Deep Generative Models Lecture 6

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Gaussian autoregressive model

Consider autoregressive model

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

with conditionals

$$p(\mathbf{x}_i|\mathbf{x}_{1:i-1},\boldsymbol{\theta}) = \mathcal{N}\left(\hat{\mu}_i(\mathbf{x}_{1:i-1}), \hat{\sigma}_i^2(\mathbf{x}_{1:i-1})\right).$$

Forward and inverse

$$egin{aligned} & \mathbf{x}_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot \mathbf{z}_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}), \quad \mathbf{z}_i \sim \mathcal{N}(0,1). \ & \mathbf{z}_i = (\mathbf{x}_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})}. \end{aligned}$$

Gaussian autoregressive model

Forward and inverse

$$\mathbf{x} = g(\mathbf{z}, \boldsymbol{\theta}); \quad x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}), \quad z_i \sim \mathcal{N}(0, 1).$$

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

Jacobian

$$\log \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right| = -\log \left| \det \left(\frac{\partial g(\mathbf{z}, \boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right| = -\sum_{i=1}^{m} \log \hat{\sigma}_i(\mathbf{x}_{1:i-1}).$$

We get an autoregressive model with tractable (triangular) Jacobian, which is easily invertible. It is a flow!

Inverse autoregressive flow (IAF)

Gaussian autoregressive model ($z \rightarrow x$)

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}).$$

$$z_i = (x_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})}.$$

This process is sequential.

Let use the following reparametrization: $\sigma=rac{1}{\hat{\sigma}}; \quad \mu=-rac{\hat{\mu}}{\hat{\sigma}}.$

Inverse transform $(x \rightarrow z)$

$$z_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot x_i + \mu_i(\mathbf{x}_{1:i-1}).$$

$$x_i = (z_i - \mu_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}.$$

This process is **not** sequential.

Inverse autoregressive flow (IAF)

Gaussian autoregressive model

$$x_i = \hat{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot z_i + \hat{\mu}_i(\mathbf{x}_{1:i-1}).$$

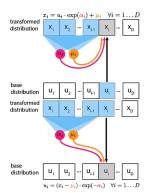
Inverse transform

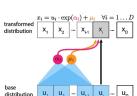
$$z_i = (x_i - \hat{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_i(\mathbf{x}_{1:i-1})};$$

$$z_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot x_i + \mu_i(\mathbf{x}_{1:i-1}).$$

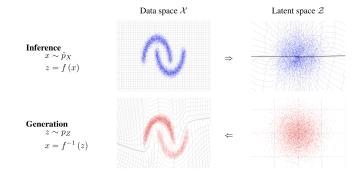
Inverse autoregressive flow

$$x_i = \sigma_i(\mathbf{z}_{1:i-1}) \cdot z_i + \mu_i(\mathbf{z}_{1:i-1}).$$





Flows



- ► Inference mode in autoregressive flows is used for density estimation task.
- Generation mode in autoregressive flows (IAF) is used for stochastic variational inference to get more flexible posterior distribution.

Inverse autoregressive flow (IAF)

Inverse transform $(\mathbf{x} \to \mathbf{z})$

$$z_i = \sigma_i(\mathbf{x}_{1:i-1}) \cdot x_i + \mu_i(\mathbf{x}_{1:i-1}).$$

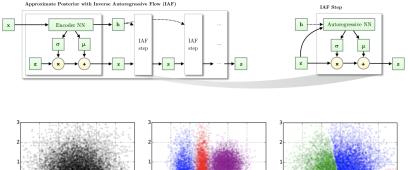
$$x_i = (z_i - \mu_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{x}_{1:i-1})}.$$

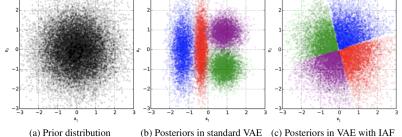
Inverse autoregressive flow use such inverted autoregressive model as a flow in VAE:

$$egin{aligned} \mathbf{z}_0 &= \sigma(\mathbf{x}) \cdot \epsilon + \mu(\mathbf{x}), \quad \epsilon \sim \mathcal{N}(0,1); \quad \sim q(\mathbf{z}_0|\mathbf{x},\phi). \ \\ \mathbf{z}_k &= \sigma_k(\mathbf{z}_{k-1}) \cdot \mathbf{z}_{k-1} + \mu_k(\mathbf{z}_{k-1}), \quad k \geq 1; \quad \sim q_k(\mathbf{z}_k|\mathbf{x},\phi,\{\phi_j\}_{j=1}^k). \end{aligned}$$

https://arxiv.org/pdf/1606.04934.pdf

Inverse autoregressive flow (IAF)



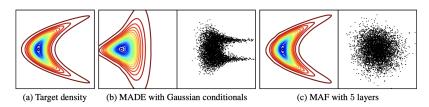


Masked autoregressive flow (MAF)

Gaussian autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{m} p(x_i|\mathbf{x}_{1:i-1},\boldsymbol{\theta}) = \prod_{i=1}^{m} \mathcal{N}\left(x_i|\mu_i(\mathbf{x}_{1:i-1}),\sigma_i^2(\mathbf{x}_{1:i-1})\right).$$

We could use MADE (masked autoencoder) as conditional model. The sampling order could be crucial.

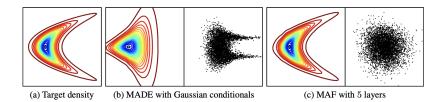


Samples from the base distribution could be an indicator of how good the flow was fitted.

Masked autoregressive flow (MAF)

Gaussian autoregressive model

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{i=1}^{m} p(x_i|\mathbf{x}_{1:i-1},\boldsymbol{\theta}) = \prod_{i=1}^{m} \mathcal{N}\left(x_i|\mu_i(\mathbf{x}_{1:i-1}),\sigma_i^2(\mathbf{x}_{1:i-1})\right).$$



MAF is just a stacked MADE model.

https://arxiv.org/pdf/1705.07057.pdf

Sampling and inverse transform in MAF

$$x_{i} = \hat{\sigma}_{i}(\mathbf{x}_{1:i-1}) \cdot z_{i} + \hat{\mu}_{i}(\mathbf{x}_{1:i-1}).$$

$$z_{i} = (x_{i} - \hat{\mu}_{i}(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\hat{\sigma}_{i}(\mathbf{x}_{1:i-1})}.$$

- ► Sampling is slow (sequential).
- Density estimation is fast.

Sampling and inverse transform in IAF

$$x_i = \sigma_i(\mathbf{z}_{1:i-1}) \cdot z_i + \mu_i(\mathbf{z}_{1:i-1}).$$

$$z_i = (x_i - \mu_i(\mathbf{z}_{1:i-1})) \cdot \frac{1}{\sigma_i(\mathbf{z}_{1:i-1})}.$$

- Sampling is fast.
- ▶ Density estimation is slow (sequential).

Theorem

Training a MAF with maximum likelihood corresponds to fitting an implicit IAF with stochastic variational inference where the posterior is taken to be the base density $\pi(\mathbf{z})$:

$$\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) \quad \Leftrightarrow \quad \min_{\boldsymbol{\theta}} \mathit{KL}\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right).$$

- \blacktriangleright $\pi(\mathbf{z})$ is a base distribution; $\pi(\mathbf{x})$ is a data distribution.
- $ightharpoonup z = f(x, \theta)$ MAF model; $x = g(z, \theta)$ IAF model.

$$\log p(\mathbf{z}|\boldsymbol{\theta}) = \log \pi(g(\mathbf{z},\boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial g(\mathbf{z},\boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right|$$

$$\log p(\mathbf{z}|\boldsymbol{\theta}) = \log \pi(g(\mathbf{z},\boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{z}} \right) \right|$$

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \pi(f(\mathbf{x}, \boldsymbol{\theta})) + \log \left| \det \left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}} \right) \right|$$

Theorem

Training a MAF with maximum likelihood corresponds to fitting an implicit IAF with stochastic variational inference where the posterior is taken to be the base density $\pi(\mathbf{z})$:

$$\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) \quad \Leftrightarrow \quad \min_{\boldsymbol{\theta}} \mathit{KL}\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right).$$

Proof

$$\begin{split} & \mathit{KL}\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right) = \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})} \big[\log p(\mathbf{z}|\boldsymbol{\theta}) - \log \pi(\mathbf{z})\big] = \\ & = \mathbb{E}_{p(\mathbf{z}|\boldsymbol{\theta})} \left[\log \pi(g(\mathbf{z},\boldsymbol{\theta})) + \log \left|\det \left(\frac{\partial g(\mathbf{z},\boldsymbol{\theta})}{\partial \mathbf{z}}\right)\right| - \log \pi(\mathbf{z})\right] = \\ & = \mathbb{E}_{\pi(\mathbf{x})} \left[\log \pi(\mathbf{x}) - \log \left|\det \left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log \pi(f(\mathbf{x},\boldsymbol{\theta}))\right]. \end{split}$$

Proof (continued)

$$\begin{split} & \mathsf{KL}\left(p(\mathbf{z}|\boldsymbol{\theta})||\pi(\mathbf{z})\right) = \\ & = \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log\left|\det\left(\frac{\partial f(\mathbf{x},\boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log \pi(f(\mathbf{x},\boldsymbol{\theta}))\right] = \\ & = \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\boldsymbol{\theta})\right] = \mathsf{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})). \end{split}$$

$$\begin{split} \arg\min_{\boldsymbol{\theta}} \mathit{KL}(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) &= \arg\min_{\boldsymbol{\theta}} \mathbb{E}_{\pi(\mathbf{x})} \left[\log \pi(\mathbf{x}) - \log p(\mathbf{x}|\boldsymbol{\theta})\right] \\ &= \arg\max_{\boldsymbol{\theta}} \mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) \end{split}$$

Unbiased estimator is MLE:

$$\mathbb{E}_{\pi(\mathbf{x})} \log p(\mathbf{x}|\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

MAF vs IAF vs RealNVP

MAF

$$\mathbf{x} = \hat{\boldsymbol{\sigma}}(\mathbf{x}) \odot \mathbf{z} + \hat{\boldsymbol{\mu}}(\mathbf{x}).$$

- ► Calculating the density $p(\mathbf{x}|\theta)$ 1 pass.
- ► Sampling *m* passes.

IAF

$$\mathsf{x} = \sigma(\mathsf{z}) \odot \mathsf{z} + \mu(\mathsf{z}).$$

- ▶ Calculating the density $p(\mathbf{x}|\theta)$ m passes.
- Sampling 1 pass.

RealNVP

$$x_{1:d} = z_{1:d};$$

$$\mathbf{x}_{d:m} = \mathbf{z}_{d:m} \odot \exp(c_1(\mathbf{z}_{1:d}, \boldsymbol{\theta})) + c_2(\mathbf{x}_{1:d}, \boldsymbol{\theta}).$$

MAF vs IAF vs RealNVP

RealNVP

$$egin{aligned} \mathbf{x}_{1:d} &= \mathbf{z}_{1:d}; \ \mathbf{x}_{d:m} &= \mathbf{z}_{d:m} \odot \exp\left(c_1(\mathbf{z}_{1:d}, oldsymbol{ heta})\right) + c_2(\mathbf{x}_{1:d}, oldsymbol{ heta}). \end{aligned}$$

- ▶ Calculating the density $p(\mathbf{x}|\theta)$ 1 pass.
- Sampling 1 pass.

RealNVP is a special case of MAF and IAF:

MAF

$$\begin{cases} \hat{\mu}_i = \hat{\sigma}_i = 0, \ i = 1, \dots, d; \\ \hat{\mu}_i, \hat{\sigma}_i - \text{functions of } \mathbf{x}_{1:d}, \ i = d+1, \dots, m. \end{cases}$$

IAF

$$\begin{cases} \mu_i = \sigma_i = 0, \ i = 1, \dots, d; \\ \mu_i, \sigma_i - \text{functions of } \mathbf{z}_{1:d}, \ i = d+1, \dots, m. \end{cases}$$

MAF/IAF pros and cons

MAF

- ► Sampling is slow.
- Likelihood evaluation is fast.

IAF

- ► Sampling is fast.
- Likelihood evaluation is slow.

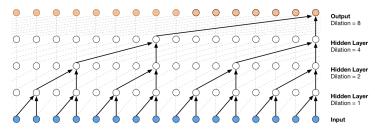
How to take the best of both worlds?

WaveNet (2016)

Autoregressive model for raw audio waveforms generation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{t=1}^{T} p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta}).$$

The model uses causal dilated convolutions.



https://arxiv.org/pdf/1609.03499.pdf

Parallel WaveNet, 2017

Previous WaveNet model

- raw audio is high-dimensional (e.g. 16000 samples per second for 16kHz audio);
- WaveNet encodes 8-bit signal with 256-way categorical distribution.

Goal

- improved fidelity (24kHz instead of 16kHz) → increase dilated convolution filter size from 2 to 3;
- ▶ 16-bit signals → mixture of logistics instead of categorical distribution.

https://arxiv.org/pdf/1711.10433.pdf

Parallel WaveNet, 2017

Probability density distillation

- 1. Train usual WaveNet (MAF) via MLE (teacher network).
- 2. Train IAF WaveNet model (student network), which attempts to match the probability of its own samples under the distribution learned by the teacher.

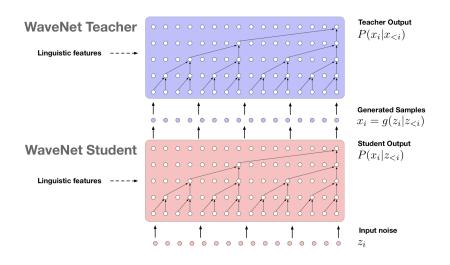
Student objective

$$KL(p_s||p_t) = H(p_s, p_t) - H(p_s).$$

More than 1000x speed-up relative to original WaveNet!

https://arxiv.org/pdf/1711.10433.pdf

Parallel WaveNet, 2017



https://arxiv.org/pdf/1711.10433.pdf

Summary

- ► Flows is a continuous model. To use it for discrete distribution, the data should be dequantized.
- Original VAE model has lot of limitations. One of them is a restricted class of variational posteriors.
- Using flows in a latent space of VAE could give more flexible posterior distribution.
- Gaussian autoregressive model is a special type of flow (RealNVP model is a special type of this autoregressive model)
- ► MAF is an example of such model which is suitable for density estimation tasks.
- ► IAF used the inverse autoregressive transformation for variational inference task.

VAE limitations

Poor variational posterior distribution (encoder)

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

Poor prior distribution

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

Poor probabilistic model (decoder)

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

Loose lower bound

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



$$\mathcal{L}(q, heta) = \int q(\mathbf{Z}|\mathbf{X}) \log rac{p(\mathbf{X}, \mathbf{Z}| heta)}{q(\mathbf{Z}|\mathbf{X})} d\mathbf{Z}.$$

ELBO interpretations

► Evidence minus posterior KL

$$\mathcal{L}(q, \theta) = \log p(\mathbf{X}|\theta) - KL(q(\mathbf{Z}|\mathbf{X})||p(\mathbf{Z}|\mathbf{X}, \theta)).$$

Average negative energy plus entropy

$$\mathcal{L}(q, \theta) = \mathbb{E}_{q(\mathbf{Z}|\mathbf{X})} p(\mathbf{X}, \mathbf{Z}|\theta) + \mathbb{H}[q(\mathbf{Z}|\mathbf{X})].$$

▶ Average term-by-term reconstruction minus KL to prior

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

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

Theorem

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

where i is treated as random variable:

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

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

http://approximate inference.org/accepted/Hoffman Johnson 2016.pdf



Theorem

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

Proof

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

Theorem

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

Proof (continued)

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

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

Theorem

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

ELBO revisiting

$$\begin{split} \mathcal{L}(q, \boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} \left[\mathbb{E}_{q(\mathbf{z}_{i} | \mathbf{x}_{i})} \log p(\mathbf{x}_{i} | \mathbf{z}_{i}, \boldsymbol{\theta}) - KL(q(\mathbf{z}_{i} | \mathbf{x}_{i}) || p(\mathbf{z}_{i})) \right] = \\ &= \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_{i} | \mathbf{x}_{i})} \log p(\mathbf{x}_{i} | \mathbf{z}_{i}, \boldsymbol{\theta}) - \mathbb{I}_{q(i, \mathbf{z})}[i, \mathbf{z}] - KL(q(\mathbf{z}) || p(\mathbf{z})) = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}_{i} | \mathbf{x}_{i})} \log p(\mathbf{x}_{i} | \mathbf{z}_{i}, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{O} - \text{Mutual info} < \log n} - \underbrace{KL(q(\mathbf{z}) || p(\mathbf{z}))}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{E}_{q(\mathbf{z})} \mathbb{H} \left[q(i | \mathbf{z})\right]\right)}_{\text{Marginal KL}} - \underbrace{\left(\log n - \mathbb{$$

ELBO revisiting

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

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

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

$$\log n \approx 11.0021$$

VAE prior

ELBO revisiting

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

How to choose the optimal p(z)?

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

^(*) https://arxiv.org/abs/1611.02648

 $^{(**)\} https://pdfs.semanticscholar.org/f6fe/5e8e25994c188ba6a124462e2cc55f2c5a67.pdf$

References

► IAF: Improving Variational Inference with Inverse Autoregressive Flow https://arxiv.org/abs/1606.04934
Summary: Introduce inverse autoregressive flow (IAF). Models each autoregressive conditional as gaussian with autoregressive means and covariances. Inverse transformation allows to parallelize sampling.

MAF: Masked Autoregressive Flow for Density Estimation https://arxiv.org/pdf/1705.07057.pdf
Summary: Similar to IAF. Give comprehensive overview with link to IAF and RealNVP. MAF is suitable for density estimation, IAF as a recognition network.

Parallel WaveNet: Fast High-Fidelity Speech Synthesis https://arxiv.org/pdf/1711.10433.pdf
Summary: WaveNet is MAF (sequential generation). To exploit IAF fast sampling, knowledge distillation used. Teacher network is large WaveNet, student - is a IAF small WaveNet (generate samples from noise is parallel). The loss is KL divergence between student and teacher distributions. The additional perceptual, contrastive and power losses used to create more natural sounds.

ELBO surgery: yet another way to carve up the variational evidence lower bound http://approximateinference.org/accepted/HoffmanJohnson2016.pdf
Summary: Propose the decomposition of standard ELBO into 3 terms. The prior distribution should be close to average posterior. Show empirically that weak prior has a significant impact on ELBO value.