Deep Generative Models
Lecture 6

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Ozon Masters

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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

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

Forward and inverse

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

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

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 ($\mathbf{z} \rightarrow \mathbf{x}$)

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

This process is sequential.
Let use the following reparametrization: $\boldsymbol{\sigma} = \frac{1}{\hat{\boldsymbol{\sigma}}}; \quad \boldsymbol{\mu} = -\frac{\hat{\boldsymbol{\mu}}}{\hat{\boldsymbol{\sigma}}}$.

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

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

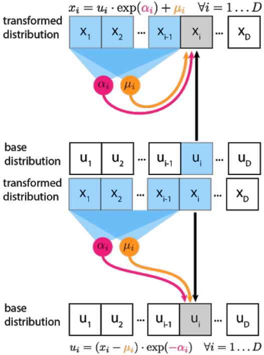
This process is **not** sequential.

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

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

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

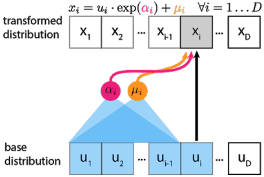


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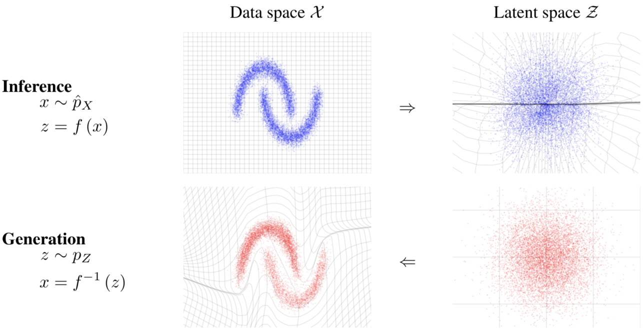
image credit: https://blog.evjang.com/2018/01/nf2.html

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.

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

Inverse autoregressive flow (IAF)

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

$$
\begin{aligned}
z_i &= \boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1}) \cdot x_i + \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1}). \\
x_i &= (z_i - \boldsymbol{\mu}_i(\mathbf{x}_{1:i-1})) \cdot \frac{1}{\boldsymbol{\sigma}_i(\mathbf{x}_{1:i-1})}.
\end{aligned}
$$

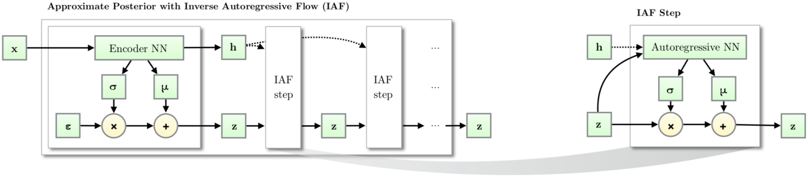
Inverse autoregressive flow use such inverted autoregressive model as a flow in VAE:

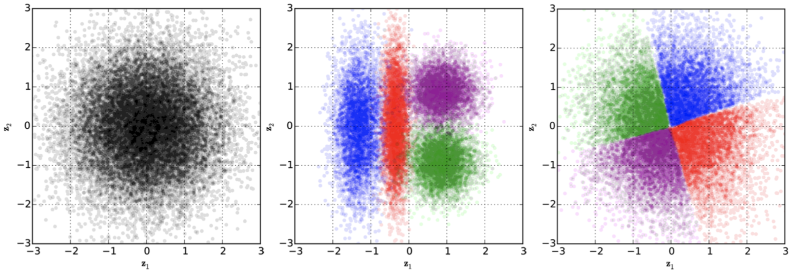
$$
\mathbf{z}_0 = \boldsymbol{\sigma}(\mathbf{x}) \cdot \boldsymbol{\epsilon} + \boldsymbol{\mu}(\mathbf{x}), \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, 1); \quad \sim q(\mathbf{z}_0 | \mathbf{x}, \boldsymbol{\phi}).
$$

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

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

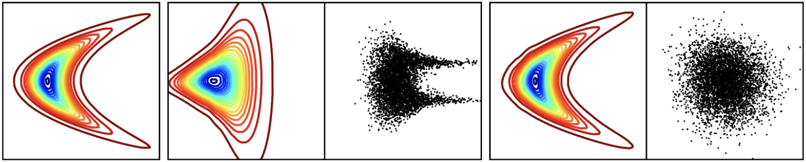
Kingma D. P. et al. Improving Variational Inference with Inverse Autoregressive Flow, 2016

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.



(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

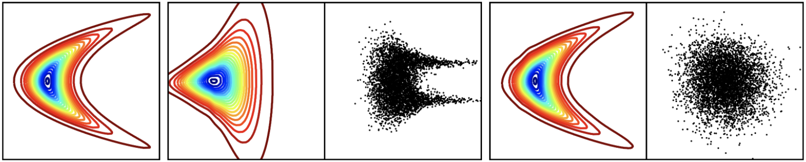
Samples from the base distribution could be an indicator of how good the flow was fitted.

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

Masked autoregressive flow (MAF)

Gaussian autoregressive model

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



(a) Target density (b) MADE with Gaussian conditionals (c) MAF with 5 layers

MAF is just a stacked MADE model.

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF

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).

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF

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 $\pi(\mathbf{z})$:

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

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

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

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

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

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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 $\pi(\mathbf{z})$:

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

Proof

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

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

$$= \mathbb{E}_{\pi(\mathbf{x})}\left[\log \pi(\mathbf{x}) - \log \left|\det\left(\frac{\partial f(\mathbf{x}, \boldsymbol{\theta})}{\partial \mathbf{x}}\right)\right| - \log \pi(f(\mathbf{x}, \boldsymbol{\theta}))\right].$$

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF

Proof (continued)

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

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

Unbiased estimator is MLE:

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

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF vs RealNVP

MAF

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

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

IAF

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

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

RealNVP

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

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF vs IAF vs RealNVP

RealNVP

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

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

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

Papamakarios G., Pavlakou T., Murray I. Masked Autoregressive Flow for Density Estimation, 2017

MAF/IAF pros and cons

MAF

- Sampling is slow.
- Likelihood evaluation is fast.

IAF

- Sampling is fast.
- Likelihood evaluation is slow.

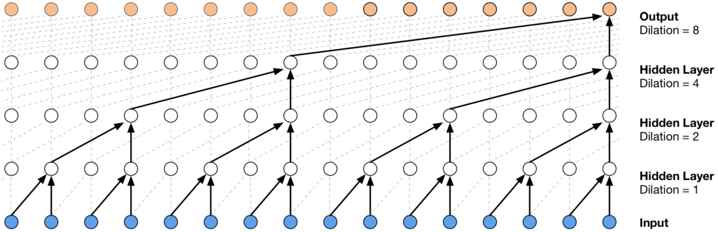
How to take the best of both worlds?

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.



Oord A. et al. Wavenet: A generative model for raw audio, 2016

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) $\rightarrow$ increase dilated convolution filter size from 2 to 3;
- 16-bit signals $\rightarrow$ mixture of logistics instead of categorical distribution.

Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

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.

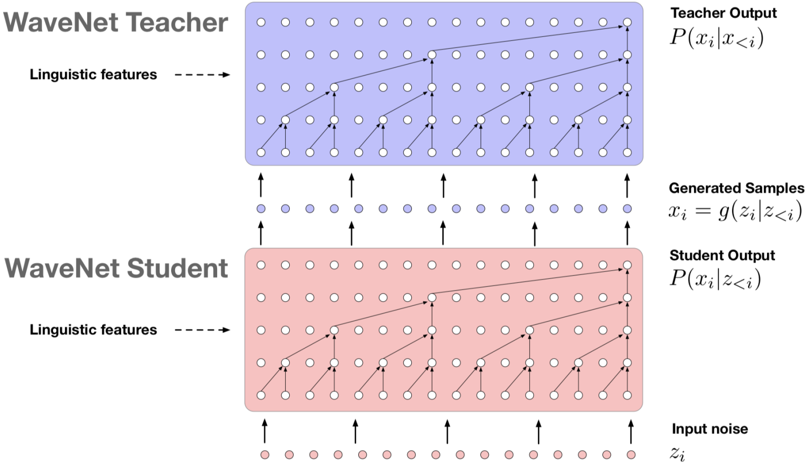
Student objective

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

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

Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

Parallel WaveNet, 2017



Oord A. et al. Parallel WaveNet: Fast High-Fidelity Speech Synthesis, 2017

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)

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

- 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

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

ELBO surgery, 2016

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

ELBO interpretations

- Evidence minus posterior KL

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

- Average negative energy plus entropy

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

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

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

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

ELBO surgery, 2016

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

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:

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

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

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

ELBO surgery, 2016

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

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

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

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

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

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

ELBO surgery, 2016

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)

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

$$\mathbb{I}_{q(i,\mathbf{z})}[i, \mathbf{z}] = \mathbb{E}_{q(i,\mathbf{z})} \log \frac{q(i,\mathbf{z})}{q(i)q(\mathbf{z})} = \mathbb{E}_{q(\mathbf{z})}\mathbb{E}_{q(i|\mathbf{z})} \log \frac{q(i|\mathbf{z})q(\mathbf{z})}{q(i)q(\mathbf{z})} =$$

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

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

ELBO surgery, 2016

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

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

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

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

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

ELBO surgery, 2016

ELBO revisiting

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

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

	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

$$\log n \approx 11.0021$$

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

VAE prior

ELBO revisiting

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

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

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

(*) Dilokthanakul N. et al. Deep Unsupervised Clustering with Gaussian Mixture Variational Autoencoders, 2016
(**) Nalisnick E., Hertel L., Smyth P. Approximate Inference for Deep Latent Gaussian Mixtures, 2016

Summary