

Deep Generative Models

Lecture 2

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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 $p(\mathbf{x}|\theta) \approx \pi(\mathbf{x})$.

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

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

Recap of previous lecture

Forward KL

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

Reverse KL

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

Maximum likelihood estimation (MLE)

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

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

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

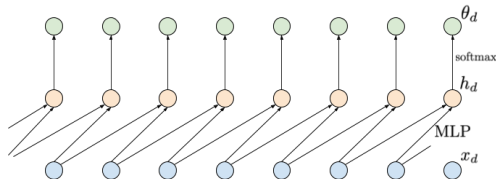
Sampling

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

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

Recap of previous lecture

Autoregressive MLP



Autoregressive CNN

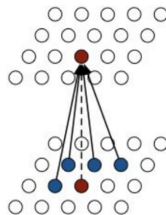
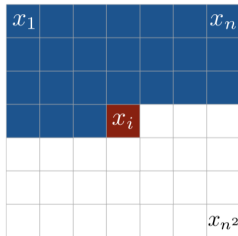
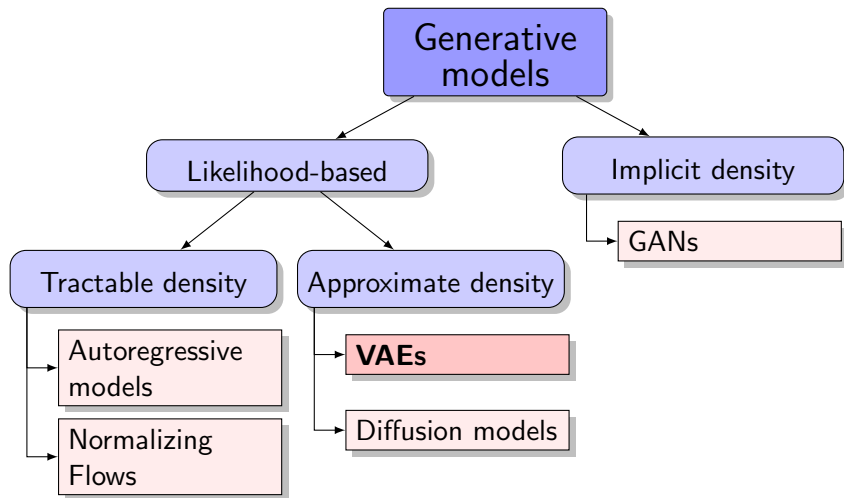


image credit: https://jmtomczak.github.io/blog/2/2_ARM.html

Outline

1. Bayesian framework
2. Latent variable models (LVM)
3. Variational lower bound (ELBO)
4. EM-algorithm, amortized inference

Generative models zoo



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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 θ .

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

Posterior distribution

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

Bayesian inference

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

Note the difference from

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

Bayesian framework

Posterior distribution

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

Bayesian inference

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

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

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

Bayesian framework

MAP estimation

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

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

Dirac delta function

$$\delta(x) = \begin{cases} +\infty, & x = 0; \\ 0, & x \neq 0; \end{cases} \quad \int \delta(x) dx = 1; \quad \int f(x) \delta(x-y) dx = f(y).$$

MAP inference

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

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Latent variable models (LVM)

MLE problem

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

The distribution $p(\mathbf{x}|\theta)$ 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}

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

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

Motivation

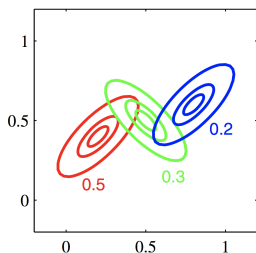
The distributions $p(\mathbf{x}|\mathbf{z}, \theta)$ and $p(\mathbf{z})$ could be quite simple.

Latent variable models (LVM)

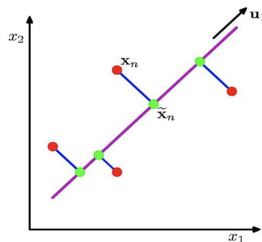
$$\log p(\mathbf{x}|\boldsymbol{\theta}) = \log \int p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})p(\mathbf{z})d\mathbf{z} \rightarrow \max_{\boldsymbol{\theta}}$$

Examples

Mixture of gaussians



PCA model

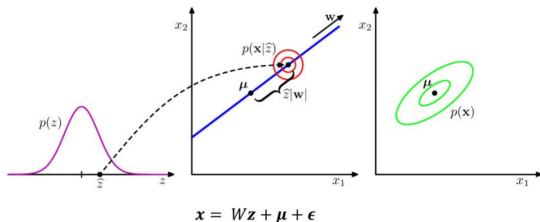


- ▶ $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$
- ▶ $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{x}|\mathbf{W}\mathbf{z} + \boldsymbol{\mu}, \sigma^2\mathbf{I})$
- ▶ $p(\mathbf{z}) = \text{Categorical}(\boldsymbol{\pi})$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

Latent variable models (LVM)

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

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



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

Maximum likelihood estimation for LVM

MLE for extended problem

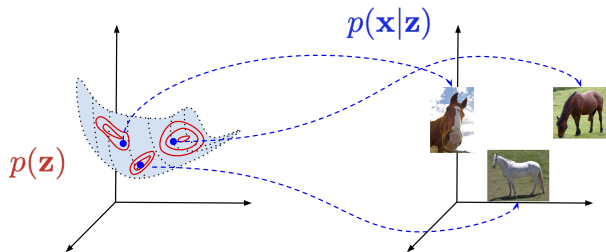
$$\begin{aligned}\theta^* &= \arg \max_{\theta} p(\mathbf{X}, \mathbf{Z} | \theta) = \arg \max_{\theta} \prod_{i=1}^n p(\mathbf{x}_i, \mathbf{z}_i | \theta) = \\ &= \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i, \mathbf{z}_i | \theta).\end{aligned}$$

However, \mathbf{Z} is unknown.

MLE for original problem

$$\begin{aligned}\theta^* &= \arg \max_{\theta} \log p(\mathbf{X} | \theta) = \arg \max_{\theta} \sum_{i=1}^n \log p(\mathbf{x}_i | \theta) = \\ &= \arg \max_{\theta} \sum_{i=1}^n \log \int p(\mathbf{x}_i, \mathbf{z}_i | \theta) d\mathbf{z}_i = \\ &= \arg \max_{\theta} \log \sum_{i=1}^n \int p(\mathbf{x}_i | \mathbf{z}_i, \theta) p(\mathbf{z}_i) d\mathbf{z}_i.\end{aligned}$$

Naive approach



Monte-Carlo estimation

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

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

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

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Variational lower bound (ELBO)

Derivation 1 (inequality)

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

Derivation 2 (equality)

$$\begin{aligned}\mathcal{L}(q, \boldsymbol{\theta}) &= \int q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}) p(\mathbf{x}|\boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\ &= \int q(\mathbf{z}) \log p(\mathbf{x}|\boldsymbol{\theta}) d\mathbf{z} + \int q(\mathbf{z}) \log \frac{p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta})}{q(\mathbf{z})} d\mathbf{z} = \\ &= \log p(\mathbf{x}|\boldsymbol{\theta}) - KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}))\end{aligned}$$

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)

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

Log-likelihood decomposition

$$\begin{aligned}\log p(\mathbf{x} | \theta) &= \mathcal{L}(q, \theta) + KL(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}, \theta)) \\ &= \mathbb{E}_q \log p(\mathbf{x} | \mathbf{z}, \theta) - KL(q(\mathbf{z}) || p(\mathbf{z})) + KL(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}, \theta)).\end{aligned}$$

- Instead of maximizing incomplete likelihood, maximize ELBO

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

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

$$\arg \max_q \mathcal{L}(q, \theta) \equiv \arg \min_q KL(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}, \theta)).$$

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EM-algorithm

$$\begin{aligned}\mathcal{L}(q, \theta) &= \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \theta) - KL(q(\mathbf{z})||p(\mathbf{z})) = \\ &= \mathbb{E}_q \left[\log p(\mathbf{x}|\mathbf{z}, \theta) - \log \frac{q(\mathbf{z})}{p(\mathbf{z})} \right] d\mathbf{z} \rightarrow \max_{q, \theta}.\end{aligned}$$

Block-coordinate optimization

- ▶ Initialize θ^* ;
- ▶ **E-step** ($\mathcal{L}(q, \theta) \rightarrow \max_q$)

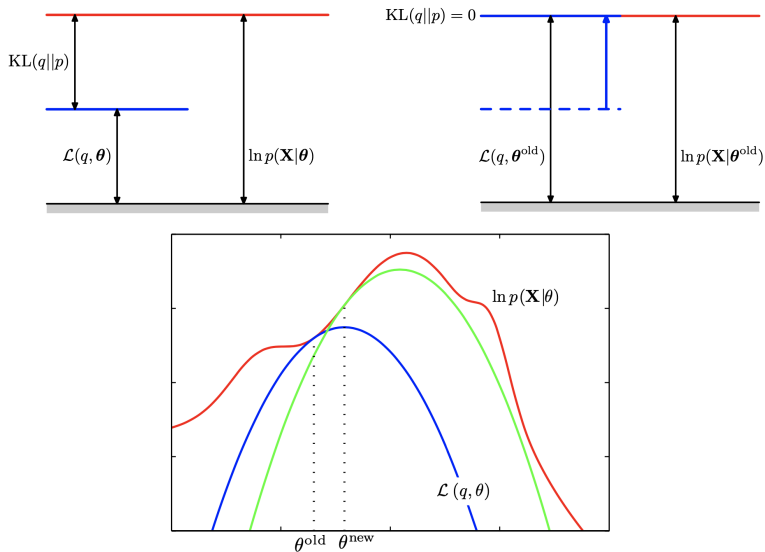
$$\begin{aligned}q^*(\mathbf{z}) &= \arg \max_q \mathcal{L}(q, \theta^*) = \\ &= \arg \min_q KL(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x}, \theta^*)) = p(\mathbf{z}|\mathbf{x}, \theta^*);\end{aligned}$$

- ▶ **M-step** ($\mathcal{L}(q, \theta) \rightarrow \max_\theta$)

$$\theta^* = \arg \max_\theta \mathcal{L}(q^*, \theta);$$

- ▶ Repeat E-step and M-step until convergence.

EM-algorithm illustration



Amortized variational inference

E-step

$$q(\mathbf{z}) = \arg \max_q \mathcal{L}(q, \theta^*) = \arg \min_q KL(q||p) = p(\mathbf{z}|\mathbf{x}, \theta^*).$$

- ▶ $q(\mathbf{z})$ approximates true posterior distribution $p(\mathbf{z}|\mathbf{x}, \theta^*)$, that is why it is called **variational posterior**;
- ▶ $p(\mathbf{z}|\mathbf{x}, \theta^*)$ could be **intractable**;
- ▶ $q(\mathbf{z})$ is different for each object \mathbf{x} .

Idea

Restrict a family of all possible distributions $q(\mathbf{z})$ to a parametric class $q(\mathbf{z}|\mathbf{x}, \phi)$ conditioned on samples \mathbf{x} with parameters ϕ .

Variational Bayes

- ▶ E-step

$$\phi_k = \phi_{k-1} + \eta \nabla_{\phi} \mathcal{L}(\phi, \theta_{k-1})|_{\phi=\phi_{k-1}}$$

- ▶ M-step

$$\theta_k = \theta_{k-1} + \eta \nabla_{\theta} \mathcal{L}(\phi_k, \theta)|_{\theta=\theta_{k-1}}$$

Variational EM-algorithm

ELBO

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

► E-step

$$\boldsymbol{\phi}_k = \boldsymbol{\phi}_{k-1} + \eta \nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}_{k-1})|_{\boldsymbol{\phi}=\boldsymbol{\phi}_{k-1}},$$

where $\boldsymbol{\phi}$ – parameters of variational posterior distribution $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$.

► M-step

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} + \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}_k, \boldsymbol{\theta})|_{\boldsymbol{\theta}=\boldsymbol{\theta}_{k-1}},$$

where $\boldsymbol{\theta}$ – parameters of the generative distribution $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$.

Now all we have to do is to obtain two gradients $\nabla_{\boldsymbol{\phi}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta})$, $\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta})$.

Challenge: Number of samples n could be huge (we need to derive unbiased stochastic gradients).

Summary

- ▶ 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.
- ▶ The general variational EM algorithm maximizes ELBO objective for LVM model to find MLE for parameters θ .