Deep Generative Models

Lecture 7

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Recap of previous lecture

Gaussian AR NF

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

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

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

Inverse gaussian AR NF

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

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

- 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

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

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	$\phi, \boldsymbol{\theta}$	$\boldsymbol{\theta} \equiv \phi$

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

$\log p(x)$ $\mathcal{L}_k$

Outline

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Discrete data vs continuous model

Let our data **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.

$= \mathcal{N}(\mu(x, \theta), \sigma(x, \theta))$

Discrete model

- Use **discrete** model (e.x. $P(\mathbf{y}|\boldsymbol{\theta}) = \text{Cat}(\boldsymbol{\pi}(\boldsymbol{\theta}))$).
- Minimize any suitable divergence measure $D(\Pi, P)$. $\{0, \dots, 255\}$
- 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

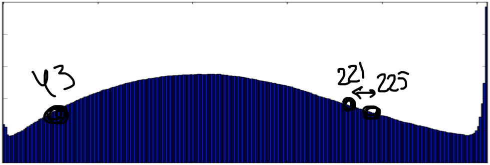
Discrete data vs continuous model

$$\begin{array}{ccc}\{\Pi(y)\} & \longrightarrow & \{\pi(x)\}\\ \updownarrow & & \updownarrow \\ \{P(y|\theta)\} & \longleftarrow & \{p(x|\theta)\}\end{array}$$

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

Discretization of continuous distribution

$p(x|\theta) \to P(y|\theta)$

Model discretization through CDF

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

$\sigma\left(\frac{x-\mu}{s}\right)$ $\quad P(y)$

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++

$F(y+0.5) = \sum \pi_k \sigma\left(\frac{y+0.5-\mu_k}{s_k}\right)$ $\quad \boxed{\text{PixelCNN}} \to \{\pi, \mu, s\}$

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

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 $\underbrace{-\infty}$, and for 255 replace $x + 0.5$ by $\underbrace{+\infty}$.

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

Outline

dequantization

Uniform ~~discretization~~

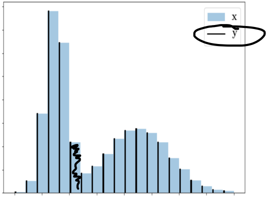
(+) $\pi(x) \leftrightarrow p(x|\theta)$

Let dequantize 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

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

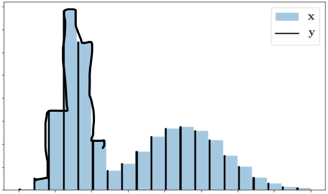
$$\leq \sum \Pi(\mathbf{y}) \log \int_{U[0,1]} p(\mathbf{y} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u} =$$

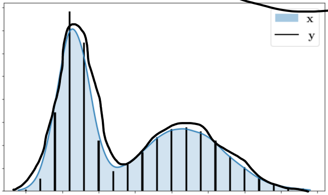
$$= \sum \Pi(\mathbf{y}) \log P(\mathbf{y}|\boldsymbol{\theta}) = \boxed{\mathbb{E}_\Pi \log P(\mathbf{y}|\boldsymbol{\theta}).}$$

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

Variational dequantization

$y + u \sim q(u|y)$





- $p(\mathbf{x}|\boldsymbol{\theta})$ 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

$y \to u$

$x \quad z$

$y+u$

Variational lower bound

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

$$\geq \underbrace{\int \underbrace{q(\mathbf{u}|\mathbf{y})}_{1} \log \frac{p(\mathbf{y}+\mathbf{u}|\boldsymbol{\theta})}{q(\mathbf{u}|\mathbf{y})} d\mathbf{u}} = \mathcal{L}(q, \boldsymbol{\theta}).$$

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

Flow++: flow-based variational dequantization

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

$g \triangleq f^{-1}$

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

$f \triangleq g^{-1}$

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

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

Outline

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

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

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

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

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

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

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

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

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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**

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

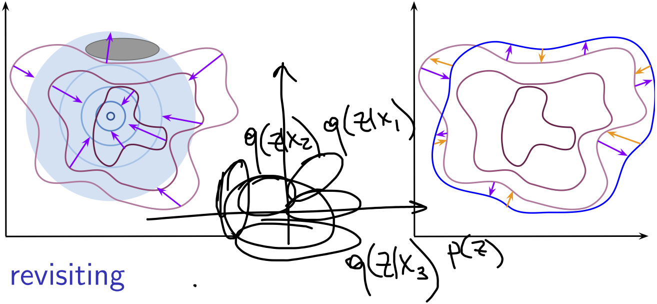
- Poor variational posterior distribution (encoder)

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

Optimal VAE prior

- 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.

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



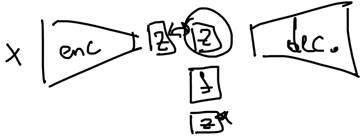
ELBO revisiting

$$\frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_i(q, \boldsymbol{\theta}) = \text{RL} - \text{MI} - KL(q_{\text{agg}}(\mathbf{z}) || p(\mathbf{z}|\boldsymbol{\lambda}))$$

It is Forward KL with respect to $p(\mathbf{z}|\boldsymbol{\lambda})$.

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

Flow-based VAE prior



Flow model in latent space

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

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

- RealNVP with coupling layers.
- Autoregressive flow (fast $f(\mathbf{z}, \boldsymbol{\lambda})$, slow $g(\mathbf{z}^*, \boldsymbol{\lambda})$).
- Is it OK to use IAF for VAE prior?

ELBO with flow-based VAE prior

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

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

Is it possible to use non-invertible model in VAE prior?

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 decomposition

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

- E-step of EM-algorithm: $KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})) = 0$. (In this case the lower bound is tight $\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathcal{L}(q, \boldsymbol{\theta})$).
- $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_\phi(\mathbf{x}), \boldsymbol{\sigma}^2_\phi(\mathbf{x}))$ is a unimodal distribution (not expressive enough).
- NF convert a simple distribution to a complex one. Let use NF 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.

Summary

- Lots of data are discrete. We able to discretize the model or to dequantize our data to use continuous model.
- Uniform dequantization is the simplest form of dequantization. Variational dequantization is a more natural type that uses variational inference.
- 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 (even autoregressive).
- We could use flows to make variational posterior more expressive.