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

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

IWAE objective

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

Theorem

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

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

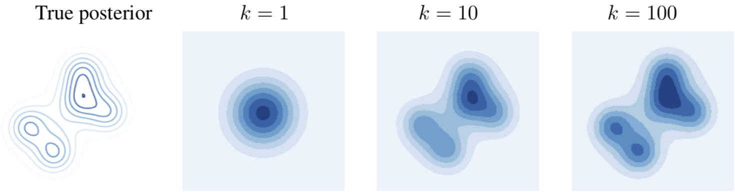
$\mathcal{L}(q^*, \boldsymbol{\theta}) = \mathcal{L}_K(q, \boldsymbol{\theta})$ for the following variational distribution

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

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

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

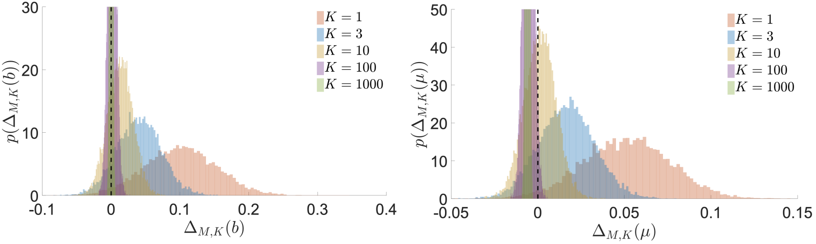
Hence, increasing K vanishes gradient signal of inference network $q(\mathbf{z}|\mathbf{x}, \phi)$.

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

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

- Average reconstruction loss with regularizer (prior KL)

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

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

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.

Optimal VAE 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 $p(\mathbf{z})$ is the aggregated posterior $q(\mathbf{z})$.

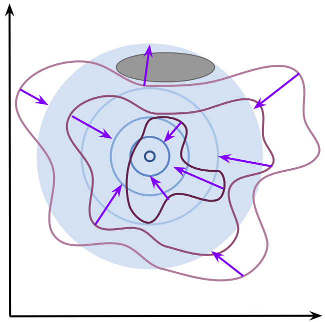
Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

Optimal VAE prior

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

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

Non learnable prior $p(\mathbf{z})$



Learnable prior $p(\mathbf{z}|\boldsymbol{\lambda})$

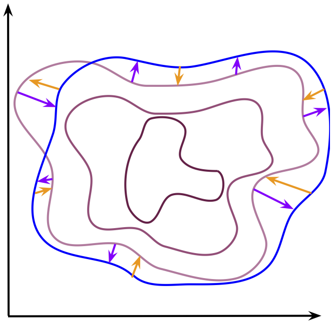


image credit: https://jmtomczak.github.io/blog/7/7_priors.html

Learnable VAE prior

Optimal prior

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

Mixture of Gaussians

$$p(\mathbf{z}|\boldsymbol{\lambda}) = \sum_{k=1}^{K} w_k \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_k, \boldsymbol{\sigma}_k^2), \quad \boldsymbol{\lambda} = \{w_k, \boldsymbol{\mu}_k, \boldsymbol{\sigma}_k\}_{k=1}^{K}.$$

Variational Mixture of posteriors (VampPrior)

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

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

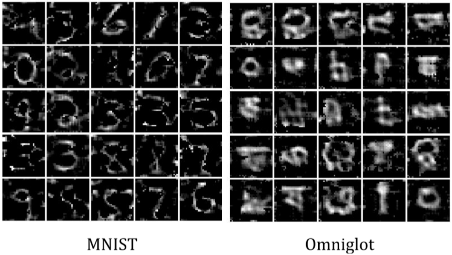
- Multimodal $\Rightarrow$ prevents over-regularization;.
- $K \ll n \Rightarrow$ prevents from potential overfitting + less expensive to train.

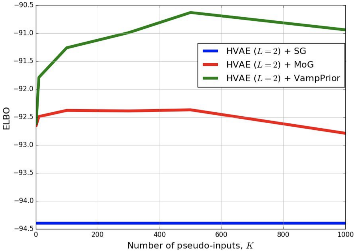
Tomczak J. M., Welling M. VAE with a VampPrior, 2017

VampPrior

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

Results





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-based VAE prior

Flow model in latent space

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

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

- RealNVP flow.
- Autoregressive flow (MAF).

Why it is not a good idea to use IAF for VAE prior?

ELBO with flow-based VAE prior

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

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

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 posterior?

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.
- We could use flow-based prior in VAE (moreover, autoregressive) as well as flow-based posterior (next lecture).