Deep Generative Models

Lecture 7

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Recap of previous lecture

LVM

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z}$$

- More powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ leads to more powerful generative model $p(\mathbf{x}|\boldsymbol{\theta})$.
- Too powerful $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ could lead to posterior collapse: $q(\mathbf{z}|\mathbf{x})$ will not carry any information about $\mathbf{x}$ and close to prior $p(\mathbf{z})$.

Autoregressive decoder

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \prod_{i=1}^{n} p(x_i|\mathbf{x}_{1:i-1}, \mathbf{z}, \boldsymbol{\theta})$$

- Global structure is captured by latent variables.
- Local statistics are captured by limited receptive field autoregressive model.

Gulrajani I. et al. PixelVAE: A Latent Variable Model for Natural Images, 2016

Recap of previous lecture

Decoder weakening

- Powerful decoder $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ makes the model expressive, but posterior collapse is possible.
- PixelVAE model uses the autoregressive PixelCNN model with small number of layers to limit receptive field.

KL annealing

$$\mathcal{L}(q, \boldsymbol{\theta}, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))$$

Start training with $\beta = 0$, increase it until $\beta = 1$ during training.

Free bits

Ensure the use of less than λ bits of information:

$$\mathcal{L}(q, \boldsymbol{\theta}, \lambda) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \max(\lambda, KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z}))).$$

This results in $KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \geq \lambda$.

Recap of previous lecture

VAE objective

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

IWAE objective

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

Theorem

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

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.

$$
\begin{aligned}
\mathcal{L}_K(q, \boldsymbol{\theta}) &= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \left(\frac{1}{K} \sum_{k=1}^{K} \frac{p(\mathbf{x}, \mathbf{z}_k|\boldsymbol{\theta})}{q(\mathbf{z}_k|\mathbf{x})} \right) = \\
&= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \log \mathbb{E}_{k_1, \dots, k_M} \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})} \right) \geq \\
&\geq \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_K} \mathbb{E}_{k_1, \dots, k_m} \log \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_{k_m}|\boldsymbol{\theta})}{q(\mathbf{z}_{k_m}|\mathbf{x})} \right) = \\
&= \mathbb{E}_{\mathbf{z}_1, \dots, \mathbf{z}_M} \log \left(\frac{1}{M} \sum_{m=1}^{M} \frac{p(\mathbf{x}, \mathbf{z}_m|\boldsymbol{\theta})}{q(\mathbf{z}_m|\mathbf{x})} \right) = \mathcal{L}_M(q, \boldsymbol{\theta})
\end{aligned}
$$

$$
\frac{a_1 + \dots + a_K}{K} = \mathbb{E}_{k_1, \dots, k_M} \frac{a_{k_1} + \dots + a_{k_M}}{M}, \quad k_1, \dots, k_M \sim U[1, K]
$$

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.

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

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

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

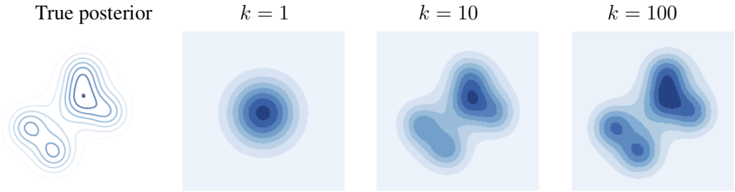
$\mathcal{L}(q_{EW}, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$ for the following variational distribution

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

where

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

IWAE posterior



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

IWAE

Objective

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

Gradient

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

Theorem

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

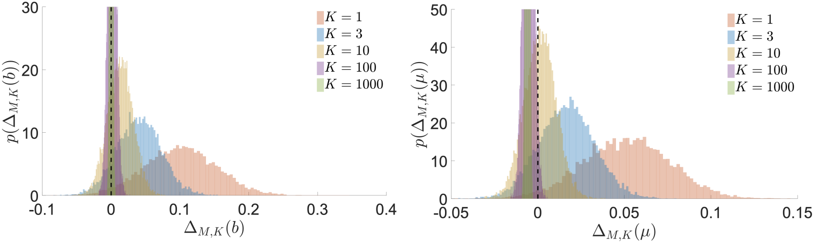
Hence, increasing K vanishes gradient signal of inference network $q(\mathbf{z}|\mathbf{x}, \phi)$.

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

IWAE

Theorem

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



- 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)

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

- 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

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

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

- Evidence minus posterior KL

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

- Average reconstruction loss with regularizer (prior KL)

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

ELBO surgery

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

Theorem

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

- $q(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i)$ – **aggregated** posterior distribution.
- $\mathbb{I}_q[\mathbf{x}, \mathbf{z}]$ – mutual information between $\mathbf{x}$ and $\mathbf{z}$ under empirical data distribution and distribution $q(\mathbf{z}|\mathbf{x})$.
- First term pushes $q(\mathbf{z})$ towards the prior $p(\mathbf{z})$.
- Second term reduces the amount of information about $\mathbf{x}$ stored in $\mathbf{z}$.

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

ELBO surgery

Theorem

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

Proof

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

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

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

Without proof:

$$\mathbb{I}_q[\mathbf{x}, \mathbf{z}] = \frac{1}{n}\sum_{i=1}^{n} KL(q(\mathbf{z}|\mathbf{x}_i)||q(\mathbf{z})) \in [0, \log n].$$

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

ELBO surgery

Theorem

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

ELBO revisiting

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

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

Prior distribution $p(\mathbf{z})$ is only in the last term.

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

ELBO surgery

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

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

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.
How to choose the optimal $p(\mathbf{z})$?

- Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, I) \Rightarrow$ over-regularization;
- Parametrized distribution $p(\mathbf{z}|\boldsymbol{\lambda})$;
- $p(\mathbf{z}) = q(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i) \Rightarrow$ overfitting and highly expensive.

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

VampPrior

Optimal prior

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

The optimal prior distribution $p(\mathbf{z})$ is aggregated posterior $q(\mathbf{z})$.

Variational Mixture of posteriors

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

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

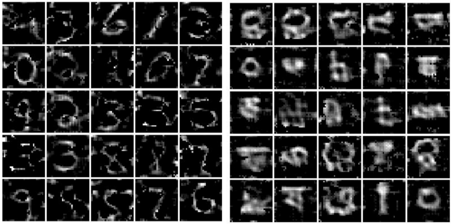
- Multimodal $\Rightarrow$ prevents over-regularization;.
- $K \ll n \Rightarrow$ prevents from potential overfitting + less expensive to train.

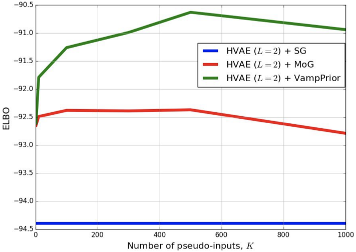
Tomczak J. M., Welling M. VAE with a VampPrior, 2017

VampPrior

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

Results





MNIST   Omniglot

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

Flows in VAE prior

ELBO revisiting

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

VampPrior

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

where $\mathbf{u}_1, \dots, \mathbf{u}_K$ are 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

VAE limitations

- Poor variational posterior distribution (encoder)

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

- 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

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

Variational posterior

ELBO

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

- In E-step of EM-algorithm we wish $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = 0$.
  (In this case the lower bound is tight $\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$).
- Normal variational distribution $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x}))$ is poor (e.g. has only one mode).
- Flows models convert a simple base distribution to a complex one using invertible transformation with simple Jacobian. How to use flows in VAE?

Flows in VAE posterior

Apply a sequence of transformations to the random variable

$$\mathbf{z}_0 \sim q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x})).$$

Here, $q(\mathbf{z}|\mathbf{x}, \phi)$ (which is a VAE encoder) plays a role of a base distribution.

$$\mathbf{z}_0 \xrightarrow{g_1} \mathbf{z}_1 \xrightarrow{g_2} \dots \xrightarrow{g_K} \mathbf{z}_K, \quad \mathbf{z}_K = g(\mathbf{z}_0), \quad g = g_K \circ \dots \circ g_1.$$

Each g_k is a flow transformation (e.g. planar, coupling layer) parameterized by ϕ_k.

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi, \{\phi_k\}_{k=1}^K) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^K \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows in VAE posterior

ELBO

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

Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Let use $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$, $\phi_* = \{\phi, \phi_1, \dots, \phi_K\}$ as a variational distribution. Here ϕ – encoder parameters, $\{\phi_k\}_{k=1}^K$ – flow parameters.

- Encoder outputs base distribution $q(\mathbf{z}_0|\mathbf{x}, \phi)$.
- Flow model $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$ transforms the base distribution $q(\mathbf{z}_0|\mathbf{x}, \phi)$ to the distribution $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$.
- Distribution $q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)$ is used as a variational distribution for ELBO maximization.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows in VAE posterior

Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| .$$

ELBO objective

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

The second term in ELBO is reverse KL divergence. Planar flows was originally proposed for variational inference in VAE.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows in VAE posterior

Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| .$$

ELBO objective

$$\begin{aligned}
\mathcal{L}(\phi, \boldsymbol{\theta}) &= \mathbb{E}_{q_K(\mathbf{z}_K|\mathbf{x},\phi_*)} \bigl[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)\bigr] \\
&= \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x},\phi)} \bigl[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*)\bigr] \Bigr|_{\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)} \\
&= \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x},\phi)} \Biggl[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \phi) + \\
&\qquad + \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| \Biggr] .
\end{aligned}$$

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Flows in VAE posterior

Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x}, \phi_*) = \log q(\mathbf{z}_0|\mathbf{x}, \phi) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| .$$

ELBO objective

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x},\phi)} \Bigg[\log p(\mathbf{x}, \mathbf{z}_K|\boldsymbol{\theta}) - \log q(\mathbf{z}_0|\mathbf{x}, \phi) + \\ + \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial g_k(\mathbf{z}_{k-1}, \phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right| \Bigg] .$$

- Obtain samples $\mathbf{z}_0$ from the encoder.
- Apply flow model $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$.
- Compute likelihood for $\mathbf{z}_K$ using the decoder, base distribution for $\mathbf{z}_0$ and the Jacobian.
- We do not need inverse flow function, if we use flows in variational inference.

Rezende D. J., Mohamed S. Variational Inference with Normalizing Flows, 2015

Inverse autoregressive flow (IAF)

$$\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \quad \Rightarrow \quad x_i = \tilde{\sigma}_i(\mathbf{z}_{1:i-1}) \cdot z_i + \tilde{\mu}_i(\mathbf{z}_{1:i-1}).$$

$$\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad \Rightarrow \quad z_i = (x_i - \tilde{\mu}_i(\mathbf{z}_{1:i-1})) \cdot \frac{1}{\tilde{\sigma}_i(\mathbf{z}_{1:i-1})}.$$

Reverse KL for flow model

$$KL(p||\pi) = \mathbb{E}_{p(\mathbf{z})} \left[\log p(\mathbf{z}) - \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| - \log \pi(g(\mathbf{z}, \boldsymbol{\theta})) \right]$$

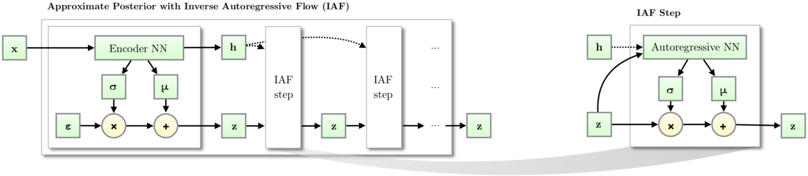
- We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.
- Inverse autoregressive flow is a natural choice for using flows in VAE:

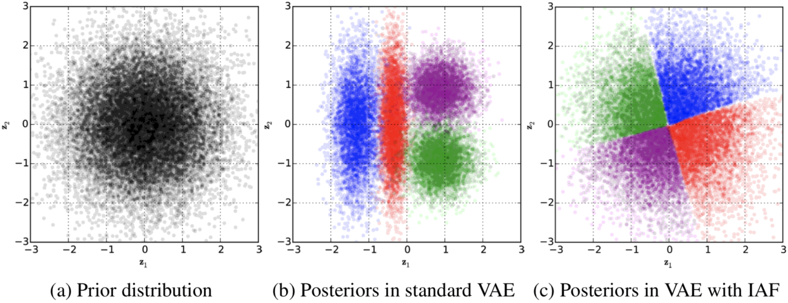
$$\mathbf{z}_0 = \boldsymbol{\sigma}(\mathbf{x}) \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}_0|\mathbf{x}, \phi).$$

$$\mathbf{z}_k = \tilde{\boldsymbol{\sigma}}_k(\mathbf{z}_{k-1}) \odot \mathbf{z}_{k-1} + \tilde{\boldsymbol{\mu}}_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k|\mathbf{x}, \phi, \{\phi_j\}_{j=1}^k).$$

Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Inverse autoregressive flow (IAF)





Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

Flows in VAE prior

Theorem

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

Proof

$$
\begin{aligned}
\mathcal{L}(q, \boldsymbol{\theta}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\left(\log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{AF prior}} - \log q(\mathbf{z}|\mathbf{x})\right] \\
&= \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\left(\log q(\mathbf{z}|\mathbf{x}) - \log \left|\det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}}\right|\right)}_{\text{IAF posterior}}\right]
\end{aligned}
$$

Flows in VAE posterior

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

Chen X. et al. Variational Lossy Autoencoder, 2016

Flows in VAE prior

Autoregressive flow prior

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

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

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

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

- The IWAE could get the tighter lower bound to the likelihood, but the training of such model becomes more difficult.

- 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.