Monotonic Alpha-divergence Minimisation

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Joint work with Randal Douc and François Roueff

Outline

Bayesian statistics

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

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

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

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

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

$$q^\star = \operatorname{arginf}_{q \in \mathcal{Q}} D(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}}) ,$$

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

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Important aspects in Variational Inference

$$q^\star = \mathrm{arginf}_{q \in \mathcal{Q}} D(\mathbb{Q}||\mathbb{P}_{|\mathscr{D}})$$

- Choice of the approximating family $\mathcal{Q}$
- Choice of the measure of dissimilarity D

Goal : construct a theoretically-sound Variational Inference (VI) framework

- that enables mixture models optimisation in its most general form
- by performing α-divergence minimisation

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The α-divergence family

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

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

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

where

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

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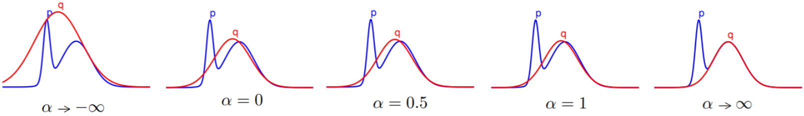
$\rightarrow$ A flexible family of divergences...

Figure: The Gaussian q which minimizes α-divergence to p (a mixture of two Gaussian), for varying α



Adapted from **Divergence Measures and Message Passing**. T. Minka (2005). Technical Report MSR-TR-2005-173]

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Conditions for a systematic decrease

We consider

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

and we want to construct $(\boldsymbol{\lambda}_n, \Theta_n)_{n \geqslant 1}$ such that the α-divergence decreases at each step

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

Assume (A1) and let $\alpha \in [0, 1)$. Then, choosing $(\boldsymbol{\lambda}_n, \Theta_n)_{n \geqslant 1}$ so that: $\forall n \geqslant 1$,

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

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

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

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

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Infinite-dimensional gradient-based descent for alpha-divergence minimisation.

K. Daudel, R. Douc and F. Portier (2021). *To appear in the Annals of Statistics.*

Core insight :

The mixture weights update is gradient-based, η_n plays the role of a learning rate

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- Maximisation approach

$$\theta_{j,n+1} = \operatorname{argmax}_{\theta_j \in \mathsf{T}} \int_{\mathsf{Y}} \gamma_{j,\alpha}^n(y) \log(k(\theta_j, y)) \nu(\mathrm{d}y) \;, \quad j = 1 \ldots J$$

- Gradient-based approach :

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

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

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

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

Question

How do these newly-found simultaneous updates for mixture model optimisation relate to / improve on the existing literature?

Outline

The M-PMC algorithm a.k.a 'Integrated EM'

(Weights) and (Components) hold for $\boldsymbol{\lambda}_{n+1}$ and Θ_{n+1} such that

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

$$\theta_{j,n+1} = \operatorname{argmax}_{\theta_j \in \mathsf{T}} \int_{\mathsf{Y}} \gamma_{j,\alpha}^n(y) \log(k(\theta_j, y))\nu(\mathrm{d}y) \;, \quad j = 1 \ldots J$$

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

$\rightarrow$ We recover the M-PMC algorithm when $\alpha = 0$, $\eta_n = 1$ and $\kappa = 0$

We have generalised an integrated EM algorithm for mixture models optimisation

1. We introduce η_n and κ, where η_n acts as a learning rate
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Application to GMMs

→ Gaussian kernels : $k(\theta_j, y) = \mathcal{N}(y; m_j, \Sigma_j)$ with $\theta_j = (m_j, \Sigma_j) \in \mathsf{T}$

Algorithm 1: α-divergence minimisation for GMMs

At iteration n,
For all $j = 1 \dots J$, set

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→ In practice : M i.i.d samples generated from q_n at iteration n

$$\hat{\gamma}_{j,\alpha}^n(y) = \frac{k(\theta_{j,n}, y)}{q_n(y)} \left(\frac{\mu_{\boldsymbol{\lambda}_n, \Theta_n} k(y)}{p(y)} \right)^{\alpha - 1}$$

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Improving on the M-PMC algorithm

Target : $p(y) = 2 \times \left[0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})\right]$, $d = 16$

<u>Parameters</u>
$\alpha = 0$, $\eta_n = \eta$
$M = 200$, $J = 100$
$q_n(y) = \sum_{j=1}^{J} \lambda_{j,n} k(\theta_{j,n}, y)$
$\rightarrow$ varying η and κ

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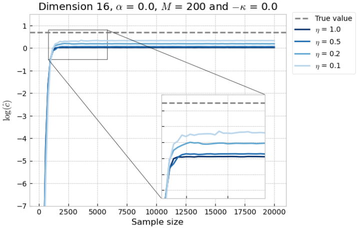

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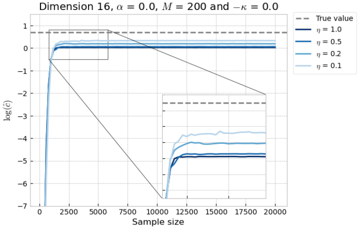

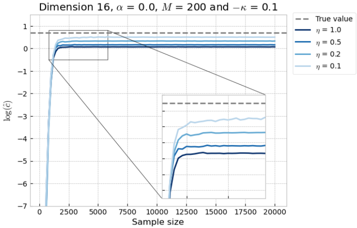

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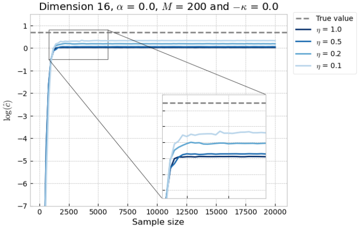

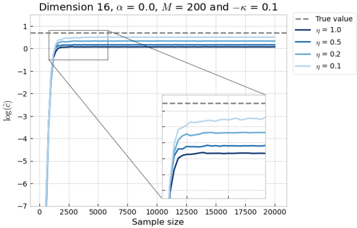

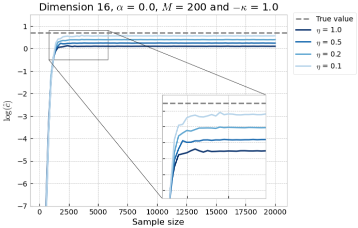

Outline

Gradient-based approach and Gradient Descent

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

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

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

Set $p = p(\cdot, \mathscr{D})$, $\gamma_{j,n} := \gamma_n \in (0,1]$. Usual gradient descent steps on Θ for

- α-divergence minimisation : $c_{j,n} = \lambda_{j,n}$
- Rényi's α-divergence minimisation : $c_{j,n} = \lambda_{j,n} (\int_{\mathsf{Y}} \mu_{\boldsymbol{\lambda}_n, \Theta_n} k(y)^\alpha p(y)^{1-\alpha} \nu(\mathrm{d}y))^{-1}$

$\rightarrow$ Problem : $\lambda_{j,n}$ appears as a multiplicative factor, which could prevent learning!

$\rightarrow$ Solution enabled by our framework : $c_{j,n} = (\int_{\mathsf{Y}} \gamma_{j,\alpha}^n(y) \nu(\mathrm{d}y))^{-1}$

Gradient-based approach and Gradient Descent

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

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Gradient-based approach and Gradient Descent

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

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

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

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

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

Set $p = p(\cdot,\mathscr{D})$, $\gamma_{j,n} := \gamma_n \in (0,1]$. Usual gradient descent steps on Θ for

- α-divergence minimisation : $c_{j,n} = \lambda_{j,n}$
- Rényi's α-divergence minimisation :
$c_{j,n} = \lambda_{j,n}(\int_{\mathsf{Y}} \mu_{\boldsymbol{\lambda}_n,\Theta_n} k(y)^\alpha p(y)^{1-\alpha}\nu(\mathrm{d}y))^{-1}$

$\to$ Problem : $\lambda_{j,n}$ appears as a multiplicative factor, which could prevent learning!

$\to$ Solution enabled by our framework : $c_{j,n} = (\int_{\mathsf{Y}} \gamma^n_{j,\alpha}(y)\nu(\mathrm{d}y))^{-1}$

Application to GMMs (2)

→ Gaussian kernels $k(\theta_j, y) = \mathcal{N}(y; \theta_j, \sigma^2 \boldsymbol{I_d})$ with $\Theta \in \mathsf{T}^J$, $\mathsf{T} = \mathbb{R}^d$ and $\sigma^2 > 0$

- Case 1 : $c_{j,n} = \lambda_{j,n} (\int_{\mathsf{Y}} \mu_{\boldsymbol{\lambda}_n, \Theta_n} k(y)^\alpha p(y)^{1-\alpha} \nu(\mathrm{d}y))^{-1}$ with $\beta_{j,n} = \sigma^{-2}(1-\alpha)^{-1}$
- Case 2 : $c_{j,n} = (\int_{\mathsf{Y}} \gamma_{j,\alpha}^n(y) \nu(\mathrm{d}y))^{-1}$ with $\beta_{j,n} = \sigma^{-2}(1-\alpha)^{-1}$

→ In practice : M i.i.d samples generated from q_n at iteration n

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Improving on Gradient Descent updates

Target : $p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]\ ,\ d = 16$

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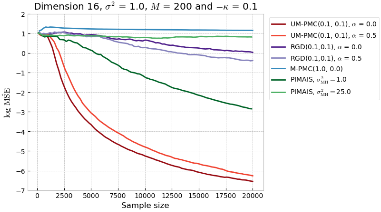

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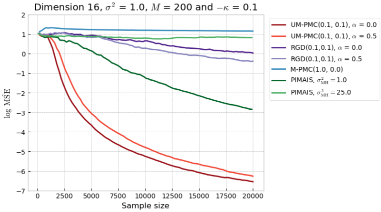

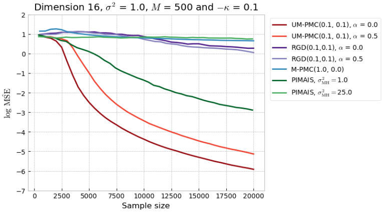

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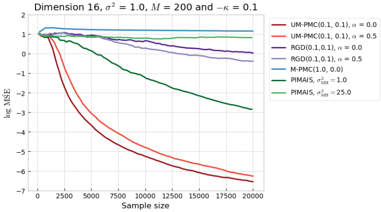

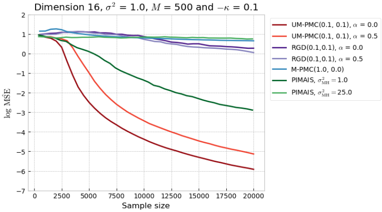

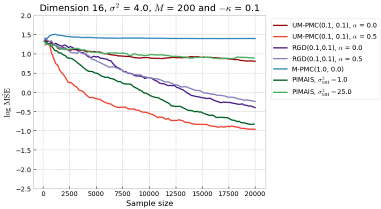

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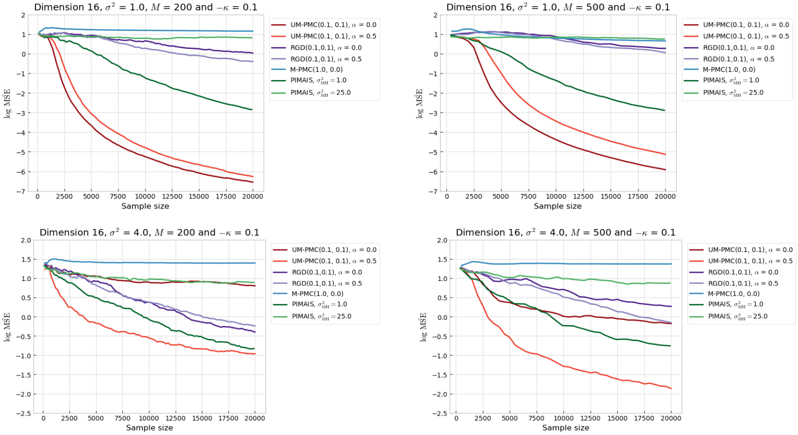

Outline

Conclusion

Novel framework for monotonic α-divergence minimisation

- applicable to mixture models optimisation,
- mixture weights and mixture components parameters can be updated simultaneously,
- empirical benefits of our general framework compared to gradient-based approaches and to the M-PMC algorithm

Thank you for your attention!

Monotonic Alpha-divergence Minimisation

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

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Practical algorithm for GMMs optimisation

→ Gaussian kernels : $k(\theta_j, y) = \mathcal{N}(y; \theta_j, \sigma^2 \boldsymbol{I}_d)$ with $\theta_j \in \mathsf{T} = \mathbb{R}^d$ and $\sigma^2 > 0$

Algorithm 3: α-divergence minimisation for GMMs (constant σ^2)

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

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

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$$\hat{\gamma}_{j,\alpha}^n(y) = \frac{k(\theta_{j,n}, y)}{q_n(y)} \left(\frac{\mu_{\boldsymbol{\lambda}_n, \Theta_n} k(y)}{p(y)} \right)^{\alpha - 1}$$

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Additionnal Numerical Experiments

Target : $p(y) = 2 \times [0.5\mathcal{N}(\boldsymbol{y}; -2\boldsymbol{u_d}, \boldsymbol{I_d}) + 0.5\mathcal{N}(\boldsymbol{y}; 2\boldsymbol{u_d}, \boldsymbol{I_d})]$, $d = 16$

Parameters

$\alpha = 0$, $\eta_n = \eta$, $M = 200$

$q_n(y) = \sum_{j=1}^J \lambda_{j,n} k(\theta_{j,n}, y)$

vs

$q_n(y) = J^{-1} \sum_{j=1}^J k(\theta_{j,n}, y)$

$\rightarrow$ varying η and κ

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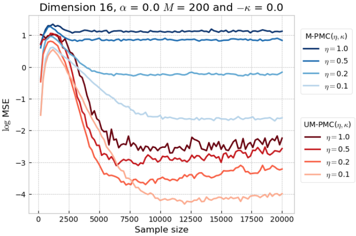

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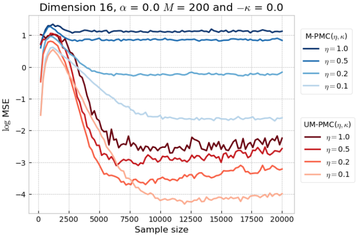

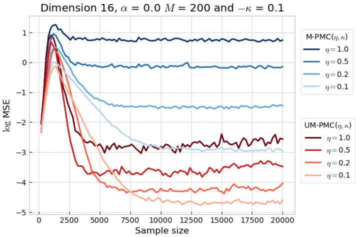

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