

Deep Generative Models

Lecture 9

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Recap of previous lecture

Disentanglement learning

A disentangled representation is 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

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

Recap of previous lecture

Likelihood-free learning

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

Imagine we have two sets of samples

- ▶ $\mathcal{S}_1 = \{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ – real samples;
- ▶ $\mathcal{S}_2 = \{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\theta)$ – generated (or fake) samples.

Two sample test

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

If test statistic $T(\mathcal{S}_1, \mathcal{S}_2) < \alpha$, then accept H_0 , else reject it.

- ▶ $p(\mathbf{x}|\theta)$ minimizes the value of test statistic $T(\mathcal{S}_1, \mathcal{S}_2)$.
- ▶ It is hard to find an appropriate test statistic in high dimensions. $T(\mathcal{S}_1, \mathcal{S}_2)$ could be learnable.

Recap of previous lecture

- ▶ **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.

GAN optimality theorem

The minimax game

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

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

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

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.

Outline

1. Vanishing gradients and mode collapse
2. Adversarial variational Bayes
3. Wasserstein distance
4. Wasserstein GAN

Outline

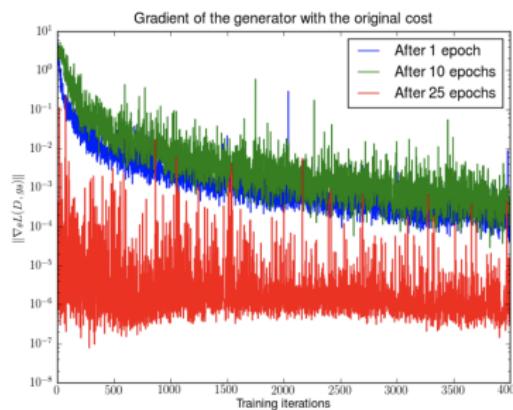
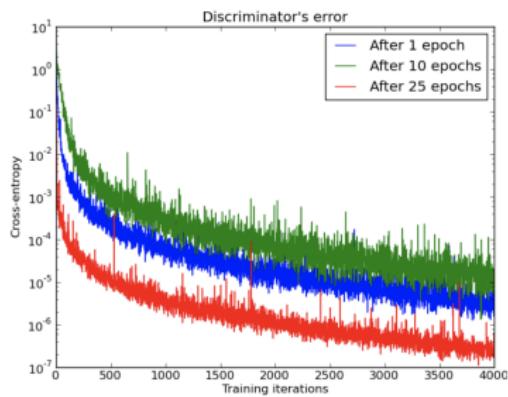
1. Vanishing gradients and mode collapse
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Vanishing gradients

Objective

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

Early in learning, G is poor, D can reject samples with high confidence. In this case, $\log(1 - D(G(\mathbf{z}, \theta), \phi))$ saturates.



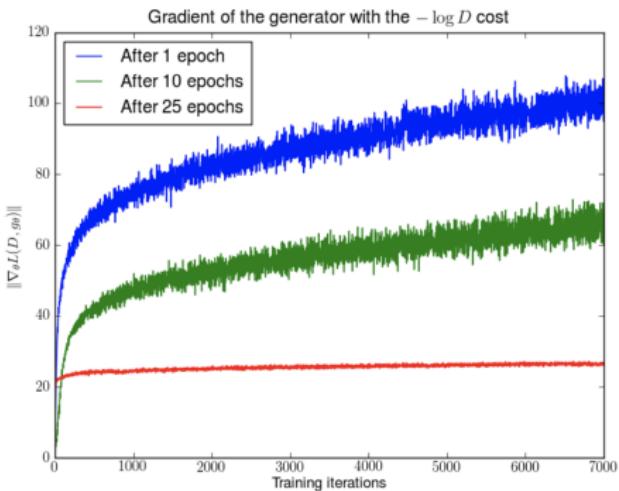
Vanishing gradients

Objective

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

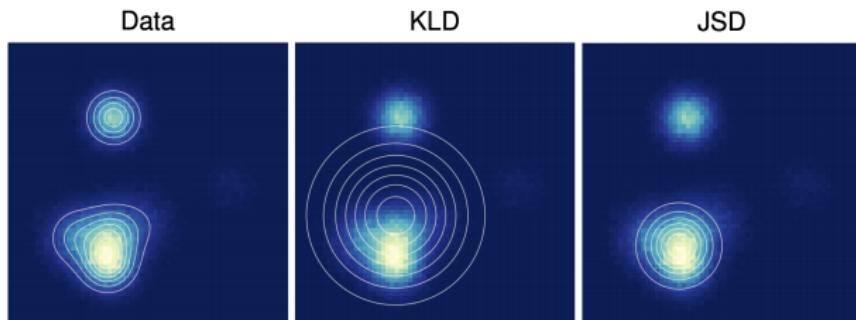
Non-saturating GAN

- ▶ Maximize $\log D(G(z))$ instead of minimizing $\log(1 - D(G(z)))$.
- ▶ Gradients are getting much stronger, but the training is unstable (with increasing mean and variance).



Mode collapse

The phenomena where the generator of a GAN collapses to one or few distribution modes.



Alternate architectures, adding regularization terms, injecting small noise perturbations and other millions bags and tricks are used to avoid the mode collapse.

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

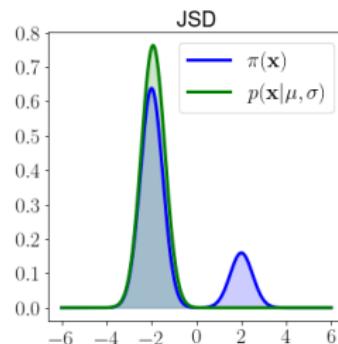
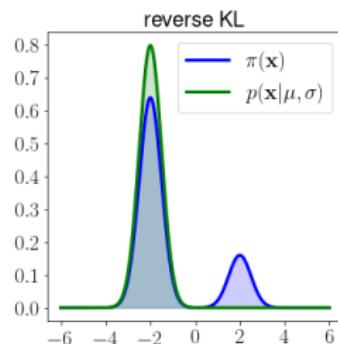
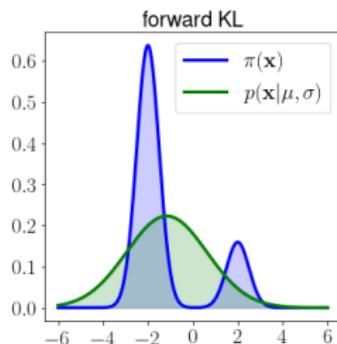
Metz L. et al. Unrolled Generative Adversarial Networks, 2016

Jensen-Shannon vs Kullback-Leibler

Mode covering vs mode seeking

$$KL(\pi||p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad KL(p||\pi) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

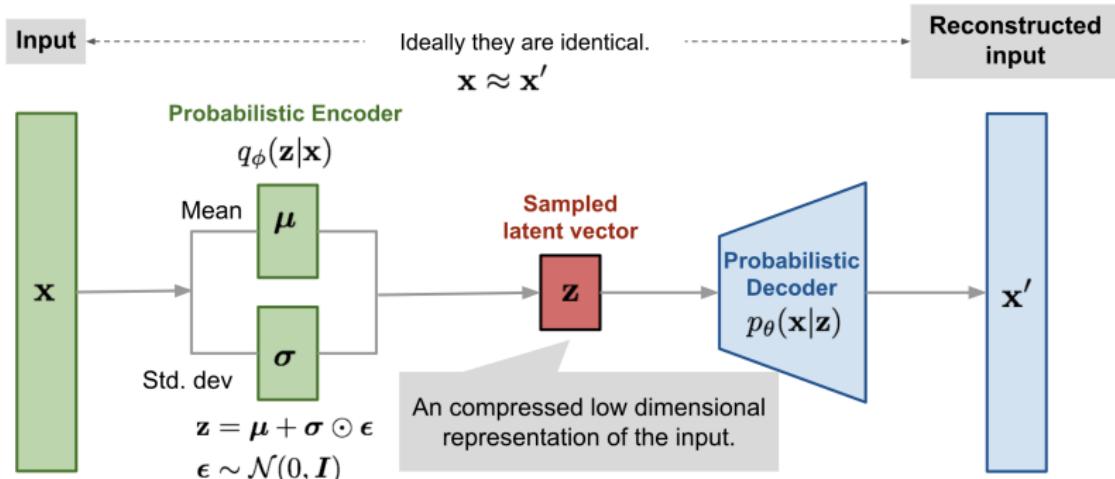
$$JSD(\pi||p) = \frac{1}{2} \left[KL \left(\pi(\mathbf{x}) || \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2} \right) + KL \left(p(\mathbf{x}) || \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2} \right) \right]$$



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VAE recap



- ▶ Encoder $q(\mathbf{z}|\mathbf{x}, \phi) = \mathcal{N}(\mathbf{z}|\mu_\phi(\mathbf{x}), \sigma_\phi(\mathbf{x}))$.
- ▶ Variational posterior $q(\mathbf{z}|\mathbf{x}, \phi)$ originally approximates the true posterior $p(\mathbf{z}|\mathbf{x}, \theta)$.
- ▶ Which methods are you already familiar with to make the posterior more flexible?

image credit:

<https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html>

Adversarial Variational Bayes

ELBO objective

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

What is the problem to make the variational posterior model an implicit model?

- ▶ The first term is reconstruction loss that needs only samples from $q(z|x, \phi)$ to evaluate.
- ▶ Reparametrization trick allows to get gradients of reconstruction loss

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

where $\epsilon^* \sim r(\epsilon)$, $z = g(x, \epsilon, \phi)$, $z \sim q(z|x, \phi)$.

Adversarial Variational Bayes

ELBO objective

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

What is the problem to make the variational posterior model an implicit model?

- ▶ The third term requires the explicit value of $q(z|x, \phi)$.
- ▶ We could join second and third terms:

$$KL(q(z|x, \phi) || p(z)) = \mathbb{E}_{q(z|x, \phi)} \log \frac{q(z|x, \phi)}{p(z)} = \mathbb{E}_{q(z|x, \phi)} \log \frac{q(z|x, \phi)\pi(x)}{p(z)\pi(x)}.$$

- ▶ We have to estimate density ratio

$$r(x, z) = \frac{q_1(x, z)}{q_2(x, z)} = \frac{q(z|x, \phi)\pi(x)}{p(z)\pi(x)}.$$

Density ratio trick

Consider two distributions $q_1(\mathbf{x})$, $q_2(\mathbf{x})$ and probabilistic model

$$p(\mathbf{x}|y) = \begin{cases} q_1(\mathbf{x}), & \text{if } y = 1, \\ q_2(\mathbf{x}), & \text{if } y = 0, \end{cases} \quad y \sim \text{Bern}(0.5).$$

Density ratio

$$\begin{aligned} \frac{q_1(\mathbf{x})}{q_2(\mathbf{x})} &= \frac{p(\mathbf{x}|y=1)}{p(\mathbf{x}|y=0)} = \frac{p(y=1|\mathbf{x})p(\mathbf{x})}{p(y=1)} \Big/ \frac{p(y=0|\mathbf{x})p(\mathbf{x})}{p(y=0)} = \\ &= \frac{p(y=1|\mathbf{x})}{p(y=0|\mathbf{x})} = \frac{p(y=1|\mathbf{x})}{1 - p(y=1|\mathbf{x})} = \frac{D(\mathbf{x})}{1 - D(\mathbf{x})} \end{aligned}$$

Here $D(\mathbf{x})$ is a discriminator model the output of which is a probability that \mathbf{x} is a sample from $q_1(\mathbf{x})$ rather than from $q_2(\mathbf{x})$.

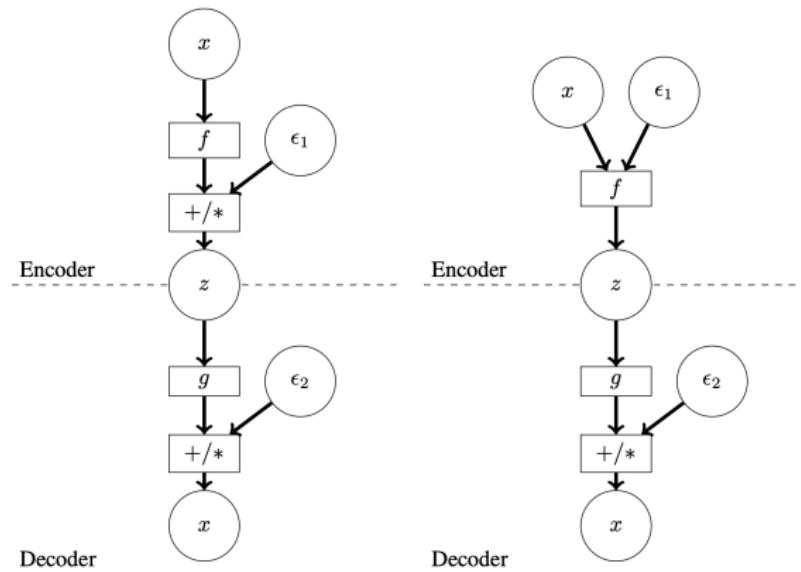
Adversarial Variational Bayes

$$\max_D \left[\mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \log D(\mathbf{x}, \mathbf{z}) + \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{p(\mathbf{z})} \log(1 - D(\mathbf{x}, \mathbf{z})) \right]$$

Adversarial Variational Bayes

ELBO objective

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

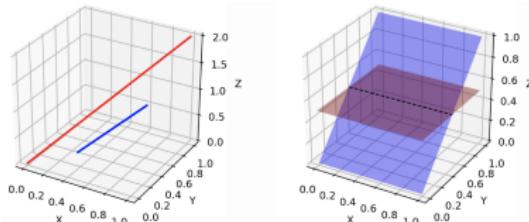


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Informal theoretical results

- ▶ Since \mathbf{z} usually has lower dimensionality compared to \mathbf{x} , manifold $G(\mathbf{z}, \theta)$ has a measure 0 in \mathbf{x} space. Hence, support of $p(\mathbf{x}|\theta)$ lies on low-dimensional manifold.
- ▶ Distribution of real images $\pi(\mathbf{x})$ is also concentrated on a low dimensional manifold.



- ▶ If $\pi(\mathbf{x})$ and $p(\mathbf{x}|\theta)$ have disjoint supports, then there is a smooth optimal discriminator. We are not able to learn anything by backproping through it.
- ▶ For such low-dimensional disjoint manifolds

$$KL(\pi||p) = KL(p||\pi) = \infty, \quad JSD(\pi||p) = \log 2$$

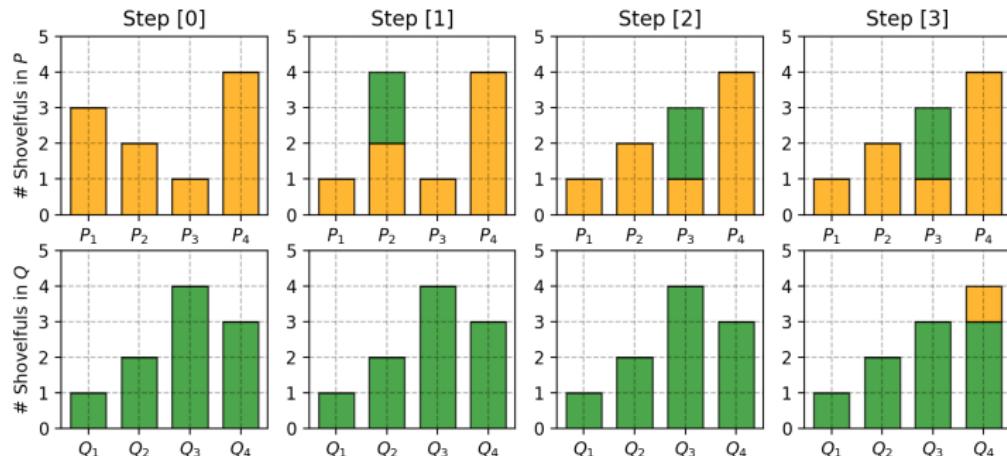
- ▶ Adding continuous noise to the inputs of the discriminator smoothes the distributions of the probability mass.

Weng L. From GAN to WGAN, 2019

Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

Wasserstein distance (discrete)

Also called Earth Mover's distance. The minimum cost of moving and transforming a pile of dirt in the shape of one probability distribution to the shape of the other distribution.



$$W(P, Q) = 2(\text{step 1}) + 2(\text{step 2}) + 1(\text{step 3}) = 5$$

Wasserstein distance (continuous)

$$W(\pi, p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} \|\mathbf{x} - \mathbf{y}\| = \inf_{\gamma \in \Gamma(\pi, p)} \int \|\mathbf{x} - \mathbf{y}\| \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$

- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ – transportation plan (the amount of "dirt" that should be transported from point \mathbf{x} to point \mathbf{y})

$$\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} = p(\mathbf{y}); \quad \int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \pi(\mathbf{x}).$$

- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ – the amount, $\|\mathbf{x} - \mathbf{y}\|$ – the distance.
- ▶ $\Gamma(\pi, p)$ – the set of all joint distributions $\Gamma(\mathbf{x}, \mathbf{y})$ with marginals π and p .

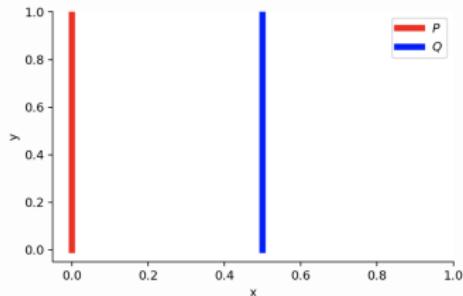
For better understanding of transportation plan function γ , try to write down the plan for previous discrete case.

Wasserstein distance vs KL vs JSD

Consider 2d distributions

$$\pi(x, y) = (0, U[0, 1])$$

$$p(x, y|\theta) = (\theta, U[0, 1])$$



- $\theta = 0$. Distributions are the same

$$KL(\pi||p) = KL(p||\pi) = JSD(p||\pi) = W(\pi, p) = 0$$

- $\theta \neq 0$

$$KL(\pi||p) = \int_{U[0,1]} 1 \log \frac{1}{0} dy = \infty = KL(p||\pi)$$

$$JSD(\pi||p) = \frac{1}{2} \left(\int_{U[0,1]} 1 \log \frac{1}{1/2} dy + \int_{U[0,1]} 1 \log \frac{1}{1/2} dy \right) = \log 2$$

$$W(\pi, p) = |\theta|$$

Wasserstein distance vs KL vs JSD

Theorem 1

Let $G(\mathbf{z}, \theta)$ be (almost) any feedforward neural network, and $p(\mathbf{z})$ a prior over \mathbf{z} such that $\mathbb{E}_{p(\mathbf{z})} \|\mathbf{z}\| < \infty$. Then therefore $W(\pi, p)$ is continuous everywhere and differentiable almost everywhere.

Theorem 2

Let π be a distribution on a compact space \mathcal{X} and $\{p_t\}_{t=1}^{\infty}$ be a sequence of distributions on \mathcal{X} .

$$KL(\pi || p_t) \rightarrow 0 \text{ (or } KL(p_t || \pi) \rightarrow 0) \quad (1)$$

$$JSD(\pi || p_t) \rightarrow 0 \quad (2)$$

$$W(\pi || p_t) \rightarrow 0 \quad (3)$$

Then, considering limits as $t \rightarrow \infty$, (1) implies (2), (2) implies (3).

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Wasserstein GAN

Wasserstein distance

$$W(\pi||p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} \|\mathbf{x} - \mathbf{y}\| = \inf_{\gamma \in \Gamma(\pi, p)} \int \|\mathbf{x} - \mathbf{y}\| \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y}$$

The infimum across all possible joint distributions in $\Gamma(\pi, p)$ is intractable.

Theorem (Kantorovich-Rubinstein duality)

$$W(\pi||p) = \frac{1}{K} \max_{\|f\|_L \leq K} [\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x})],$$

where $\|f\|_L \leq K$ are K -Lipschitz continuous functions
 $(f : \mathcal{X} \rightarrow \mathbb{R})$

$$|f(\mathbf{x}_1) - f(\mathbf{x}_2)| \leq K \|\mathbf{x}_1 - \mathbf{x}_2\|, \quad \text{for all } \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}.$$

Wasserstein GAN

Theorem (Kantorovich-Rubinstein duality)

$$W(\pi || p) = \frac{1}{K} \max_{\|f\|_L \leq K} [\mathbb{E}_{\pi(x)} f(x) - \mathbb{E}_{p(x)} f(x)],$$

- ▶ Now we have to ensure that f is K -Lipschitz continuous.
- ▶ Let $f(x, \phi)$ be a feedforward neural network parametrized by ϕ .
- ▶ If parameters ϕ lie in a compact set Φ then $f(x, \phi)$ will be K -Lipschitz continuous function.
- ▶ Let the parameters be clamped to a fixed box $\Phi \in [-0.01, 0.01]^d$ after each gradient update.

$$\begin{aligned} K \cdot W(\pi || p) &= \max_{\|f\|_L \leq K} [\mathbb{E}_{\pi(x)} f(x) - \mathbb{E}_{p(x)} f(x)] \geq \\ &\geq \max_{\phi \in \Phi} [\mathbb{E}_{\pi(x)} f(x, \phi) - \mathbb{E}_{p(x)} f(x, \phi)] \end{aligned}$$

Wasserstein GAN

Vanilla GAN objective

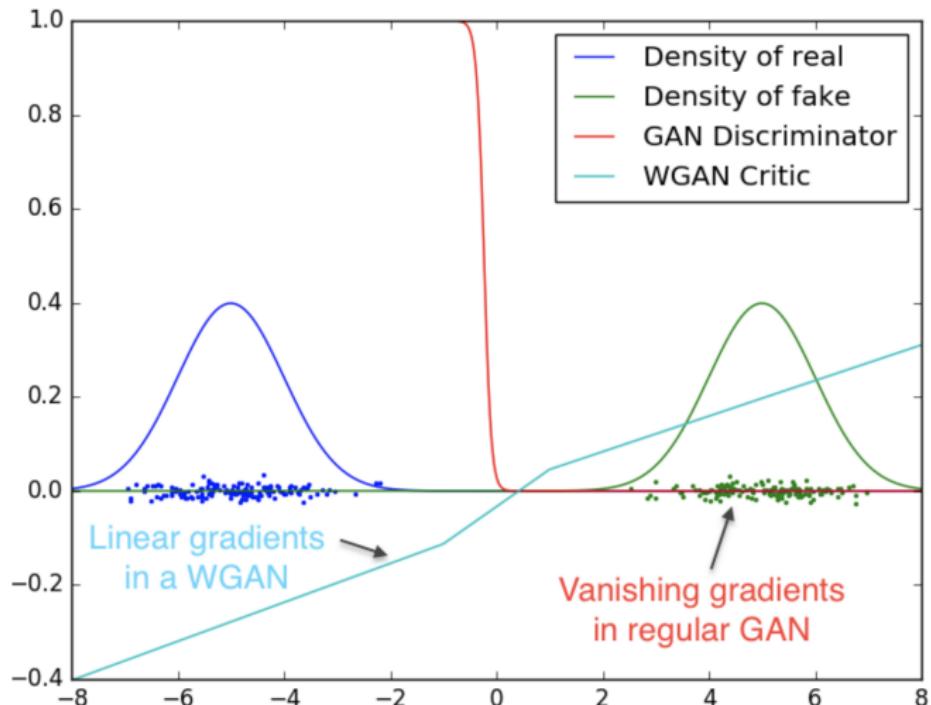
$$\min_{\theta} \max_{\phi} \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}, \phi) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z}, \theta), \phi))$$

WGAN objective

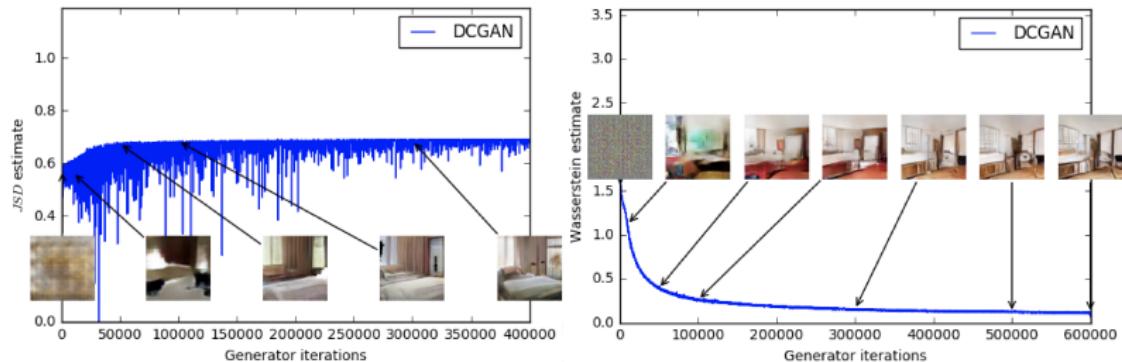
$$\min_{\theta} W(\pi || p) \approx \min_{\theta} \max_{\phi \in \Phi} [\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}, \phi) - \mathbb{E}_{p(\mathbf{z})} f(G(\mathbf{z}, \theta), \phi)] .$$

- ▶ Discriminator D is similar to the function f , but not the same (it is not a classifier anymore). In the WGAN model, function f is usually called *critic*.
- ▶ "Weight clipping is a clearly terrible way to enforce a Lipschitz constraint". If the clipping parameter is large, it is hard to train the critic till optimality. If the clipping parameter is too small, it could lead to vanishing gradients.

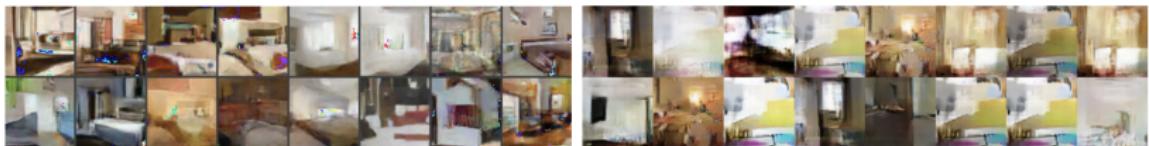
Wasserstein GAN



Wasserstein GAN



- ▶ JSD correlates poorly with the sample quality. Stays constant nearly maximum value $\log 2 \approx 0.69$.
- ▶ W is highly correlated with the sample quality.



"In no experiment did we see evidence of mode collapse for the WGAN algorithm."

Summary

- ▶ Mode collapse and vanishing gradients are the two main problems of vanilla GAN. Lots of tips and tricks has to be used to make the GAN training is stable and scalable.
- ▶ KL and JS divergences work poorly as model objective in the case of disjoint supports.
- ▶ Adversarial Variational Bayes uses density ratio trick to get more powerful variational posterior.
- ▶ Earth-Mover distance is a more appropriate objective function for distribution matching problem.
- ▶ Wasserstein GAN uses Kantorovich-Rubinstein duality to obtain EM distance.