Deep Generative Models

Lecture 3

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Recap of previous lecture

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

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

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

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)

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

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

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)

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

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

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

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EM-algorithm

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

Block-coordinate optimization

- Initialize $\boldsymbol{\theta}^*$;
- E-step

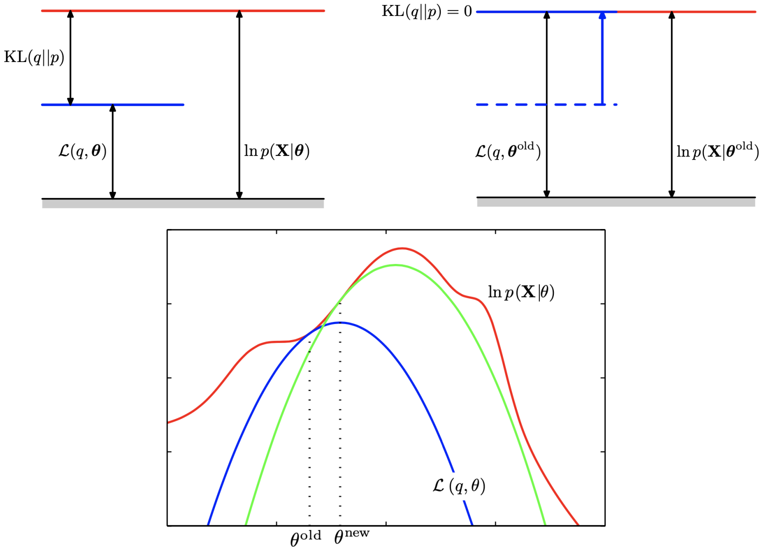
$$q^*(\mathbf{z}) = \arg\max_q \mathcal{L}(q, \boldsymbol{\theta}^*) =$$
$$= \arg\min_q KL(q(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$

- M-step

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

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

EM illustration



$\mathrm{KL}(q||p)$
$\mathcal{L}(q,\boldsymbol{\theta})$
$\ln p(\mathbf{X}|\boldsymbol{\theta})$
$\mathrm{KL}(q||p)=0$
$\mathcal{L}(q,\boldsymbol{\theta}^{\mathrm{old}})$
$\ln p(\mathbf{X}|\boldsymbol{\theta}^{\mathrm{old}})$
$\ln p(\mathbf{X}|\theta)$
$\mathcal{L}\left(q,\theta\right)$
θ^{old}
θ^{new}

Bishop C. Pattern Recognition and Machine Learning, 2006

Amortized variational inference

E-step

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

- $q(\mathbf{z})$ approximates true posterior distribution $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)$, that is why it is called **variational posterior**;
- $p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*)$ 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

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

- M-step

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

Variational EM-algorithm

ELBO

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

- E-step

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

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

- M-step

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

  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 heed to derive unbiased stochastic gradients).

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

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

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

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

$$\approx \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}|\mathbf{z}^*, \boldsymbol{\theta}), \quad \mathbf{z}^* \sim q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi}).$$

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

The variational posterior $q(\mathbf{z}|\mathbf{x}, \boldsymbol{\phi})$ 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, $\nabla_{\phi}\mathcal{L}(\phi, \boldsymbol{\theta})$)

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

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:

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

Reparametrization trick

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

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

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

$$\nabla_{\phi}\mathcal{L}(\phi, \boldsymbol{\theta}) = \nabla_{\phi} \int q(\mathbf{z}|\mathbf{x}, \phi) \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta}) d\mathbf{z} - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

$$= \int r(\epsilon) \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon, \phi), \boldsymbol{\theta}) d\epsilon - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

$$\approx \nabla_{\phi} \log p(\mathbf{x}|g(\mathbf{x}, \epsilon^*, \phi), \boldsymbol{\theta}) - \nabla_{\phi} \text{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))$$

Variational assumption

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

$$\mathbf{z} = g(\mathbf{x}, \epsilon, \phi) = \boldsymbol{\sigma}_{\phi}(\mathbf{x}) \cdot \epsilon + \boldsymbol{\mu}_{\phi}(\mathbf{x}).$$

Here $\boldsymbol{\mu}_{\phi}(\cdot), \boldsymbol{\sigma}_{\phi}(\cdot)$ 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 $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I})$.
- $p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})$ - generative distibution. Since it is a parameterized function let it be neural network with parameters $\boldsymbol{\theta}$.

Summary

- LVM maximizes variational evidence lower bound (ELBO) to find MLE for the parameters.
- The general variational EM algorithm maximizes ELBO objective.
- Amortized 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.