# Deep Generative Models Lecture 2

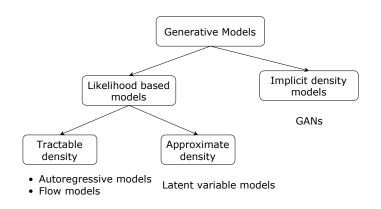
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#### Generative models zoo



# Bayesian framework

- x samples;
- y − target variables;
- ightharpoonup heta model parameters.

#### Discriminative

$$p(\mathbf{y}, \boldsymbol{\theta} | \mathbf{x}) = p(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}) p(\boldsymbol{\theta})$$

- Find conditional probability of y given x.
- ► Samples **x** are given.
- Used for classification, regression.

#### Generative

$$p(\mathbf{y}, \mathbf{x}, \boldsymbol{\theta}) = p(\mathbf{y}, \mathbf{x} | \boldsymbol{\theta}) p(\boldsymbol{\theta})$$

- Find joint probability of (x, y).
- Samples x should be modelled.
- Generation of new samples (x, y).

#### Generative models

We age given samples  $\{\mathbf{x}_i\}_{i=1}^n \in X$  from unknown distribution  $p(\mathbf{x})$ .

#### Goal

We would like to learn a distribution p(x) for

- evaluating  $p(\mathbf{x})$  for new samples;
- ightharpoonup sampling from p(x).

#### Challenge

Data is complex and high-dimensional (curse of dimensionality).

#### Solution

Fix probabilistic model  $p(\mathbf{x}|\theta)$  – the set of parameterized distributions .

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

# Latent variable models (LVM)

Suppose that our probabilistic model is  $p(\mathbf{x}, \mathbf{z}|\theta)$  instead of  $p(\mathbf{x}|\theta)$ .

- Here z are latent variables.
- ► We observe only samples x.
- Latent variables **z** are unknown.
- $\triangleright$  Parameters  $\theta$  are not random.

#### MLE problem for LVM

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

What if  $\theta$  are random variables with distribution  $p(\theta)$ ?

# Bayesian framework

What if  $\theta$  are random variables with distribution  $p(\theta)$ ?

Before we get any data, we do not know anything about  $\theta$  except the **prior** distribution  $p(\theta)$ .

When we get data, we could change the **prior** distribution to the **posterior**.

#### Bayes theorem

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

#### Full Bayesian inference

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

# Bayesian framework

#### Full Bayesian inference

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

Maximum a posteriori (MAP)

$$egin{aligned} m{ heta}^* &= rg\max_{m{ heta}} p(m{ heta}|\mathbf{X},\mathbf{Z}) = rg\max_{m{ heta}} ig(\log p(\mathbf{X},\mathbf{Z}|m{ heta}) + \log p(m{ heta})ig) \ p(\mathbf{x}^*|\mathbf{X},\mathbf{Z}) &= \int p(\mathbf{x}^*|m{ heta}) p(m{ heta}|\mathbf{X},\mathbf{Z}) dm{ heta} pprox p(\mathbf{x}^*|m{ heta}^*). \end{aligned}$$

#### Latent variable models

#### MLE problem

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

#### Challenge

 $p(\mathbf{x}|\boldsymbol{\theta})$  could be intractable.

#### Extend probabilistic model

Introduce latent variable z for each sample 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

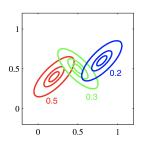
The distributions  $p(\mathbf{x}|\mathbf{z}, \theta)$  and  $p(\mathbf{z})$  could be quite simple.

#### Latent variable models

$$\log p(\mathbf{x}|oldsymbol{ heta}) = \log \int p(\mathbf{x}|\mathbf{z},oldsymbol{ heta}) p(\mathbf{z}) d\mathbf{z} 
ightarrow \max_{oldsymbol{ heta}}$$

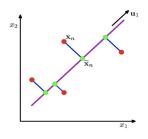
#### **Examples**

Mixture of gaussians



- $ho(\mathbf{x}|\mathbf{z}, oldsymbol{ heta}) = \mathcal{N}(\mathbf{x}|oldsymbol{\mu}_{\mathbf{z}}, oldsymbol{\Sigma}_{\mathbf{z}})$
- $p(z) = \text{Categorical}(z|\pi)$

#### PCA model

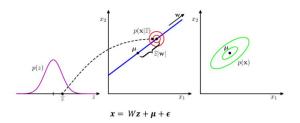


- $\qquad \qquad \rho(\mathsf{x}|\mathsf{z},\boldsymbol{\theta}) = \mathcal{N}(\mathsf{x}|\mathsf{Wz} + \boldsymbol{\mu},\boldsymbol{\Sigma}_{\mathsf{z}})$
- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0,\mathbf{I})$

#### Latent variable models

$$\log p(\mathbf{x}|oldsymbol{ heta}) = \log \int p(\mathbf{x}|\mathbf{z},oldsymbol{ heta}) p(\mathbf{z}) d\mathbf{z} 
ightarrow \max_{oldsymbol{ heta}}$$

**PCA goal:** Project original data **X** onto low latent space while maximizing the variance of the projected data.



- $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|0,\mathbf{I})$

### Incomplete likelihood

**MLE** 

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

Since **Z** is unknown, maximize **incomplete likelihood**.

#### MILE problem

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

#### Variational lower bound

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

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

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

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

#### Kullback-Leibler divergence

- $KL(q||p) = \int q(\mathbf{z}) \log \frac{q(\mathbf{z})}{p(\mathbf{z})} d\mathbf{z};$
- $KL(q||p) \geq 0$ ;
- $\mathsf{KL}(q||p) = 0 \Leftrightarrow q \equiv p.$

#### Variational lower bound

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

#### Evidence Lower Bound (ELBO)

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

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

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

Instead of maximizing incomplete likelihood, maximize ELBO (equivalently minimize KL)

$$\max_{ heta} p(\mathbf{x}|oldsymbol{ heta}) \quad o \quad \max_{q, heta} \mathcal{L}(q,oldsymbol{ heta}) \equiv \min_{q, heta} \mathit{KL}(q(\mathbf{z})||p(\mathbf{z}|\mathbf{x},oldsymbol{ heta})).$$

# EM-algorithm

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

#### Block-coordinate optimization

- Initialize θ\*;
- E-step

$$q(\mathbf{z}) = \underset{q}{\operatorname{arg max}} \mathcal{L}(q, \boldsymbol{\theta}^*) = \underset{q}{\operatorname{arg min}} \mathit{KL}(q||p) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*);$$

M-step

$$oldsymbol{ heta}^* = rg\max_{oldsymbol{ heta}} \mathcal{L}(oldsymbol{q}, oldsymbol{ heta});$$

Repeat E-step and M-step until convergence.

# Ugly pic

#### Amortized variational inference

#### E-step

$$q(\mathbf{z}) = rg \max_{q} \mathcal{L}(q, \boldsymbol{\theta}^*) = rg \min_{q} \mathit{KL}(q||p) = p(\mathbf{z}|\mathbf{x}, \boldsymbol{\theta}^*).$$

could be intractable.

#### Idea

Restrict a family of all possible distributions  $q(\mathbf{z})$  to a particular parametric class conditioned on sample:  $q(\mathbf{z}|\mathbf{x}, \phi)$ .

#### 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**

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

E-step

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

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

M-step

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

where  $\theta$  – parameters of likelihood  $p(\mathbf{x}|\mathbf{z},\theta)$ .

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

**Difficulty:** number of samples n.

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \theta) - \mathit{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z})) \to \max_{\phi, \theta}.$$

Optimization w.r.t.  $\theta$ : **mini-batching** (1) + **Monte-Carlo** estimation (2)

$$\nabla_{\theta} \mathcal{L}(\phi, \theta) = \sum_{i=1}^{n} \int q(\mathbf{z}_{i}|\mathbf{x}_{i}, \phi) \nabla_{\theta} \log p(\mathbf{x}_{i}|\mathbf{z}_{i}, \theta) d\mathbf{z}_{i}$$

$$\stackrel{(1)}{\approx} n \int q(\mathbf{z}_{i}|\mathbf{x}_{i}, \phi) \nabla_{\theta} \log p(\mathbf{x}_{i}|\mathbf{z}_{i}, \theta) d\mathbf{z}_{i}, \quad i \sim U[1, n]$$

$$\stackrel{(2)}{\approx} n \nabla_{\theta} \log p(\mathbf{x}_{i}|\mathbf{z}_{i}^{*}, \theta), \quad \mathbf{z}_{i}^{*} \sim q(\mathbf{z}_{i}|\mathbf{x}_{i}, \phi).$$

Monte-Carlo estimation (2):

$$\int q(\mathbf{z})f(\mathbf{z})d\mathbf{z}pprox f(\mathbf{z}^*), ext{where } \mathbf{z}^*\sim q(\mathbf{z}).$$

$$\mathcal{L}(\phi, \theta) = \mathbb{E}_q \log p(\mathbf{x}|\mathbf{z}, \theta) - \mathit{KL}(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z})) 
ightarrow \max_{\phi, \theta}.$$

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

$$abla_{\phi}\mathcal{L}(\phi, oldsymbol{ heta}) = \int 
abla_{\phi}q(\mathbf{z}|\mathbf{x}, \phi)\log p(\mathbf{x}|\mathbf{z}, oldsymbol{ heta})d\mathbf{z} - 
abla_{\phi}KL$$

#### Log-derivative trick

$$abla_{\xi} q(\eta|\xi) = q(\eta|\xi) \left(rac{
abla_{\xi} q(\eta|\xi)}{q(\eta|\xi)}
ight) = q(\eta|\xi) 
abla_{\xi} \log q(\eta|\xi).$$

$$abla_{\phi} q(\mathbf{z}|\mathbf{x}, \phi) = q(\mathbf{z}|\mathbf{x}, \phi) \nabla_{\phi} \log q(\mathbf{z}|\mathbf{x}, \phi).$$

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

$$= \int q(\mathbf{z}|\mathbf{x}, \phi) [\nabla_{\phi} \log q(\mathbf{z}|\mathbf{x}, \phi) \log p(\mathbf{x}|\mathbf{z}, \theta)] d\mathbf{z} - \nabla_{\phi} KL$$

After applying the log-reparametrization trick, we are able to use the Monte-Carlo estimation:

$$abla_{\phi} \mathcal{L}(\phi, m{ heta}) pprox n 
abla_{\phi} \log q(\mathbf{z}_i^* | \mathbf{x}_i, \phi) \log p(\mathbf{x}_i | \mathbf{z}_i^*, m{ heta}) - 
abla_{\phi} KL, 
onumber \ \mathbf{z}_i^* \sim q(\mathbf{z}_i | \mathbf{x}_i, \phi).$$

#### **Problem**

Unstable solution with huge variance.

#### Solution

Reparametrization trick

#### Reparametrization trick

$$f(\xi) = \int q(\eta|\xi)h(\eta)d\eta$$

Let  $\eta = g(\xi, \epsilon)$ , where g is a deterministic function,  $\epsilon$  is a random variable with a density function  $r(\epsilon)$ .

$$egin{aligned} 
abla_{\xi} \int q(\eta|\xi)h(\eta)d\eta &= 
abla_{\xi} \int r(\epsilon)h(g(\xi,\epsilon))d\epsilon \ &pprox 
abla_{\xi}h(g(\xi,\epsilon^*)), \quad \epsilon^* \sim r(\epsilon). \end{aligned}$$

#### Example

$$q(\eta|\xi) = \mathcal{N}(\eta|\mu, \sigma^2), \quad r(\epsilon) = \mathcal{N}(\epsilon|0, 1), \quad \eta = \sigma \cdot \epsilon + \mu, \quad \xi = [\mu, \sigma].$$

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

$$\approx n \nabla_{\phi} \int r(\epsilon) \log p(\mathbf{x}_{i}|g(\mathbf{x}_{i}, \epsilon, \phi), \theta) d\epsilon - \nabla_{\phi} KL$$

$$\approx n \nabla_{\phi} \log p(\mathbf{x}_{i}|g(\mathbf{x}_{i}, \epsilon^{*}, \phi), \theta) - \nabla_{\phi} KL, \quad \epsilon^{*} \sim r(\epsilon).$$

#### Variational assumption

$$egin{aligned} q(\mathbf{z}|\mathbf{x},\phi) &= \mathcal{N}(\mu(\mathbf{x}),\mathbf{\Sigma}(\mathbf{x})). \ \mathbf{z} &= g(\mathbf{x},\epsilon,\phi) &= \sqrt{\mathbf{\Sigma}(\mathbf{x})} \cdot \epsilon + \mu(\mathbf{x}). \end{aligned}$$

 $\nabla_{\phi} \mathit{KL}(q(\mathbf{z}|\mathbf{x},\phi)||p(\mathbf{z}))$  has an analytical solution.

# Variational autoencoder (VAE)

#### Final algorithm

- ▶ pick  $i \sim U[1, n]$ ;
- ightharpoonup compute stochastic gradient w.r.t.  $\phi$

$$\nabla_{\phi} \mathcal{L}(\phi, \theta) = n \nabla_{\phi} \log p(\mathbf{x}_i | g(\mathbf{x}_i, \epsilon^*, \phi), \theta) - \\ - \nabla_{\phi} KL(q(\mathbf{z}_i | \mathbf{x}_i, \phi) || p(\mathbf{z}_i)), \quad \epsilon^* \sim r(\epsilon);$$

ightharpoonup compute stochastic gradient w.r.t. heta

$$\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\phi}, \boldsymbol{\theta}) = n \nabla_{\boldsymbol{\theta}} \log p(\mathbf{x}_i | \mathbf{z}_i^*, \boldsymbol{\theta}), \quad \mathbf{z}_i^* \sim q(\mathbf{z}_i | \mathbf{x}_i, \boldsymbol{\phi});$$

• update  $\theta$ ,  $\phi$  according to the selected optimization method (SGD, Adam, RMSProp).

# Variational autoencoder (VAE)

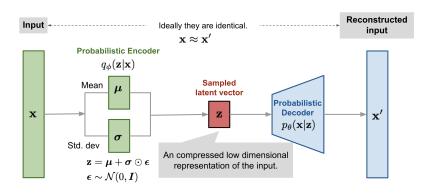
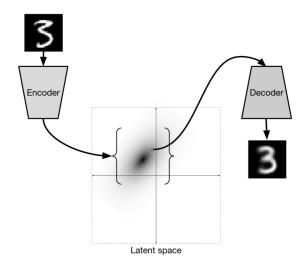


image credit:

#### Variational Autoencoder



#### Variational Autoencoder

Generation objects by sampling the latent space  $\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$ 

# Bayesian framework

#### Bayes theorem

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

- x observed variables;
- ▶ t unobserved variables (latent variables/parameters);
- $p(\mathbf{x}|\mathbf{t})$  likelihood;
- p(x) evidence;
- p(t) − prior;
- $ightharpoonup p(\mathbf{t}|\mathbf{x})$  posterior.

# Summary