Deep Generative Models

Lecture 7

Roman Isachenko

AI Masters

Autumn, 2022

Recap of previous lecture

Gaussian AR NF

$$
\begin{aligned}
\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \quad &\Rightarrow \quad x_j = \sigma_j(\mathbf{x}_{1:j-1}) \cdot z_j + \mu_j(\mathbf{x}_{1:j-1}). \\
\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad &\Rightarrow \quad z_j = (x_j - \mu_j(\mathbf{x}_{1:j-1})) \cdot \frac{1}{\sigma_j(\mathbf{x}_{1:j-1})}.
\end{aligned}
$$

- Sampling is sequential, density estimation is parallel.
- Forward KL is a natural loss.

Inverse gaussian AR NF

$$
\begin{aligned}
\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}) \quad &\Rightarrow \quad x_j = \tilde{\sigma}_j(\mathbf{z}_{1:j-1}) \cdot z_j + \tilde{\mu}_j(\mathbf{z}_{1:j-1}) \\
\mathbf{z} = f(\mathbf{x}, \boldsymbol{\theta}) \quad &\Rightarrow \quad z_j = (x_j - \tilde{\mu}_j(\mathbf{z}_{1:j-1})) \cdot \frac{1}{\tilde{\sigma}_j(\mathbf{z}_{1:j-1})}.
\end{aligned}
$$

- Sampling is parallel, density estimation is sequential.
- Reverse KL is a natural loss.

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

Recap of previous lecture

Let split $\mathbf{x}$ and $\mathbf{z}$ in two parts:

$$\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2] = [\mathbf{x}_{1:d}, \mathbf{x}_{d+1:m}]; \quad \mathbf{z} = [\mathbf{z}_1, \mathbf{z}_2] = [\mathbf{z}_{1:d}, \mathbf{z}_{d+1:m}].$$

Coupling layer

$$\begin{cases} \mathbf{x}_1 = \mathbf{z}_1; \\ \mathbf{x}_2 = \mathbf{z}_2 \odot \boldsymbol{\sigma}(\mathbf{z}_1, \boldsymbol{\theta}) + \boldsymbol{\mu}(\mathbf{z}_1, \boldsymbol{\theta}). \end{cases} \quad \begin{cases} \mathbf{z}_1 = \mathbf{x}_1; \\ \mathbf{z}_2 = (\mathbf{x}_2 - \boldsymbol{\mu}(\mathbf{x}_1, \boldsymbol{\theta})) \odot \frac{1}{\boldsymbol{\sigma}(\mathbf{x}_1, \boldsymbol{\theta})}. \end{cases}$$

Estimating the density takes 1 pass, sampling takes 1 pass!

Jacobian

$$\det \left(\frac{\partial \mathbf{z}}{\partial \mathbf{x}} \right) = \det \begin{pmatrix} \mathbf{I}_d & 0_{d \times m-d} \\ \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_1} & \frac{\partial \mathbf{z}_2}{\partial \mathbf{x}_2} \end{pmatrix} = \prod_{j=1}^{m-d} \frac{1}{\sigma_j(\mathbf{x}_1, \boldsymbol{\theta})}.$$

Coupling layer is a special case of autoregressive flow.

Dinh L., Sohl-Dickstein J., Bengio S. Density estimation using Real NVP, 2016

Recap of previous lecture

	VAE	**NF**
Objective	ELBO $\mathcal{L}$	Forward KL/MLE
Encoder	stochastic $\mathbf{z} \sim q(\mathbf{z}\|\mathbf{x}, \phi)$	deterministic $\mathbf{z} = f(\mathbf{x}\|\boldsymbol{\theta})$ $q(\mathbf{z}\|\mathbf{x}, \boldsymbol{\theta}) = \delta(\mathbf{z} - f(\mathbf{x}, \boldsymbol{\theta}))$
Decoder	stochastic $\mathbf{x} \sim p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta})$	deterministic $\mathbf{x} = g(\mathbf{z}\|\boldsymbol{\theta})$ $p(\mathbf{x}\|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - g(\mathbf{z}, \boldsymbol{\theta}))$
Parameters	$\boldsymbol{\phi}, \boldsymbol{\theta}$	$\boldsymbol{\theta} \equiv \boldsymbol{\phi}$

Theorem

MLE for normalizing flow is equivalent to maximization of ELBO for VAE model with deterministic encoder and decoder:

$$p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \delta(\mathbf{x} - f^{-1}(\mathbf{z}, \boldsymbol{\theta})) = \delta(\mathbf{x} - g(\mathbf{z}, \boldsymbol{\theta}));$$

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

Nielsen D., et al. SurVAE Flows: Surjections to Bridge the Gap between VAEs and Flows, 2020

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

Discrete data vs continuous model

Let our data $\mathbf{y}$ comes from discrete distribution $\Pi(\mathbf{y})$ and we have continuous model $p(\mathbf{x}|\boldsymbol{\theta}) = \text{NN}(\mathbf{x}, \boldsymbol{\theta})$.

- Images (and not only images) are discrete data, pixels lie in the integer domain ($\{0, 255\}$).
- By fitting a continuous density model $p(\mathbf{x}|\boldsymbol{\theta})$ to discrete data $\Pi(\mathbf{y})$, one can produce a degenerate solution with all probability mass on discrete values.

Discrete model

- Use **discrete** model (e.x. $P(\mathbf{y}|\boldsymbol{\theta}) = \text{Cat}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Minimize any suitable divergence measure $D(\Pi, P)$.
- NF works only with continuous data $\mathbf{x}$ (there are discrete NF, see papers below).
- If pixel value is not presented in the train data, it won't be predicted.

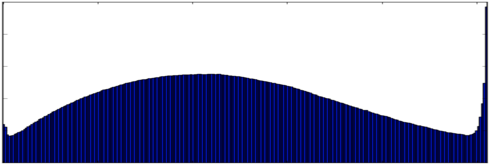
Hoogeboom E. et al. Integer discrete flows and lossless compression
Tran D. et al. Discrete flows: Invertible generative models of discrete data

Discrete data vs continuous model

Continuous model

- Use **continuous** model (e.x. $p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{\theta}}(\mathbf{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\theta}}(\mathbf{x}))$), but
  - **discretize** model (make the model outputs discrete): transform $p(\mathbf{x}|\boldsymbol{\theta})$ to $P(\mathbf{y}|\boldsymbol{\theta})$;
  - **dequantize** data (make the data continuous): transform $\Pi(\mathbf{y})$ to $\pi(\mathbf{x})$.
- Continuous distribution know numerical relationships.

CIFAR-10 pixel values distribution



Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

Discretization of continuous distribution

Model discretization through CDF

$$F(\mathbf{x}|\boldsymbol{\theta}) = \int_{-\infty}^{\mathbf{x}'} p(\mathbf{x}'|\boldsymbol{\theta}) d\mathbf{x}'; \quad P(\mathbf{y}|\boldsymbol{\theta}) = F(\mathbf{y} + 0.5|\boldsymbol{\theta}) - F(\mathbf{y} - 0.5|\boldsymbol{\theta})$$

Mixture of logistic distributions

$$p(x|\mu, s) = \frac{\exp^{-(x-\mu)/s}}{s(1 + \exp^{-(x-\mu)/s})^2}; \quad p(x|\boldsymbol{\pi}, \boldsymbol{\mu}, \mathbf{s}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k, s_k).$$

PixelCNN++

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{m} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}); \quad p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}) = \sum_{k=1}^{K} \pi_k p(x|\mu_k, s_k).$$

Here, $\pi_k = \pi_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$, $\mu_k = \mu_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$, $s_k = s_{k,\boldsymbol{\theta}}(\mathbf{x}_{1:j-1})$.

For the pixel edge cases of 0, replace $x - 0.5$ by $-\infty$, and for 255 replace $x + 0.5$ by $+\infty$.

Salimans T. et al. PixelCNN++: Improving the PixelCNN with Discretized Logistic Mixture Likelihood and Other Modifications, 2017

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

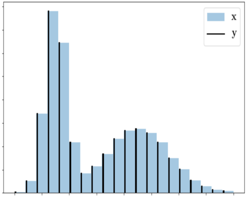
Uniform discretization

Let discrete discrete distribution $\Pi(\mathbf{y})$ to continuous distribution $\pi(\mathbf{x})$ in the following way: $\mathbf{x} = \mathbf{y} + \mathbf{u}$, where $\mathbf{u} \sim U[0,1]$.

Theorem

Fitting continuous model $p(\mathbf{x}|\boldsymbol{\theta})$ on uniformly dequantized data is equivalent to maximization of a lower bound on log-likelihood for a discrete model:

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



Proof

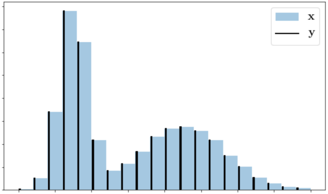
$$\mathbb{E}_\pi \log p(\mathbf{x}|\boldsymbol{\theta}) = \int \pi(\mathbf{x}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{y} = \sum \Pi(\mathbf{y}) \int_{U[0,1]} \log p(\mathbf{y}+\mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} \leq$$

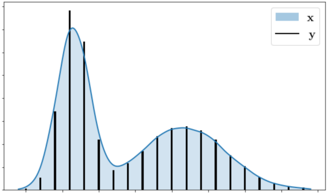
$$\leq \sum \Pi(\mathbf{y}) \log \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} =$$

$$= \sum \Pi(\mathbf{y}) \log P(\mathbf{y}|\boldsymbol{\theta}) = \mathbb{E}_\Pi \log P(\mathbf{y}|\boldsymbol{\theta}).$$

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

Variational dequantization





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

Introduce variational dequantization noise distribution $q(\mathbf{u}|\mathbf{y})$, which tells what kind of noise we have to add to our discrete data. Treat it as an approximate posterior as in VAE model.

Variational dequantization

Variational lower bound

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

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

Uniform dequantization is a special case of variational dequantization ($q(\mathbf{u}|\mathbf{x}) = U[0, 1]$).

Flow++: flow-based variational dequantization

Let $\mathbf{u} = g(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\lambda})$ is a flow model with base distribution $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$:

$$q(\mathbf{u}|\mathbf{x}) = p(f(\mathbf{u}, \mathbf{x}, \boldsymbol{\lambda})) \cdot \left|\det \frac{\partial f(\mathbf{u}, \mathbf{x}, \boldsymbol{\lambda})}{\partial \mathbf{u}}\right|.$$

$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \mathcal{L}(\boldsymbol{\lambda}, \boldsymbol{\theta}) = \int p(\boldsymbol{\epsilon}) \log \left(\frac{p(\mathbf{x} + g(\boldsymbol{\epsilon}, \mathbf{x}, \boldsymbol{\lambda})|\boldsymbol{\theta})}{p(\boldsymbol{\epsilon}) \cdot |\det \mathbf{J}_g|^{-1}}\right) d\boldsymbol{\epsilon}.$$

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

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

ELBO surgery

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

Theorem

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

- $q_{\text{agg}}(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}_i)$ – **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 $q_{\text{agg}}(\mathbf{z})$ 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

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

Proof

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

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

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

Without proof:

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

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

ELBO surgery

ELBO revisiting

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

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

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

Optimal VAE prior

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

The optimal prior $p(\mathbf{z})$ is the aggregated posterior $q_{\text{agg}}(\mathbf{z})$!

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

Outline

Outline

1. Discrete data vs continuous model
   - Discretization of continuous distribution
   - Dequantization of discrete data
2. ELBO surgery
3. VAE limitations
   - VAE prior
   - VAE posterior

VAE limitations

- Poor generative distribution (decoder)

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

- Loose lower bound

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

- **Poor prior distribution**

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

- Poor variational posterior distribution (encoder)

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

Optimal VAE prior

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

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

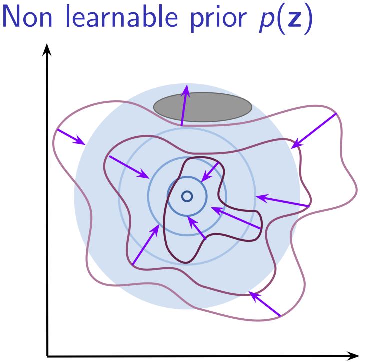


image credit: https://jmtomczak.github.io/blog/7/7_priors.html

Flows-based VAE prior

Flow model in latent space

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\mathbf{z}^*) + \log \left| \det \left(\frac{d\mathbf{z}^*}{d\mathbf{z}} \right) \right| = \log p(g(\mathbf{z}, \boldsymbol{\lambda})) + \log |\det(\mathbf{J}_g)|$$

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

- RealNVP flow.
- Autoregressive flow (MAF).

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

ELBO with flow-based VAE prior

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x}, \phi) \right]$$
$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \Bigg[\log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \underbrace{\Big(\log p(g(\mathbf{z}, \boldsymbol{\lambda})) + \log |\det(\mathbf{J}_g)| \Big)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \phi) \Bigg]$$

Chen X. et al. Variational Lossy Autoencoder, 2016

Outline

VAE limitations

- Poor generative distribution (decoder)

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

- Loose lower bound

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

- Poor prior distribution

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

- **Poor variational posterior distribution (encoder)**

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

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?

Flows in VAE posterior

Apply a sequence of transformations to the random variable

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

Let $q(\mathbf{z}|\mathbf{x}, \phi)$ (VAE encoder) be a base distribution for a flow model.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right) \right|$$

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

Here $g(\mathbf{z}, \boldsymbol{\lambda})$ is a flow model (e.g. stack of planar/coupling/AR layers) parameterized by $\boldsymbol{\lambda}$.
Let use $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$ as a variational distribution. Here ϕ – encoder parameters, $\boldsymbol{\lambda}$ – flow parameters.

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

Flows-based VAE posterior

- Encoder outputs base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$.
- Flow model $\mathbf{z}^* = g(\mathbf{z}, \boldsymbol{\lambda})$ transforms the base distribution $q(\mathbf{z}|\mathbf{x}, \phi)$ to the distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$.
- Distribution $q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})$ is used as a variational distribution for ELBO maximization.

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right) \right|$$

ELBO with flow-based VAE posterior

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

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-based VAE posterior

Flow model in latent space

$$\log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) = \log q(\mathbf{z}|\mathbf{x}, \phi) + \log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \right) \right|$$

ELBO objective

$$\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda})} \bigl[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) \bigr] =$$
$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left. \bigl[\log p(\mathbf{x}, \mathbf{z}^*|\boldsymbol{\theta}) - \log q(\mathbf{z}^*|\mathbf{x}, \phi, \boldsymbol{\lambda}) \bigr] \right|_{\mathbf{z}^* = g(\mathbf{z}, \boldsymbol{\lambda})} =$$
$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \Bigl[\log p(\mathbf{x}, g(\mathbf{z}, \boldsymbol{\lambda})|\boldsymbol{\theta}) - \log q(\mathbf{z}|\mathbf{x}, \phi) - \log |\det(\mathbf{J}_g)| \Bigr].$$

- Obtain samples $\mathbf{z}$ from the encoder $q(\mathbf{z}|\mathbf{x}, \phi)$.
- Apply flow model $\mathbf{z}^* = g(\mathbf{z}, \boldsymbol{\lambda})$.
- Compute likelihood for $\mathbf{z}^*$ using the decoder, base distribution for $\mathbf{z}^*$ and the Jacobian.

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

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

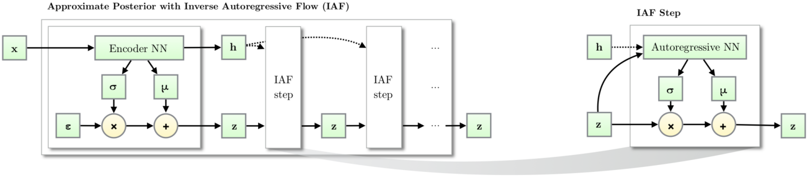
- We don't need to think about computing the function $f(\mathbf{x}, \boldsymbol{\theta})$.
- Inverse autoregressive flow is a natural choice for using flows in VAE:

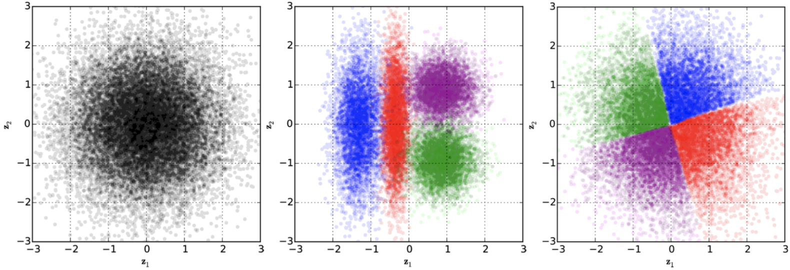
$$\mathbf{z} = \boldsymbol{\sigma}(\mathbf{x}) \odot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}|\mathbf{x}, \phi).$$

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

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

Inverse autoregressive flow (IAF)





(a) Prior distribution (b) Posteriors in standard VAE (c) Posteriors in VAE with IAF

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

Flows-based VAE prior vs posterior

Theorem

VAE with the flow-based prior for latent code $\mathbf{z}$ is equivalent to VAE with flow-based posterior for latent code $\mathbf{z}$.

Proof

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}, \boldsymbol{\lambda}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \underbrace{KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}) || p(\mathbf{z}|\boldsymbol{\lambda}))}_{\text{flow-based prior}} \\
&= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - \underbrace{KL(q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}, \boldsymbol{\lambda}) || p(\mathbf{z}))}_{\text{flow-based posterior}}
\end{aligned}
$$

(Here we use Flow KL duality theorem from Lecture 5)

Flows in VAE posterior

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

Chen X. et al. Variational Lossy Autoencoder, 2016

Flows-based VAE prior vs posterior

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

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.

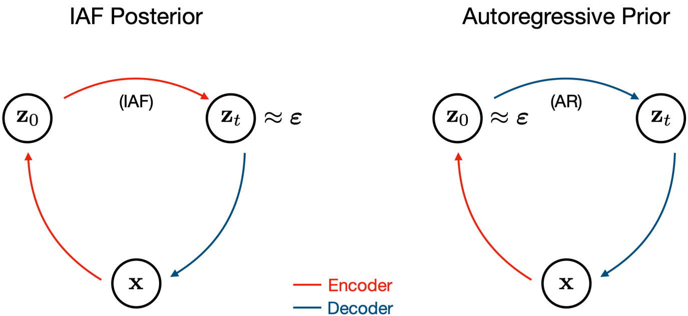


image credit: https://courses.cs.washington.edu/courses/cse599i/20au

VAE limitations

- Poor generative distribution (decoder)

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

- Loose lower bound

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

- Poor prior distribution

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

- Poor variational posterior distribution (encoder)

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

Summary

- Dequantization allows to fit discrete data using continuous model.
- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that was proposed in Flow++ model.
- The ELBO surgery reveals insights about a prior distribution in VAE. The optimal prior is the aggregated posterior.
- We could use flow-based prior in VAE (moreover, autoregressive).
- We could use flows to make variational posterior more expressive. This is equivalent to the flow-based prior.