

Infinite-dimensional α -divergence minimisation for Variational Inference

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Joint work with Randal Douc and François Portier

Outline

- ① Introduction
- ② Infinite-dimensional α -divergence minimisation
- ③ Numerical experiments
- ④ Conclusion

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Bayesian statistics

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

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

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

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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

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

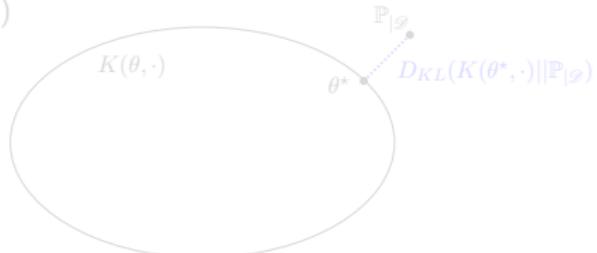
where D is a measure of dissimilarity between the variational distribution \mathbb{Q} and the posterior distribution $\mathbb{P}_{|\mathcal{D}}$

→ Typically, D : exclusive Kullback-Leibler (KL)

divergence and \mathcal{Q} : parametric family

(e.g. Mean-field)

$$\begin{cases} D_{KL}(\mathbb{Q} || \mathbb{P}) = \int_Y \log \left(\frac{q(y)}{p(y)} \right) q(y) \nu(dy) \\ \mathcal{Q} = \{q : y \mapsto k(\theta, y) : \theta \in \Theta\} \end{cases}$$



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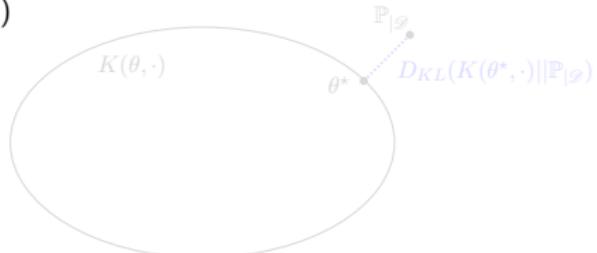
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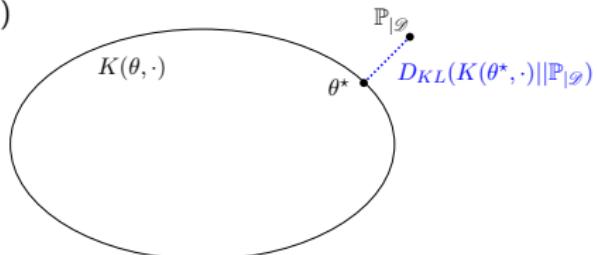
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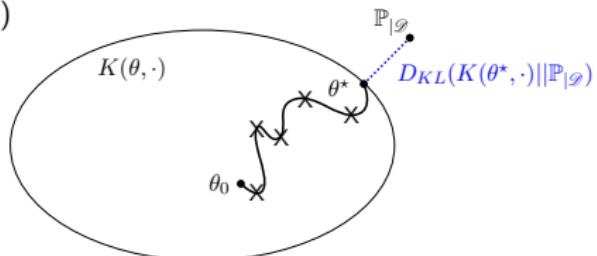
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Core question in Variational Inference

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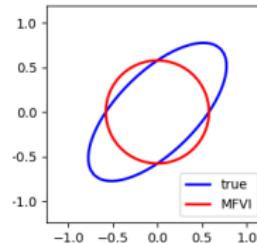
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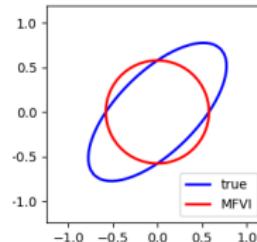
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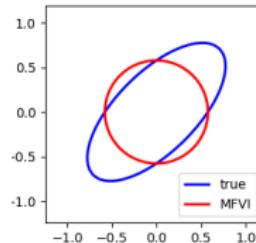
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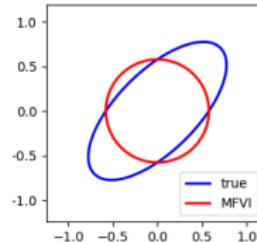
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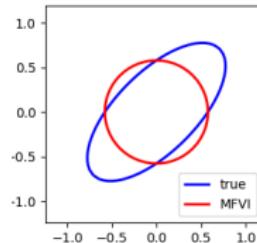
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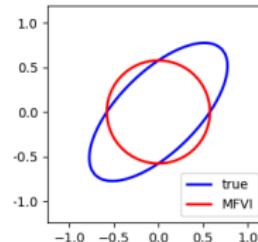
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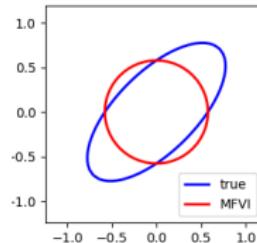
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Variational Inference with the α -divergence family

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

\mathbb{Q} and \mathbb{P} : $\mathbb{Q} \preceq \nu$, $\mathbb{P} \preceq \nu$ with $\frac{d\mathbb{Q}}{d\nu} = q$, $\frac{d\mathbb{P}}{d\nu} = p$.

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

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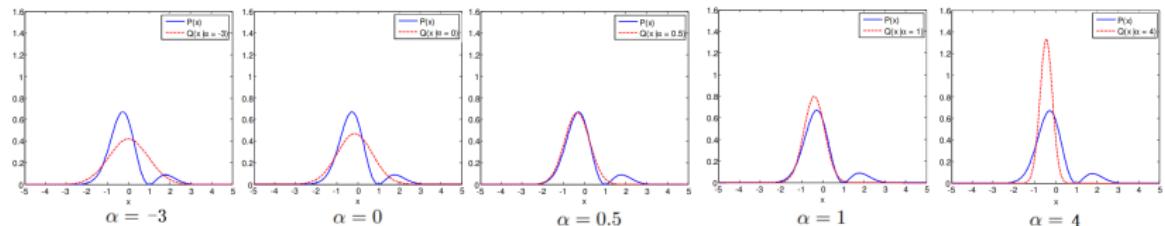
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- ① A **flexible** family of divergences...

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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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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Mixture weights optimisation for Alpha-Divergence Variational Inference.

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Idea : Extend the traditional variational parametric family

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by putting a prior on the variational parameter θ

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

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

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

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

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Optimisation problem

$$\inf_{\mu \in M} \Psi_\alpha(\mu k; p) \quad \text{with} \quad \Psi_\alpha(\mu k; p) := \int_Y f_\alpha \left(\frac{\mu k(y)}{p(y)} \right) p(y) \nu(dy)$$

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

(A1) For all $(\theta, y) \in T \times Y$, $k(\theta, y) > 0$, $p(y) \geq 0$ and $\int_Y p(y)\nu(dy) < \infty$.

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

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

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Assume (A1) and (A2). Let $\mu \in M_1(T)$ be such that $\Psi_\alpha(\mu k) < \infty$ and $\mu(\Gamma(b_{\mu,\alpha} + \kappa)) < \infty$. Then,

- ① $\Psi_\alpha(\mathcal{I}_\alpha(\mu)k) \leq \Psi_\alpha(\mu k)$
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$$\mu_{n+1}(d\theta) = \frac{\mu_n(d\theta) \cdot \Gamma(b_{\mu_n, \alpha}(\theta) + \kappa)}{\mu_n(\Gamma(b_{\mu_n, \alpha} + \kappa))}, \quad n \geq 1$$

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

- Entropic Mirror Descent : $\Gamma(v) = e^{-\eta v}$ with $\eta \in (0, \frac{1}{|\alpha-1||b|_{\infty, \alpha}+1})$, any α, κ
- Power Descent : $\Gamma(v) = [(\alpha - 1)v + 1]^{\eta/(1-\alpha)}$ with $\eta \in (0, 1]$, $\alpha > 1$, $\kappa > 0$

→ The case $\alpha < 1$ for the Power Descent is trickier... $\eta \in (0, 1]$, $\kappa \leq 0$

Under additionnal assumptions on Ψ_α and $b_{\mu, \alpha}$, if $(\mu_n)_{n \geq 1}$ weakly converges to μ^* , then :

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The special case of finite mixture models

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

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

Let $\Theta = (\theta_1, \dots, \theta_J) \in \mathbb{T}^J$, $\boldsymbol{\lambda}_1 = (\lambda_{1,1}, \dots, \lambda_{J,1}) \in S_J$ and denote

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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

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e.g. Entropic Mirror Descent: when $\alpha = 1$, we have for all $\eta \in (0, 1)$

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Towards a practical implementation

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Let $\Theta = (\theta_1, \dots, \theta_J) \in \mathcal{T}^J$ be **fixed** and let $\lambda_1 \in \mathcal{S}_J$. At time $n \geq 1$, define

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

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Outline

- 1 Introduction
- 2 Infinite-dimensional α -divergence minimisation
- 3 Numerical experiments
- 4 Conclusion

Numerical experiments

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

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

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

- Toy example

$$p(\mathbf{y}) = Z \times [0.5\mathcal{N}(\mathbf{y}; -2\mathbf{u}_d, \mathbf{I}_d) + 0.5\mathcal{N}(\mathbf{y}; 2\mathbf{u}_d, \mathbf{I}_d)], Z = 2$$

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

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

Numerical experiments

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

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

Algorithm

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

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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 : $[1/J, \dots, 1/J]$, $N = 10$, $T = 20$

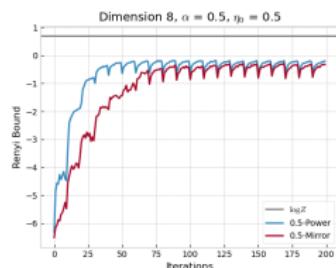
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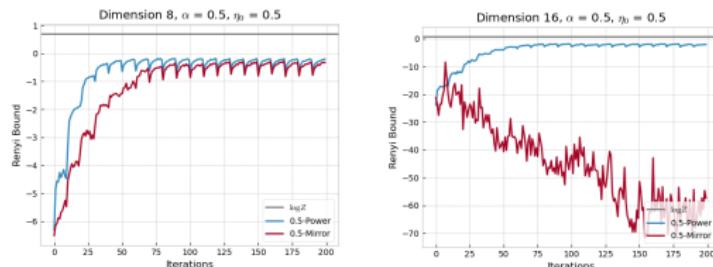


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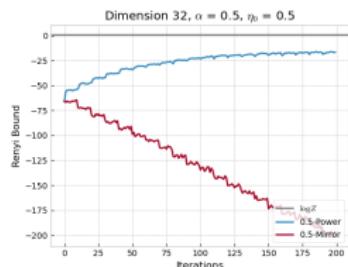
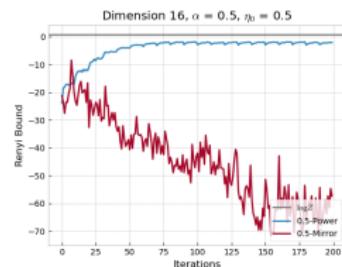
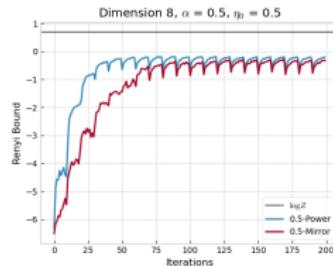


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Toy example : the case $\alpha = 1$

Comparison between:

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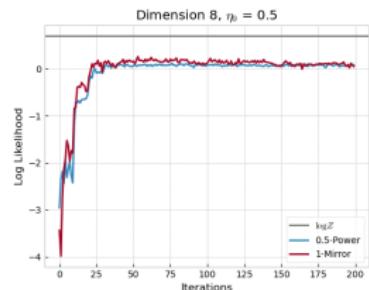
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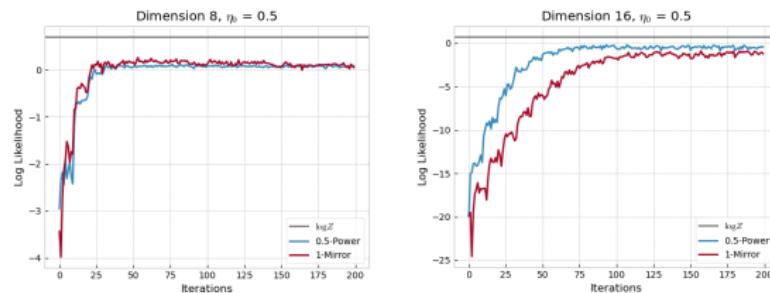


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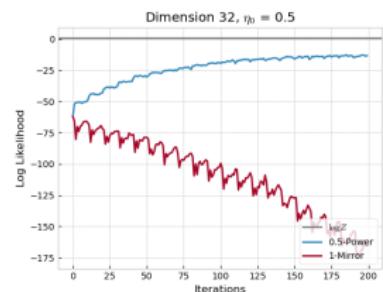
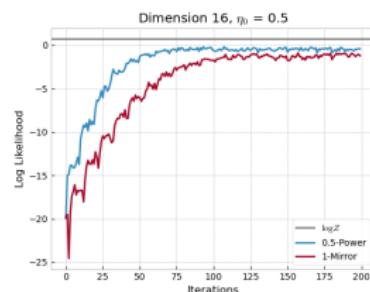
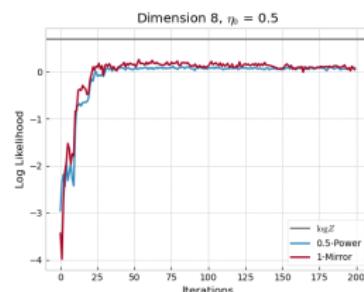


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Bayesian Logistic Regression

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

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

$$p_0(\beta) = \text{Gamma}(\beta; a, b),$$

$$p_0(w_l | \beta) = \mathcal{N}(w_l; 0, \beta^{-1}), \quad 1 \leq l \leq L$$

$$p(c_i = 1 | \mathbf{x}_i, \mathbf{w}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}_i}}, \quad 1 \leq i \leq I$$

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

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

→ Quantity of interest : $p(y|\mathcal{D})$ with $y = [\mathbf{w}, \log \beta]$

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

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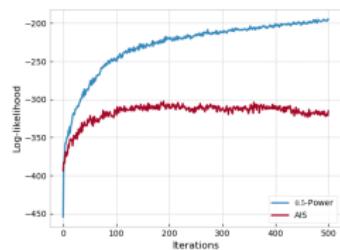
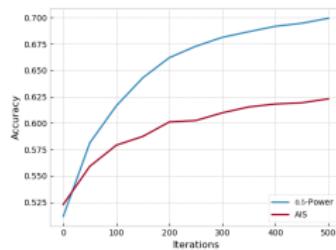
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Outline

- 1 Introduction
- 2 Infinite-dimensional α -divergence minimisation
- 3 Numerical experiments
- 4 Conclusion

Summary

General framework for infinite-dimensional α -divergence minimisation over

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

- recovers the Entropic Mirror Descent algorithm
- novel Power Descent algorithm
- conditions for a systematic decrease + convergence results
- applicable to mixture models :

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

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