

Deep Generative Models

Lecture 3

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Recap of previous lecture

MLE problem for autoregressive model

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

Sampling

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

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

Masking helps to make neural network autoregressive.

- ▶ **MADE** - masked autoencoder (MLP).
- ▶ **WaveNet** - masked 1D convolutions.
- ▶ **PixelCNN** - masked 2D convolutions.

PixelCNN++ uses discretized mixture of logistic distribution to make the output distribution more natural.

Recap of previous lecture

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

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

Maximum a posteriori (MAP) estimation

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

MAP inference

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

Recap of previous lecture

Latent variable models (LVM)

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

MLE problem for LVM

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

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

Outline

1. Variational lower bound (ELBO)
2. EM-algorithm, amortized inference
3. ELBO gradients, reparametrization trick

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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

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

- ▶ Instead of maximizing incomplete likelihood, maximize ELBO

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

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

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

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3. ELBO gradients, reparametrization trick

EM-algorithm

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

Block-coordinate optimization

- ▶ Initialize θ^* ;
- ▶ E-step

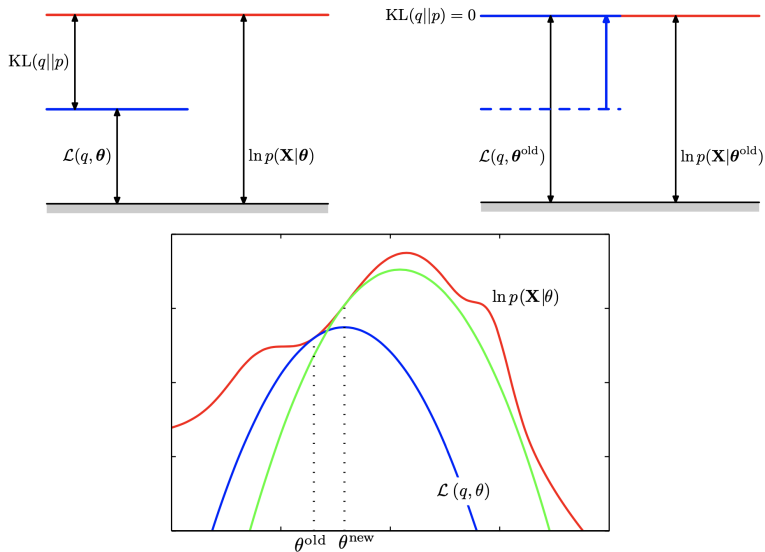
$$\begin{aligned} q^*(\mathbf{z}) &= \arg \max_q \mathcal{L}(q, \theta^*) = \\ &= \arg \min_q KL(q(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}, \theta^*)) = p(\mathbf{z}|\mathbf{x}, \theta^*); \end{aligned}$$

- ▶ M-step

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

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

EM 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).

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ELBO gradients, (M-step, $\nabla_{\theta} \mathcal{L}(\phi, \theta)$)

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) - \log \frac{q(\mathbf{z}|\mathbf{x}, \phi)}{p(\mathbf{z})} \right] \rightarrow \max_{\phi, \theta}.$$

M-step: $\nabla_{\theta} \mathcal{L}(\phi, \theta)$

$$\begin{aligned} \nabla_{\theta} \mathcal{L}(\phi, \theta) &= \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}, \theta) d\mathbf{z} \approx \\ &\approx \nabla_{\theta} \log p(\mathbf{x}|\mathbf{z}^*, \theta), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \phi). \end{aligned}$$

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

The variational posterior $q(\mathbf{z}|\mathbf{x}, \phi)$ assigns typically more probability mass in a smaller region than the prior $p(\mathbf{z})$.

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

ELBO gradients, (E-step, $\nabla_{\phi} \mathcal{L}(\phi, \theta)$)

E-step: $\nabla_{\phi} \mathcal{L}(\phi, \theta)$

Difference from M-step: density function $q(\mathbf{z}|\mathbf{x}, \phi)$ depends on the parameters ϕ , it is impossible to use the Monte-Carlo estimation:

$$\begin{aligned}\nabla_{\phi} \mathcal{L}(\phi, \theta) &= \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \phi)} \right] d\mathbf{z} \\ &\neq \int q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\phi} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \log \frac{p(\mathbf{z})}{q(\mathbf{z}|\mathbf{x}, \phi)} \right] d\mathbf{z}\end{aligned}$$

Reparametrization trick

- ▶ $r(x) = \mathcal{N}(x|0, 1)$, $y = \sigma \cdot x + \mu$, $p_Y(y|\theta) = \mathcal{N}(y|\mu, \sigma^2)$,
 $\theta = [\mu, \sigma]$.
- ▶ $\epsilon^* \sim r(\epsilon)$, $\mathbf{z} = g(\mathbf{x}, \epsilon, \phi)$, $\mathbf{z} \sim q(\mathbf{z}|\mathbf{x}, \phi)$

$$\begin{aligned}\nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) f(\mathbf{z}) d\mathbf{z} &= \nabla_{\phi} \int r(\epsilon) f(\mathbf{z}) d\epsilon \\ &= \int r(\epsilon) \nabla_{\phi} f(g(\mathbf{x}, \epsilon, \phi)) d\epsilon \approx \nabla_{\phi} f(g(\mathbf{x}, \epsilon^*, \phi))\end{aligned}$$

ELBO gradient (E-step, $\nabla_{\phi} \mathcal{L}(\phi, \theta)$)

$$\begin{aligned}\nabla_{\phi} \mathcal{L}(\phi, \theta) &= \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) \log p(\mathbf{x}|\mathbf{z}, \theta) d\mathbf{z} - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z})) \\ &= \int r(\epsilon) \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon, \phi), \theta) d\epsilon - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z})) \\ &\approx \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon^*, \phi), \theta) - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi) || p(\mathbf{z}))\end{aligned}$$

Variational assumption

$$r(\epsilon) = \mathcal{N}(0, \mathbf{I}); \quad q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mu_{\phi}(\mathbf{x}), \sigma_{\phi}^2(\mathbf{x})).$$

$$\mathbf{z} = g(\mathbf{x}, \epsilon, \phi) = \sigma_{\phi}(\mathbf{x}) \cdot \epsilon + \mu_{\phi}(\mathbf{x}).$$

Here $\mu_{\phi}(\cdot), \sigma_{\phi}(\cdot)$ are parameterized functions (outputs of neural network).

- ▶ $p(\mathbf{z})$ – prior distribution on latent variables \mathbf{z} . We could specify any distribution that we want. Let say $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.
- ▶ $p(\mathbf{x}|\mathbf{z}, \theta)$ – generative distribution. Since it is a parameterized function let it be neural network with parameters θ .

Summary

- ▶ LVM maximizes variational evidence lower bound (ELBO) to find MLE for the parameters.
- ▶ The general variational EM algorithm maximizes ELBO objective.
- ▶ Amortized variational inference allows to efficiently compute the stochastic gradients for ELBO using Monte-Carlo estimation.
- ▶ The reparametrization trick gets unbiased gradients w.r.t to the variational posterior distribution.