

Deep Generative Models

Lecture 8

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Recap of previous lecture

Gumbel-max trick

Let $g_k \sim \text{Gumbel}(0, 1)$ for $k = 1, \dots, K$. Then

$$c = \arg \max_k [\log \pi_k + g_k]$$

has a categorical distribution $c \sim \text{Categorical}(\pi)$.

Gumbel-softmax relaxation

Concrete distribution = continuous + discrete

$$\hat{c}_k = \frac{\exp\left(\frac{\log q(k|\mathbf{x}, \phi) + g_k}{\tau}\right)}{\sum_{j=1}^K \exp\left(\frac{\log q(j|\mathbf{x}, \phi) + g_j}{\tau}\right)}, \quad k = 1, \dots, K.$$

Reparametrization trick

$$\nabla_{\phi} \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x}|\mathbf{e}_c, \theta) = \mathbb{E}_{\text{Gumbel}(0,1)} \nabla_{\phi} \log p(\mathbf{x}|\mathbf{z}, \theta),$$

where $\mathbf{z} = \sum_{k=1}^K \hat{c}_k \mathbf{e}_k$ (all operations are differentiable now).

Maddison C. J., Mnih A., Teh Y. W. *The Concrete distribution: A continuous relaxation of discrete random variables*, 2016

Jang E., Gu S., Poole B. *Categorical reparameterization with Gumbel-Softmax*, 2016

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

Let define discriminative model (classifier):

$$p(y = 1|\mathbf{x}) = P(\{\mathbf{x} \sim \pi(\mathbf{x})\}); \quad p(y = 0|\mathbf{x}) = P(\{\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta})\})$$

Assumption

Generative distribution $p(\mathbf{x}|\boldsymbol{\theta})$ equals to the true distribution $\pi(\mathbf{x})$ if we can not distinguish them using discriminative model $p(y|\mathbf{x})$. It means that $p(y = 1|\mathbf{x}) = 0.5$ for each sample \mathbf{x} .

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

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

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

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

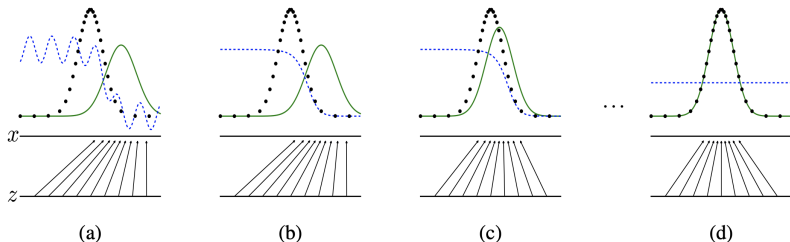
If the generator could be **any** function and the discriminator is **optimal** at every step, then the generator is **guaranteed to converge** to the data distribution.

Recap of previous lecture

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

Objective

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



Outline

1. Wasserstein distance
2. Wasserstein GAN
3. Lipschitzness of Wasserstein GAN critic
 - WGAN with Gradient Penalty
 - Spectral Normalization GAN

Outline

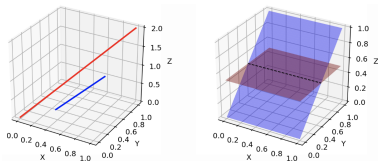
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Informal theoretical results

- ▶ Since \mathbf{z} usually has lower dimensionality compared to \mathbf{x} , manifold $G_{\theta}(\mathbf{z})$ 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.



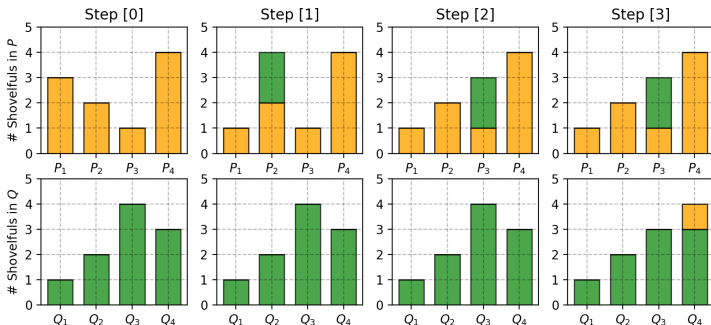
- ▶ If $\pi(\mathbf{x})$ and $p(\mathbf{x}|\theta)$ have disjoint supports, then there is a smooth optimal discriminator. We are not able to learn anything by backproping through it.
- ▶ For such low-dimensional disjoint manifolds
$$KL(\pi||p) = KL(p||\pi) = \infty, \quad JSD(\pi||p) = \log 2$$
- ▶ Adding 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)

A.k.a. **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})

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

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

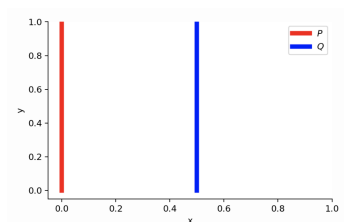
For better understanding of transportation plan function γ , try to write down the plan for previous discrete case.

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

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

- $\theta \neq 0$

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

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

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

Weng L. From GAN to WGAN, 2019

Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

Wasserstein distance vs KL vs JSD

Theorem 1

Let $G_{\theta}(\mathbf{z})$ 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
($f : \mathcal{X} \rightarrow \mathbb{R}$)

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

Now we need only samples to get Monte Carlo estimate for $W(\pi||p)$.

Wasserstein GAN

Theorem (Kantorovich-Rubinstein duality)

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

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

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

Wasserstein GAN

Standard GAN objective

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

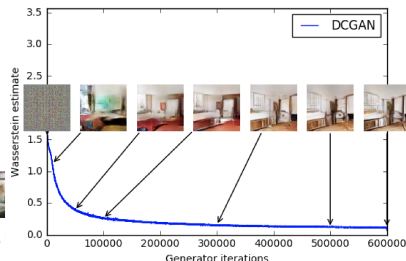
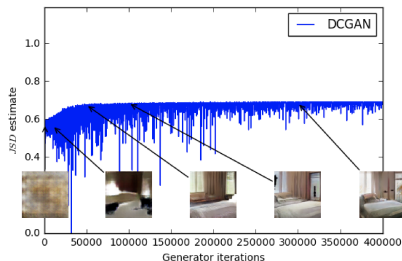
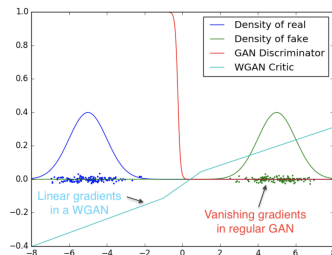
WGAN objective

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

- ▶ 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 c is too large, it is hard to train the critic till optimality. If the clipping parameter c is too small, it could lead to vanishing gradients.

Wasserstein GAN

- ▶ WGAN has non-zero gradients for disjoint supports.
- ▶ $JSD(\pi||p)$ correlates poorly with the sample quality. Stays constant nearly maximum value $\log 2 \approx 0.69$.
- ▶ $W(\pi||p)$ is highly correlated with the sample quality.



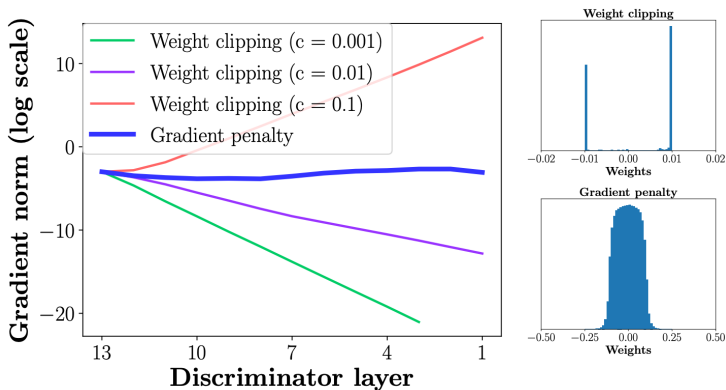
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Wasserstein GAN with Gradient Penalty



Weight clipping analysis

- ▶ The gradients either grow or decay exponentially.
- ▶ Gradient penalty makes the gradients more stable.

Wasserstein GAN with Gradient Penalty

Theorem

Let $\pi(\mathbf{x})$ and $p(\mathbf{x})$ be two distributions in \mathcal{X} , a compact metric space. Let γ be the optimal transportation plan between $\pi(\mathbf{x})$ and $p(\mathbf{x})$. Then

1. there is 1-Lipschitz function f^* which is the optimal solution of

$$\max_{\|f\|_L \leq 1} \left[\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x}) \right].$$

2. if f^* is differentiable, $\gamma(\mathbf{y} = \mathbf{z}) = 0$ and $\hat{\mathbf{x}}_t = t\mathbf{y} + (1-t)\mathbf{z}$ with $\mathbf{y} \sim \pi(\mathbf{x})$, $\mathbf{z} \sim p(\mathbf{x}|\boldsymbol{\theta})$, $t \in [0, 1]$ it holds that

$$\mathbb{P}_{(\mathbf{y}, \mathbf{z}) \sim \gamma} \left[\nabla f^*(\hat{\mathbf{x}}_t) = \frac{\mathbf{z} - \hat{\mathbf{x}}_t}{\|\mathbf{z} - \hat{\mathbf{x}}_t\|} \right] = 1.$$

Corollary

f^* has gradient norm 1 almost everywhere under $\pi(\mathbf{x})$ and $p(\mathbf{x})$.

Wasserstein GAN with Gradient Penalty

A differentiable function is 1-Lipschitz if and only if it has gradients with norm at most 1 everywhere.

Gradient penalty

$$W(\pi||p) = \underbrace{\mathbb{E}_{\pi(\mathbf{x})}f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})}f(\mathbf{x})}_{\text{original critic loss}} + \lambda \underbrace{\mathbb{E}_{U[0,1]} \left[(\|\nabla f(\hat{\mathbf{x}})\|_2 - 1)^2 \right]}_{\text{gradient penalty}},$$

- ▶ Samples $\hat{\mathbf{x}}_t = t\mathbf{y} + (1 - t)\mathbf{z}$ with $t \in [0, 1]$ are uniformly sampled along straight lines between pairs of points: \mathbf{y} from the data distribution $\pi(\mathbf{x})$ and \mathbf{z} from the generator distribution $p(\mathbf{x}|\theta)$.
- ▶ Enforcing the unit gradient norm constraint everywhere is intractable, it turns out to be sufficient to enforce it only along these straight lines.

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Spectral Normalization GAN

Definition

$\|\mathbf{A}\|_2$ is a *spectral norm* of matrix \mathbf{A} :

$$\|\mathbf{A}\|_2 = \max_{\mathbf{h} \neq 0} \frac{\|\mathbf{A}\mathbf{h}\|_2}{\|\mathbf{h}\|_2} = \max_{\|\mathbf{h}\|_2 \leq 1} \|\mathbf{A}\mathbf{h}\|_2 = \sqrt{\lambda_{\max}(\mathbf{A}^T \mathbf{A})},$$

where $\lambda_{\max}(\mathbf{A}^T \mathbf{A})$ is the largest eigenvalue value of $\mathbf{A}^T \mathbf{A}$.

Statement 1

if \mathbf{g} is a K-Lipschitz vector function then

$$\|\mathbf{g}\|_L \leq K = \sup_{\mathbf{x}} \|\nabla \mathbf{g}(\mathbf{x})\|_2.$$

Statement 2

Lipschitz norm of superposition is bounded above by product of Lipschitz norms

$$\|\mathbf{g}_1 \circ \mathbf{g}_2\|_L \leq \|\mathbf{g}_1\|_L \cdot \|\mathbf{g}_2\|_L$$

Spectral Normalization GAN

Let consider the critic $f_\phi(\mathbf{x})$ of the following form:

$$f_\phi(\mathbf{x}) = \mathbf{W}_{K+1} \sigma_K(\mathbf{W}_K \sigma_{K-1}(\dots \sigma_1(\mathbf{W}_1 \mathbf{x}) \dots)).$$

This feedforward network is a superposition of simple functions.

- ▶ σ_k is a pointwise nonlinearities. We assume that $\|\sigma_k\|_L = 1$ (it holds for ReLU).
- ▶ $\mathbf{g}(\mathbf{x}) = \mathbf{W}^T \mathbf{x}$ is a linear transformation ($\nabla \mathbf{g}(\mathbf{x}) = \mathbf{W}$).

$$\|\mathbf{g}\|_L \leq \sup_{\mathbf{x}} \|\nabla \mathbf{g}(\mathbf{x})\|_2 = \|\mathbf{W}\|_2.$$

Critic spectral norm

$$\|f\|_L \leq \|\mathbf{W}_{K+1}\|_2 \cdot \prod_{k=1}^K \|\sigma_k\|_L \cdot \|\mathbf{W}_k\|_2 = \prod_{k=1}^{K+1} \|\mathbf{W}_k\|_2.$$

If we replace the weights in the critic $f_\phi(\mathbf{x})$ by $\mathbf{W}_k^{SN} = \mathbf{W}_k / \|\mathbf{W}_k\|_2$, we will get $\|f\|_L \leq 1$.

Spectral Normalization GAN

How to compute $\|\mathbf{W}\|_2 = \sqrt{\lambda_{\max}(\mathbf{W}^T \mathbf{W})}$?

We are not able to apply SVD at each iteration.

Power iteration (PI) method

- ▶ \mathbf{u}_0 – random vector.
- ▶ for $m = 0, \dots, M - 1$: (M is a fixed number of steps)

$$\mathbf{v}_{m+1} = \frac{\mathbf{W}^T \mathbf{u}_m}{\|\mathbf{W}^T \mathbf{u}_m\|}, \quad \mathbf{u}_{m+1} = \frac{\mathbf{W} \mathbf{v}_{m+1}}{\|\mathbf{W} \mathbf{v}_{m+1}\|}.$$

- ▶ approximate the spectral norm

$$\|\mathbf{W}\|_2 = \sqrt{\lambda_{\max}(\mathbf{W}^T \mathbf{W})} \approx \mathbf{u}_M^T \mathbf{W} \mathbf{v}_M.$$

SNGAN gradient update

- ▶ Apply PI method to get approximation of spectral norm.
- ▶ Normalize weights $\mathbf{W}_k^{SN} = \mathbf{W}_k / \|\mathbf{W}_k\|_2$.
- ▶ Apply gradient rule to \mathbf{W} .

Summary

- ▶ KL and JS divergences work poorly as model objective in the case of disjoint supports.
- ▶ Earth-Mover distance is a more appropriate objective function for distribution matching problem.
- ▶ Kantorovich-Rubinstein duality gives the way to calculate the EM distance using only samples.
- ▶ Wasserstein GAN uses Kantorovich-Rubinstein duality for getting Earth Mover distance as model objective.
- ▶ Weight clipping is a terrible way to enforce Lipschitzness. Gradient Penalty adds regularizer to loss that uses necessary conditions for optimal critic.
- ▶ Spectral normalization is a weight normalization technique to enforce Lipschitzness, which is helpful for generator and critic.