variational Inference :** Two possible objective functions

$$\Psi_\alpha(q;p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$$
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When $\mathcal{Q}$ is parametric,

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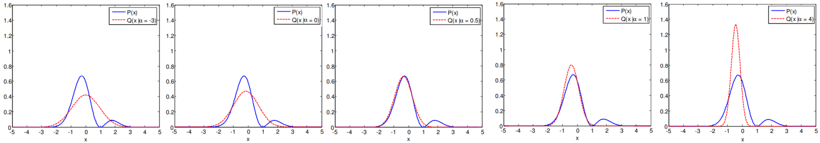

$\alpha = -3$ $\alpha = 0$ $\alpha = 0.5$ $\alpha = 1$ $\alpha = 4$

Outline

1. Infinite-dimensional Alpha-divergence minimisation
2. Numerical experiments
3. Conclusion of Part 2

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Infinite-dimensional gradient-based descent for alpha-divergence minimisation.
K. Daudel, R. Douc and F. Portier. Ann. Statist. 49 (4) 2250 - 2270, August 2021.
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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 $\int_{\mathsf{Y}} p(y)\nu(\mathrm{d}y) < \infty$.

(A2) The function $\Gamma : \mathrm{Dom}_\alpha \to \mathbb{R}_{>0}$ is decreasing, continuously differentiable and satisfies the inequality

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

Theorem

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,

1. $\Psi_\alpha(\mathcal{I}_\alpha(\mu)k) \leqslant \Psi_\alpha(\mu k)$
2. $\Psi_\alpha(\mathcal{I}_\alpha(\mu)k) = \Psi_\alpha(\mu k)$ if and only if $\mu = \mathcal{I}_\alpha(\mu)$

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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Proof : 1) Proving a general lower bound

Let $\mu, \zeta \in \mathrm{M}_1(\mathsf{T})$ s.t $\zeta \preceq \mu$ and $\Psi_\alpha(\mu k) < \infty$. Denote by g the density of ζ w.r.t μ.

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and equality holds iif $\zeta = \mu$.

By definition $\Psi_\alpha(\mu k) = \int_{\mathsf{Y}} f_\alpha\left(\frac{\mu k(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$ with f_α convex.

First idea

By convexity of f_α,

$$f_\alpha\left(\frac{\mu k(y)}{p(y)}\right) \geqslant f_\alpha\left(\frac{\zeta k(y)}{p(y)}\right) + f'_\alpha\left(\frac{\zeta k(y)}{p(y)}\right)\frac{\mu k(y) - \zeta k(y)}{p(y)}$$

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By convexity of f_α : for all $y \in \mathsf{Y}$

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$\to$ Next, we integrate w.r.t to $\frac{\mu(\mathrm{d}\theta)k(\theta,y)}{\mu k(y)}$,

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Choice of A_α

We take $\quad A_\alpha := \int_{\mathsf{Y}} \nu(\mathrm{d}y) \int_{\mathsf{T}} \mu(\mathrm{d}\theta) k(\theta, y) f_\alpha'\left(\frac{g(\theta)\mu k(y)}{p(y)}\right) [1 - g(\theta)]$

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Setting $g \propto \Gamma(b_{\mu,\alpha} + \kappa)$, we have that

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The proof is complete if we prove that $A_\alpha \geqslant 0$.

Proving that $A_\alpha \geqslant 0 \to$ We treat the case $\alpha \in \mathbb{R} \setminus \{1\}$.

In this case $f'_\alpha(u) = \frac{1}{\alpha - 1}[u^{\alpha-1} - 1]$ and

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$$\begin{aligned} A_\alpha &= \mathbb{E}\left(\left[V - \kappa + \frac{1}{\alpha - 1} \right] \tilde{\Gamma}^{\alpha-1}(V) \left[1 - \tilde{\Gamma}(V) \right] \right) \\ &= \mathbb{C}\mathrm{ov}\left(\left[V - \kappa + \frac{1}{\alpha - 1} \right] \tilde{\Gamma}^{\alpha-1}(V), 1 - \tilde{\Gamma}(V) \right) \quad \text{since} \quad \mathbb{E}[1 - \tilde{\Gamma}(V)] = 0 \end{aligned}$$

(A2) The function $\Gamma : \mathrm{Dom}_\alpha \rightarrow \mathbb{R}_{>0}$ is decreasing, continuously differentiable and satisfies the inequality

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

Conclusion: $A_\alpha \geqslant 0$! □

Proof : 2) take $g \propto \Gamma(b_{\mu,\alpha} + \kappa)$ and show that $A_\alpha \geqslant 0$

Proving that $A_\alpha \geqslant 0 \rightarrow$ We treat the case $\alpha \in \mathbb{R} \setminus \{1\}$.

We have obtained that

$$A_\alpha = \int_{\mathsf{T}} \mu(\mathrm{d}\theta) \left[b_{\mu,\alpha}(\theta) + \frac{1}{\alpha - 1} \right] g(\theta)^{\alpha-1} \left[1 - g(\theta)\right]$$

It's time to use that $g \propto \Gamma(b_{\mu,\alpha} + \kappa)$!

(i) Let V be the random variable $V(\theta) = b_{\mu,\alpha}(\theta) + \kappa$ (probability space $(\mathsf{T}, \mathcal{T}, \mu)$)

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Reminder : 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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Theorem

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,

1. $\Psi_\alpha(\mathcal{I}_\alpha(\mu)k) \leqslant \Psi_\alpha(\mu k)$
2. $\Psi_\alpha(\mathcal{I}_\alpha(\mu)k) = \Psi_\alpha(\mu k)$ if and only if $\mu = \mathcal{I}_\alpha(\mu)$

Examples satisfying (A2)

(A2) The function $\Gamma : \mathrm{Dom}_\alpha \to \mathbb{R}_{>0}$ is decreasing, continuously differentiable and satisfies the inequality

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- Entropic Mirror Descent : $\eta \in (0,1]$, $\kappa \in \mathbb{R}$ and $\alpha = 1$

$$\Gamma(v) = e^{-\eta v}$$

$$\mu_{n+1}(\mathrm{d}\theta) \propto \mu_n(\mathrm{d}\theta)\exp\left[-\eta\int_{\mathsf{Y}} k(\theta,y)\log\left(\frac{\mu_n k(y)}{p(y)}\right)\nu(\mathrm{d}y)\right]$$

$\to$ NB : η corresponds to the learning rate

- Power descent : $\eta \in (0,1]$, $(\alpha-1)\kappa \geqslant 0$ and $\alpha \neq 1$

$$\Gamma(v) = [(\alpha-1)\,v+1]^{\frac{\eta}{1-\alpha}}$$

$$\mu_{n+1}(\mathrm{d}\theta) \propto \mu_n(\mathrm{d}\theta)\left[\int_{\mathsf{Y}} k(\theta,y)\left(\frac{\mu_n k(y)}{p(y)}\right)^{\alpha-1}\nu(\mathrm{d}y)+(\alpha-1)\kappa\right]^{\frac{\eta}{1-\alpha}}$$

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Convergence results

$$\mu_{n+1}(\mathrm{d}\theta) = \frac{\mu_n(\mathrm{d}\theta) \cdot \Gamma(b_{\mu_n,\alpha}(\theta) + \kappa)}{\mu_n(\Gamma(b_{\mu_n,\alpha} + \kappa))}, \quad n \geqslant 1$$

Assume (A1) and that $|b|_{\infty,\alpha} = \sup_{\theta \in \mathsf{T}, \mu \in \mathrm{M}_1(\mathsf{T})} |b_{\mu,\alpha}(\theta)| < \infty$

$\to O(1/N)$ convergence rates when Γ is L-smooth and $-\log \Gamma$ is concave increasing

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The special case of finite mixture models

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

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Then, $\mu_n = \underbrace{\mathcal{I}_\alpha \circ \cdots \circ \mathcal{I}_\alpha}_{n \text{ times}}(\mu_{\boldsymbol{\lambda}_1})$ is of the form $\mu_n = \sum_{j=1}^J \lambda_{j,n} \delta_{\theta_j}$ with

$$\lambda_{j,n+1} = \frac{\lambda_{j,n} \Gamma(b_{\mu_n,\alpha}(\theta_j) + \kappa)}{\sum_{i=1}^J \lambda_{i,n} \Gamma(b_{\mu_n,\alpha}(\theta_i) + \kappa)}, \quad j = 1 \ldots J,\ n \geqslant 1$$

NB : $\mu_n k(y) = \sum_{j=1}^J \lambda_{j,n} k(\theta_j, y)$

$$\mathcal{Q} = \left\{ q : y \mapsto \mu_{\boldsymbol{\lambda}} k(y) = \sum_{j=1}^J \lambda_j k(\theta_j, y) \ : \ \boldsymbol{\lambda} \in \mathcal{S}_J \right\}$$

Convergence results for finite mixture models

$$\lambda_{j,n+1} = \frac{\lambda_{j,n}\Gamma(b_{\mu_n,\alpha}(\theta_j) + \kappa)}{\sum_{i=1}^J \lambda_{i,n}\Gamma(b_{\mu_n,\alpha}(\theta_i) + \kappa)}, \quad j = 1 \ldots J,\ n \geqslant 1$$

Assume (A1) and that $|b|_{\infty,\alpha} = \sup_{\theta\in\mathsf{T},\mu\in\mathrm{M}_1(\mathsf{T})} |b_{\mu,\alpha}(\theta)| < \infty$

$\rightarrow O(1/N)$ convergence rates when Γ is L-smooth and $-\log\Gamma$ is concave increasing
e.g. Entropic Mirror Descent: when $\alpha = 1$, we have for all $\eta \in (0,1)$

$$\Psi_\alpha(\mu_{\boldsymbol{\lambda}_n} k) - \Psi_\alpha(\mu^\star k) \leqslant \frac{\log J}{\eta N} + \frac{\sqrt{2\log J}|b|_{\infty,1}}{(1-\eta)N}$$

$\rightarrow$ The case $\alpha < 1$ for the Power Descent is trickier... $\eta \in (0,1]$, $\kappa \geqslant 0$
Under additionnal assumptions on Ψ_α and $b_{\mu,\alpha}$, if $\{K(\theta_1,\cdot),\ldots K(\theta_J,\cdot)\}$ are linearly independent, then :

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Towards a practical implementation

Algorithm

Let $\Theta = (\theta_1, ..., \theta_J) \in \mathsf{T}^J$ be fixed and let $\boldsymbol{\lambda}_1 \in \mathcal{S}_J$. At time $n \geqslant 1$, define

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$\to$ Monte Carlo approximations to estimate $b_{\mu_n,\alpha}(\theta_j)$, e.g.

$$\hat{b}_{\mu_n,\alpha,M}(\theta_j) = \frac{1}{M}\sum_{m=1}^{M} \frac{k(\theta_j, Y_{m,n})}{\mu_n k(Y_{m,n})} f'_\alpha\left(\frac{\mu_n k(Y_{m,n})}{p(Y_{m,n})}\right),$$

with $Y_{1,n}, ..., Y_{M,n} \overset{\text{i.i.d}}{\sim} \mu_n k$.

$\to$ Exploitation step not requiring any information on the distribution of $\theta_1, ..., \theta_J$

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Outline

Numerical experiments

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

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

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

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Toy example : Entropic Mirror Descent vs Power Descent

Comparison between

- 0.5-Mirror descent : $\Gamma(v) = e^{-\eta v}$ and $\alpha = 0.5$,
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$J = M = 100$, initial mixture weights : $[1/J, ..., 1/J]$, $N = 10$, $T = 20$
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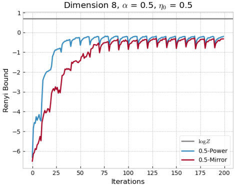

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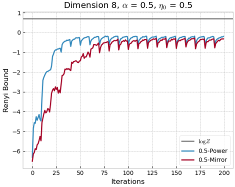

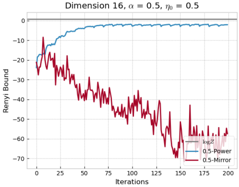

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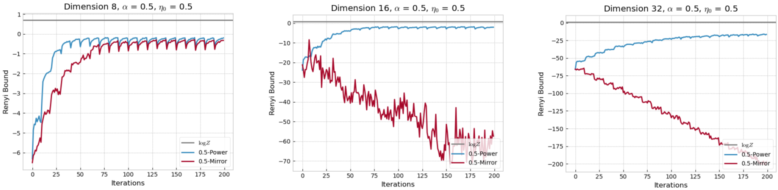

Toy example : the case $\alpha = 1$

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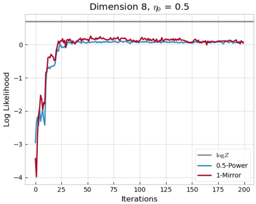

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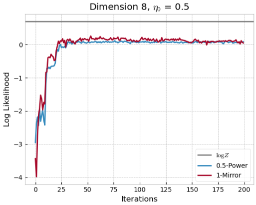

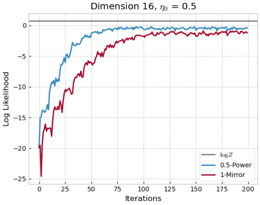

Toy example : the case $\alpha = 1$

Comparison between:

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

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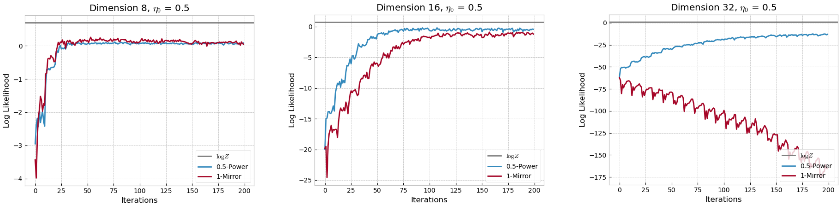

Bayesian Logistic Regression

$\rightarrow$ $\mathscr{D} = \{\boldsymbol{c}, \boldsymbol{x}\}$: 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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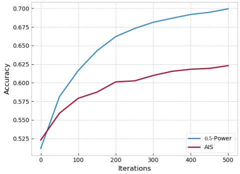

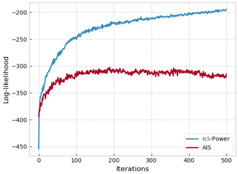

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Outline

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K. Daudel and R. Douc (2021). To appear in NeurIPS2021

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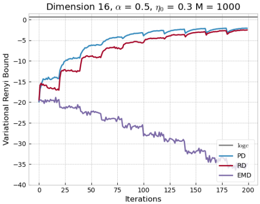

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  Some answers in Part 3!

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Variational Inference
Foundations and recent advances
(Part 3)

Kamélia Daudel

University of Bristol – 09/03/2022

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Alpha-Divergence Variational Inference : Two possible objective functions

$$\Psi_\alpha(q;p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$$

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$$\Psi_\alpha(q;p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$$

$$-\alpha^{-1}\mathcal{L}_\alpha(q;p) = \frac{1}{\alpha(\alpha-1)} \log\left(\int_{\mathsf{Y}} q(y)^\alpha p(y)^{1-\alpha}\nu(\mathrm{d}y)\right)$$

with $p = p(\cdot, \mathscr{D})$ and

$$f_\alpha(u) = \begin{cases} \frac{1}{\alpha(\alpha-1)}\left[u^\alpha - 1 - \alpha(u-1)\right], & \text{if } \alpha \in \mathbb{R}\setminus\{0,1\}, \\ u\log(u) + 1 - u, & \text{if } \alpha = 1 \text{ (Exclusive KL)}, \\ -\log(u) + u - 1, & \text{if } \alpha = 0 \text{ (Inclusive KL)}. \end{cases}$$

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

Stochastic Gradient Descent w.r.t θ on $\Psi_\alpha(q;p)$ (resp. $-\alpha^{-1}\mathcal{L}_\alpha(q;p)$)

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

Power Descent, Entropic Mirror Descent on $\Psi_\alpha(q;p)$ (resp. $-\alpha^{-1}\mathcal{L}_\alpha(q;p)$)

$\rightarrow$ applies to $\mathcal{Q} = \left\{q : y \mapsto \sum_{j=1}^J \lambda_j k(\theta_j, y) \;:\; \boldsymbol{\lambda} \in \mathcal{S}_J\right\}$

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Question : Can we propose valid updates for

$$\mathcal{Q} = \left\{ q : y \mapsto \sum_{j=1}^{J} \lambda_j k(\theta_j, y) \ : \ \boldsymbol{\lambda} \in \mathcal{S}_J, \Theta \in \mathsf{T}^J \right\} ?$$

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Outline

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Monotonic Alpha-Divergence Minimisation

Monotonic Alpha-divergence Minimisation.
K. Daudel, R. Douc and F. Roueff (2021). https://arxiv.org/abs/2103.05684

Idea : Extend the typical variational parametric family

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

by considering the mixture model variational family

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

and propose an update formula for $(\boldsymbol{\lambda}, \Theta)$ that ensures a systematic decrease in the alpha-divergence (i.e. Ψ_α) at each step.

$\rightarrow$ Optimising w.r.t $\boldsymbol{\lambda}$ and Θ is the novelty compared to Part 2!

Conditions for a monotonic decrease

Optimisation problem

$$\inf_{\boldsymbol{\lambda} \in \mathcal{S}_J, \Theta \in \mathsf{T}^J} \Psi_\alpha(\mu_{\boldsymbol{\lambda},\Theta} k; p) \quad \text{with} \quad \Psi_\alpha(\mu_{\boldsymbol{\lambda},\Theta} k; p) = \int_{\mathsf{Y}} f_\alpha\left(\frac{\mu_{\boldsymbol{\lambda},\Theta} k(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$$

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

Theorem

Assume (A1). Let $\alpha \in [0, 1)$, $J \in \mathbb{N}^\star$. Then, choosing $(\boldsymbol{\lambda}_n, \Theta_n)_{n \geqslant 1}$ so that: $\Psi_\alpha(\mu_{\boldsymbol{\lambda}_1,\Theta_1} k) < \infty$ and $\forall n \geqslant 1$,

$$\int_{\mathsf{Y}} \sum_{j=1}^{J} \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log\left(\frac{\lambda_{j,n+1}}{\lambda_{j,n}}\right) \nu(\mathrm{d}y) \geqslant 0 \qquad \text{(Weights)}$$

$$\int_{\mathsf{Y}} \sum_{j=1}^{J} \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log\left(\frac{k(\theta_{j,n+1}, y)}{k(\theta_{j,n}, y)}\right) \nu(\mathrm{d}y) \geqslant 0 \qquad \text{(Components)}$$

where $\varphi_{j,n}^{(\alpha)}(y) = k(\theta_{j,n}, y) \left(\frac{\mu_{\boldsymbol{\lambda}_n,\Theta_n} k(y)}{p(y)}\right)^{\alpha-1}$, yields a systematic decrease in Ψ_α at each step.

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$$\inf_{\boldsymbol{\lambda}\in\mathcal{S}_J,\Theta\in\mathsf{T}^J} \Psi_\alpha(\mu_{\boldsymbol{\lambda},\Theta}k\cancel{;p}) \quad \text{with} \quad \Psi_\alpha(\mu_{\boldsymbol{\lambda},\Theta}k\cancel{;p}) = \int_{\mathsf{Y}} f_\alpha\left(\frac{\mu_{\boldsymbol{\lambda},\Theta}k(y)}{p(y)}\right)p(y)\nu(\mathrm{d}y)$$

(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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Proof : 1) Proving a general lower bound - 1

Let $q, q' \in \mathcal{Q}$ and assume that $\Psi_\alpha(q') < \infty$. For all $\alpha \in [0,1)$, it holds that

$$\frac{1}{1-\alpha} \int_{\mathsf{Y}} q'(y)^\alpha p(y)^{1-\alpha} \log\left(\frac{q(y)}{q'(y)}\right) \nu(\mathrm{d}y) \leqslant \Psi_\alpha(q') - \Psi_\alpha(q)$$

By definition $\Psi_\alpha(q) = \int_{\mathsf{Y}} f_\alpha\left(\frac{q(y)}{p(y)}\right) p(y)\nu(\mathrm{d}y)$.

$\rightarrow$ **Case** $\alpha = 0$ **:** $f_0(u) = -\log(u) + u - 1$

$$\Psi_\alpha(q) = \int_{\mathsf{Y}} \left(-\log\left(\frac{q(y)}{p(y)}\right) + \frac{q(y)}{p(y)} - 1\right) p(y)\nu(\mathrm{d}y)$$

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To finish the proof :

(i) multiply by $(\mu_n k(y))^\alpha p(y)^{1-\alpha}$ on both sides ($\varphi_{j,n}^{(\alpha)}(y) = k(\theta_{j,n},y)\left(\frac{p(y)}{\mu_n k(y)}\right)^{1-\alpha}$)

(ii) integrate with respect to $\nu(\mathrm{d}y)$

Commenting the conditions for a monotonic decrease

$$\int_{\mathsf{Y}} \sum_{j=1}^{J} \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log\left(\frac{\lambda_{j,n+1}}{\lambda_{j,n}}\right) \nu(\mathrm{d}y) \geqslant 0 \qquad \text{(Weights)}$$

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1. (Weights) and (Components) permit separate/simultaneous updates
2. They are satified for $\boldsymbol{\lambda}_{n+1} = \boldsymbol{\lambda}_n$ and $\Theta_{n+1} = \Theta_n$ respectively
3. The dependency is **simpler** in (Weights)

   $\rightarrow$ (Weights) holds for $\boldsymbol{\lambda}_{n+1}$ such that

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Towards simultaneous updates

$$\int_{\mathsf{Y}} \sum_{j=1}^{J} \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log\left(\frac{k(\theta_{j,n+1}, y)}{k(\theta_{j,n}, y)}\right) \nu(\mathrm{d}y) \geqslant 0 \qquad \text{(Components)}$$

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Two questions at this stage

1. Can we derive practical updates from the maximisation / gradient-based approaches?

2. Do those approaches relate to the existing litterature?

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Outline

Maximisation approach

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For all $j = 1 \dots J$, $b_{j,n} \geqslant 0$ and

$$\theta_{j,n+1} = \mathrm{argmax}_{\theta \in \mathsf{T}} \int_{\mathsf{Y}} \left[\varphi_{j,n}^{(\alpha)}(y) + b_{j,n} k(\theta_{j,n}, y)\right] \log\left(\frac{k(\theta, y)}{k(\theta_{j,n}, y)}\right) \nu(\mathrm{d}y)$$

$\rightarrow$ We have added a regularisation term!

Maximisation approach for GMMs

Set $k(\theta, y) = \mathcal{N}(y; m, \Sigma)$ with $\theta = (m, \Sigma)$ and $\check{\varphi}_{j,n}^{(\alpha)} = \varphi_{j,n}^{(\alpha)} / \int \varphi_{j,n}^{(\alpha)} \mathrm{d}\nu$.

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Interpretation : tradeoff between

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- an update close to $\theta_{j,n} = (m_{j,n}, \Sigma_{j,n})$ $[\gamma_{j,n} \to 0]$
- an update that chooses the Gaussian with the same mean and covariance matrix as $\check{\varphi}_{j,n}^{(\alpha)}$ $[\gamma_{j,n} = 1]$

Why does it matter? In practice, Monte Carlo approximations!

Maximisation approach for GMMs

Set $k(\theta, y) = \mathcal{N}(y; m, \Sigma)$ with $\theta = (m, \Sigma)$ and $\check{\varphi}_{j,n}^{(\alpha)} = \varphi_{j,n}^{(\alpha)} / \int \varphi_{j,n}^{(\alpha)} \mathrm{d}\nu$.

For all $j = 1 \ldots J$,

$$\lambda_{j,n+1} = \frac{\lambda_{j,n} \left[\int_{\mathsf{Y}} \varphi_{j,n}^{(\alpha)}(y) \nu(\mathrm{d}y) + (\alpha - 1)\kappa \right]^{\eta_n}}{\sum_{\ell=1}^{J} \lambda_{\ell,n} \left[\int_{\mathsf{Y}} \varphi_{\ell,n}^{(\alpha)}(y) \nu(\mathrm{d}y) + (\alpha - 1)\kappa \right]^{\eta_n}}$$

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where $\tilde{\Sigma}_{j,n} = \Sigma_{j,n} + (m_{j,n+1} - m_{j,n})(m_{j,n+1} - m_{j,n})^T$ and $\gamma_{j,n}$ depends on $b_{j,n}$.

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$\rightarrow$ The M-PMC algorithm a.k.a 'Integrated EM' for GMMs

Adaptive importance sampling in general mixture classes. O. Cappé, R. Douc, A. Guillin, J-M Marin and C. P Robert (2008). Statistics and Computing, 18(4):447–459

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Outline

Gradient-based approach

$$\int_{\mathsf{Y}} \sum_{j=1}^{J} \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log \left(\frac{k(\theta_{j,n+1}, y)}{k(\theta_{j,n}, y)} \right) \nu(\mathrm{d}y) \geqslant 0 \qquad \text{(Components)}$$

For all $j = 1 \ldots J$, $\gamma_{j,n} \in (0,1]$

$$\theta_{j,n+1} = \theta_{j,n} - \frac{\gamma_{j,n}}{\beta_{j,n}} \nabla g_{j,n}(\theta)|_{\theta=\theta_{j,n}}$$

where $g_{j,n}$ is assumed to be $\beta_{j,n}$-smooth on $\mathsf{T} = \mathbb{R}^d$ with

$$g_{j,n}(\theta) = \int_{\mathsf{Y}} \frac{\varphi_{j,n}^{(\alpha)}(y)}{\alpha - 1} \log \left(\frac{k(\theta, y)}{k(\theta_{j,n}, y)} \right) \nu(\mathrm{d}y) \; .$$

We have that

$$\nabla g_{j,n}(\theta)|_{\theta=\theta_{j,n}} = \int_{\mathsf{Y}} \frac{\varphi_{j,n}^{(\alpha)}(y)}{\alpha - 1} \frac{\partial \log k(\theta, y)}{\partial \theta} \bigg|_{(\theta,y)=(\theta_{j,n},y)} \nu(\mathrm{d}y)$$

$\rightarrow$ There might be links with Gradient Descent steps...

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Gradient-based approach for GMMs

Set $k(\theta, y) = \mathcal{N}(y; m, \sigma^2 \boldsymbol{I}_d)$ with $\theta = m$, fixed $\sigma > 0$ and $\check{\varphi}_{j,n}^{(\alpha)} = \varphi_{j,n}^{(\alpha)} / \int \varphi_{j,n}^{(\alpha)} \mathrm{d}\nu$

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where $\gamma_{j,n} \in (0, 1]$

$\rightarrow$ Interpretation :

1. Maximisation and gradient-based approach coincide when $\Sigma = \sigma^2 \boldsymbol{I}_d$ with σ fixed
2. We recognise Gradient Descent steps w.r.t Θ on $-\alpha^{-1} \mathcal{L}_\alpha(\mu k; p)$ by setting

$$\gamma_{j,n} = \gamma'_{j,n} \frac{\lambda_{j,n} \int_{\mathsf{Y}} \varphi_{j,n}^{(\alpha)}(y) \nu(\mathrm{d}y)}{\int_{\mathsf{Y}} (\mu_n k(y))^\alpha p(y)^{1-\alpha} \nu(\mathrm{d}y)} \quad \text{with} \quad \gamma'_{j,n} \in (0, 1]$$

Compatibility between Gradient Descent steps w.r.t Θ and mixture weights updates (and even covariance matrices updates)!

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Gradient-based approach for GMMs

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For all $j = 1 \dots J$,

$$\lambda_{j,n+1} = \frac{\lambda_{j,n} \left[\int_{\mathsf{Y}} \varphi^{(\alpha)}_{j,n}(y) \nu(\mathrm{d}y) + (\alpha - 1)\kappa \right]^{\eta_n}}{\sum_{\ell=1}^{J} \lambda_{\ell,n} \left[\int_{\mathsf{Y}} \varphi^{(\alpha)}_{\ell,n}(y) \nu(\mathrm{d}y) + (\alpha - 1)\kappa \right]^{\eta_n}}$$

$$m_{j,n+1} = (1 - \gamma_{j,n}) m_{j,n} + \gamma_{j,n} \int_{\mathsf{Y}} \check{\varphi}^{(\alpha)}_{j,n}(y) \; y \; \nu(\mathrm{d}y)$$

where $\gamma_{j,n} \in (0, 1]$

→ Interpretation :

1. Maximisation and gradient-based approach coincide when $\Sigma = \sigma^2 \boldsymbol{I}_d$ with σ fixed
2. We recognise Gradient Descent steps w.r.t Θ on $-\alpha^{-1} \mathcal{L}_\alpha(\mu k; p)$ by setting

$$\gamma_{j,n} = \gamma'_{j,n} \frac{\lambda_{j,n} \int_{\mathsf{Y}} \varphi^{(\alpha)}_{j,n}(y) \nu(\mathrm{d}y)}{\int_{\mathsf{Y}} (\mu_n k(y))^\alpha p(y)^{1-\alpha} \nu(\mathrm{d}y)} \quad \text{with} \quad \gamma'_{j,n} \in (0, 1]$$

Compatibility between Gradient Descent steps w.r.t Θ and mixture weights updates (and even covariance matrices updates)!

At this stage

We expressed conditions on $\boldsymbol{\lambda}$ and Θ ensuring a systematic decrease in $\Psi_\alpha(\mu_{\boldsymbol{\lambda},\Theta})$:

1. Updates on $\boldsymbol{\lambda}$ linked to the gradient-based Power Descent
2. Updates on Θ :
   - Maximisation approach : generalises an Integrated EM
   - Gradient-based approach : links with Gradient Descent algorithms

	Improvements of our framework
Gradient Descent w.r.t Θ on $-\alpha^{-1}\mathcal{L}_\alpha(\mu k; p)$	Simultaneous optimisation w.r.t $(\boldsymbol{\lambda}_n)_{n\geqslant 1}$ $\lambda_{j,n}$ needs not to be as a factor in the means updates Covariance matrices update formulas
Power Descent	Simultaneous optimisation w.r.t $(\Theta_n)_{n\geqslant 1}$ Convergence towards a local optimum of the full algorithm
M-PMC algorithm	$\alpha \in [0,1)$ (prev. $\alpha = 0$) $\eta_n \in (0,1]$ and $(\alpha-1)\kappa_n \geqslant 0$ (prev. $\eta_n = 1,\ \kappa_n = 0$) $b_{j,n} \geqslant 0$ (prev. $b_{j,n} = 0$)

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Outline

Monte Carlo approximations

Algorithm 1: Gaussian Mixture Models optimisation

At iteration n,

1. Draw independently M samples $(Y_{m,n})_{1 \leqslant m \leqslant M}$ from the proposal q_n.
2. For all $j = 1 \ldots J$, set:

$$\lambda_{j,n+1} = \frac{\lambda_{j,n} \left[\sum_{m=1}^M \hat{\varphi}_{j,n}^{(\alpha)}(Y_{m,n}) + (\alpha - 1)\kappa_n\right]^{\eta_n}}{\sum_{\ell=1}^J \lambda_{\ell,n} \left[\sum_{m=1}^M \hat{\varphi}_{\ell,n}^{(\alpha)}(Y_{m,n}) + (\alpha - 1)\kappa_n\right]^{\eta_n}}$$

$$(RGD) \quad m_{j,n+1} = m_{j,n} + \gamma_n \frac{\lambda_{j,n} \sum_{m=1}^M \hat{\varphi}_{j,n}^{(\alpha)}(Y_{m,n}) \cdot (Y_{m,n} - \theta_{j,n})}{\sum_{j=1}^J \sum_{m=1}^M \lambda_{j,n} \hat{\varphi}_{j,n}^{(\alpha)}(Y_{m,n})}$$

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→ 2 possible algorithms :

- RGD : updates derived from Gradient Descent steps w.r.t Θ on $-\alpha^{-1}\mathcal{L}_\alpha(\mu k; p)$
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→ 2 possible samplers : $q_n = \mu_{\boldsymbol{\lambda}_n, \Theta_n}$ (IS-n) and $q_n = J^{-1} \sum_{j=1}^J k(\theta_{j,n}, \cdot)$ (IS-unif).

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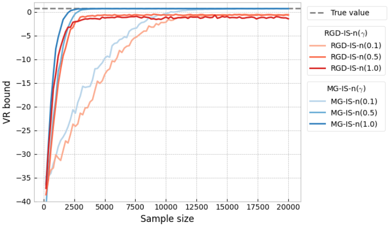
Comparing RGD to MG (fixed $\boldsymbol{\lambda}$)

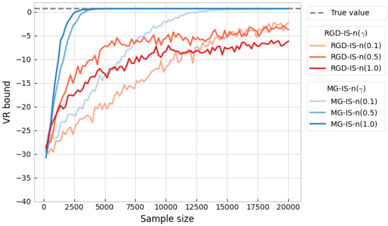
$$\text{Target :} \quad p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$$

- MC estimate of the VR Bound averaged over 30 trials for RGD and MG. [Here, $\alpha = 0.2$, $d = 16$, $M = 200$, $\kappa_n = 0$, $\eta_n = 0$. and $q_n = \mu_n k$.]

$J = 10$



$J = 50$



- LogMSE averaged over 30 trials for RGD and MG.

	$J = 10$			$J = 50$		
	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
RGD-IS-n(γ)	-0.081	-0.076	-0.218	-1.640	-1.673	-1.560
MG-IS-n(γ)	**-3.702**	**-1.875**	**-2.711**	**-2.760**	**-2.771**	**-2.788**

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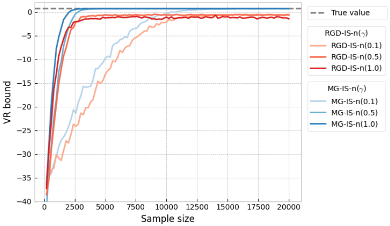

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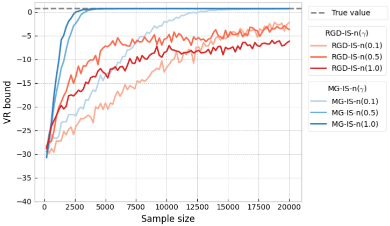

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Comparing RGD to MG (varying $\boldsymbol{\lambda}$)

Target : $\quad p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$

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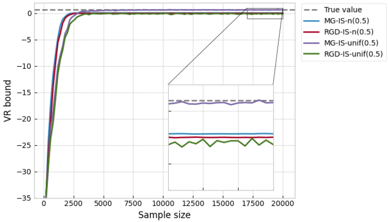

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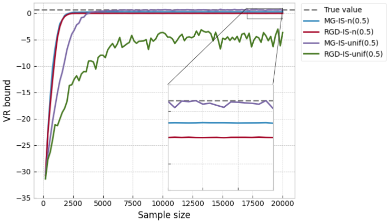

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	$J = 10$			$J = 50$		
	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
RGD-IS-n(γ)	0.372	0.510	0.384	-0.616	-0.713	-0.778
MG-IS-n(γ)	1.104	1.074	0.387	1.135	-0.077	-0.060
RGD-IS-unif(γ)	0.359	0.469	0.458	-0.688	-0.670	-0.583
MG-IS-unif(γ)	**-0.200**	**-0.229**	**-0.515**	**-1.500**	**-1.462**	**-1.246**

Comparing RGD to MG (varying $\boldsymbol{\lambda}$)

Target : $\quad p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$

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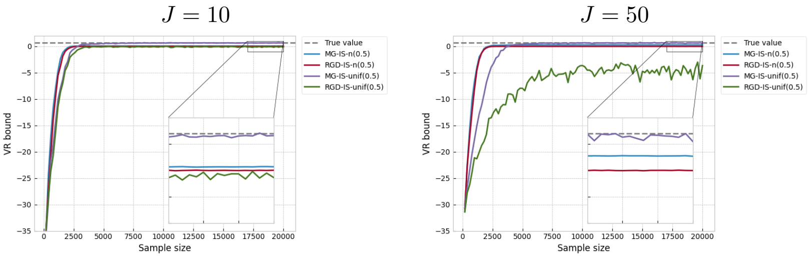

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Comparing RGD to MG (varying $\boldsymbol{\lambda}$) - 2

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

- LogMSE averaged over 30 trials for RGD and MG.

[Here, $\alpha = 0.2$, $d = 16$, $M = 200$, $\gamma = 0.5$, $\kappa_n = 0$.]

		$J = 10$			$J = 50$	
	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$
RGD-IS-n(γ)	0.045	0.510	1.299	-1.355	-0.713	0.924
MG-IS-n(γ)	0.087	1.074	1.343	-1.205	-0.077	1.329
RGD-IS-unif(γ)	-0.018	0.469	1.328	-1.385	-0.670	0.928
MG-IS-unif(γ)	**-1.244**	**-0.229**	**1.100**	**-2.524**	**-1.462**	**0.309**

Comparing RGD to MG (varying $\boldsymbol{\lambda}$) - 2

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

- LogMSE averaged over 30 trials for RGD and MG.

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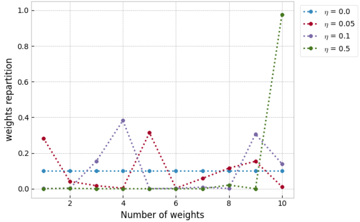
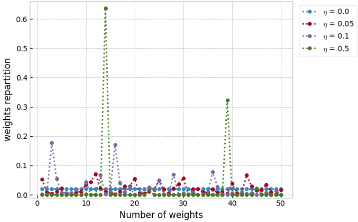
	$J = 10$			$J = 50$		
	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$
RGD-IS-n(γ)	0.045	0.510	1.299	-1.355	-0.713	0.924
MG-IS-n(γ)	0.087	1.074	1.343	-1.205	-0.077	1.329
RGD-IS-unif(γ)	-0.018	0.469	1.328	-1.385	-0.670	0.928
MG-IS-unif(γ)	**-1.244**	**-0.229**	**1.100**	**-2.524**	**-1.462**	**0.309**

$J = 10$



$J = 50$



Outline

Conclusion of Part 3

Novel framework for monotonic alpha-divergence minimisation

- applicable to mixture models optimisation
- mixture weights and mixture components parameters can be updated simultaneously
- links with an Integrated EM algorithm and with gradient-based approaches
- empirical benefits of our general framework

Some perspectives

- Additionnal convergence results
- Hyperparameters tuning
- ML applications...

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  MFVI, BBVI, Alpha-divergence VI.

- **Part 2.** *Infinite-dimensional Alpha-divergence minimisation :*
  Mixture weights optimisation to **increase expressiveness**
  Links with the Entropic Mirror Descent algorithm

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  Mixture models optimisation with **convergence guarantees**
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There is still a lot to do in Variational Inference regarding :

1. the expressiveness of the variational family
2. the choice of the measure of dissimilarity
3. the theory of Variational Inference
4. the interface between Variational Inference and Monte Carlo methods
5. and so much more!

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