Challenges and Opportunities in Scalable Alpha-divergence Variational Inference: Application to IWAEs

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CRiSM seminar – 19/10/2022

Joint work with Joe Benton, Arnaud Doucet and Yuyang Shi

Outline

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Introduction

- Setting :
  1. We consider a model with joint distribution $p_\theta(x, z)$ parameterized by θ, where x is an observation and z is a latent variable valued in $\mathbb{R}^d$
  2. In that case, the **marginal log-likelihood** of x is given by

$$\ell(\theta; x) := \log p_\theta(x) = \log \left(\int p_\theta(x, z) \mathrm{d}z \right)$$

- Goal : find θ which best describes the observation x

$$\theta^\star = \text{argmax}_\theta \ \ell(\theta; x)$$

  (more generally $\theta^\star = \text{argmax}_\theta \ \sum_{i=1}^T \ell(\theta; x_i)$)

- Problem : finding the optimal θ via maximum likelihood estimation is in general an intractable optimization problem

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Variational Inference (VI)

- Idea : construct variational bounds, i.e. surrogate objective functions to the marginal log-likelihood that are more amenable to optimization.

- Common examples :

→ **Evidence Lower BOund (ELBO)** : rely on a variational probability density $q_\phi(z|x)$ parameterized by ϕ

$$\mathrm{ELBO}(\theta, \phi; x) = \int q_\phi(z|x) \log\left(w_{\theta,\phi}(z;x)\right) \mathrm{d}z \quad \text{where} \quad w_{\theta,\phi}(z;x) = \frac{p_\theta(x,z)}{q_\phi(z|x)}$$

with $\mathrm{ELBO}(\theta, \phi; x) \leq \ell(\theta; x)$

→ **Importance Weighted Auto-Encoder (IWAE) bound** (Burda et al., 2016)

$$\ell_N^{(\mathrm{IWAE})}(\theta, \phi; x) = \int \int \prod_{i=1}^{N} q_\phi(z_i|x) \log\left(\frac{1}{N}\sum_{j=1}^{N} w_{\theta,\phi}(z_j;x)\right) \mathrm{d}z_{1:N}, \quad N \in \mathbb{N}^\star$$

with $\ell_N^{(\mathrm{IWAE})}(\theta, \phi; x) \leq \ell(\theta; x)$ and the unbiased Monte Carlo estimate

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Training procedure for the IWAE bound

- **Reparameterization trick** $z = f(\varepsilon, \phi; x) \sim q_\phi(\cdot|x)$ where $\varepsilon \sim q$ so that

$$\frac{\partial}{\partial \phi}\left[\int q_\phi(z|x) h(z) \mathrm{d}z\right] = \frac{\partial}{\partial \phi}\left[\int q(\varepsilon) h(f(\varepsilon, \phi; x)) \mathrm{d}\varepsilon\right] = \int q(\varepsilon) \, \frac{\partial}{\partial \phi}\left[h(f(\varepsilon, \phi; x))\right] \mathrm{d}\varepsilon$$
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- **Reparameterized** gradient estimator (Burda et al., 2016)

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$\rightarrow$ Unbiased SGD steps w.r.t. (θ, ϕ)

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Another interesting variational bound

The Variational Rényi (VR) bound (Li and Turner, 2016) : for all $\alpha \in \mathbb{R} \setminus \{1\}$,

$$\mathcal{L}^{(\alpha)}(\theta, \phi; x) = \frac{1}{1-\alpha} \log \left(\int q_\phi(z|x) \; w_{\theta,\phi}(z;x)^{1-\alpha} \; \mathrm{d}z \right)$$
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→ Lower bound on $\ell(\theta; x)$ for $\alpha > 0$ (upper for $\alpha < 0$)

→ Flexible family of variational bounds indexed by α which recovers the ELBO when $\alpha \to 1$ (also has ties to the α-divergence)

Training procedure using the **reparameterized** gradient estimator

$$\frac{\partial}{\partial \phi} \mathcal{L}^{(\alpha)}(\theta, \phi; x) = \frac{\int q(\varepsilon) \; w_{\theta,\phi}(z;x)^{1-\alpha} \; \frac{\partial}{\partial \phi} \log w_{\theta,\phi}(f(\varepsilon, \phi; x); x) \; \mathrm{d}\varepsilon}{\int q(\varepsilon) \; w_{\theta,\phi}(z;x)^{1-\alpha} \; \mathrm{d}\varepsilon}$$

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Recovers SGD with the IWAE bound for $\alpha = 0$ (resp. ELBO for $\alpha = 1$)

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→ However

1. The VR bound can only be estimated using biased MC estimators
2. The VR bound does not recover the IWAE bound when $\alpha = 0$
3. No theoretical justification as SGD with the VR bound resorts to biased estimators on top of the reparameterization trick (unless $\alpha \in \{0,1\}$)

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1. The VR bound can only be estimated using biased MC estimators
2. The VR bound does not recover the IWAE bound when $\alpha = 0$
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- Li and Turner (Theorem 2, 2016) further looked into the biased approximation of the VR bound

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- They investigated the expectation of the biased MC approximation, i.e.

$$\frac{1}{1-\alpha} \int \int \prod_{i=1}^{N} q_\phi(z_i|x) \log \left(\frac{1}{N} \sum_{j=1}^{N} w_{\theta,\phi}(z_j;x)^{1-\alpha} \right) \mathrm{d}z_{1:N}$$

e.g. they showed that it is non-decreasing with N when $\alpha \leq 1$.

- Question Could this expectation be seen as a variational bound?

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Outline

The VR-IWAE bound

For all $\alpha \in [0,1)$ and all $N \in \mathbb{N}^\star$

$$\ell_N^{(\alpha)}(\theta,\phi;x) := \frac{1}{1-\alpha} \int \int \prod_{i=1}^{N} q_\phi(z_i|x) \log \left(\frac{1}{N} \sum_{j=1}^{N} w_{\theta,\phi}(z_j;x)^{1-\alpha} \right) \mathrm{d}z_{1:N}$$

The VR-IWAE bound is a **lower bound** on the marginal log-likelihood that

1. Can be estimated using unbiased MC estimators
2. Recovers the IWAE objective function when $\alpha = 0$
3. Leads to the same SGD procedure as the VR bound in the reparameterized case, but this time using unbiased estimators

$$\begin{aligned}
&\frac{\partial}{\partial \phi} \ell_N^{(\alpha)}(\theta,\phi;x) \\
&\quad = \int \int \prod_{i=1}^{N} q(\varepsilon_i) \left(\sum_{j=1}^{N} \frac{w_{\theta,\phi}(z_j)^{1-\alpha}}{\sum_{k=1}^{N} w_{\theta,\phi}(z_k)^{1-\alpha}} \frac{\partial}{\partial \phi} \log w_{\theta,\phi}(f(\varepsilon_j,\phi)) \right) \mathrm{d}\varepsilon_{1:N}. \\
&\quad \approx \sum_{j=1}^{N} \frac{w_{\theta,\phi}(z_j)^{1-\alpha}}{\sum_{k=1}^{N} w_{\theta,\phi}(z_k)^{1-\alpha}} \frac{\partial}{\partial \phi} \log w_{\theta,\phi}(f(\varepsilon_j,\phi)), \quad \varepsilon_j \sim q, \quad j = 1 \ldots N
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The VR-IWAE bound (cont'd)

→ The VR-IWAE bound is the **theoretically-sound** extension of the IWAE bound originating from the α-divergence VI methodology

→ It provides **theoretical guarantees** behind various VR-bound gradient-based schemes previously proposed in the α-divergence VI community

→ Other notable advantages of the VR-IWAE bound :

- Setting $\alpha > 0$ instead of $\alpha = 0$ (IWAE bound) can improve on the SNR for the reparameterized estimated gradients of the VR-IWAE bound

$$\mathrm{SNR}_{\theta_\ell} = \Theta(\sqrt{N})$$

$$\mathrm{SNR}_{\phi_{\ell'}} = \begin{cases} \Theta(\sqrt{1/N}) & \text{if } \alpha = 0 \text{ (Rainforth et al., 2018)}, \\ \Theta(\sqrt{N}) & \text{if } \alpha \in (0,1). \end{cases}$$

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→ Quantity of interest : variational gap

$$\Delta_N^{(\alpha)}(\theta, \phi; x) := \ell_N^{(\alpha)}(\theta, \phi; x) - \ell(\theta; x), \quad \alpha \in [0, 1)$$

$$= \frac{1}{1-\alpha} \int \int \prod_{i=1}^{N} q_\phi(z_i|x) \log \left(\frac{1}{N} \sum_{j=1}^{N} \overline{w}_{\theta,\phi}(z_j; x)^{1-\alpha} \right) \mathrm{d}z_{1:N}$$

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Outline

N goes to infinity and d is fixed

→ Maddison et al. (2017) followed by Domke and Sheldon (2018) looked into the variational gap for the IWAE bound ($\alpha = 0$)

Informally, Domke and Sheldon (2018, Theorem 3) states that

$$\Delta_N^{(0)}(\theta, \phi; x) = -\frac{\gamma_0^2}{2N} + o\left(\frac{1}{N}\right)$$

where γ_0 is the variance of the relative weights, i.e.

$$\gamma_0^2 := \mathbb{V}_{Z \sim q_\phi}(\overline{w}_{\theta,\phi}(Z))$$

→ Comments :

- N is very beneficial to reduce $\Delta_N^{(0)}(\theta, \phi; x)$ (goes to 0 at a fast $1/N$ rate)
- Question What about $\Delta_N^{(\alpha)}(\theta, \phi; x)$, $\alpha \in [0, 1)$?

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$$\Delta_N^{(\alpha)}(\theta, \phi; x) = \mathcal{L}^{(\alpha)}(\theta, \phi; x) - \ell(\theta; x) - \frac{\gamma_\alpha^2}{2N} + o\left(\frac{1}{N}\right).$$

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1. A term going to zero at a fast $1/N$ rate that depends on γ_α^2
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The hyperparameter α balances between these two terms meaning that a proper tuning of α may be beneficial in practice

$\rightarrow$ "*some conditions*"

- generalize the conditions from Domke and Sheldon (2018)
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Log-normal distribution of the relative weights

Let $\sigma > 0$, $S_1, \ldots, S_N$ be i.i.d. normal r.v and assume that the distribution of the relative weights $\overline{w}_{\theta,\phi}(z_1), \ldots, \overline{w}_{\theta,\phi}(z_N)$ is log-normal of the form

$$\log \overline{w}_{\theta,\phi}(z_i) = -\frac{\sigma^2 d}{2} - \sigma\sqrt{d} S_i, \quad i = 1 \ldots N.$$

Then, for all $\alpha \in [0, 1)$,

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Log-normal distribution of the relative weights

Let $\sigma > 0$, $S_1, \ldots, S_N$ be i.i.d. normal r.v and assume that the distribution of the relative weights $\overline{w}_{\theta,\phi}(z_1), \ldots, \overline{w}_{\theta,\phi}(z_N)$ is log-normal of the form

$$\log \overline{w}_{\theta,\phi}(z_i) = -\frac{\sigma^2 d}{2} - \sigma\sqrt{d} S_i, \quad i = 1 \ldots N.$$

Then, for all $\alpha \in [0, 1)$,

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Outline

$N, d \to \infty$ with either $\frac{\log N}{d} \to 0$ or $\frac{\log N}{d^{1/3}} \to 0$

$\to$ Key intuition : it is typically possible to approximate the distribution of the relative weights by a **log-normal distribution** of the form

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2. Approximate log-normal case : $d, N \to \infty$ with $\frac{\log N}{d^{1/3}} \to 0$

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Set $p_\theta(z|x) = \mathcal{N}(z; \theta, \boldsymbol{I}_d)$ and $q_\phi(z) = \mathcal{N}(z; \phi, \boldsymbol{I}_d)$, with $\theta = 0 \cdot \boldsymbol{u}_d$ and $\phi = \boldsymbol{u}_d$, where $\boldsymbol{u}_d$ is the d-dimensional vector whose coordinates are all equal to 1. Then

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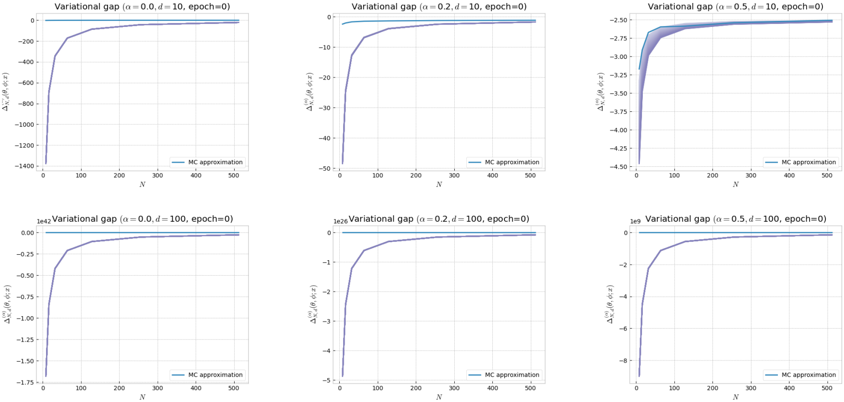
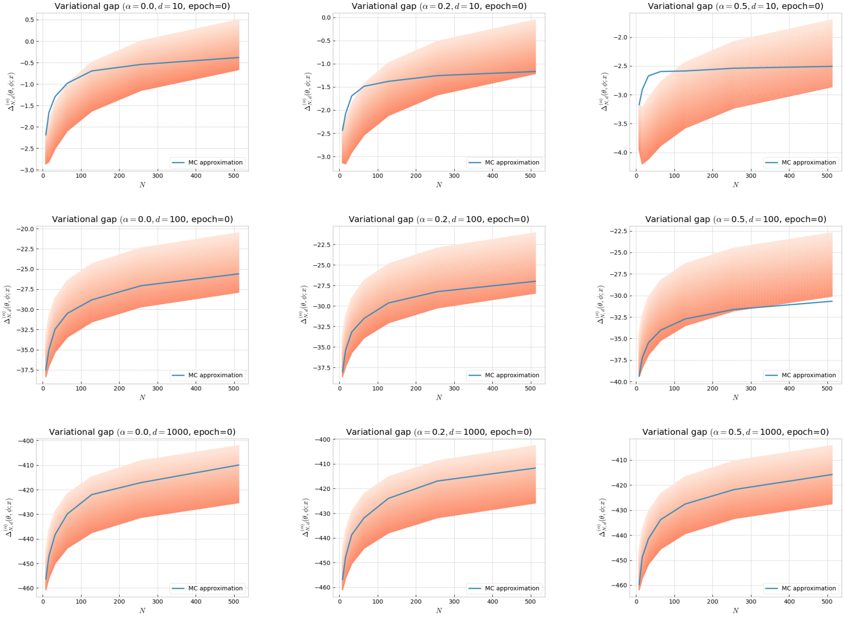


Empirical verification (cont'd)



Main result in the approximate log-normal case

(A1) For all $i = 1 \dots N$,

1. $\xi_{i,1}, \dots, \xi_{i,d}$ are i.i.d. random variables which are absolutely continuous with respect to the Lebesgue measure and satisfy $\mathbb{E}(\xi_{i,1}) = 0$ and $\mathbb{V}(\xi_{i,1}) = \sigma^2 < \infty$.
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$\rightarrow$ NB : $-da = -\log \mathbb{E}(\exp(-\sigma\sqrt{d} S_1))$

Main result in the approximate log-normal case (cont'd)

→ Let $S_1, \dots, S_N$ be such that :

$$S_i = \frac{1}{\sigma\sqrt{d}} \sum_{j=1}^{d} \xi_{i,j}, \quad i = 1 \dots N.$$

Theorem

Assume (A1). Set $a := \log \mathbb{E}(\exp(-\xi_{1,1}))$ and further assume that

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→ Weight collapse phenomenon : for all $\alpha \in [0, 1)$,

$$\Delta_{N,d}^{(\alpha)}(\theta, \phi; x) \approx \mathrm{ELBO}(\theta, \phi; x) - \ell(\theta; x), \quad \text{as } N, d \to \infty \text{ with } \frac{\log N}{d^{1/3}} \to 0.$$

The condition that N should grow at least exponentially with d has been replaced by the less restrictive yet still stringent condition that N should grow at least sub-exponentially with $d^{1/3}$.

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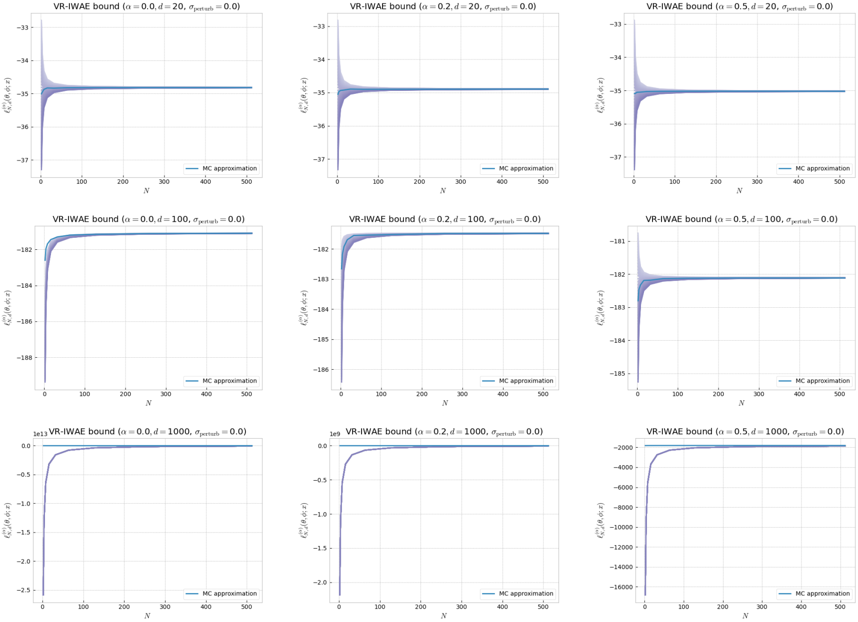
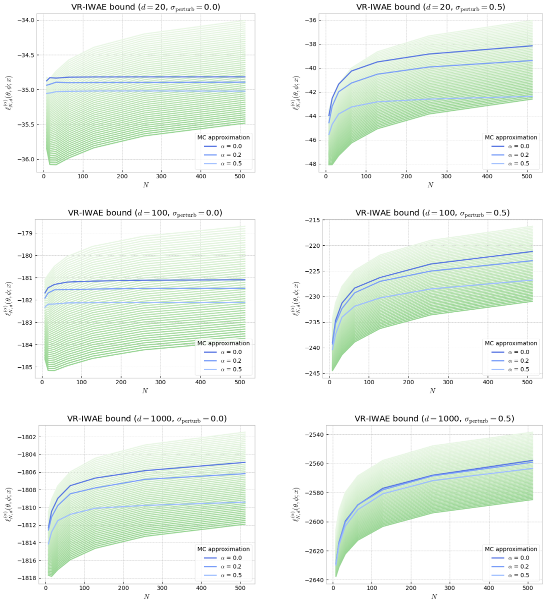
Outline

1. Introduction
2. The VR-IWAE bound
3. Theoretical study of the VR-IWAE bound
4. Numerical experiments
5. Conclusion

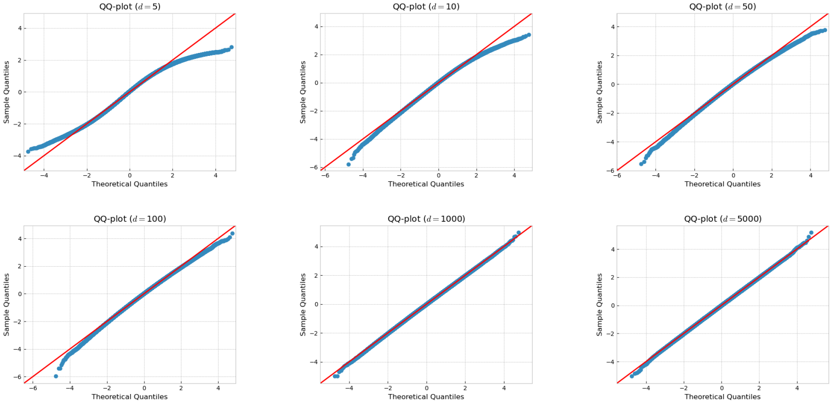
Linear Gaussian example



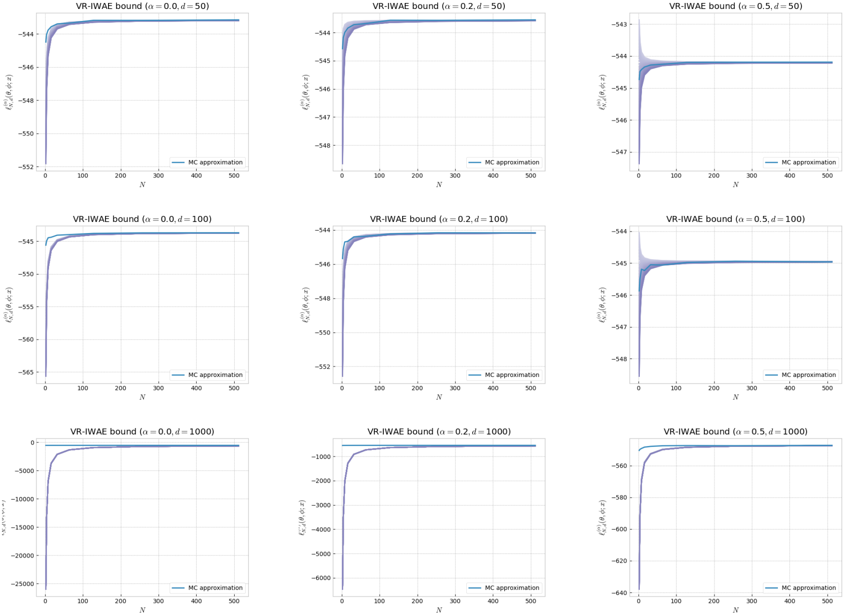
Linear Gaussian example (cont'd)



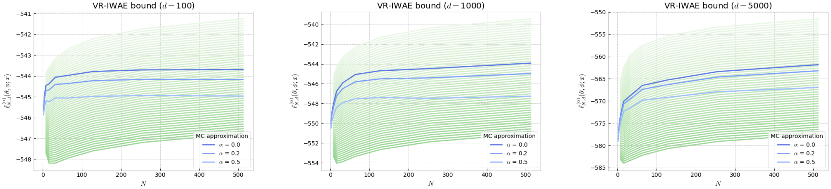
Variational auto-encoder on MNIST



Variational auto-encoder on MNIST (cont'd)



Variational auto-encoder on MNIST (cont'd - 2)



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→ Further work:

- Does the weight collapse behavior apply beyond the cases highlighted here?
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   - Theoretically-sound extension of the IWAE bound ($\alpha = 0$)
   - Provides theoretical guarantees behind various VR bound-based schemes proposed in the α-Divergence VI community
   - Enjoys other additional desirable properties of this bound (SNR, doubly-reparameterized)

2. We provided two complementary analyses of the VR-IWAR bound
   - Shed light on the conditions behind the success or failure of the VR-IWAE bound methodology
   - Encompass the case of the IWAE bound

3. Empirical verification of our theoretical results

$\rightarrow$ Further work:

- Does the weight collapse behavior apply beyond the cases highlighted here?
- How does the weight collapse affect the gradient descent procedures?
- Can we further use the fact that the VR-IWAE bound extends the IWAE bound?