# Deep Generative Models

Lecture 9

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## Autoregressive flow prior

$$\log p(\mathbf{z}|\boldsymbol{\lambda}) = \log p(\epsilon) + \log \det \left| \frac{d\epsilon}{d\mathbf{z}} \right|; \quad \mathbf{z} = g(\epsilon, \boldsymbol{\lambda}) = f^{-1}(\epsilon, \boldsymbol{\lambda})$$

#### **Theorem**

VAE with the AF prior for latent code z is equivalent to using the IAF posterior for latent code  $\epsilon$ .

$$\begin{split} \mathcal{L}(q, \theta) &= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \bigg[ \log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\bigg( \log p(f(\mathbf{z}, \boldsymbol{\lambda})) + \log \bigg| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \bigg| \bigg)}_{\text{AF prior}} - \log q(\mathbf{z}|\mathbf{x}) \bigg] \\ &= \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z}|\mathbf{x})} \bigg[ \log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(f(\mathbf{z}, \boldsymbol{\lambda})) - \underbrace{\bigg( \log q(\mathbf{z}|\mathbf{x}) - \log \bigg| \det \frac{\partial f(\mathbf{z}, \boldsymbol{\lambda})}{\partial \mathbf{z}} \bigg| \bigg)}_{\text{IAF posterior}} \bigg] \end{split}$$

#### **ELBO**

$$p(\mathbf{x}|oldsymbol{ heta}) \geq \mathcal{L}(oldsymbol{\phi},oldsymbol{ heta}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},oldsymbol{\phi})} \log rac{p(\mathbf{x},\mathbf{z}|oldsymbol{ heta})}{q(\mathbf{z}|\mathbf{x},oldsymbol{\phi})} 
ightarrow \max_{oldsymbol{\phi},oldsymbol{ heta}}.$$

- Normal variational distribution  $q(\mathbf{z}|\mathbf{x},\phi) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}_{\phi}(\mathbf{x}), \boldsymbol{\sigma}_{\phi}^2(\mathbf{x}))$  is poor (e.g. has only one mode).
- ► Flows models convert a simple base distribution to a compex one using an invertible transformation with simple Jacobian.

## Flow model in latent space

$$\log q_K(\mathbf{z}_K|\mathbf{x},\phi_*) = \log q(\mathbf{z}_0|\mathbf{x},\phi) - \sum_{k=1}^K \log \left| \det \left( \frac{\partial g_k(\mathbf{z}_{k-1},\phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

Let's use  $q_K(\mathbf{z}_K|\mathbf{x},\phi_*),\ \phi_*=\{\phi,\phi_1,\ldots,\phi_K\}$  as a variational distribution. Here,  $\phi$  – encoder parameters,  $\{\phi_k\}_{k=1}^K$  – flow parameters.

#### Variational distribution

$$\log q_K(\mathbf{z}_K|\mathbf{x},\phi_*) = \log q(\mathbf{z}_0|\mathbf{x},\phi) - \sum_{k=1}^K \log \left| \det \left( \frac{\partial g_k(\mathbf{z}_{k-1},\phi_k)}{\partial \mathbf{z}_{k-1}} \right) \right|.$$

## **ELBO** objective

$$egin{aligned} \mathcal{L}(\phi, oldsymbol{ heta}) &= \mathbb{E}_{q(\mathbf{z}_0|\mathbf{x}, oldsymbol{\phi})} igg[ \log p(\mathbf{x}, \mathbf{z}_K | oldsymbol{ heta}) - \log q(\mathbf{z}_0 | \mathbf{x}, oldsymbol{\phi}) + \\ &+ \sum_{k=1}^K \log \left| \det \left( rac{\partial g_k(\mathbf{z}_{k-1}, oldsymbol{\phi}_k)}{\partial \mathbf{z}_{k-1}} 
ight) 
ight| igg]. \end{aligned}$$

- $\triangleright$  Obtain samples  $\mathbf{z}_0$  from the encoder.
- Apply flow model  $\mathbf{z}_K = g(\mathbf{z}_0, \{\phi_k\}_{k=1}^K)$ .
- ▶ Compute likelihood for  $\mathbf{z}_K$  using the decoder, base distribution for  $\mathbf{z}_0$  and the Jacobian.
- ▶ We do not need an inverse flow function if we use flows in variational inference.

Images are discrete data flow is a continuous model. We need to convert a discrete data distribution to a continuous one.

# Uniform dequantization bound

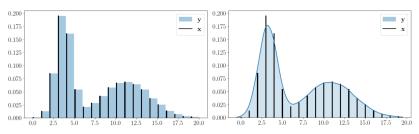
$$\mathbf{x} \sim \mathsf{Categorical}(\boldsymbol{\pi}), \quad \mathbf{u} \sim U[0,1], \quad \mathbf{y} = \mathbf{x} + \mathbf{u} \sim \mathsf{Continuous}$$
 
$$\log P(\mathbf{x}|\boldsymbol{\theta}) \geq \int_{U[0,1]} \log p(\mathbf{x} + \mathbf{u}|\boldsymbol{\theta}) d\mathbf{u}.$$

# Variational dequantization bound

Introduce variational dequantization noise distribution  $q(\mathbf{u}|\mathbf{x})$  and treat it as an approximate posterior.

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

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019



# Flow model for dequantization

$$q(\mathbf{u}|\mathbf{x}) = p(h^{-1}(\mathbf{u}, \phi)) \cdot \left| \det \frac{\partial h^{-1}(\mathbf{u}, \phi)}{\partial \mathbf{u}} \right|.$$

# Variational dequantization bound

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

Ho J. et al. Flow++: Improving Flow-Based Generative Models with Variational Dequantization and Architecture Design, 2019

# Disentanglement learning

A disentangled representation is a one where single latent units are sensitive to changes in single generative factors, while being invariant to changes in other factors.

**β-VAE** 

$$\mathcal{L}(q, \theta, \beta) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})} \log p(\mathbf{x}|\mathbf{z}, \theta) - \beta \cdot KL(q(\mathbf{z}|\mathbf{x})||p(\mathbf{z})).$$

Representations becomes disentangled by setting a stronger constraint with  $\beta>1$ . However, it leads to poorer reconstructions and a loss of high frequency details.

# **ELBO** surgery

$$\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{i}(q, \boldsymbol{\theta}, \beta) = \underbrace{\frac{1}{n} \sum_{i=1}^{n} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_{i})} \log p(\mathbf{x}_{i}|\mathbf{z}, \boldsymbol{\theta})}_{\text{Reconstruction loss}} - \beta \cdot \underbrace{\mathbb{I}_{q}[\mathbf{x}, \mathbf{z}] - \beta \cdot \underbrace{KL(q(\mathbf{z})||p(\mathbf{z}))}_{\text{Marginal KL}}$$

#### **DIP-VAE**

# Disentangled aggregated variational posterior

$$q(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^{n} q(\mathbf{z}|\mathbf{x}) = \prod_{j=1}^{d} q(z_j)$$

#### **DIP-VAE Objective**

$$\begin{split} \mathcal{L}_{\mathsf{DIP}}(q, \boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{i}(q, \boldsymbol{\theta}) - \lambda \cdot \mathsf{KL}(q(\mathbf{z}) || p(\mathbf{z})) = \\ &= \frac{1}{n} \sum_{i=1}^{n} \left[ \mathbb{E}_{q(\mathbf{z} | \mathbf{x}_{i})} \log p(\mathbf{x}_{i} | \mathbf{z}, \boldsymbol{\theta}) - \mathsf{KL}(q(\mathbf{z} | \mathbf{x}_{i}) || p(\mathbf{z})) \right] - \lambda \cdot \mathsf{KL}(q(\mathbf{z}) || p(\mathbf{z})) = \\ &= \underbrace{\frac{1}{n} \sum_{i=1}^{n} \left[ \mathbb{E}_{q(\mathbf{z} | \mathbf{x}_{i})} \log p(\mathbf{x}_{i} | \mathbf{z}, \boldsymbol{\theta}) \right] - \mathbb{I}_{q}[\mathbf{x}, \mathbf{z}] - (1 + \lambda) \cdot \underbrace{\mathsf{KL}(q(\mathbf{z}) || p(\mathbf{z}))}_{\mathsf{Marginal} \; \mathsf{KL}} \right]}_{\mathsf{Reconstruction \; loss} \end{split}$$

#### **DIP-VAE**

$$\mathcal{L}_{\mathsf{DIP}}(q, oldsymbol{ heta}) = rac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{i}(q, oldsymbol{ heta}) - \lambda \cdot \underbrace{\mathcal{K}\!\mathcal{L}\!(q(\mathbf{z})||p(\mathbf{z}))}_{\mathsf{intractable}}$$

Let match the moments of q(z) and p(z):

$$\mathsf{cov}_{q(\mathsf{z})}(\mathsf{z}) = \mathbb{E}_{q(\mathsf{z})}\left[ (\mathsf{z} - \mathbb{E}_{q(\mathsf{z})}(\mathsf{z}))(\mathsf{z} - \mathbb{E}_{q(\mathsf{z})}(\mathsf{z}))^T 
ight]$$

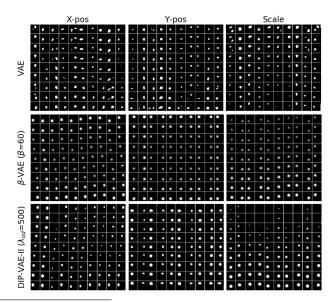
DIP-VAE regularizes  $cov_{q(z)}(z)$  to be close to the identity matrix.

## Objective

$$\max_{q,\boldsymbol{\theta}} \left[ \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}_{i}(q,\boldsymbol{\theta}) - \lambda_{1} \sum_{i \neq i} \left[ \mathsf{cov}_{q(\mathbf{z})}(\mathbf{z}) \right]_{ij}^{2} - \lambda_{2} \sum_{i} \left( \left[ \mathsf{cov}_{q(\mathbf{z})}(\mathbf{z}) \right]_{ii} - 1 \right)^{2} \right]$$

Kumar A., Sattigeri P., Balakrishnan A. Variational Inference of Disentangled Latent Concepts from Unlabeled Observations, 2017

#### DIP-VAE



Kumar A., Sattigeri P., Balakrishnan A. Variational Inference of Disentangled Latent Concepts from Unlabeled Observations, 2017

Whether unsupervised disentanglement learning is even possible for arbitrary generative models?

#### **Theorem**

For d > 1, let  $\mathbf{z} \sim P$  denote any distribution which admits a density  $p(\mathbf{z}) = \prod_{i=1}^d p(z_i)$ . Then, there exists an infinite family of bijective functions  $f : \operatorname{supp}(\mathbf{z}) \to \operatorname{supp}(\mathbf{z})$  such that

- ▶  $\frac{\partial f_i(\mathbf{z})}{\partial z_j} \neq 0$  almost everywhere for all i and j (i.e.,  $\mathbf{z}$  and  $f(\mathbf{z})$  are completely entangled);
- ▶ and  $P(\mathbf{z} \le \mathbf{u}) = P(f(\mathbf{z}) \le \mathbf{u})$  for all  $\mathbf{u} \in \text{supp}(\mathbf{z})$  (i.e., they have the same marginal distribution).

Theorem claims that unsupervised disentanglement learning is impossible for arbitrary generative models with a factorized prior.

Assume we have  $p(\mathbf{z})$  and some  $p(\mathbf{x}|\mathbf{z})$  defining a generative model. Consider any unsupervised disentanglement method and assume that it finds a representation that is perfectly disentangled with respect to  $\mathbf{z}$  in the generative model.

- ► Theorem claims that  $\exists \ \hat{\mathbf{z}} = f(\mathbf{z})$  where  $\hat{\mathbf{z}}$  is completely entangled with respect to  $\mathbf{z}$ .
- ➤ Since the (unsupervised) disentanglement method only has access to observations x, it hence cannot distinguish between the two equivalent generative models and thus has to be entangled to at least one of them

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

# Proof (1)

1. Consider the function  $g : \text{supp}(\mathbf{z}) \to [0, 1]^d$ :

$$g_i(\mathbf{u}) = P(z_i \leq u_i), \quad i = 1, \ldots, d.$$

- ightharpoonup g is bijective (since  $p(\mathbf{z}) = \prod_{i=1}^d p(z_i)$ ).
- $ightharpoonup \frac{\partial g_i(\mathbf{u})}{\partial u_i} \neq 0$ , for all i and  $\frac{\partial g_i(\mathbf{u})}{\partial u_i} = 0$  for all  $i \neq j$ .
- $ightharpoonup g(\mathbf{z})$  is an independent d-dimensional uniform distribution.
- 2. Consider  $h:(0,1]^d \to \mathbb{R}^d$

$$h_i(\mathbf{u}) = \psi^{-1}(u_i), \quad i = 1, \dots, d.$$

Here  $\psi$  denotes the CDF of a standard normal distribution.

- h is bijective.
- ▶  $\frac{\partial h_i(\mathbf{u})}{\partial u_i} \neq 0$ , for all i and  $\frac{\partial h_i(\mathbf{u})}{\partial u_i} = 0$  for all  $i \neq j$ .
- h(g(z)) is a d-dimensional standard normal distribution.

# Proof (2)

Let  $\mathbf{A} \in \mathbb{R}^{d \times d}$  be an arbitrary orthogonal matrix with  $A_{ij} \neq 0$  for all i, j. The family of such matrices is infinite.

- ► **A** is orthogonal, it is invertible and thus defines a bijective linear operator.
- ▶  $\mathbf{A}h(g(\mathbf{z})) \in \mathbb{R}^d$  is hence an independent, multivariate standard normal distribution.
- ▶  $h^{-1}(\mathbf{A}h(g(\mathbf{z}))) \in \mathbb{R}^d$  is an independent d-dimensional uniform distribution.

Define  $f : \text{supp}(\mathbf{z}) \rightarrow \text{supp}(\mathbf{z})$ :

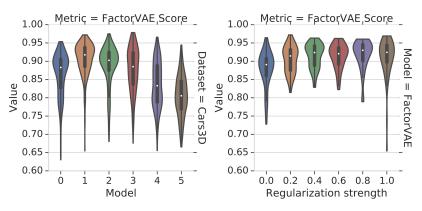
$$f(\mathbf{u}) = g^{-1}(h^{-1}(\mathbf{A}h(g(\mathbf{z})))).$$

By definition f(z) has the same marginal distribution as z:

$$P(\mathbf{z} \leq \mathbf{u}) = P(f(\mathbf{z}) \leq \mathbf{u}) \text{ and } \frac{\partial f_i(\mathbf{z})}{\partial \mathbf{z}_i} \neq 0.$$

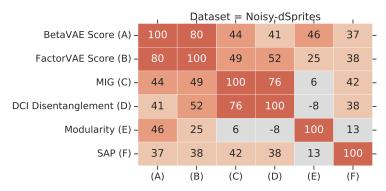
Locatello F. et al. Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations, 2018

# Importance of different models and hyperparameters for disentanglement

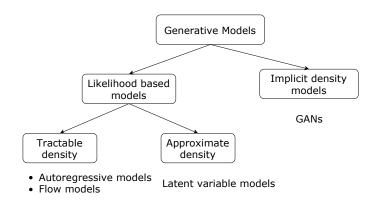


Locatello F. et al. Challenging Common Assumptions in the Unsupervised Learning of Disentangled Representations, 2018

# Agreement of different disentanglement metrics



#### Generative models zoo



# Likelihood based models

Is likelihood a good measure of model quality?

Poor likelihood Great samples

$$p_1(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \mathcal{N}(\mathbf{x} | \mathbf{x}_i, \epsilon \mathbf{I})$$

For small  $\epsilon$  this model will generate samples with great quality, but likelihood will be very poor.

Great likelihood Poor samples

$$p_2(\mathbf{x}) = 0.01p(\mathbf{x}) + 0.99p_{\mathsf{noise}}(\mathbf{x})$$

$$egin{aligned} \log\left[0.01p(\mathbf{x})+0.99p_{\mathsf{noise}}(\mathbf{x})
ight] \geq \\ \geq \log\left[0.01p(\mathbf{x})
ight] = \log p(\mathbf{x}) - \log 100 \end{aligned}$$

Noisy irrelevant samples, but for high dimensions  $\log p(\mathbf{x})$  becomes proportional to m.

# Likelihood-free learning

- Likelihood is not a perfect measure quality measure for generative model.
- Likelihood could be intractable.

#### Where did we start

We would like to approximate true data distribution  $\pi(\mathbf{x})$ . Instead of searching true  $\pi(\mathbf{x})$  over all probability distributions, learn function approximation  $p(\mathbf{x}|\theta) \approx \pi(\mathbf{x})$ .

Imagine we have two sets of samples

- $\triangleright$   $S_1 = \{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$  real samples;
- $\triangleright$   $S_2 = \{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\boldsymbol{\theta})$  generated (or fake) samples.

# Two sample test

$$H_0: \pi(\mathbf{x}) = \rho(\mathbf{x}|\boldsymbol{\theta}), \quad H_1: \pi(\mathbf{x}) \neq \rho(\mathbf{x}|\boldsymbol{\theta})$$

Define test statistic  $T(S_1, S_2)$ . The test statistic is likelihood free. If  $T(S_1, S_2) < \alpha$ , then accept  $H_0$ , else reject it.

# Likelihood-free learning

## Two sample test

$$H_0: \pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta}), \quad H_1: \pi(\mathbf{x}) \neq p(\mathbf{x}|\boldsymbol{\theta})$$

#### Desired behaviour

- $\triangleright$   $p(\mathbf{x}|\theta)$  minimizes the value of test statistic  $T(S_1, S_2)$ .
- ▶ It is hard to find an appropriate test statistic in high dimensions.  $T(S_1, S_2)$  could be learnable.

# **GAN** objective

$$\min_{G} \max_{D} V(G, D) = \min_{G} \max_{D} \left[ \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(G(\mathbf{z}))) \right]$$

- ▶ **Generator:** generative model  $\mathbf{x} = G(\mathbf{z})$ , which makes generated sample more realistic.
- **Discriminator:** a classifier  $D(\mathbf{x}) \in [0, 1]$ , which distinguishes real samples from generated samples.

# Vanilla GAN optimality

#### **Theorem**

The minimax game

$$\min_{G} \max_{D} V(G, D) = \min_{G} \max_{D} \left[ \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(G(\mathbf{z}))) \right]$$

has the global optimum  $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$ , in this case  $D^*(\mathbf{x}) = 0.5$ .

# Proof (fixed G)

$$V(G, D) = \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\theta)} \log(1 - D(\mathbf{x}))$$

$$= \int \underbrace{\left[\pi(\mathbf{x}) \log D(\mathbf{x}) + p(\mathbf{x}|\theta) \log(1 - D(\mathbf{x})\right]}_{y(D)} d\mathbf{x}$$

$$\frac{dy(D)}{dD} = \frac{\pi(\mathbf{x})}{D(\mathbf{x})} - \frac{p(\mathbf{x}|\theta)}{1 - D(\mathbf{x})} = 0 \quad \Rightarrow \quad D^*(\mathbf{x}) = \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)}$$

# Vanilla GAN optimality

Proof confitnued (fixed  $D = D^*$ )

$$V(G, D^*) = \mathbb{E}_{\pi(\mathbf{x})} \log \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)} + \mathbb{E}_{p(\mathbf{x}|\theta)} \log \frac{p(\mathbf{x}|\theta)}{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)}$$

$$= KL\left(\pi(\mathbf{x})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)}{2}\right) + KL\left(p(\mathbf{x}|\theta)||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\theta)}{2}\right) - 2\log 2$$

$$= 2JSD(\pi(\mathbf{x})||p(\mathbf{x}|\theta)) - 2\log 2.$$

Jensen-Shannon divergence (symmetric KL divergence)

$$JSD(\pi(\mathbf{x})||p(\mathbf{x}|\boldsymbol{\theta})) = \frac{1}{2} \left[ KL\left(\pi(\mathbf{x})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right) + KL\left(p(\mathbf{x}|\boldsymbol{\theta})||\frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2}\right) \right]$$

Could be used as a distance measure!

$$V(G^*, D^*) = -2 \log 2$$
,  $\pi(\mathbf{x}) = p(\mathbf{x}|\theta)$ .

# Vanilla GAN optimality

#### Theorem

The minimax game

$$\min_{G} \max_{D} V(G, D) = \min_{G} \max_{D} \left[ \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(G(\mathbf{z}))) \right]$$

has the global optimum  $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$ , in this case  $D^*(\mathbf{x}) = 0.5$ .

#### Proof

for fixed G:

$$D^*(\mathbf{x}) = \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + \rho(\mathbf{x}|\boldsymbol{\theta})}$$

for fixed  $D = D^*$ :

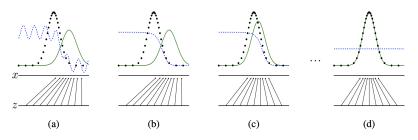
$$\min_{G} V(G, D^*) = \min_{G} \left[ 2JSD(\pi||p) - \log 4 \right] = -\log 4, \quad \pi(\mathbf{x}) = p(\mathbf{x}|\theta).$$

If the generator could be any function and the discriminator is optimal at every step, then the generator is guaranteed to converge to the data distribution.

## Vanilla GAN

# Objective

$$\min_{G} \max_{D} V(G, D) = \min_{G} \max_{D} \left[ \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(G(\mathbf{z}))) \right]$$



- Generator updates are made in parameter space.
- ▶ Discriminator is not optimal at every step.
- Generator and discriminator loss keeps oscillating during GAN training.

# Summary

- Majority of disentanglement learning models use heuristic objective or regularizers to achieve the goal, but the task itself could not be solved without good inductive bias.
- Likelihood is not a perfect criteria to measure quality of generative model.
- Adversarial learning suggest to solve minimax problem to match the distributions.
- Vanilla GAN tries to optimize Jensen-Shannon divergence (in theory).