Monotonic Alpha-Divergence Variational Inference

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Joint work with Randal Douc and François Roueff

Outline

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Bayesian inference

- Goal : compute / sample from 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 normalisation constant constant $p(\mathscr{D})$

$\rightarrow$ Variational Inference : inference is seen as an optimisation problem

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 $\mathbb{P}_{|\mathscr{D}}$

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

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Challenges in Variational Inference

→ Typically, D is the exclusive Kullback-Leibler (KL) divergence

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

1. The exclusive Kullback-Leibler tends to underestimate the posterior variance
2. The approximative family $\mathcal{Q}$ can be too restrictive
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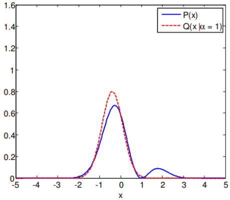

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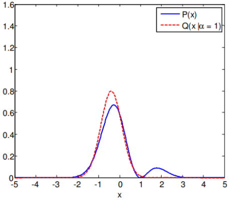

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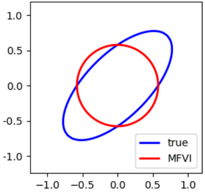

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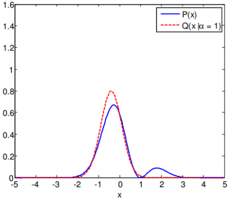

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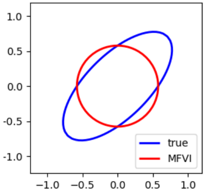

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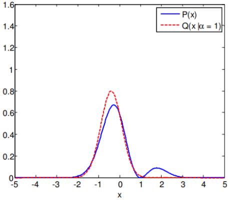

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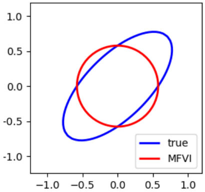

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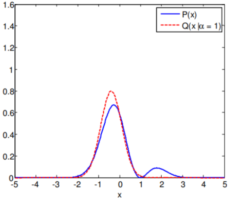

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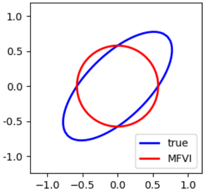

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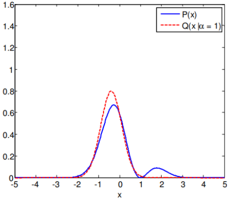

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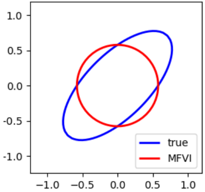

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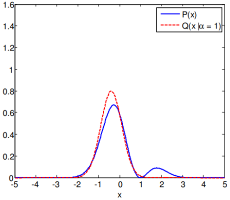

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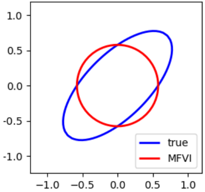

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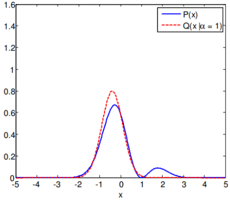

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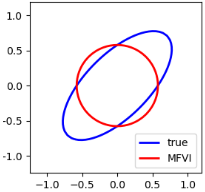

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$\rightarrow$ Can we derive algorithms with theoretical guarantees?

Choice of D: 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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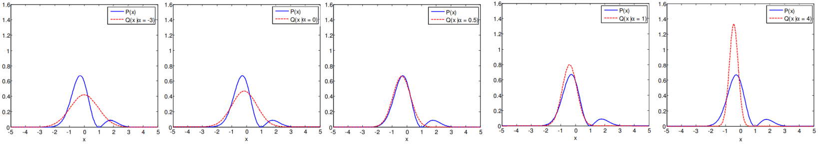

$\alpha = -3$ $\alpha = 0$ $\alpha = 0.5$ $\alpha = 1$ $\alpha = 4$

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

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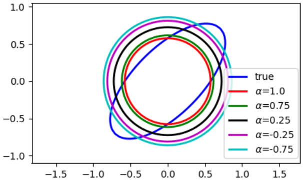

Adapted from **Rényi divergence variational inference.** Y. Li and R. E Turner. (2016). NeurIPS

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

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

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

NB : One may also use the **VR bound** $\mathcal{L}_\alpha(q;p)$ as an objective function.

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

Choice of $\mathcal{Q}$

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

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

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

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Question :

Can we enlarge the variational family $\mathcal{Q}$ and with what theoretical guarantees?

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Outline

Monotonic Alpha-Divergence Minimisation

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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 iterative update formulas for $(\boldsymbol{\lambda}, \Theta)$ that ensures a **systematic decrease in the α-divergence** (i.e. in Ψ_α) at each step, with $\alpha \in [0, 1)$.

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Conditions for a monotonic decrease

- Goal : Given $(\boldsymbol{\lambda}_n, \Theta_n)$ find $(\boldsymbol{\lambda}_{n+1}, \Theta_{n+1})$ such that

$$\Psi_\alpha(\mu_{\boldsymbol{\lambda}_{n+1},\Theta_{n+1}} k; p) \leqslant \Psi_\alpha(\mu_{\boldsymbol{\lambda}_n,\Theta_n} k; p)$$

- Key idea : simplify the problem by writing conditions enabling separate (and simultaneous!) updates for $\boldsymbol{\lambda}_{n+1}$ and Θ_{n+1}

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

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\end{aligned}$$

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

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

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An example : GMMs, $k(\theta_j, y) = \mathcal{N}(y; m_j, \Sigma_j)$

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At this stage...

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1. Possible updates for the mixture weights $\boldsymbol{\lambda}_{n+1}$

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   where $\eta_n \in (0, 1]$ and κ_n is such that $(\alpha - 1)\kappa_n \geqslant 0$

2. Possible updates for the mixture components parameters Θ_{n+1}
   - Maximisation approach
   - Gradient-based approach

3. Applicable to GMMs with the maximisation approach providing covariance matrices updates.

At this stage...

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Outline

1) GD for (Rényi's) α-divergence minimisation

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where $r_{j,n} > 0$ is the learning rate.

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Core insights :

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   $\rightarrow$ Compatibility between GD steps and mixture weights updates

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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.
https://doi.org/10.1214/20-AOS2035.

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

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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

We recover this algorithm by setting :
- $\alpha = 0$
- $\eta_n = 1$, $\kappa_n = 0$ in the mixture weights update
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Core insights :

We have generalised an integrated EM algorithm for mixture models optimisation

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NB : Why do the learning rate aspects matter? In pratice, Monte Carlo approximations!

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We recover this algorithm by setting :
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Core insights :

We have generalised an integrated EM algorithm for mixture models optimisation

1. We extend the systematic decrease property to $\alpha \in [0, 1)$
2. We introduce η_n and κ_n, where η_n acts as a learning rate
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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 $j = 1 \dots J$, set:

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

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

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→ Here $\hat{\varphi}_{j,n}^{(\alpha)}(y) = \frac{\varphi_{j,n}^{(\alpha)}(y)}{q_n(y)}$, $\gamma_{j,n} := \gamma_n \in (0,1]$ (simultaneity matters!)

→ RGD : updates derived from GD steps w.r.t. Θ applied to the VR bound

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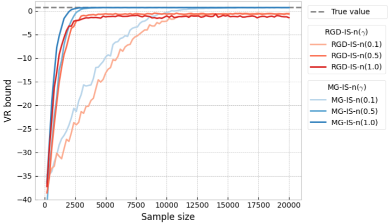
Comparing RGD to MG (fixed $\boldsymbol{\lambda}$)

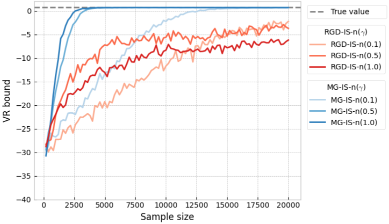
$$\text{Target}: \quad p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$$

- 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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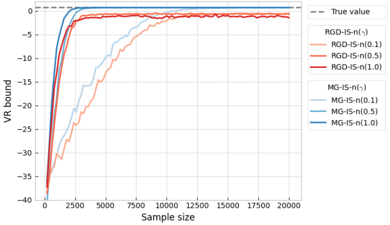

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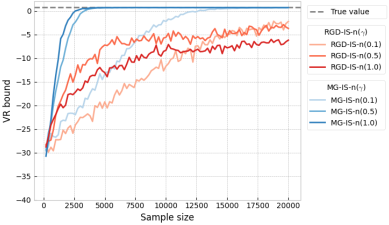

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Comparing RGD to MG (varying $\boldsymbol{\lambda}$)

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

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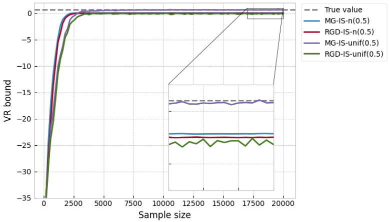

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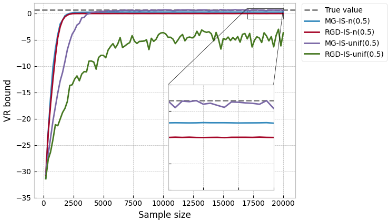

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	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
RGD-IS-n(γ)	0.372	0.510	0.384	-0.616	-0.713	-0.778
MG-IS-n(γ)	1.104	1.074	0.387	1.135	-0.077	-0.060
RGD-IS-unif(γ)	0.359	0.469	0.458	-0.688	-0.670	-0.583
MG-IS-unif(γ)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

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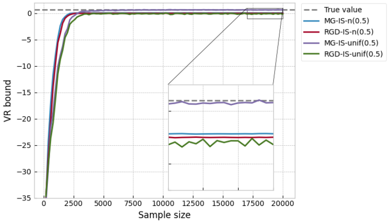

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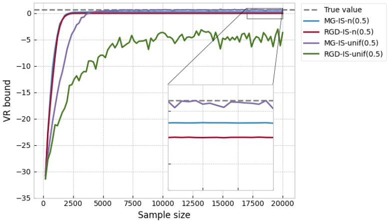

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	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$	$\eta = 0.05$	$\eta = 0.1$	$\eta = 0.5$
RGD-IS-n(γ)	0.045	0.510	1.299	-1.355	-0.713	0.924
MG-IS-n(γ)	0.087	1.074	1.343	-1.205	-0.077	1.329
RGD-IS-unif(γ)	-0.018	0.469	1.328	-1.385	-0.670	0.928
MG-IS-unif(γ)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

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

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- LogMSE averaged over 30 trials for RGD and MG.

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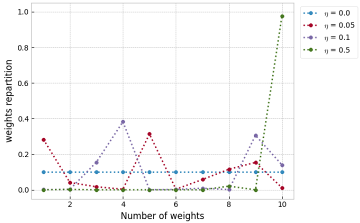

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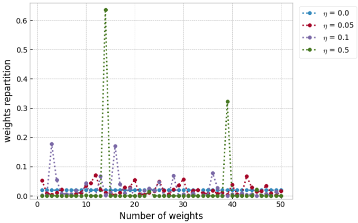

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Conclusion

Novel framework for monotonic alpha-divergence minimisation

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

Some perspectives

- Additional convergence results
- Hyperparameters tuning...

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Thank you for your attention!

Summary

	Improvements of our framework
Gradient Descent	Simultaneous optimisation w.r.t $(\boldsymbol{\lambda}, \Theta)$ (prev. mixture weights optimisation $\boldsymbol{\lambda}$ not considered) For GMMs : maximisation approach encompasses Rényi Gradient Descent and provides covariance matrices updates
Power Descent	Simultaneous optimisation w.r.t $(\boldsymbol{\lambda}, \Theta)$ (prev. $(\Theta_n)_{n \geqslant 1}$ constant)
M-PMC algorithm	Extension of an Integrated EM algorithm to: $\alpha \in [0, 1)$, $\eta_n \in (0, 1]$ and $(\alpha - 1)\kappa_n \geqslant 0$ and $b_{j,n} \geqslant 0$ (prev. $\alpha = 0$, $\eta_n = 1$, $\kappa_n = 0$ and $b_{j,n} = 0$)

This is done while maintaining theoretical guarantees!