Deep Generative Models

Lecture 2

Roman Isachenko

AI Masters

Autumn, 2022

Recap of previous lecture

We are given i.i.d. samples $\{\mathbf{x}_i\}_{i=1}^n \in \mathcal{X}$ (e.g. $\mathcal{X} = \mathbb{R}^m$) from unknown distribution $\pi(\mathbf{x})$.

Goal

We would like to learn a distribution $\pi(\mathbf{x})$ for

- evaluating $\pi(\mathbf{x})$ for new samples (how likely to get object $\mathbf{x}$?);
- sampling from $\pi(\mathbf{x})$ (to get new objects $\mathbf{x} \sim \pi(\mathbf{x})$).

Instead of searching true $\pi(\mathbf{x})$ over all probability distributions, learn function approximation $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Divergence

- $D(\pi||p) \geq 0$ for all $\pi, p \in \mathcal{S}$;
- $D(\pi||p) = 0$ if and only if $\pi \equiv p$.

Divergence minimization task

$$\min_{\boldsymbol{\theta}} D(\pi||p).$$

Recap of previous lecture

Forward KL

$$KL(\pi||p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x}|\boldsymbol{\theta})} d\mathbf{x} \rightarrow \min_{\boldsymbol{\theta}}$$

Reverse KL

$$KL(p||\pi) = \int p(\mathbf{x}|\boldsymbol{\theta}) \log \frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x})} d\mathbf{x} \rightarrow \min_{\boldsymbol{\theta}}$$

Maximum likelihood estimation (MLE)

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

Maximum likelihood estimation is equivalent to minimization of the Monte-Carlo estimate of forward KL.

Recap of previous lecture

Likelihood as product of conditionals

Let $\mathbf{x} = (x_1, \dots, x_m)$, $\mathbf{x}_{1:j} = (x_1, \dots, x_j)$. Then

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

MLE problem for autoregressive model

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \sum_{j=1}^{m} \log p(x_{ij}|\mathbf{x}_{i,1:j-1}\boldsymbol{\theta}).$$

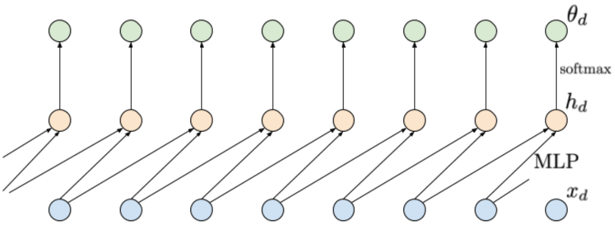
Sampling

$$\hat{x}_1 \sim p(x_1|\boldsymbol{\theta}), \quad \hat{x}_2 \sim p(x_2|\hat{x}_1, \boldsymbol{\theta}), \dots, \quad \hat{x}_m \sim p(x_m|\hat{\mathbf{x}}_{1:m-1}, \boldsymbol{\theta})$$

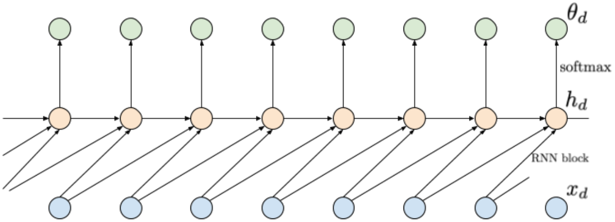
New generated object is $\hat{\mathbf{x}} = (\hat{x}_1, \hat{x}_2, \dots, \hat{x}_m)$.

Recap of previous lecture

Autoregressive MLP



Autoregressive RNN



---

image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Outline

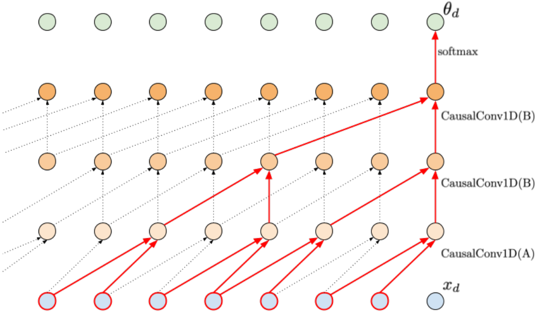
1. Autoregressive models (WaveNet, PixelCNN)
2. Bayesian framework
3. Latent variable models (LVM)
4. Variational lower bound (ELBO)

Outline

1. Autoregressive models (WaveNet, PixelCNN)
2. Bayesian framework
3. Latent variable models (LVM)
4. Variational lower bound (ELBO)

Autoregressive models

- Convolutions could be used for autoregressive models, but they have to be **causal**.
- Try to find and understand the difference between Conv A/B.



- Could learn long-range dependecies.
- Do not suffer from gradient issues.
- Easy to estimate probability for given input, but hard generation of new samples (the sequential process).

---

image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

WaveNet

Goal

Efficient generation of raw audio waveforms with natural sounds.

Solution

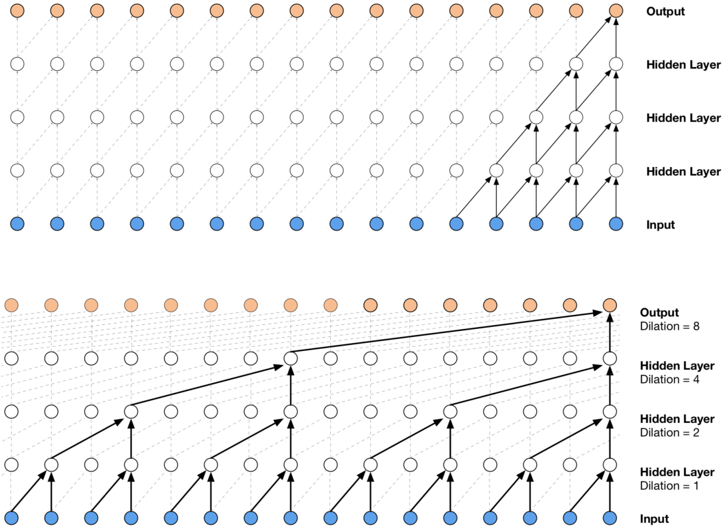
Autoregressive model

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

- Each conditional $p(x_t|\mathbf{x}_{1:t-1}, \boldsymbol{\theta})$ models the distribution for the timestamp t.
- The model uses **causal** dilated convolutions.

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

WaveNet



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

PixelCNN

Goal

Model a distribution $\pi(\mathbf{x})$ of natural images.

Solution

Autoregressive model on 2D pixels

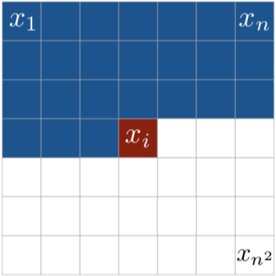
$$p(\mathbf{x}|\boldsymbol{\theta}) = \prod_{j=1}^{\text{width} \times \text{height}} p(x_j|\mathbf{x}_{1:j-1}, \boldsymbol{\theta}).$$

- We need to introduce the ordering of image pixels.
- The convolution should be **masked** to make them causal.
- The image has RGB channels, these dependencies could be addressed.

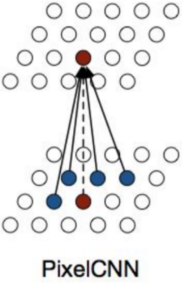
Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

PixelCNN

Raster ordering

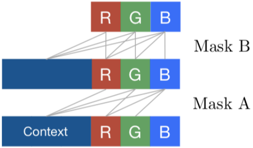


Dependencies between pixels



Mask for the convolution kernel

1	1	1
1	0	0
0	0	0



Oord A., Kalchbrenner N., Kavukcuoglu K. Pixel recurrent neural networks, 2016

Outline

1. Autoregressive models (WaveNet, PixelCNN)
2. Bayesian framework
3. Latent variable models (LVM)
4. Variational lower bound (ELBO)

Bayesian framework

Bayes theorem

$$p(\mathbf{t}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{p(\mathbf{x})} = \frac{p(\mathbf{x}|\mathbf{t})p(\mathbf{t})}{\int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}}$$

- $\mathbf{x}$ – observed variables, $\mathbf{t}$ – unobserved variables (latent variables/parameters);
- $p(\mathbf{x}|\mathbf{t})$ – likelihood;
- $p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{t})p(\mathbf{t})d\mathbf{t}$ – evidence;
- $p(\mathbf{t})$ – prior distribution, $p(\mathbf{t}|\mathbf{x})$ – posterior distribution.

Meaning

We have unobserved variables $\mathbf{t}$ and some prior knowledge about them $p(\mathbf{t})$. Then, the data $\mathbf{x}$ has been observed. Posterior distribution $p(\mathbf{t}|\mathbf{x})$ summarizes the knowledge after the observations.

Bayesian framework

Let consider the case, where the unobserved variables $\mathbf{t}$ is our model parameters $\boldsymbol{\theta}$.

- $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ – observed samples;
- $p(\boldsymbol{\theta})$ – prior parameters distribution (we treat model parameters $\boldsymbol{\theta}$ as random variables).

Posterior distribution

$$p(\boldsymbol{\theta}|\mathbf{X}) = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathbf{X})} = \frac{p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\mathbf{X}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}}$$

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

Note the difference from

$$p(\mathbf{x}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}.$$

Bayesian framework

Bayesian inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta}$$

If evidence $p(\mathbf{X})$ is intractable (due to multidimensional integration), we can't get posterior distribution and perform the precise inference.

Maximum a posteriori (MAP) estimation

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \big(\log p(\mathbf{X}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})\big)$$

Estimated $\boldsymbol{\theta}^*$ is a deterministic variable, but we could treat it as a random variable with density $p(\boldsymbol{\theta}|\mathbf{X}) = \delta(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$.

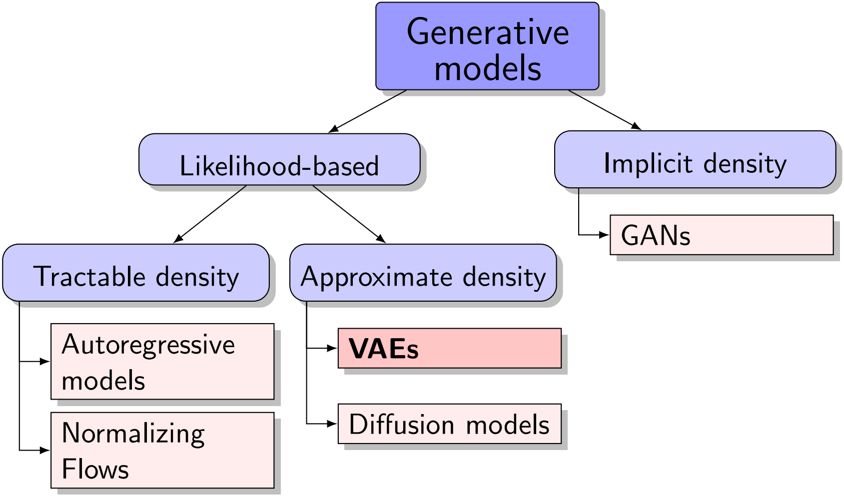
MAP inference

$$p(\mathbf{x}|\mathbf{X}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{X})d\boldsymbol{\theta} \approx p(\mathbf{x}|\boldsymbol{\theta}^*).$$

Outline

1. Autoregressive models (WaveNet, PixelCNN)
2. Bayesian framework
3. Latent variable models (LVM)
4. Variational lower bound (ELBO)

Generative models zoo



Latent variable models (LVM)

MLE problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}).$$

The distribution $p(\mathbf{x}|\boldsymbol{\theta})$ could be very complex and intractable (as well as real distribution $\pi(\mathbf{x})$).

Extended probabilistic model

Introduce latent variable $\mathbf{z}$ for each sample $\mathbf{x}$

$$p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}); \quad \log p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) = \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) + \log p(\mathbf{z}).$$

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z}) d\mathbf{z}.$$

Motivation

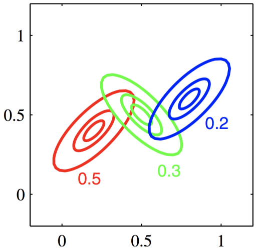
The distributions $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ and $p(\mathbf{z})$ could be quite simple.

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

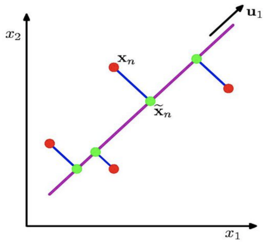
Examples

Mixture of gaussians



- $p(\mathbf{x}|z, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- $p(z) = \text{Categorical}(\boldsymbol{\pi})$

PCA model



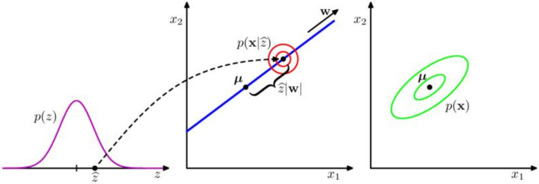
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$

Bishop C. Pattern Recognition and Machine Learning, 2006

Latent variable models (LVM)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} \to \max_{\boldsymbol{\theta}}$$

PCA projects original data $\mathbf{X}$ onto a low dimensional latent space while maximizing the variance of the projected data.



$$\boldsymbol{x} = W\boldsymbol{z} + \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0, \mathbf{I})$
- $p(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I})$
- $p(\mathbf{z}|\mathbf{x}) = \mathcal{N}\big(\mathbf{M}^{-1}\mathbf{W}^T(\mathbf{x} - \boldsymbol{\mu}), \sigma^2\mathbf{M}\big)$, where $\mathbf{M} = \mathbf{W}\mathbf{W}^T + \sigma^2\mathbf{I}$

Maximum likelihood estimation for LVM

MLE for extended problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}).$$

However, $\mathbf{Z}$ is unknown.

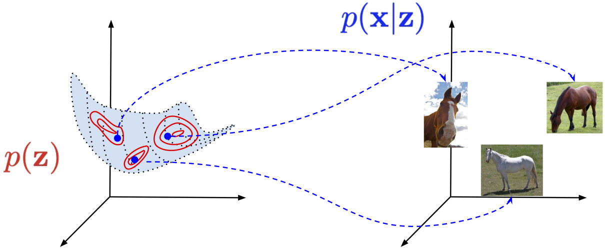
MLE for original problem

$$\boldsymbol{\theta}^* = \arg\max_{\boldsymbol{\theta}} \log p(\mathbf{X}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}_i|\boldsymbol{\theta}) =$$

$$= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log \int p(\mathbf{x}_i, \mathbf{z}_i|\boldsymbol{\theta}) d\mathbf{z}_i =$$

$$= \arg\max_{\boldsymbol{\theta}} \log \sum_{i=1}^{n} \int p(\mathbf{x}_i|\mathbf{z}_i, \boldsymbol{\theta}) p(\mathbf{z}_i) d\mathbf{z}_i.$$

Naive approach



Monte-Carlo estimation

$$p(\mathbf{x}|\boldsymbol{\theta}) = \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z} = \mathbb{E}_{p(\mathbf{z})} p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) \approx \frac{1}{K} \sum_{k=1}^{K} p(\mathbf{x}|\mathbf{z}_k, \boldsymbol{\theta}),$$

where each $\mathbf{z}_k \sim p(\mathbf{z})$.

Challenge: to cover the space properly, the number of samples grows exponentially with respect to dimensionality of $\mathbf{z}$.

image credit: https://jmtomczak.github.io/blog/4/4_VAE.html

Outline

1. Autoregressive models (WaveNet, PixelCNN)
2. Bayesian framework
3. Latent variable models (LVM)
4. Variational lower bound (ELBO)

Variational lower bound (ELBO)

Derivation 1 (inequality)

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} = \log \int \frac{q(\mathbf{z})}{q(\mathbf{z})} p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta}) d\mathbf{z} =$$

$$= \log \mathbb{E}_q \left[\frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} \right] \geq \mathbb{E}_q \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} = \mathcal{L}(q, \boldsymbol{\theta})$$

Derivation 2 (equality)

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

$$= \int q(\mathbf{z}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} =$$

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

Variational decomposition

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

Variational lower bound (ELBO)

$$\mathcal{L}(q, \boldsymbol{\theta}) = \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} =$$
$$= \int q(\mathbf{z}) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z})}{q(\mathbf{z})} d\mathbf{z}$$
$$= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z}))$$

Log-likelihood decomposition

$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z})) + KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

- Instead of maximizing incomplete likelihood, maximize ELBO

$$\max_{\boldsymbol{\theta}} p(\mathbf{x}|\boldsymbol{\theta}) \quad \rightarrow \quad \max_{q, \boldsymbol{\theta}} \mathcal{L}(q, \boldsymbol{\theta})$$

- Maximization of ELBO by variational distribution q is equivalent to minimization of KL

$$\max_{q} \mathcal{L}(q, \boldsymbol{\theta}) \equiv \min_{q} KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})).$$

Summary

- WaveNet and PixelCNN models use masked causal convolutions (1D or 2D) to get autoregressive model.
- Bayesian inference is a generalization of most common machine learning tasks. It allows to construct MLE, MAP and bayesian inference, to compare models complexity and many-many more cool stuff.
- LVM introduces latent representation of observed samples to make model more interpretable.
- LVM maximizes variational evidence lower bound (ELBO) to find MLE for the parameters.