

# Monotonic Alpha-Divergence Variational Inference

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Joint work with Randal Douc and François Roueff

# Introduction

- Bayesian Inference : complex posterior density  $p(y|\mathcal{D})$  only known **up to a constant**
- Variational Inference :
  - ① Posit a **simpler variational family**  $\mathcal{Q}$
  - ② Find the best approximation to the posterior density belonging to  $\mathcal{Q}$  : solve an optimisation problem involving a **measure of dissimilarity**  $D$

$$\inf_{q \in \mathcal{Q}} D(q \parallel p(\cdot|\mathcal{D}))$$

- Typically,  $D$  is the *exclusive* Kullback-Leibler (KL) divergence and  $\mathcal{Q}$  is parametric

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

with  $\theta$  for example being optimised via stochastic gradient descent.

- **Yet**, the exclusive KL has some known **limitations** (e.g. posterior variance underestimation, cannot capture multimodality) and  $\mathcal{Q}$  might also be **too restrictive**

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# An idea

Instead of the exclusive KL divergence and  $\mathcal{Q}$  of the form

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

consider the  $\alpha$ -divergence and choose  $\mathcal{Q}$  of the form

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

→ Why is that a good idea?

- ① The  $\alpha$ -divergence family is more general and permits to bypass some issues of the exclusive KL divergence when  $\alpha < 1$
- ② Optimising w.r.t.  $\lambda$  and  $\Theta$  expands the traditional parametric variational family → Optimising w.r.t.  $\lambda$  enables to select the mixture components according to their overall importance in the set of component parameters  $\Theta$

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- ① The optimisation w.r.t  $\lambda$  is over a **constrained space** (the simplex)
- ② How do we establish **theoretical guarantees**?

## Monotonic Alpha-divergence Minimisation for Variational Inference.

K. Daudel, R. Douc and F. Roueff (2021). <https://arxiv.org/abs/2103.05684>

Goal : Propose valid update formulas for  $(\lambda, \Theta)$  that ensures a **systematic decrease in the  $\alpha$ -divergence**  $D_\alpha(\mu_{\lambda, \Theta} k \parallel p(\cdot | \mathcal{D}))$  at each step, with  $\alpha \in [0, 1)$ .

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# Monotonic Alpha-Divergence Minimisation

- Goal : Given  $(\lambda_n, \Theta_n)$  find  $(\lambda_{n+1}, \Theta_{n+1})$  such that

$$D_\alpha(\mu_{\lambda_{n+1}, \Theta_{n+1}} k \parallel p(\cdot | \mathcal{D})) \leq D_\alpha(\mu_{\lambda_n, \Theta_n} k \parallel p(\cdot | \mathcal{D}))$$

- Core step : simplify the problem by writing conditions enabling **separate** (and simultaneous!) updates for  $\lambda_{n+1}$  and  $\Theta_{n+1}$

$$\int_Y \sum_{j=1}^J \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log \left( \frac{\lambda_{j,n+1}}{\lambda_{j,n}} \right) \nu(dy) \geq 0 \quad (\text{Weights})$$

$$\int_Y \sum_{j=1}^J \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log \left( \frac{k(\theta_{j,n+1}, y)}{k(\theta_{j,n}, y)} \right) \nu(dy) \geq 0 \quad (\text{Components})$$

$$\text{where } \varphi_{j,n}^{(\alpha)}(y) = k(\theta_{j,n}, y) \left( \frac{\mu_{\lambda_n, \Theta_n} k(y)}{p(y, \mathcal{D})} \right)^{\alpha-1}$$

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# Updating the mixture weights $\lambda_{n+1}$

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→ (Weights) holds for  $\lambda_{n+1}$  such that

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

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$$\int_Y \sum_{j=1}^J \lambda_{j,n} \varphi_{j,n}^{(\alpha)}(y) \log \left( \frac{k(\theta_{j,n+1}, y)}{k(\theta_{j,n}, y)} \right) \nu(dy) \geq 0 \quad (\text{Components})$$

- Maximisation approach : for all  $j = 1 \dots J$ ,

$$\theta_{j,n+1} = \operatorname{argmax}_{\theta \in \mathcal{T}} \int_Y \varphi_{j,n}^{(\alpha)}(y) \log \left( \frac{k(\theta, y)}{k(\theta_{j,n}, y)} \right) \nu(dy)$$

- Gradient-based approach : for all  $j = 1 \dots J$ ,  $\gamma_{j,n} \in (0, 1]$

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

- Maximisation approach with  $\theta_j = (m_j, \Sigma_j)$  : for all  $j = 1 \dots J$ ,

$$m_{j,n+1} = (1 - \gamma_{j,n})m_{j,n} + \gamma_{j,n} \frac{\int_Y \varphi_{j,n}^{(\alpha)}(y) y \nu(dy)}{\int_Y \varphi_{j,n}^{(\alpha)}(y) \nu(dy)}$$
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Considering all possible values of  $b_{j,n}$ , we have  $\gamma_{j,n} \in (0, 1]$

- Gradient-based approach with  $\theta_j = m_j$  : for all  $j = 1 \dots J$

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where  $\gamma_{j,n} \in (0, 1]$ , and  $\Sigma_j = \sigma_j^2 \mathbf{I}_d$  with  $\sigma_j > 0$  fixed

(here  $g_{j,n}$  is  $\beta_{j,n}$ -smooth with  $\beta_{j,n} = \sigma_j^{-2}(1 - \alpha)^{-1} \int \varphi_{j,n}^{(\alpha)} d\nu$ )



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$$\Sigma_{j,n+1} = (1 - \gamma_{j,n})\tilde{\Sigma}_{j,n} + \gamma_{j,n} \frac{\int_Y \varphi_{j,n}^{(\alpha)}(y)(y - m_{j,n+1})(y - m_{j,n+1})^T \nu(dy)}{\int_Y \varphi_{j,n}^{(\alpha)}(y) \nu(dy)}$$

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  $b_{j,n}$

Considering all possible values of  $b_{j,n}$ , we have  $\gamma_{j,n} \in (0, 1]$

- Gradient-based approach with  $\theta_j = m_j$  : for all  $j = 1 \dots J$

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where  $\gamma_{j,n} \in (0, 1]$ , and  $\Sigma_j = \sigma_j^2 \mathbf{I}_d$  with  $\sigma_j > 0$  fixed

(here  $g_{j,n}$  is  $\beta_{j,n}$ -smooth with  $\beta_{j,n} = \sigma_j^{-2}(1 - \alpha)^{-1} \int \varphi_{j,n}^{(\alpha)} d\nu$ )

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

**Variational inference via  $\chi$ -upper bound minimization.** A. Dieng, D. Tran, R. Ranganath, J. Paisley, and D. Blei (2017). NeurIPS

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Recall that in the GMM case, we obtained: for all  $j = 1 \dots J$ ,

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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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**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 :

- $\alpha = 0$
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We have **generalised** an integrated EM algorithm for mixture models optimisation

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

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- $b_{j,n} = 0$  in the maximisation approach

#### 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  $\eta_n$  and  $\kappa_n$ , where  $\eta_n$  acts as a **learning rate**
- ③ In the GMM case, we introduce  $\gamma_{j,n}$  via  $b_{j,n}$ , which acts as a **learning rate**

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

# Monte Carlo approximations

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**Algorithm 1:** Gaussian Mixture Models optimisation

---

**At iteration  $n$ ,**

- ➊ Draw independently  $M$  samples  $(Y_{m,n})_{1 \leq m \leq M}$  from the proposal  $q_n$ .
- ➋ For all  $j = 1 \dots J$ , set:

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

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

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

---

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

→ RGD : updates derived from GD steps w.r.t.  $\Theta$  applied to Rényi's  $\alpha$ -divergence

→ 2 possible samplers :  $q_n = \mu_{\lambda_n, \Theta_n}$  (IS- $n$ ) and  $q_n = J^{-1} \sum_{j=1}^J k(\theta_{j,n}, \cdot)$  (IS-unif).

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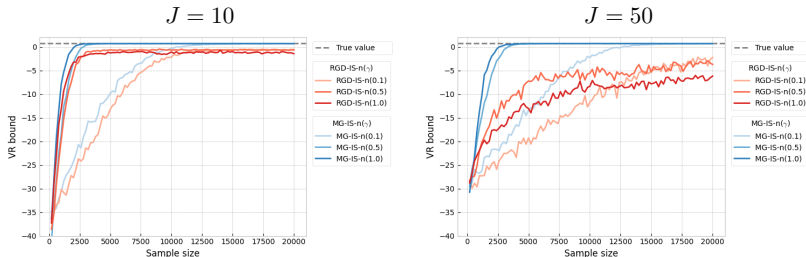
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# Comparing RGD to MG (fixed $\lambda$ )

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

- 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  $q_n = \mu_n k$ .]



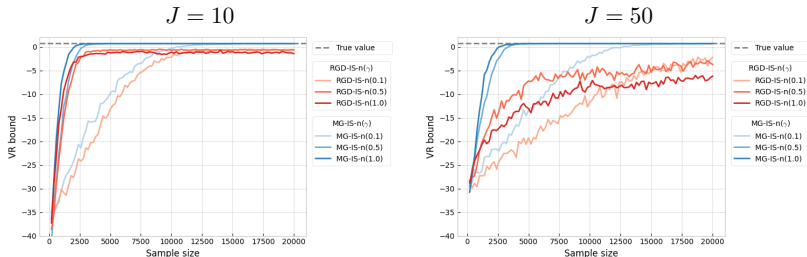
- LogMSE averaged over 30 trials for RGD and MG.

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

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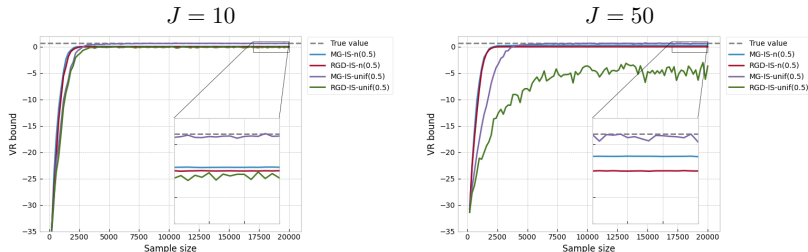
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# Comparing RGD to MG (varying $\lambda$ )

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- LogMSE averaged over 30 trials for RGD and MG.

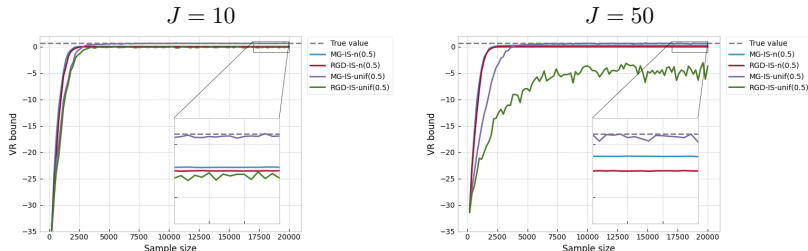
	$J = 10$			$J = 50$		
	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$	$\gamma = 0.1$	$\gamma = 0.5$	$\gamma = 1.0$
RGD-IS-n( $\gamma$ )	0.372	0.510	0.384	-0.616	-0.713	-0.778
MG-IS-n( $\gamma$ )	1.104	1.074	0.387	1.135	-0.077	-0.060
RGD-IS-unif( $\gamma$ )	0.359	0.469	0.458	-0.688	-0.670	-0.583
MG-IS-unif(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



# Comparing RGD to MG (varying $\lambda$ )

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

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## Comparing RGD to MG (varying $\lambda$ ) - 2

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

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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( $\gamma$ )	0.045	0.510	1.299	-1.355	-0.713	0.924
MG-IS-n( $\gamma$ )	0.087	1.074	1.343	-1.205	-0.077	1.329
RGD-IS-unif( $\gamma$ )	-0.018	0.469	1.328	-1.385	-0.670	0.928
MG-IS-unif( $\gamma$ )	<b>-1.244</b>	<b>-0.229</b>	<b>1.100</b>	<b>-2.524</b>	<b>-1.462</b>	<b>0.309</b>

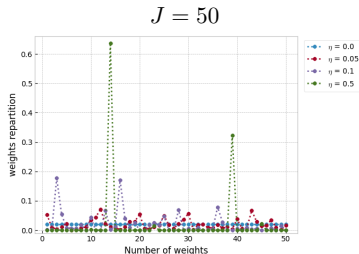
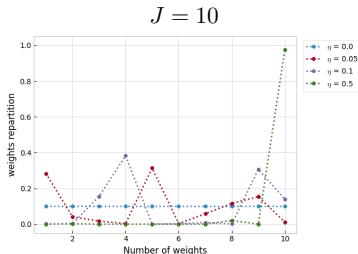
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# Conclusion

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!