Deep Generative Models
Lecture 7

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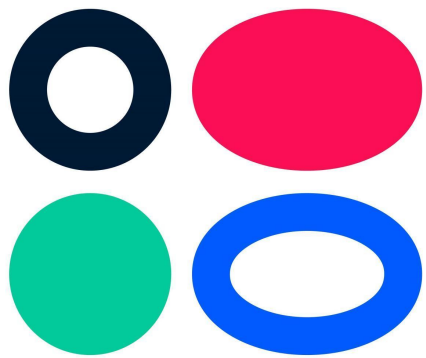


Ozon Masters

Spring, 2021

Dequantization

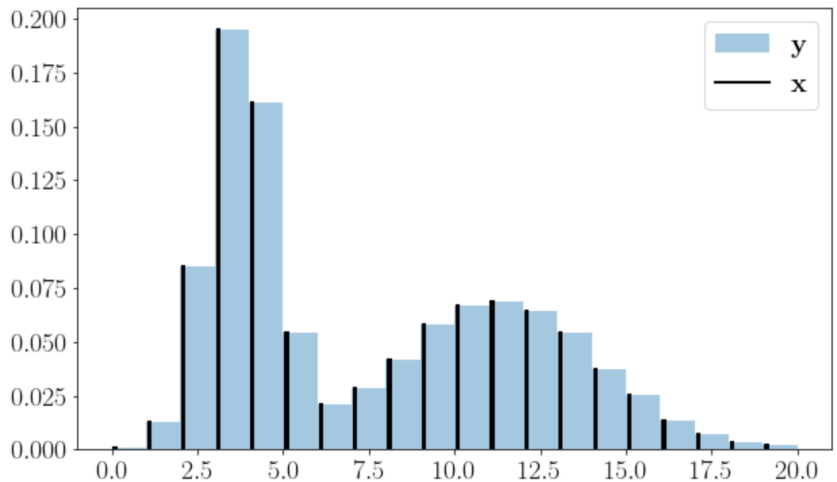
- Images are discrete data, pixels lie in the [0, 255] integer domain (the model is $P(\mathbf{x}|\boldsymbol{\theta}) = \text{Categorical}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Flow is a continuous model (it works with continuous data $\mathbf{x}$).

By fitting a continuous density model to discrete data, one can produce a degenerate solution with all probability mass on discrete values.
How to convert a discrete data distribution to a continuous one?

Uniform dequantization

$$\mathbf{x} \sim \text{Categorical}(\boldsymbol{\pi})$$
$$\mathbf{u} \sim U[0, 1]$$

$$\mathbf{y} = \mathbf{x} + \mathbf{u} \sim \text{Continuous}$$



Theis L., Oord A., Bethge M. A note on the evaluation of generative models. 2015

Uniform dequantization

Statement

Fitting continuous model $p(\mathbf{y}|\boldsymbol{\theta})$ on uniformly dequantized data $\mathbf{y} = \mathbf{x} + \mathbf{u}$, $\mathbf{u} \sim U[0, 1]$ is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

$$P(\mathbf{x}|\boldsymbol{\theta}) = \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}$$

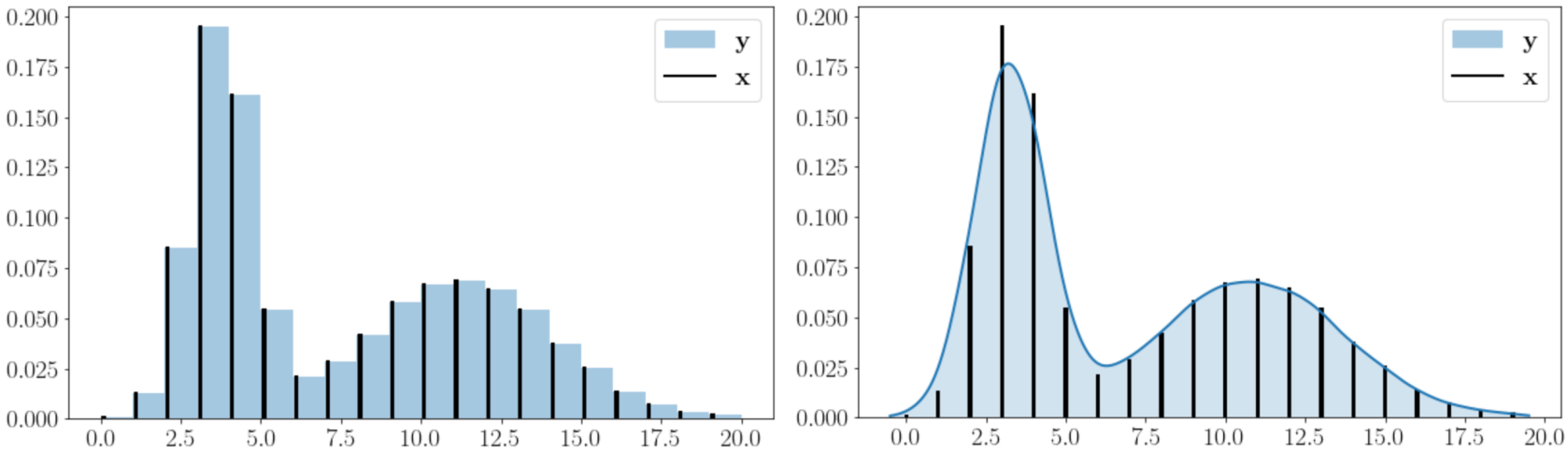
Thus, the maximisation of continuous model log-likelihood on $\mathbf{y}$ can't lead to the a collapse onto the discrete data (the objective is bounded above by the discrete model log-likelihood).

Proof

$$\log P(\mathbf{x}|\boldsymbol{\theta}) = \log \int_{U[0,1]} p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \geq$$

$$\geq \int_{U[0,1]} \log p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} = \log p(\mathbf{y}|\boldsymbol{\theta}).$$

Variational dequantization



- $p(\mathbf{y}|\boldsymbol{\theta})$ assign unifrom density to unit hypercubes $\mathbf{x} + U[0, 1]$ (left fig).
- Neural network density models are smooth function approximators (right fig).
- Smooth dequantization is more natural.

How to perform the smooth dequantization?

Flow++

Variational dequantization

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{x})$ and treat it as an approximate posterior.

Variational lower bound

$$\log P(\mathbf{x}|\boldsymbol{\theta}) = \left[\log \int q(\mathbf{u}|\mathbf{x}) \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u}\right] \geq$$

$$\geq \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u} = \mathcal{L}(q, \boldsymbol{\theta}).$$

Uniform dequantization bound

$$\log P(\mathbf{x}|\boldsymbol{\theta}) = \log \int_{U[0,1]} p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \geq$$

$$\geq \int_{U[0,1]} \log p(\mathbf{x}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} = \log p(\mathbf{y}|\boldsymbol{\theta}).$$

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Flow++

Variational lower bound

$$\mathcal{L}(q, \theta) = \int q(\mathbf{u}|\mathbf{x}) \log \frac{p(\mathbf{x} + \mathbf{u}|\theta)}{q(\mathbf{u}|\mathbf{x})} d\mathbf{u}.$$

Let $\mathbf{u} = h(\epsilon, \phi)$ is a flow model with base distribution $\epsilon \sim p(\epsilon) = \mathcal{N}(0, \mathbf{I})$:

$$q(\mathbf{u}|\mathbf{x}) = p(h^{-1}(\mathbf{u}, \phi)) \cdot \left| \det \frac{\partial h^{-1}(\mathbf{u}, \phi)}{\partial \mathbf{u}} \right|.$$

Then

$$\log P(\mathbf{x}|\theta) \geq \mathcal{L}(\phi, \theta) = \int p(\epsilon) \log \left(\frac{p(\mathbf{x} + h(\epsilon, \phi)|\theta)}{p(\epsilon) \cdot \left| \det \frac{\partial h(\epsilon, \phi)}{\partial \epsilon} \right|^{-1}} \right) d\epsilon.$$

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Flow++

Variational lower

$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{x} + h(\boldsymbol{\epsilon}, \boldsymbol{\phi}))}{p(\boldsymbol{\epsilon}) \cdot \left| \det \frac{\partial h(\boldsymbol{\epsilon}, \boldsymbol{\phi})}{\partial \boldsymbol{\epsilon}} \right|^{-1}} \right) d\boldsymbol{\epsilon}.$$

- If $p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta})$ is also a flow model, it is straightforward to calculate stochastic gradient of this ELBO.
- Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0, 1]$). The gap between $\log P(\mathbf{x}|\boldsymbol{\theta})$ and the derived ELBO is $KL(q(\mathbf{u}|\mathbf{x})||p(\mathbf{u}|\mathbf{x}))$.
- In the case of uniform dequantization the model unnaturally places uniform density over each hypercube $\mathbf{x} + U[0, 1]$ due to inexpressive distribution q.

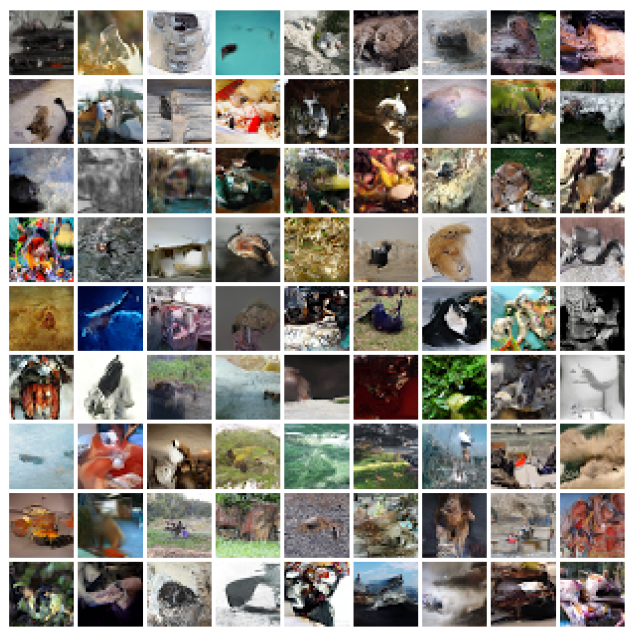
Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

Flow++

Table 1. Unconditional image modeling results in bits/dim

Model family	Model	CIFAR10	ImageNet 32x32	ImageNet 64x64
Non-autoregressive	RealNVP (Dinh et al., 2016)	3.49	4.28	–
	Glow (Kingma & Dhariwal, 2018)	3.35	4.09	3.81
	IAF-VAE (Kingma et al., 2016)	3.11	–	–
	Flow++ (ours)	**3.08**	**3.86**	**3.69**
Autoregressive	Multiscale PixelCNN (Reed et al., 2017)	–	3.95	3.70
	PixelCNN (van den Oord et al., 2016b)	3.14	–	–
	PixelRNN (van den Oord et al., 2016b)	3.00	3.86	3.63
	Gated PixelCNN (van den Oord et al., 2016c)	3.03	3.83	3.57
	PixelCNN++ (Salimans et al., 2017)	2.92	–	–
	Image Transformer (Parmar et al., 2018)	2.90	3.77	–
	PixelSNAIL (Chen et al., 2017)	2.85	3.80	3.52

(a) PixelCNN



(b) Flow++

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

VAE limitations

- Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

- Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

- Poor probabilistic model (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{z})).$$

- Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

Importance Sampling

Generative model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} \right] q(\mathbf{z}|\mathbf{x}) d\mathbf{z}$$
$$= \int f(\mathbf{x}, \mathbf{z}) q(\mathbf{z}|\mathbf{x}) d\mathbf{z} = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z})$$

Here $f(\mathbf{x}, \mathbf{z}) = \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$.

ELBO

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}) \geq \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}) =$$
$$= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = \mathcal{L}(q, \boldsymbol{\theta}).$$

Could we choose better $f(\mathbf{x}, \mathbf{z})$?

IWAE

Let define

$$f(\mathbf{x}, \mathbf{z}_1, \ldots, \mathbf{z}_K) = \frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})}$$

$$\mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}_1, \ldots, \mathbf{z}_K) = p(\mathbf{x}|\boldsymbol{\theta})$$

ELBO

$$\begin{aligned}
\log p(\mathbf{x}|\boldsymbol{\theta}) &= \log \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} f(\mathbf{x}, \mathbf{z}, \ldots, \mathbf{z}_K) \geq \\
&\geq \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log f(\mathbf{x}, \mathbf{z}, \ldots, \mathbf{z}_K) = \\
&= \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left[\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right] = \mathcal{L}_K(q, \boldsymbol{\theta}).
\end{aligned}$$

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

VAE objective

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} \to \max_{\phi, \boldsymbol{\theta}}$$

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \left(\frac{1}{K} \sum_{k=1}^{K} \log \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \to \max_{q, \boldsymbol{\theta}}.$$

IWAE objective

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) \to \max_{q, \boldsymbol{\theta}}.$$

If $K = 1$, these objectives coincide.

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}), \quad \text{for } K \geq M;$
2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K\to\infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x},\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$ is bounded.

Proof of 1.

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K} \log\left(\frac{1}{K}\sum_{k=1}^{K}\frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})}\right) =$$

$$= \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K} \log \mathbb{E}_{k_1,\ldots,k_M}\left(\frac{1}{M}\sum_{m=1}^{M}\frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})}\right) \geq$$

$$\geq \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_K}\mathbb{E}_{k_1,\ldots,k_m} \log\left(\frac{1}{M}\sum_{m=1}^{M}\frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})}\right) =$$

$$= \mathbb{E}_{\mathbf{z}_1,\ldots,\mathbf{z}_M} \log\left(\frac{1}{M}\sum_{m=1}^{M}\frac{p(\mathbf{x}, \mathbf{z}_m|\boldsymbol{\theta})}{q(\mathbf{z}_m|\mathbf{x})}\right) = \mathcal{L}_M(q, \boldsymbol{\theta})$$

$$\frac{a_1 + \cdots + a_K}{K} = \mathbb{E}_{i_1,\ldots,i_M}\frac{a_{i_1} + \cdots + a_{i_M}}{M}, \quad i_1, \ldots, i_M \sim U[1, K]$$

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

1. $\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}_M(q, \boldsymbol{\theta}), \quad \text{for} K \geq M;$
2. $\log p(\mathbf{x}|\boldsymbol{\theta}) = \lim_{K\to\infty} \mathcal{L}_K(q, \boldsymbol{\theta})$ if $\frac{p(\mathbf{x},\mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})}$ is bounded.

Proof of 2.

Consider r.v. $\xi_K = \frac{1}{K}\sum_{k=1}^{K} \frac{p(\mathbf{x},\mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})}$.

If summands are bounded, then (from the strong law of large numbers)

$$\xi_K \xrightarrow[K\to\infty]{a.s.} \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})} = p(\mathbf{x}|\boldsymbol{\theta}).$$

Hence $\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E} \log \xi_K$ converges to $\log p(\mathbf{x}|\boldsymbol{\theta})$ as $K \to \infty$.

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

$$\log p(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}_K(q, \boldsymbol{\theta}) \geq \mathcal{L}(q, \boldsymbol{\theta})$$

If $K > 1$ the bound could be tighter.

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x})};$$

$$\mathcal{L}_K(q, \boldsymbol{\theta}) = \mathbb{E}_{\mathbf{z}_1, \ldots, \mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right).$$

- $\mathcal{L}_1(q, \boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$;
- $\mathcal{L}_\infty(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$.

Which $q(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta})$?

Which $q(\mathbf{z}|\mathbf{x})$ gives $\mathcal{L}(q, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$?

Burda Y., Grosse R., Salakhutdinov R. Importance Weighted Autoencoders, 2015

IWAE

Theorem

The VAE objective is equal to IWAE objective

$$\mathcal{L}(q_{EW}, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$$

for the following variational distribution

$$q_{EW}(\mathbf{z}|\mathbf{x}) = \mathbb{E}_{\mathbf{z}_2,\dots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x})} q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}),$$

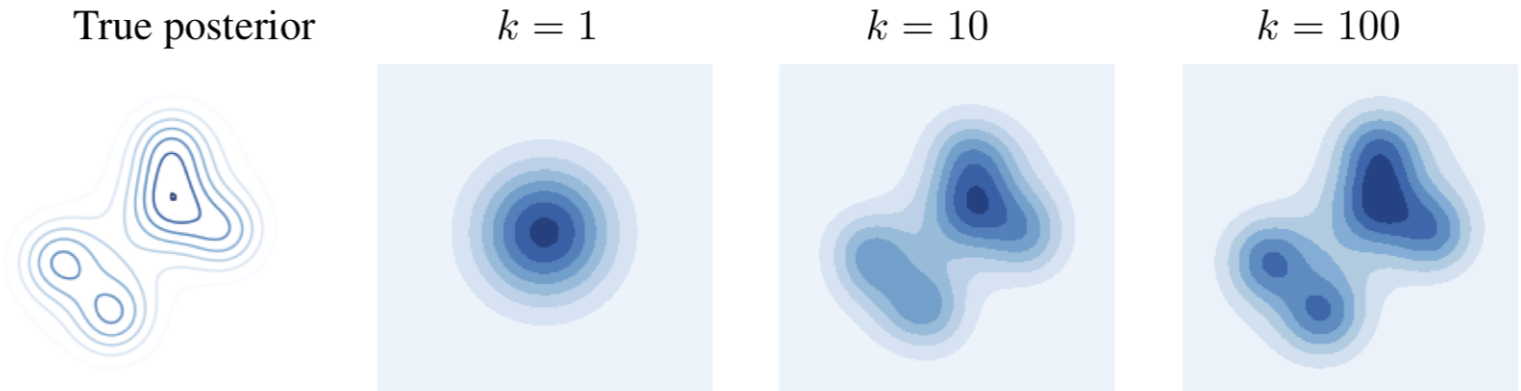
where

$$q_{IW}(\mathbf{z}|\mathbf{x}, \mathbf{z}_{2:K}) = \frac{\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})}}{\frac{1}{K}\sum_{k=1}^{K} \frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}} q(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}, \mathbf{z})}{\frac{1}{K}\left(\frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})} + \sum_{k=2}^{K} \frac{p(\mathbf{x},\mathbf{z}_k)}{q(\mathbf{z}_k|\mathbf{x})}\right)}.$$

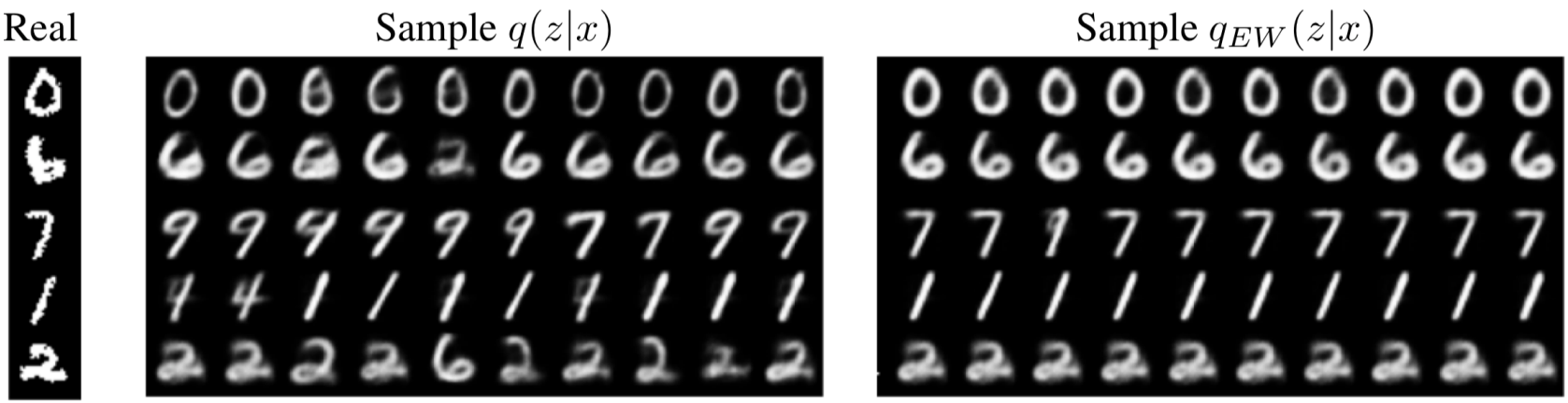
Cremer C., Morris Q., Duvenaud D. Reinterpreting Importance-Weighted Autoencoders, 2017

IWAE

IWAE posterior



IWAE samples



Cremer C., Morris Q., Duvenaud D. Reinterpreting Importance-Weighted Autoencoders, 2017

IWAE

Objective

$$\mathcal{L}_K(q, \theta) = \mathbb{E}_{\mathbf{z}_1,\dots,\mathbf{z}_K \sim q(\mathbf{z}|\mathbf{x},\phi)} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\theta)}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right) \to \max_{\phi,\theta}.$$

Gradient

$$\Delta_K = \nabla_{\theta,\phi} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\theta)}{q(\mathbf{z}_k|\mathbf{x}, \phi)} \right), \quad \mathbf{z}_k \sim q(\mathbf{z}|\mathbf{x}, \phi).$$

Theorem

$$\mathrm{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \mathrm{SNR}_K(\theta) = O(\sqrt{K}); \quad \mathrm{SNR}_K(\phi) = O\left(\sqrt{\frac{1}{K}}\right).$$

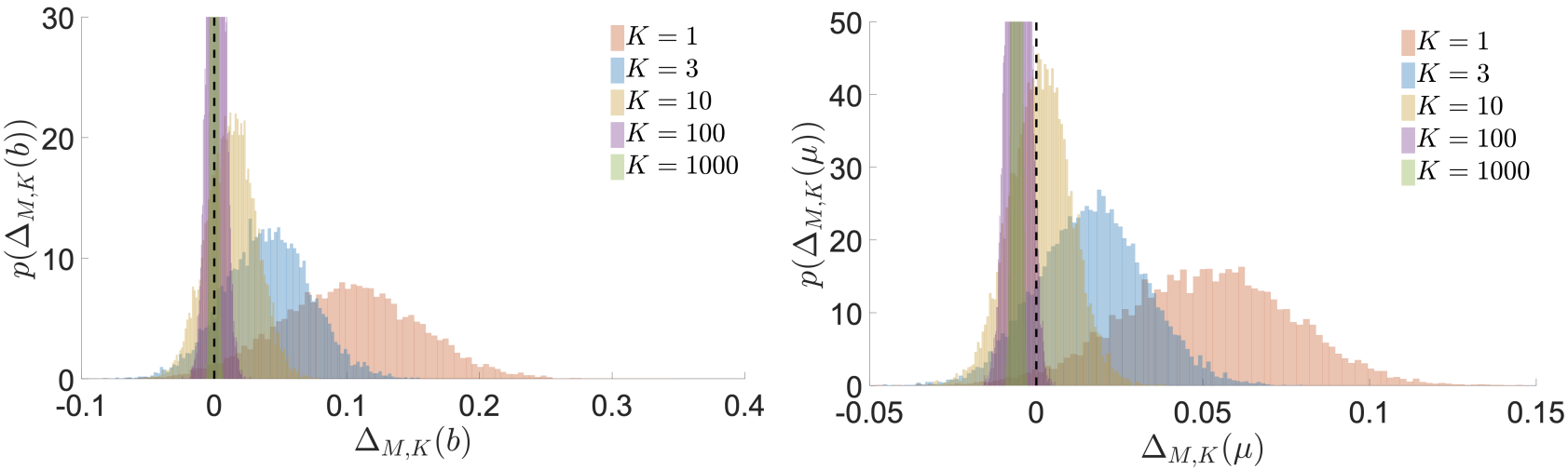
Hence, increasing K vanishes gradient signal of inference network $q(\mathbf{z}|\mathbf{x}, \phi)$.

Rainforth T. et al. Tighter variational bounds are not necessarily better, 2018

IWAE

Theorem

$$\text{SNR}_K = \frac{\mathbb{E}[\Delta_K]}{\sigma(\Delta_K)}; \quad \text{SNR}_K(\boldsymbol{\theta}) = O(\sqrt{K}); \quad \text{SNR}_K(\boldsymbol{\phi}) = O\left(\sqrt{\frac{1}{K}}\right).$$



- IWAE makes the variational bound tighter and extends the class of variational distributions.
- Gradient signal becomes really small, training is complicated.
- IWAE is very popular technique as a quality measure for VAE models.

Rainforth T. et al. Tighter variational bounds are not necessarily better, 2018

VAE limitations

- Poor variational posterior distribution (encoder)

$$q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

- Poor prior distribution

$$p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}).$$

- Poor probabilistic model (decoder)

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{z}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{z})).$$

- Loose lower bound

$$\log p(\mathbf{x}|\boldsymbol{\theta}) - \mathcal{L}(q, \boldsymbol{\theta}) = (?).$$

ELBO interpretations

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) + KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) \geq \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}).$$

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \int q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} d\mathbf{z}.$$

- Evidence minus posterior KL

$$\mathcal{L}(q, \boldsymbol{\theta}) = \log p(\mathbf{x}|\boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

- Average negative energy plus entropy

$$\begin{aligned}\mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \left[\log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) - \log q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})\right] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) + \mathbb{H}\left[q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})\right].\end{aligned}$$

- Average reconstruction minus KL to prior

$$\begin{aligned}\mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}) - \log q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})\right] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})||p(\mathbf{z})).\end{aligned}$$

ELBO surgery, 2016

$$\sum_{i=1}^{n} \mathcal{L}_i(q, \theta) = \frac{1}{n} \sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta) - KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) \right].$$

Theorem

$$\frac{1}{n} \sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}],$$

where i is treated as random variable:

$$q(i, \mathbf{z}) = q(i)q(\mathbf{z}|i); \quad p(i, \mathbf{z}) = p(i)p(\mathbf{z}); \quad q(i) = p(i) = \frac{1}{n}; \quad q(\mathbf{z}|i) = q(\mathbf{z}|\mathbf{x}_i).$$

$$q(\mathbf{z}) = \sum_{i=1}^{n} q(i, \mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i); \quad \mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})} \log \frac{q(i, \mathbf{z})}{q(i)q(\mathbf{z})}.$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

ELBO surgery, 2016

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q(i,\mathbf{z})}[i,\mathbf{z}].$$

Proof

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = \sum_{i=1}^{n}\int q(i)q(\mathbf{z}|i)\log\frac{q(\mathbf{z}|i)}{p(\mathbf{z})}d\mathbf{z} =$$

$$= \sum_{i=1}^{n}\int q(i,\mathbf{z})\log\frac{q(i,\mathbf{z})}{p(\mathbf{z})p(i)}d\mathbf{z} = \int\sum_{i=1}^{n} q(i,\mathbf{z})\log\frac{q(\mathbf{z})q(i|\mathbf{z})}{p(\mathbf{z})p(i)}d\mathbf{z} =$$

$$= \int q(\mathbf{z})\log\frac{q(\mathbf{z})}{p(\mathbf{z})}d\mathbf{z} + \int\sum_{i=1}^{n} q(i|\mathbf{z})q(\mathbf{z})\log\frac{q(i|\mathbf{z})}{p(i)}d\mathbf{z} =$$

$$= KL(q(\mathbf{z})||p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n.$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

ELBO surgery, 2016

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q(i,\mathbf{z})}[i,\mathbf{z}].$$

Proof (continued)

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n$$

$$\mathbb{I}_{q(i,\mathbf{z})}[i,\mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})}\log\frac{q(i,\mathbf{z})}{q(i)q(\mathbf{z})} = \mathbb{E}_{q(\mathbf{z})}\mathbb{E}_{q(i|\mathbf{z})}\log\frac{q(i|\mathbf{z})q(\mathbf{z})}{q(i)q(\mathbf{z})} =$$

$$= \mathbb{E}_{q(\mathbf{z})}\mathbb{E}_{q(i|\mathbf{z})}\log\frac{q(i|\mathbf{z})}{q(i)} = -\mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right] + \log n.$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

ELBO surgery, 2016

Theorem

$$\frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i)) = KL(q(\mathbf{z})||p(\mathbf{z})) + \mathbb{I}_{q(i,\mathbf{z})}[i,\mathbf{z}].$$

ELBO revisiting

$$\sum_{i=1}^{n}\mathcal{L}_i(q,\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n}\left[\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)}\log p(\mathbf{x}_i|\mathbf{z}_i,\boldsymbol{\theta}) - KL(q(\mathbf{z}_i|\mathbf{x}_i)||p(\mathbf{z}_i))\right] =$$

$$= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)}\log p(\mathbf{x}_i|\mathbf{z}_i,\boldsymbol{\theta}) - \mathbb{I}_{q(i,\mathbf{z})}[i,\mathbf{z}] - KL(q(\mathbf{z})||p(\mathbf{z})) =$$

$$= \underbrace{\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)}\log p(\mathbf{x}_i|\mathbf{z}_i,\boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})}\mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0\leq\text{Mutual info}\leq\log n} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

ELBO surgery, 2016

ELBO revisiting

$$\sum_{i=1}^{n} \mathcal{L}(q, \theta) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta)}_{\text{Reconstruction loss}} -$$

$$- \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log n} \underbrace{- KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

$$KL(q(\mathbf{z})||p(\mathbf{z})) = 0 \quad \Leftrightarrow \quad p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i).$$

	ELBO	Avg. KL	Mutual info. ②	Marg. KL ③
2D latents	-129.63	7.41	7.20	0.21
10D latents	-88.95	19.17	10.82	8.35
20D latents	-87.45	20.2	10.67	9.53

$$\log n \approx 11.0021$$

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

VAE prior

ELBO revisiting

$$\sum_{i=1}^{n} \mathcal{L}(q, \theta) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta)}_{\text{Reconstruction loss}} -$$

$$- \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log n} \underbrace{- KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

How to choose the optimal $p(\mathbf{z})$?

- SG: $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$ over-regularization;
- MoG: $p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K} \sum_{k=1}^{K} \mathcal{N}(\boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^2) \Rightarrow$ (*), (**);
- $p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i) \Rightarrow$ overfitting and highly expensive.

(*) Dilokthanakul N. et al. Deep Unsupervised Clustering with Gaussian Mixture Variational Autoencoders, 2016
(**) Nalisnick E., Hertel L., Smyth P. Approximate Inference for Deep Latent Gaussian Mixtures, 2016

VampPrior

Variational Mixture of posteriors

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K}\sum_{k=1}^{K} q(\mathbf{z}|\mathbf{u}_k),$$

where $\boldsymbol{\lambda} = \{\mathbf{u}_1, \ldots, \mathbf{u}_K\}$ are trainable preudo-inputs.

- Multimodal $\Rightarrow$ prevents over-regularization;.
- $K \ll n \Rightarrow$ prevents from potential overfitting + less expensive to train.
- Pseudo-inputs are prior hyperparameters $\Rightarrow$ connection to the Empirical Bayes.

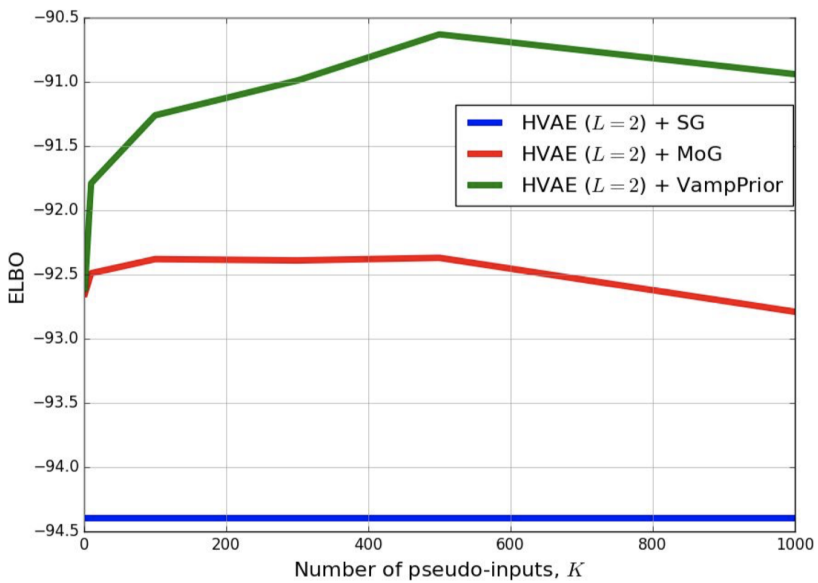
Tomczak J. M., Welling M. VAE with a VampPrior, 2017

VampPrior

- Do we equally need the multimodal prior?
- Is it beneficial to couple the prior with the variational posterior or MoG is enough?

MNIST results

Model	LL
VAE ($L=1$) + NF [32]	-85.10
VAE ($L=2$) [6]	-87.86
IWAE ($L=2$) [6]	-85.32
HVAE ($L=2$) + SG	-85.89
HVAE ($L=2$) + MoG	-85.07
HVAE ($L=2$) + VampPrior *data*	-85.71
HVAE ($L=2$) + VampPrior	$\mathbf{-83.19}$
AVB + AC ($L=1$) [28]	-80.20
VLAE [7]	$\mathbf{-79.03}$
VAE + IAF [18]	-79.88
convHVAE ($L=2$) + VampPrior	-81.09
PixelHVAE ($L=2$) + VampPrior	-79.78



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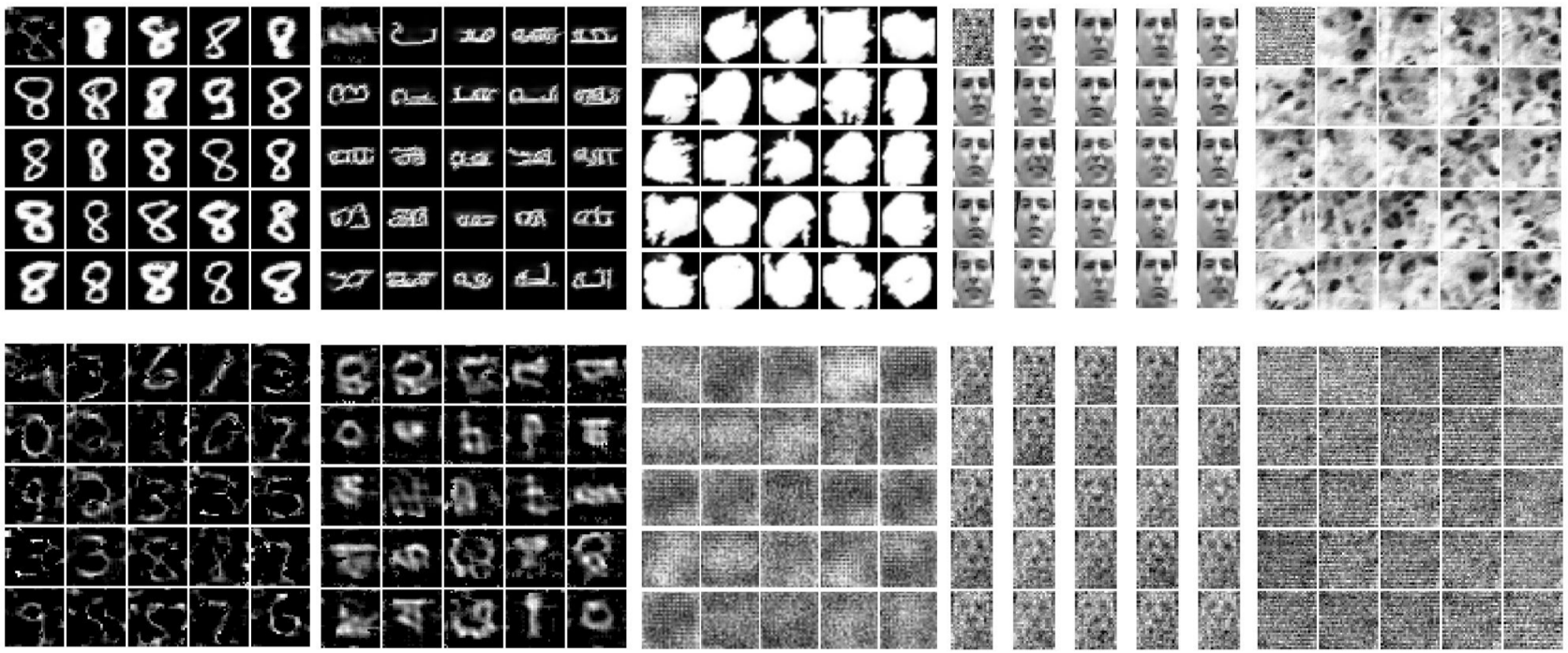
VampPrior

Top row: generated images by PixelHVAE + VampPrior for chosen pseudo-input in the left top corner.

Bottom row: pseudo-inputs for different datasets.



Tomczak J. M., Welling M. VAE with a VampPrior, 2017

Flow prior in VAE

ELBO revisiting

$$\mathcal{L}(q, \theta) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_i|\mathbf{x}_i)} \log p(\mathbf{x}_i|\mathbf{z}_i, \theta)}_{\text{Reconstruction loss}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H}\left[q(i|\mathbf{z})\right]\right)}_{0 \leq \text{Mutual info} \leq \log N} - \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

VampPrior

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \frac{1}{K} \sum_{k=1}^{K} q(\mathbf{z}|\mathbf{u}_k),$$

where $\mathbf{u}_1, \ldots \mathbf{u}_K$ is trainable preudo-inputs.

Autoregressive flow prior

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\boldsymbol{\epsilon}) + \log \det \left| \frac{d\boldsymbol{\epsilon}}{d\mathbf{z}} \right|$$

$$\mathbf{z} = g(\boldsymbol{\epsilon}, \boldsymbol{\lambda}) = f^{-1}(\boldsymbol{\epsilon}, \boldsymbol{\lambda})$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

Theorem

VAE with the AF prior for latent code $\mathbf{z}$ is equivalent to using the IAF posterior for latent code $\boldsymbol{\epsilon}$.

Proof

$$\mathcal{L}(q, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}, \boldsymbol{\lambda}) - q(\mathbf{z}|\mathbf{x})\right]$$

$$= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\left(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{AF prior}} - q(\mathbf{z}|\mathbf{x})\right]$$

$$= \mathbb{E}_{\mathbf{z}\sim q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\left(q(\mathbf{z}|\mathbf{x}) - \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{IAF posterior}}\right]$$

Flows in VAE

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x}, \boldsymbol{\phi})} \left[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \boldsymbol{\phi}) + \log \left|\det \left(\frac{\partial g(\mathbf{z}_0, \boldsymbol{\phi}_*)}{\partial \mathbf{z}_0}\right)\right|\right].$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Variational Lossy AutoEncoder, 2016

Autoregressive flow prior

$$\mathcal{L}(q, \theta) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \Big[\log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\Big(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \Big| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \Big| \Big)}_{\text{AF prior}} - q(\mathbf{z}|\mathbf{x}) \Big]$$

$$= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \Big[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\Big(q(\mathbf{z}|\mathbf{x}) - \log \Big| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \Big| \Big)}_{\text{IAF posterior}} \Big]$$

- IAF posterior decoder path: $p(\mathbf{x}|\mathbf{z}, \theta)$, $\mathbf{z} \sim p(\mathbf{z})$.
- AF prior decoder path: $p(\mathbf{x}|\mathbf{z}, \theta)$, $\mathbf{z} = g(\boldsymbol{\epsilon}, \boldsymbol{\lambda})$, $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$.

The AF prior and the IAF posterior have the same computation cost, so using the AF prior makes the model more expressive at no training time cost.

Chen X. et al. Variational Lossy Autoencoder, 2016

Summary

- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that was proposed in Flow++ model.
- The importance sampling could get the tighter lower bound to the likelihood.
- The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior.
- VampPrior proposes to use a variational mixture of posteriors as the prior to approximate the aggregated posterior.
- The autoregressive flows could be used as the prior. This is equivalent to the use of the IAF posterior.