Variational bounds in Variational Inference: how to choose them?

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UNIVERSITY OF OXFORD

CoSInES-Bayes4Health VI Masterclass – 09/11/2022

Outline

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Introduction

- 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 $\mathbb{R}^d$

- Posterior density of the latent variable z given the observation x

$$p_\theta(z|x) = \frac{p_\theta(x,z)}{\int p_\theta(x,z)\mathrm{d}z}$$

- What we would like : compute / sample from the posterior density

- Key example : maximize the **marginal log likelihood** w.r.t. θ

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

$$\nabla_\theta \ell(\theta;x) = \frac{\nabla_\theta(\int p_\theta(x,z)\mathrm{d}z)}{\int p_\theta(x,z)\mathrm{d}z} = \frac{\int \nabla_\theta(p_\theta(x,z))\mathrm{d}z}{\int p_\theta(x,z)\mathrm{d}z} = \frac{\int p_\theta(x,z)\nabla_\theta(\log p_\theta(x,z))\mathrm{d}z}{\int p_\theta(x,z)\mathrm{d}z}$$
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Variational bounds

- Variational bounds are surrogate objective functions to the marginal log likelihood that are more amenable to optimization.
- They involve a variational family of probability densities $\mathcal{Q}$

$$\text{e.g.} \quad \mathcal{Q} = \left\{ z \mapsto q_\phi(z|x) \ : \ \phi \in \mathbb{R}^L \right\}$$

- Example : **Evidence Lower BOund (ELBO)**

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

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"Traditional Variational Inference" : θ is constant, the goal is to minimize the exclusive KL divergence $\Leftrightarrow$ maximizing the ELBO

Optimisation w.r.t. (θ, ϕ): Variational Auto-Encoder (VAE) framework

Training with the ELBO

1. Unbiased Monte Carlo (MC) estimator of the ELBO

$$\begin{aligned}\mathrm{ELBO}(\theta,\phi;x) &= \int q_\phi(z|x)\log\left(w_{\theta,\phi}(z;x)\right)\mathrm{d}z \\ &\approx \frac{1}{N}\sum_{i=1}^{N}\log\left(w_{\theta,\phi}(z_i;x)\right), \quad z_i \sim q_\phi(\cdot|x), \quad i = 1\ldots N\end{aligned}$$

2. Reparameterization trick $z = f(\varepsilon,\phi;x) \sim q_\phi(\cdot|x)$ where $\varepsilon \sim q$
3. Reparameterized gradient of the ELBO:

$$\nabla_{\theta,\phi}\mathrm{ELBO}(\phi;x) = \int q(\varepsilon)\nabla_{\theta,\phi}\left(\log w_{\theta,\phi}(f(\varepsilon,\phi;x);x)\right)\mathrm{d}\varepsilon$$

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Variational Rényi (VR) bound (Li and Turner, NeurIPS 2016): for all $\alpha > 0$ and $\neq 1$

$$\mathrm{VR}^{(\alpha)}(\theta, \phi; x) := \frac{1}{1-\alpha} \log \left(\int q_\phi(z|x) w_{\theta,\phi}(z;x)^{1-\alpha} \mathrm{d}z \right), \quad w_{\theta,\phi}(z;x) = \frac{p_\theta(z,x)}{q_\phi(z|x)}$$
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where $D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x))$ is **Rényi's α-divergence**: for all $\alpha > 0$ and $\neq 1$

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- We have that $\lim_{\alpha \to 1} D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x)) = D^{(KL)}(q_\phi(\cdot|x)||p_\theta(\cdot|x))$

Proof Set $f(\alpha) = \int q_\phi(z|x) \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right)^{\alpha-1} \mathrm{d}z$

Then, $f(1) = 1$ and $f'(\alpha) = \int q_\phi(z|x) \log \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right) \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right)^{\alpha-1} \mathrm{d}z$

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where $D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x))$ is **Rényi's α-divergence**: for all $\alpha > 0$ and $\neq 1$

$$D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x)) = \frac{1}{\alpha - 1} \log \left(\int q_\phi(z|x) \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right)^{\alpha-1} \mathrm{d}z \right)$$

- We have that $\lim_{\alpha \to 1} D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x)) = D^{(KL)}(q_\phi(\cdot|x)||p_\theta(\cdot|x))$

Proof Set $f(\alpha) = \int q_\phi(z|x) \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right)^{\alpha-1} \mathrm{d}z$

Then, $f(1) = 1$ and $f'(\alpha) = \int q_\phi(z|x) \log \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right) \left(\frac{q_\phi(z|x)}{p_\theta(z|x)} \right)^{\alpha-1} \mathrm{d}z$

$$\lim_{\alpha \to 1} D^{(\alpha)}(q_\phi(\cdot|x)||p_\theta(\cdot|x)) = \lim_{\alpha \to 1} \frac{\log f(\alpha) - \log f(1)}{\alpha - 1} = \frac{f'(1)}{f(1)} = D^{(KL)}(q_\phi(\cdot|x)||p_\theta(\cdot|x))$$

The Variational Rényi (VR) bound

Variational Rényi (VR) bound (Li and Turner, NeurIPS 2016): for all $\alpha > 0$ and $\neq 1$

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- $\mathrm{VR}^{(\alpha)}(\theta, \phi; x) \leq \ell(\theta; x)$, $\mathrm{VR}^{(0)}(\theta, \phi; x) = \ell(\theta; x)$

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- Question How does the regularization term behave?

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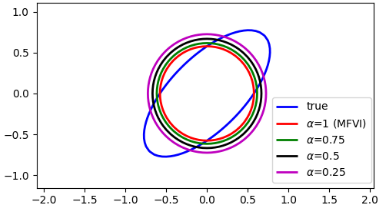
- Question How does the regularization term behave?
- Example : $D^{(\alpha)}(q||p)$ with $p(z) = \mathcal{N}(z; [0,0], [[3,-2],[-2,3]])$ and $\mathcal{Q} = \{q : z \mapsto \mathcal{N}(z_1; \mu_1, \sigma_1^2)\ \mathcal{N}(z_2; \mu_2, \sigma_2^2) : \mu_1, \mu_2 \in \mathbb{R}, \sigma_1, \sigma_2 > 0\}$



Adapted from (Li and Turner, NeurIPS 2016)

Training with the VR bound (Li and Turner, NeurIPS 2016)

1. MC estimator of the VR bound

$$\begin{aligned}\mathrm{VR}^{(\alpha)}(\theta,\phi;x) &= \frac{1}{1-\alpha}\log\left(\int q_\phi(z|x) w_{\theta,\phi}(z;x)^{1-\alpha}\mathrm{d}z\right)\\ &\approx \frac{1}{1-\alpha}\log\left(\frac{1}{N}\sum_{i=1}^{N} w_{\theta,\phi}(z_i;x)^{1-\alpha}\right), \quad z_i\sim q_\phi(\cdot|x), \quad i=1\ldots N\end{aligned}$$

2. Reparameterization trick $z = f(\varepsilon,\phi;x)\sim q_\phi(\cdot|x)$ where $\varepsilon\sim q$
3. Reparameterized gradient of the VR bound :

$$\begin{aligned}\nabla_{\theta,\phi}\mathrm{VR}^{(\alpha)}(\theta,\phi;x) &= \nabla_{\theta,\phi}\left[\frac{1}{1-\alpha}\log\left(\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon,\phi;x);x)^{1-\alpha}\mathrm{d}\varepsilon\right)\right]\\ &= \frac{1}{1-\alpha}\frac{\int q(\varepsilon)\nabla_{\theta,\phi}\left[w_{\theta,\phi}(f(\varepsilon,\phi;x);x)^{1-\alpha}\right]\mathrm{d}\varepsilon}{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon,\phi;x);x)^{1-\alpha}\mathrm{d}\varepsilon}\\ &= \frac{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon,\phi;x);x)^{-\alpha}\nabla_{\theta,\phi}\left[w_{\theta,\phi}(f(\varepsilon,\phi;x);x)\right]\mathrm{d}\varepsilon}{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon,\phi;x);x)^{1-\alpha}\mathrm{d}\varepsilon}\\ &= \frac{\int q(\varepsilon) w_{\theta,\phi}(z;x)^{1-\alpha}\nabla_{\theta,\phi}\left(\log w_{\theta,\phi}(f(\varepsilon,\phi;x);x)\right)\mathrm{d}\varepsilon}{\int q(\varepsilon) w_{\theta,\phi}(z;x)^{1-\alpha}\mathrm{d}\varepsilon}\end{aligned}$$

4. SGD w.r.t. (θ,ϕ)

$$\nabla_{\theta,\phi}\mathrm{VR}^{(\alpha)}(\theta,\phi;x) \approx \sum_{i=1}^{N}\frac{w_{\theta,\phi}(z_i;x)^{1-\alpha}}{\sum_{j=1}^{N} w_{\theta,\phi}(z_j;x)^{1-\alpha}}\nabla_{\theta,\phi}\left(\log w_{\theta,\phi}(f(\varepsilon_i,\phi;x);x)\right),\ \varepsilon_i\sim q, i=1\ldots N$$

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1. MC estimator of the VR bound

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Training with the VR bound (Li and Turner, NeurIPS 2016)

❶ MC estimator of the VR bound

$$\begin{aligned}
\mathrm{VR}^{(\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) \\
&\approx \frac{1}{1-\alpha} \log \left(\frac{1}{N} \sum_{i=1}^{N} w_{\theta,\phi}(z_i; x)^{1-\alpha} \right), \quad z_i \sim q_\phi(\cdot|x), \quad i = 1 \dots N
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❸ Reparameterized gradient of the VR bound :

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&= \frac{1}{1-\alpha} \frac{\int q(\varepsilon) \nabla_{\theta,\phi} \left[w_{\theta,\phi}(f(\varepsilon, \phi; x); x)^{1-\alpha} \right] \mathrm{d}\varepsilon}{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon, \phi; x); x)^{1-\alpha} \mathrm{d}\varepsilon} \\
&= \frac{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon, \phi; x); x)^{-\alpha} \nabla_{\theta,\phi} \left[w_{\theta,\phi}(f(\varepsilon, \phi; x); x) \right] \mathrm{d}\varepsilon}{\int q(\varepsilon) w_{\theta,\phi}(f(\varepsilon, \phi; x); x)^{1-\alpha} \mathrm{d}\varepsilon} \\
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\end{aligned}$$

❹ SGD w.r.t. (θ, ϕ)

$$\nabla_{\theta,\phi} \mathrm{VR}^{(\alpha)}(\theta, \phi; x) \approx \sum_{i=1}^{N} \frac{w_{\theta,\phi}(z_i; x)^{1-\alpha}}{\sum_{j=1}^{N} w_{\theta,\phi}(z_j; x)^{1-\alpha}} \nabla_{\theta,\phi} \left(\log w_{\theta,\phi}(f(\varepsilon_i, \phi; x); x) \right), \ \varepsilon_i \sim q, i = 1 \dots N$$

Some important comments

$$\mathrm{VR}^{(\alpha)}(\theta,\phi;x) = \frac{1}{1-\alpha}\log\left(\int q_\phi(z|x)w_{\theta,\phi}(z;x)^{1-\alpha}\mathrm{d}z\right)$$
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→ Sanity check : $\nabla_{\theta,\phi}\mathrm{VR}^{(1)}(\theta,\phi;x) = \nabla_{\theta,\phi}\mathrm{ELBO}(\theta,\phi;x)$

→ Training with $\alpha < 1$ lead to positive empirical results

→ However,

1. The VR bound can only be estimated using biased MC estimators
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→ Sanity check : $\nabla_{\theta,\phi}\mathrm{VR}^{(1)}(\theta,\phi;x) = \nabla_{\theta,\phi}\mathrm{ELBO}(\theta,\phi;x)$

→ Training with $\alpha < 1$ lead to positive empirical results

→ However,

1. The VR bound can only be estimated using biased MC estimators
2. No theoretical justification as SGD with the VR bound resorts to biased estimators on top of the reparameterization trick (unless $\alpha = 1$)

Some important comments

$$\mathrm{VR}^{(\alpha)}(\theta,\phi;x) = \frac{1}{1-\alpha}\log\left(\int q_\phi(z|x)w_{\theta,\phi}(z;x)^{1-\alpha}\mathrm{d}z\right)$$

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Problem 1

- Li and Turner (Theorem 2, NeurIPS 2016) looked into the properties of the biased approximation of the VR bound

$$\begin{aligned}\mathrm{VR}^{(\alpha)}(\theta,\phi;x) &= \frac{1}{1-\alpha}\log\left(\int q_\phi(z|x)\ w_{\theta,\phi}(z;x)^{1-\alpha}\,\mathrm{d}z\right)\\ &\approx \frac{1}{1-\alpha}\log\left(\frac{1}{N}\sum_{j=1}^{N} w_{\theta,\phi}(z_j;x)^{1-\alpha}\right), \quad z_j \sim q_\phi(z|x), \quad j = 1\ldots N\end{aligned}$$

- More precisely, they investigated the expectation of the biased MC approximation, i.e.

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

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$$\mathrm{ELBO}(\theta,\phi;x) \le \ell_N^{(\alpha)}(\theta,\phi;x) \le \ell_{N+1}^{(\alpha)}(\theta,\phi;x) \le \mathrm{VR}^{(\alpha)}(\theta,\phi;x)$$

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- VR bound : interesting generalization of the ELBO

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     $\rightarrow$ Some control of the approximation error via

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  2. The SGD with the VR bound uses biased estimators

An idea

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

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💡 Could this expectation be seen as a variational bound?

Daudel, Benton, Shi and Doucet (2022). **Alpha-divergence Variational Inference Meets Importance Weighted Auto-Encoders: Methodology and Asymptotics.**

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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. Leads to the same SGD procedure as the VR bound in the reparameterized case, but this time using unbiased estimators

$$\nabla_{\theta,\phi} \ell_N^{(\alpha)}(\theta, \phi; x)$$

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The VR-IWAE bound provides **theoretical guarantees** behind various VR-bound gradient-based schemes previously proposed in the literature

Special cases of 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 case $\alpha \to 1$

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The VR-IWAE bound recovers the **Importance Weighted Auto-encoder (IWAE) bound** (Burda et al., ICLR 2016) when $\alpha = 0$

$\rightarrow$ Extension of the ELBO also leading to positive empirical results

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→ Question Can we understand the behavior of the VR-IWAE bound as a function of $\alpha \in [0, 1)$ better?

Outline

Quantity of interest

Variational gap

For all $\alpha \in [0, 1)$,

$$\Delta_N^{(\alpha)}(\theta, \phi; x) := \ell_N^{(\alpha)}(\theta, \phi; x) - \ell(\theta; x)$$

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

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NB : we will drop the dependency in x in $\overline{w}_{\theta,\phi}(z; x)$ for convenience

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Part I

N goes to infinity and d is fixed in the variational gap

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Informally, Domke and Sheldon (Theorem 3, NeurIPS 2018) 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.

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

→ 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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Main result when $N \to \infty$ and d is fixed

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

→ Two main terms :

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

→ "*some conditions*"

- generalize the conditions from Domke and Sheldon (2018)
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💡 To the best of our knowledge, first result shedding light on how α may play a role in Rényi's α-divergence VI

Example

Example 1 : 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 $\alpha \in [0, 1)$,

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

with

$$\mathrm{VR}^{(\alpha)}(\theta, \phi; x) - \ell(\theta; x) = -\frac{\alpha\sigma^2 d}{2} \quad \text{and} \quad \gamma_\alpha^2 = \frac{\exp\left[(1-\alpha)^2\sigma^2 d\right] - 1}{1 - \alpha}.$$

→ Sanity check : $\mathbb{E}(\overline{w}_{\theta,\phi}) = \mathbb{E}(\exp(-\frac{\sigma^2 d}{2} - \sigma\sqrt{d} S_1)) = 1$

→ **Gaussian example** Set $p_\theta(z|x) = \mathcal{N}(z; \theta, \boldsymbol{I}_d)$ and $q_\phi(z|x) = \mathcal{N}(z; \phi, \boldsymbol{I}_d)$, 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 $\sigma = 1$.

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Example 1 : 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

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Gaussian example and Theorem 1 empirically

- $\Delta_N^{(\alpha)}(\theta, \phi; x)$ is estimated using the unbiased MC estimator

$$\frac{1}{1-\alpha} \log \left(\frac{1}{N} \sum_{j=1}^{N} \overline{w}_{\theta,\phi}(z_j; x)^{1-\alpha} \right), \quad z_j \sim q_\phi(\cdot|x), \quad j = 1 \dots N$$

- Theorem 1 is represented through functions of the form:

$$c \mapsto -\frac{\alpha d}{2} - \frac{\exp\left[(1-\alpha)^2 d\right] - 1}{2(1-\alpha)N} + \frac{c}{N}$$

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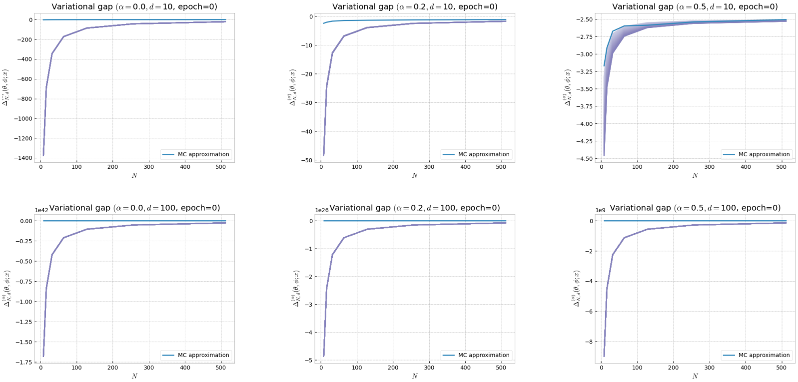

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Part II

N and d go to infinity in the variational gap

$N, d \to \infty$ in the variational gap

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

$$\log \overline{w}_{\theta,\phi}(z_i) = -\frac{\sigma^2 d}{2} - \sigma\sqrt{d} S_i, \quad S_i \sim \mathcal{N}(0,1), \quad i = 1 \dots N.$$

$\to$ Theoretical study in two steps :

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

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Part II.1

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Main result in the log-normal case

Theorem 2

Let $S_1, \ldots, S_N$ be **i.i.d. normal random variables**. Further assume that

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$$\Delta_{N,d}^{(\alpha)}(\theta,\phi;x) \approx -\frac{d\sigma^2}{2}\left(1 - 2\sqrt{\frac{2\log N}{d\sigma^2}} + \frac{1}{1-\alpha}\frac{2\log N}{d\sigma^2} + O\left(\frac{\log\log N}{\sqrt{d\log N}}\right)\right)$$

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

$$\Delta^{(\alpha)}_{N,d}(\theta, \phi; x) \approx \mathrm{ELBO}(\theta, \phi; x) - \ell(\theta; x), \quad \text{as } N, d \to \infty \text{ with } \tfrac{\log N}{d} \to 0.$$

Gaussian example revisited

Gaussian example

Set $p_\theta(z|x) = \mathcal{N}(z;\theta,\boldsymbol{I}_d)$ and $q_\phi(z|x) = \mathcal{N}(z;\phi,\boldsymbol{I}_d)$, 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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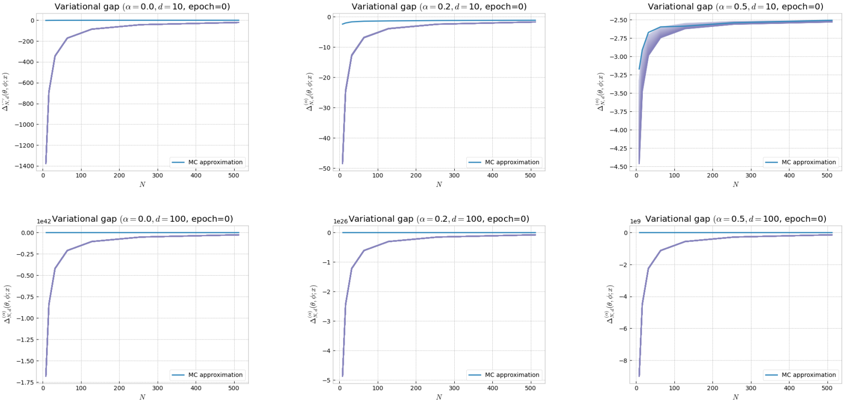
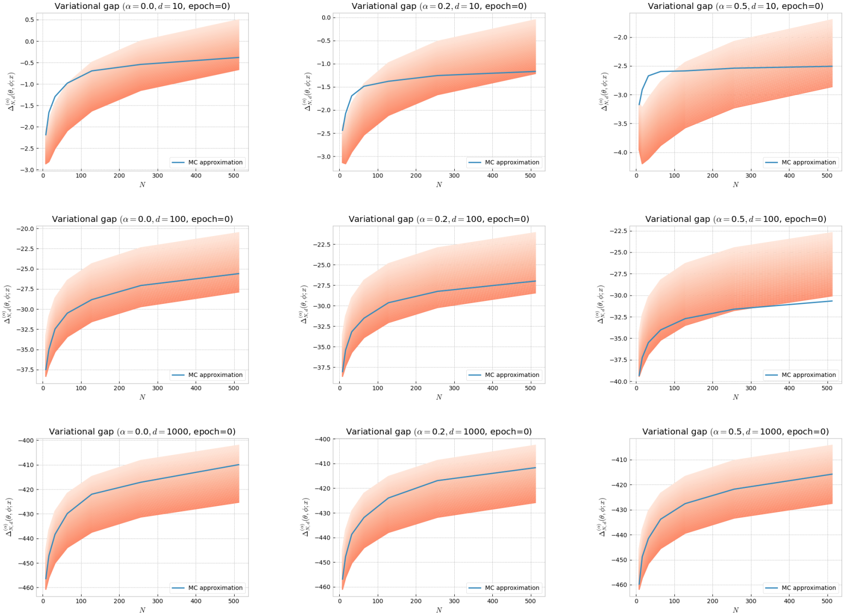
Weight collapse phenomenon might occur even for simple examples!

Gaussian example and Theorem 1 empirically



Gaussian example and Theorem 2 empirically



Part II.2

Approximate log-normal case

Assumptions

Let $S_1, \ldots, S_N$ be such that :

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

We will work under (A1) :

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

1. $\xi_{i,1}, \ldots, \xi_{i,d}$ 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 $\mathbb{V}(\xi_{i,1}) = \sigma^2 < \infty$.
2. There exists $K > 0$ such that:

$$|\mathbb{E}(\xi_{i,1}^k)| \leq k! K^{k-2} \sigma^2, \quad k \geq 3.$$

Approximate log-normal weights

$$\begin{aligned} \log \overline{w}_{\theta,\phi}(z_i) &= -\log \mathbb{E}(\exp(-\sigma\sqrt{d}S_1)) - \sigma\sqrt{d}S_i, \quad i = 1 \ldots N \\ &= -da - \sigma\sqrt{d}S_i, \quad i = 1 \ldots N \end{aligned}$$

with $a := \log \mathbb{E}(\exp(-\xi_{1,1}))$

Assumptions

Let $S_1, \ldots, S_N$ be such that :

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

We will work under (A1) :

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Main result in the approximate log-normal case

Theorem 3

Assume (A1) and that

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

Then, $a > 0$ and for all $\alpha \in [0,1)$, we have

$$\lim_{\substack{N,d\to\infty \\ \log N/d^{1/3}\to 0}} \Delta^{(\alpha)}_{N,d}(\theta,\phi;x) + da\left(1 - \frac{\sigma}{a}\sqrt{\frac{2\log N}{d}} + O\left(\frac{\log\log N}{\sqrt{d\log N}}\right)\right) = 0.$$

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

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

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 exponentially with $d^{1/3}$.

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Linear Gaussian example

Linear Gaussian example (Rainforth et al., ICML 2018)

Set $p_\theta(z) = \mathcal{N}(z; \theta, \boldsymbol{I}_d)$, $p_\theta(x|z) = \mathcal{N}(x; z, \boldsymbol{I}_d)$ with $\theta \in \mathbb{R}^d$, and $q_\phi(z|x) = \mathcal{N}(z; Ax + b, 2/3\ \boldsymbol{I}_d)$ with $A = \mathrm{diag}(\tilde{a})$ and $\phi = (\tilde{a}, b) \in \mathbb{R}^d \times \mathbb{R}^d$.
Then, we can write

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

with $\sigma^2 = \frac{1}{18} + \frac{8}{3}\lambda^2$ and $a = \lambda^2 + \frac{1}{6} + \frac{1}{2}\log(3/4)$, where $\lambda = \frac{\left\| \frac{\theta+x}{2} - Ax - b \right\|}{\sqrt{d}}$

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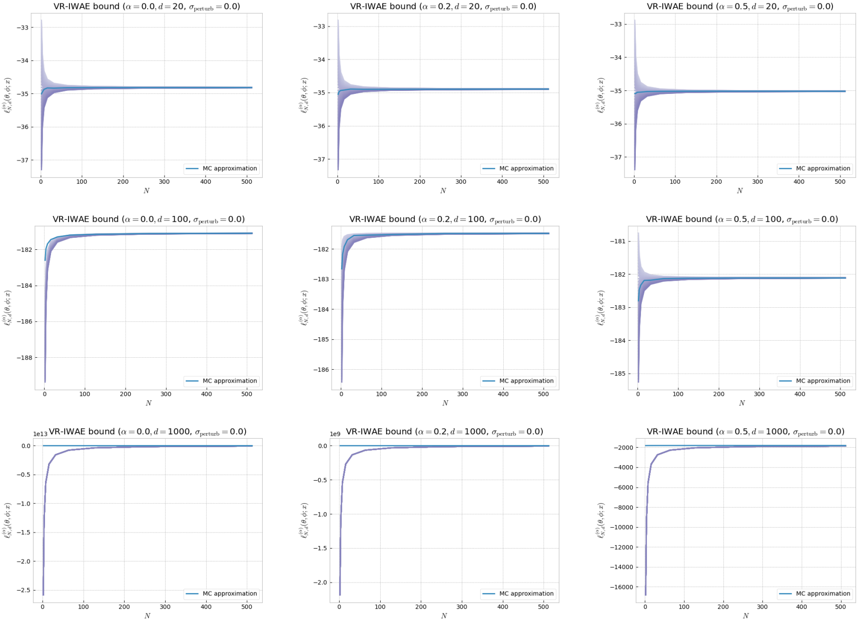
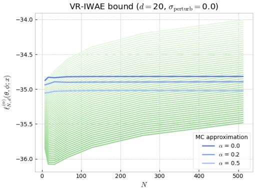
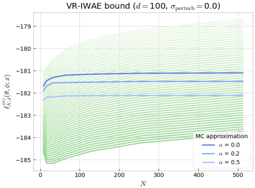
The choice of the variational approximation $q_\phi(\cdot|x)$ matters a lot!

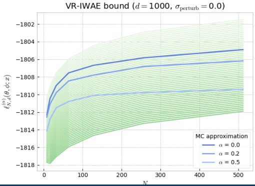
Linear Gaussian example and Theorem 1 empirically



Linear Gaussian example and Theorem 3 empirically







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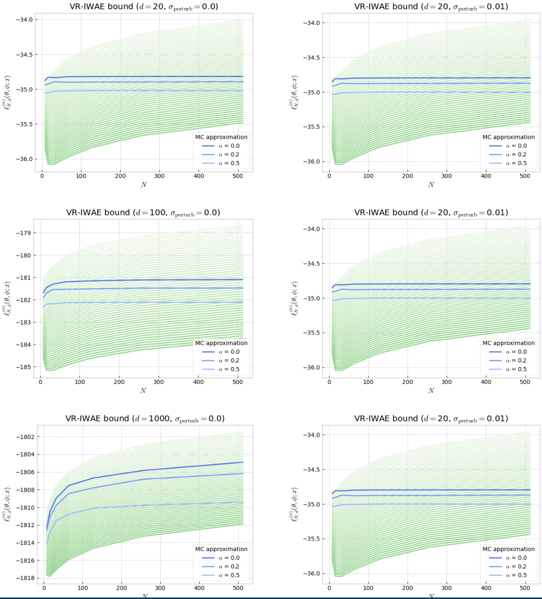

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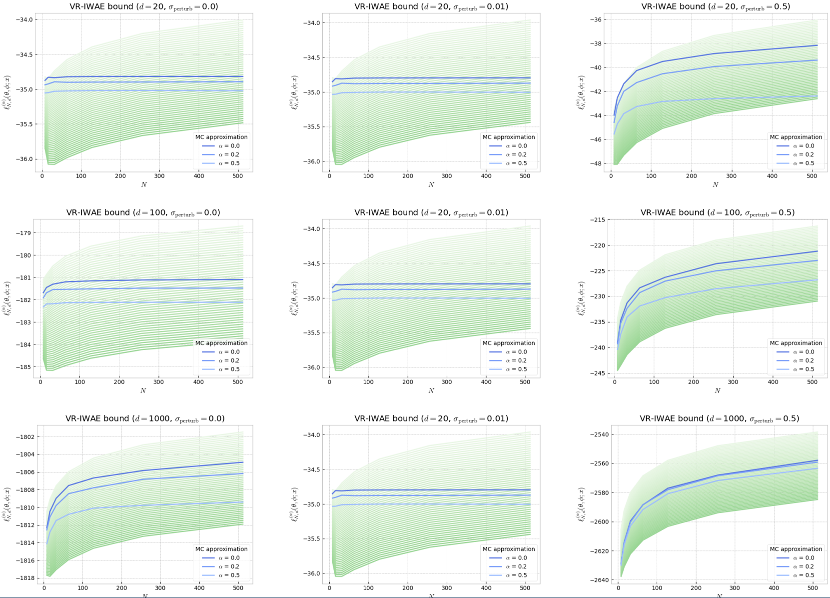

At this stage

Quantity of interest : **variational gap**

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

$\rightarrow$ Two **complementary** studies

1. When $N \to \infty$ and the dimension of the latent space d is fixed

2. When $N, d \to \infty$ with (i) $\frac{\log N}{d} \to 0$ or (ii) $\frac{\log N}{d^{1/3}} \to 0$

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From theory to practice

- $\ell_N^{(\alpha)}(\theta,\phi;x)$ is estimated using the unbiased MC estimator

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- Theorem 3 *Assuming that the weights are approximately log-normal*

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Outline

VAE on MNIST dataset

- More details about this framework in the afternoon lecture!
- Here, we only want to look at
  1. the behavior of the relative weights
  2. the behavior of the VR-IWAE bound

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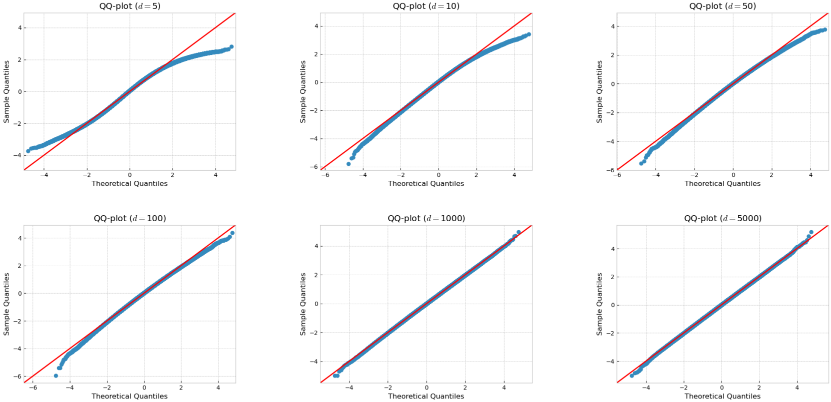
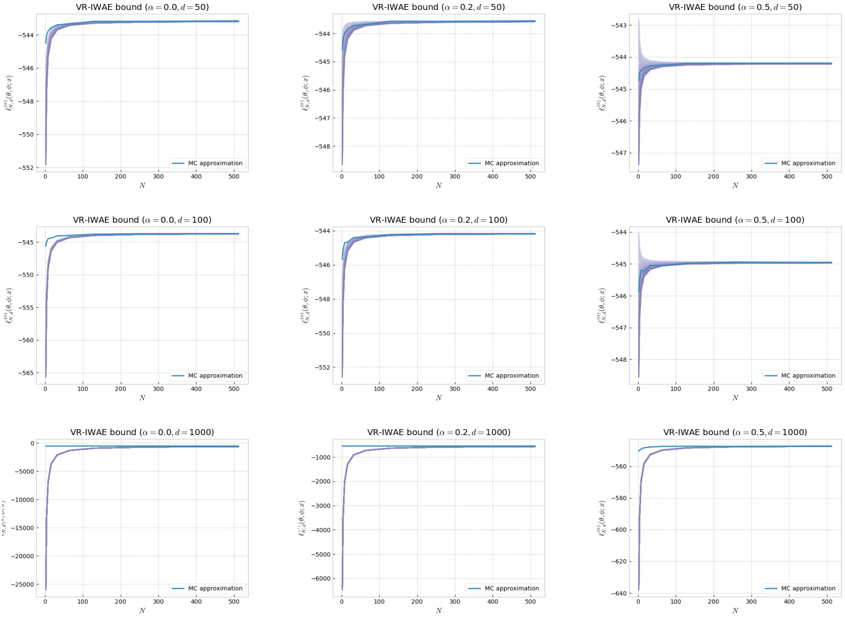
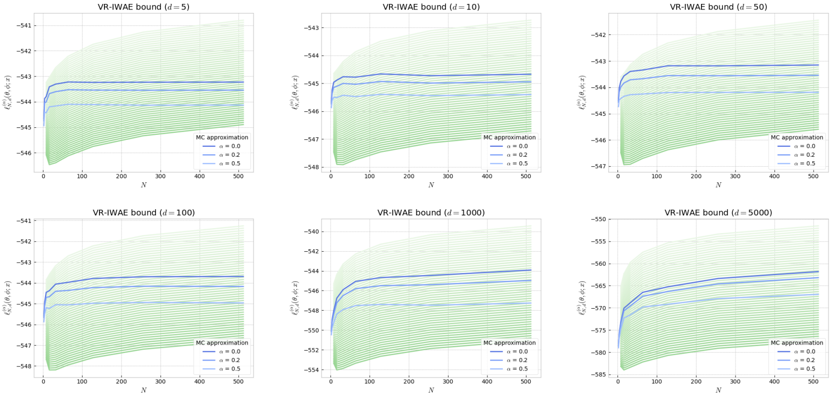


VAE on MNIST dataset and Theorem 1



VAE on MNIST dataset and Theorem 3



At this stage

→ Two complementary analyses of the VR-IWAE bound that we verified on a **real-world scenario**

1. Theorem 1 is tailored for low to medium dimensions settings
2. Theorem 3 is tailored for high-dimensional settings

Questions?

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Question Can we say something about the gradient of the VR-IWAE bound as a function of $\alpha \in [0, 1)$?

Outline

Study of the gradient(s) of the VR-IWAE bound

Quantities of interest

- MC estimates of the reparameterized gradients of the VR-IWAE bound

$$\delta_N^{(\alpha)}(\phi_\ell) = \frac{\partial}{\partial \phi_\ell} \log \left(\frac{1}{N} \sum_{j=1}^N w_{\theta,\phi}(f(\varepsilon_j, \phi; x))^{1-\alpha} \right), \quad \ell = 1 \ldots L$$

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  with $\phi = (\phi_1, \ldots, \phi_L)$, $\theta = (\theta_1, \ldots, \theta_{L'})$

- Signal-to-Noise Ratio

  Letting $X = (X_1, \ldots, X_L)$ be a random vector of dimension L,

$$\mathrm{SNR}[X] = \left(\frac{|\mathbb{E}(X_1)|}{\sqrt{\mathbb{V}(X_1)}}, \ldots, \frac{|\mathbb{E}(X_L)|}{\sqrt{\mathbb{V}(X_L)}} \right).$$

Study of the gradient(s) of the VR-IWAE bound

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SNR analysis in the reparameterized case

Theorem 4

Let $\alpha \in [0,1)$. Define $\tilde{w}_j = w_{\theta,\phi}(f(\varepsilon_j, \phi; x))$ and $\hat{Z}_{N,\alpha} = N^{-1} \sum_{j=1}^{N} \tilde{w}_j^{1-\alpha}$. Assume that the eighth moments of $\tilde{w}_1^{1-\alpha}$, $\partial \tilde{w}_1^{1-\alpha} / \partial \phi_\ell$ and $\partial \tilde{w}_1^{1-\alpha} / \partial \theta_{\ell'}$ are finite. Furthermore, assume that there exists some $N \in \mathbb{N}^\star$ for which $\mathbb{E}((1/\hat{Z}_{N,\alpha})^4) < \infty$. Lastly, assume that

$$\begin{aligned} &\partial \mathbb{V}(\tilde{w}_1^{1-\alpha}) / \partial \phi_\ell > 0, \quad \text{if } \alpha = 0 \\ &\partial \mathbb{E}(\tilde{w}_1^{1-\alpha}) / \partial \phi_\ell \neq 0, \quad \text{if } \alpha \in (0,1) \end{aligned}$$

and that $\partial \mathbb{E}(\tilde{w}_1^{1-\alpha}) / \partial \theta_{\ell'} \neq 0$. Then,

$$\begin{aligned} \mathrm{SNR}[\delta_N^{(\alpha)}(\phi_\ell)] &= \begin{cases} \Theta(\sqrt{1/N}) & \text{if } \alpha = 0, \\ \Theta(\sqrt{N}) & \text{if } \alpha \in (0,1) \end{cases} \\ \mathrm{SNR}[\delta_N^{(\alpha)}(\theta_{\ell'})] &= \Theta(\sqrt{N}). \end{aligned}$$

→ The IWAE case was already known from Rainforth et al. (ICML 2018)

→ Motivates $\alpha \in (0,1)$

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Doubly-reparameterized gradients

→ Introduced in Tucker (ICLR 2019) for the IWAE bound

Theorem 5

For all $\alpha \in [0, 1]$,

$$\frac{\partial}{\partial \phi} \ell_N^{(\alpha)}(\theta, \phi; x) = \int \int \prod_{i=1}^{N} q(\varepsilon_i) \left(\sum_{j=1}^{N} h_j(\alpha) \frac{\partial}{\partial \phi} \log w_{\theta,\phi'}(f(\varepsilon_j, \phi; x))|_{\phi'=\phi} \right) \mathrm{d}\varepsilon_{1:N}$$

with $z_j = f(\varepsilon_j, \phi; x)$ for all $j = 1 \ldots J$ and

$$h_j(\alpha) = \alpha \frac{w_{\theta,\phi}(z_j)^{1-\alpha}}{\sum_{k=1}^{N} w_{\theta,\phi}(z_k)^{1-\alpha}} + (1-\alpha) \left(\frac{w_{\theta,\phi}(z_j)^{1-\alpha}}{\sum_{k=1}^{N} w_{\theta,\phi}(z_k)^{1-\alpha}} \right)^2 .$$

An unbiased estimator of $\partial \ell_N^{(\alpha)}(\theta, \phi; x)/\partial \phi$ is then given by

$$\sum_{j=1}^{N} h_j(\alpha) \frac{\partial}{\partial \phi} \log w_{\theta,\phi'}(f(\varepsilon_j, \phi))|_{\phi'=\phi}$$

where $\varepsilon_1, \ldots, \varepsilon_N$ are i.i.d. samples generated from q and $z_j = f(\varepsilon_j, \phi; x)$ for all $j = 1 \ldots J$.

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At this stage

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

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

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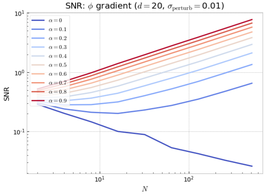
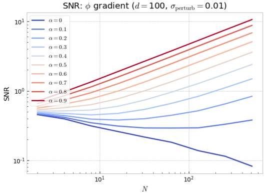
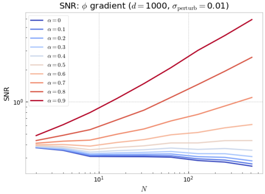
SNR analysis for the Linear Gaussian example : ϕ

Reparameterized







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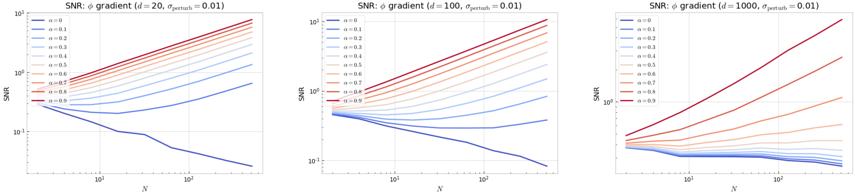
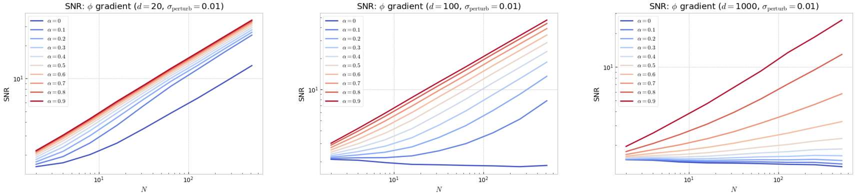
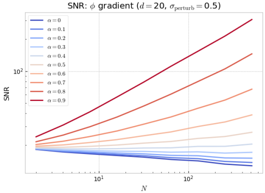


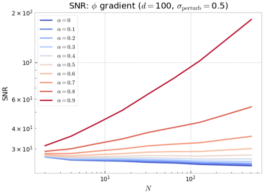
Doubly-reparameterized

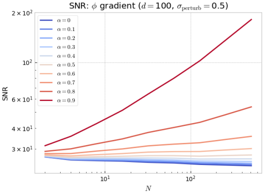


SNR analysis for the Linear Gaussian example : ϕ (cont'd)

Reparameterized

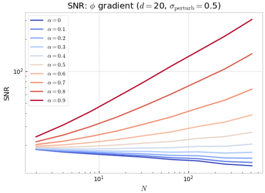


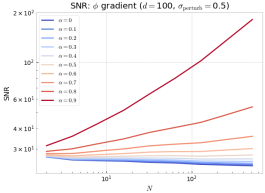


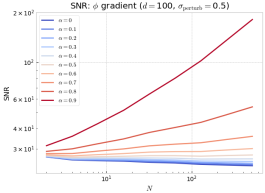


SNR analysis for the Linear Gaussian example : ϕ (cont'd)

Reparameterized







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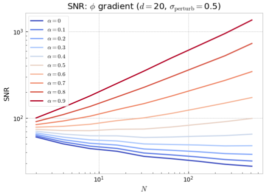
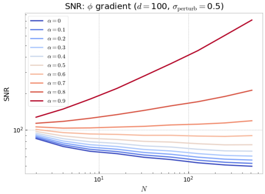
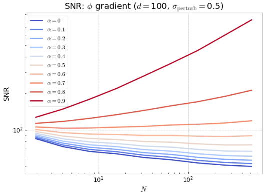
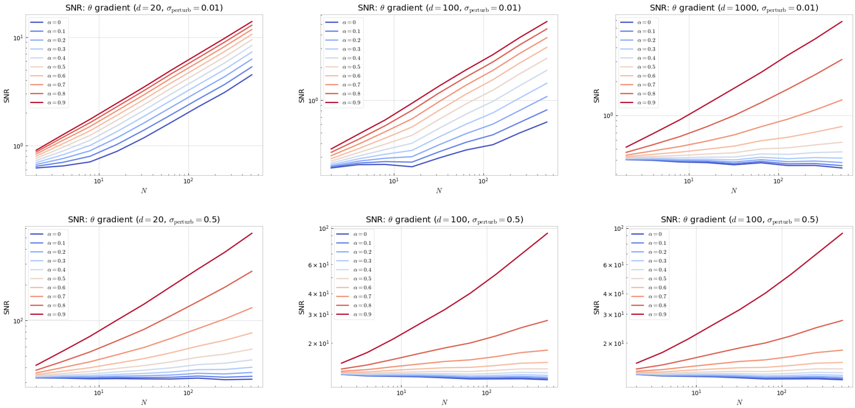




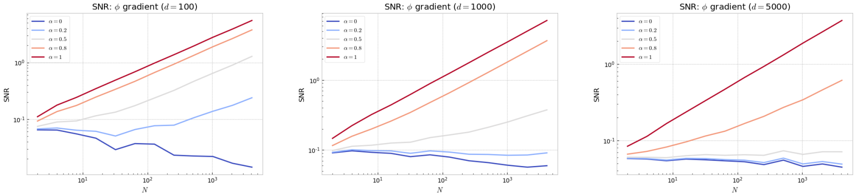


SNR analysis for the Linear Gaussian example : θ



SNR analysis for VAE with MNIST : ϕ

Reparameterized



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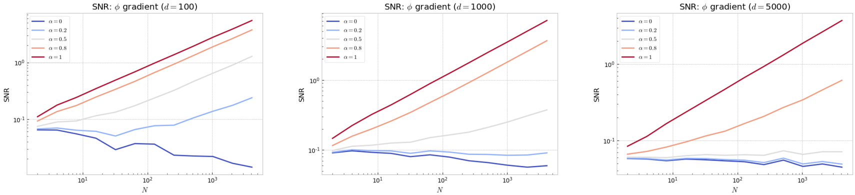
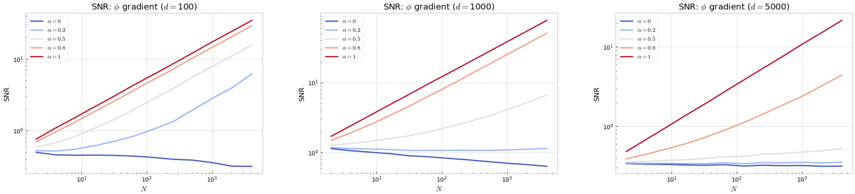
Reparameterized



Doubly-reparameterized



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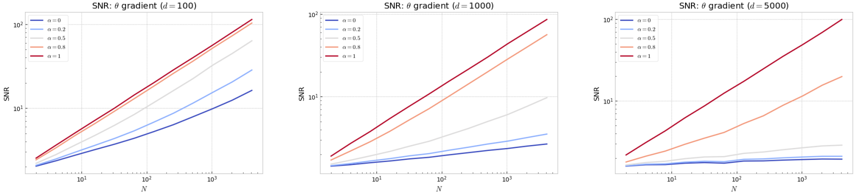
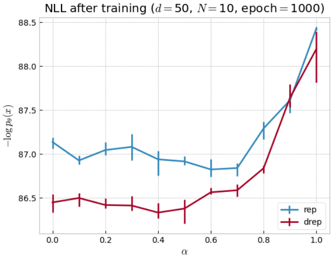
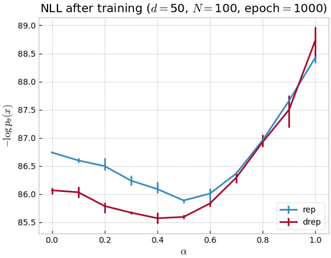


Final plots


NLL after training ($d = 50$, $N = 10$, epoch = 1000)
$-\log p_\theta(x)$
88.5
88.0
87.5
87.0
86.5
0.0
0.2
0.4
0.6
0.8
1.0
α
rep
drep


NLL after training ($d = 50$, $N = 100$, epoch = 1000)
$-\log p_\theta(x)$
89.0
88.5
88.0
87.5
87.0
86.5
86.0
85.5
0.0
0.2
0.4
0.6
0.8
1.0
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Outline

Conclusion

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   - Theoretically-sound extension of the IWAE bound ($\alpha = 0$)
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   - Shed light on the conditions behind the success or failure of the VR-IWAE bound methodology
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3. We looked into the gradient(s) of the VR-IWAE bound and found desirable properties (SNR, doubly-reparameterized)
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Perspectives

Some open questions:

- Does the weight collapse behavior apply beyond the cases highlighted here?
- How does the weight collapse affect the gradient descent procedures?
- Can we use the fact that the VR-IWAE bound extends the IWAE bound? (e.g. to build better gradient estimators / to enrich the variational family $\mathcal{Q}$)

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