Deep Generative Models

Lecture 8

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AI Masters

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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):

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

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 $\mathbf{x} = \mathbf{G}(\mathbf{z})$, 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

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

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

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

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.

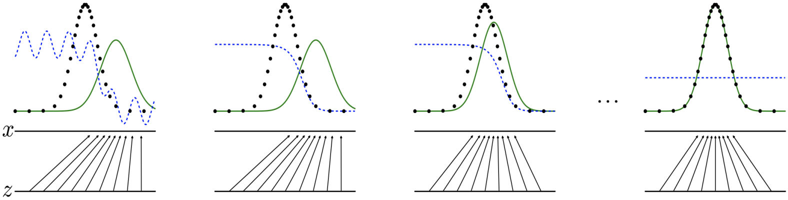
Goodfellow I. J. et al. Generative Adversarial Networks, 2014

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

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



(a) (b) (c) (d)

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

Recap of previous lecture

Main problems of standard GAN

- Vanishing gradients (solution: non-saturating GAN);
- Mode collapse (caused by Jensen-Shannon divergence).

Standard GAN

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

Informal theoretical results

The real images distribution $\pi(\mathbf{x})$ and the generated images distribution $p(\mathbf{x}|\boldsymbol{\theta})$ are low-dimensional and have disjoint supports. In this case

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

Goodfellow I. J. et al. Generative Adversarial Networks, 2014
Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

Outline

1. Wasserstein distance (continued)

2. Lipschitzness of Wasserstein GAN critic
   Wasserstein GAN
   WGAN with Gradient Penalty

3. f-divergence minimization

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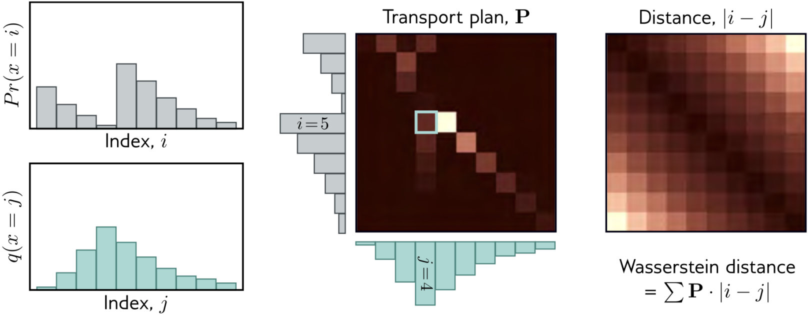
Wasserstein distance (discrete)

A.k.a. **Earth Mover's distance**.

Optimal transport formulation

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.



Simon J.D. Prince. *Understanding Deep Learning*, 2023

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.

Wasserstein metric

$$W_s(\pi, p) = \inf_{\gamma \in \Gamma(\pi, p)} \left(\mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} \|\mathbf{x} - \mathbf{y}\|^s\right)^{1/s}$$

Here we will use $W(\pi, p) = W_1(\pi, p)$ that corresponds to the optimal transport formulation.

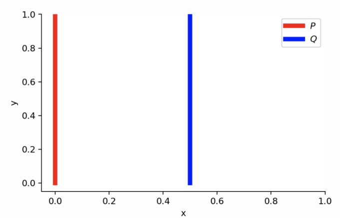
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

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 $\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z})$ 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 $\mathcal{X}$.

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

$$JSD(\pi||p_t) \rightarrow 0 \tag{2}$$

$$W(\pi||p_t) \rightarrow 0 \tag{3}$$

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

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

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2. Lipschitzness of Wasserstein GAN critic
   Wasserstein GAN
   WGAN with Gradient Penalty

3. f-divergence minimization

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)

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

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $\|f\|_L \leq K$ 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 $W(\pi||p)$.

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

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Wasserstein GAN

Theorem (Kantorovich-Rubinstein duality)

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

- 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 $\mathbf{\Phi}$ then $f_\phi(\mathbf{x})$ will be K-Lipschitz continuous function.
- Let the parameters be clamped to a fixed box $\mathbf{\Phi} \in [-c, c]^d$ (e.x. $c = 0.01$) after each gradient update.

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

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

Wasserstein GAN

Standard GAN objective

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

WGAN objective

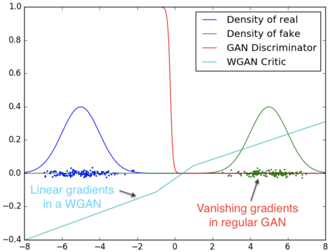
$$\min_{\boldsymbol{\theta}} W(\pi || p) \approx \min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi} \in \boldsymbol{\Phi}} \left[\mathbb{E}_{\pi(\mathbf{x})} f_{\boldsymbol{\phi}}(\mathbf{x}) - \mathbb{E}_{p(\mathbf{z})} f_{\boldsymbol{\phi}}(\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z})) \right].$$

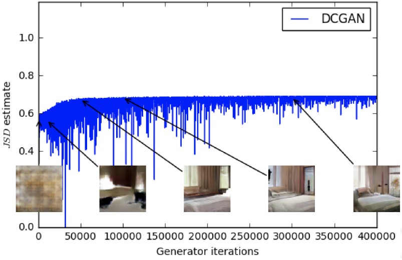
- Discriminator D is similar to the function f, but not the same (it is not a classifier anymore). In the WGAN model, function f is usually called **critic**.
- *"Weight clipping is a clearly terrible way to enforce a Lipschitz constraint"*. If the clipping parameter c is too large, it is hard to train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

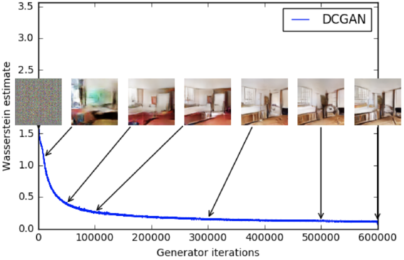
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

Wasserstein GAN

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







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

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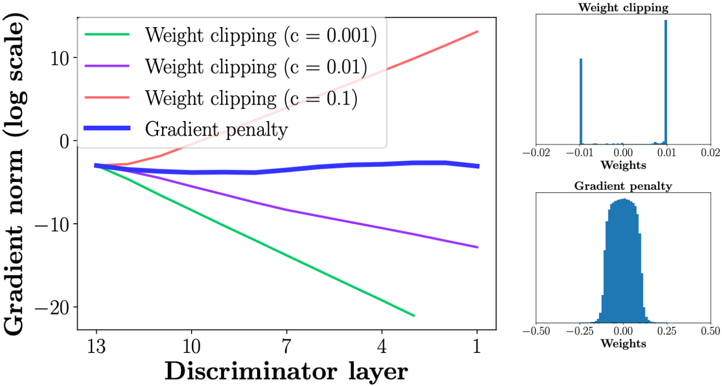
Wasserstein GAN with Gradient Penalty



Weight clipping analysis

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

Gulrajani I. et al. Improved Training of Wasserstein GANs, 2017

Wasserstein GAN with Gradient Penalty

Theorem

Let $\pi(\mathbf{x})$ and $p(\mathbf{x})$ be two distribution 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 $p(\mathbf{x})$.

Gulrajani I. et al. Improved Training of Wasserstein GANs, 2017

Wasserstein GAN with Gradient Penalty

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

Gradient penalty

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

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

Gulrajani I. et al. Improved Training of Wasserstein GANs, 2017

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Divergences

- Forward KL divergence in maximum likelihood estimation.
- Reverse KL in variational inference.
- JS divergence in standard GAN.
- Wasserstein distance in WGAN.

What is a divergence?

Let $\mathcal{P}$ be the set of all possible probability distributions. Then $D : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$ is a divergence if

- $D(\pi || p) \geq 0$ for all $\pi, p \in \mathcal{P}$;
- $D(\pi || p) = 0$ if and only if $\pi \equiv p$.

General divergence minimization task

$$\min_p D(\pi || p)$$

Chalenge

We do not know the real distribution $\pi(\mathbf{x})$!

f-divergence family

f-divergence

$$D_f(\pi||p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) = \int p(\mathbf{x}) f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) d\mathbf{x}.$$

Here $f : \mathbb{R}_+ \to \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

Name	$D_f(P\|Q)$	Generator $f(u)$
Kullback-Leibler	$\int p(x) \log \frac{p(x)}{q(x)} \, \mathrm{d}x$	$u \log u$
Reverse KL	$\int q(x) \log \frac{q(x)}{p(x)} \, \mathrm{d}x$	$-\log u$
Pearson χ^2	$\int \frac{(q(x)-p(x))^2}{p(x)} \, \mathrm{d}x$	$(u-1)^2$
Squared Hellinger	$\int \left(\sqrt{p(x)} - \sqrt{q(x)}\right)^2 \, \mathrm{d}x$	$(\sqrt{u}-1)^2$
Jensen-Shannon	$\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} \, \mathrm{d}x$	$-(u+1)\log\frac{1+u}{2} + u \log u$
GAN	$\int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} \, \mathrm{d}x - \log(4)$	$u \log u - (u+1)\log(u+1)$

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Fenchel conjugate

$$f^*(t) = \sup_{u \in \mathrm{dom}_f} (ut - f(u)), \quad f(u) = \sup_{t \in \mathrm{dom}_{f^*}} (ut - f^*(t))$$

Important property: $f^{**} = f$ for convex f.

f-divergence

$$D_f(\pi || p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) = \int p(\mathbf{x}) f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) d\mathbf{x} =$$

$$= \int p(\mathbf{x}) \sup_{t \in \mathrm{dom}_{f^*}} \left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})} t - f^*(t)\right) d\mathbf{x} =$$

$$= \int \sup_{t \in \mathrm{dom}_{f^*}} (\pi(\mathbf{x}) t - p(\mathbf{x}) f^*(t)) \, d\mathbf{x}.$$

Here we seek value of t, which gives us maximum value of $\pi(\mathbf{x}) t - p(\mathbf{x}) f^*(t)$, for each data point $\mathbf{x}$.

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

f-divergence

$$D_f(\pi||p) = \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) = \int p(\mathbf{x}) f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) d\mathbf{x}.$$

Variational f-divergence estimation

$$D_f(\pi||p) = \int \sup_{t \in \mathrm{dom}_{f^*}} (\pi(\mathbf{x})t - p(\mathbf{x})f^*(t))\, d\mathbf{x} \geq$$

$$\geq \sup_{T \in \mathcal{T}} \int (\pi(\mathbf{x})T(\mathbf{x}) - p(\mathbf{x})f^*(T(\mathbf{x})))\, d\mathbf{x} =$$

$$= \sup_{T \in \mathcal{T}} \left[\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))\right]$$

This is a lower bound because of Jensen inequality and restricted class of functions $\mathcal{T} : \mathcal{X} \to \mathbb{R}$.

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Variational divergence estimation

$$D_f(\pi||p) \geq \sup_{T \in \mathcal{T}} \left[\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))\right]$$

The lower bound is tight for $T^*(\mathbf{x}) = f'\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right)$.

Example (JSD)

- Let define function f and its conjugate f^*

$$f(u) = u \log u - (u+1)\log(u+1), \quad f^*(t) = -\log(1 - e^t).$$

- Let reparametrize $T(\mathbf{x}) = \log D(\mathbf{x})$.

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

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Variational divergence estimation

$$D_f(\pi || p) \geq \sup_{T \in \mathcal{T}} \left[\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))\right]$$

Note: To evaluate lower bound we only need samples from $\pi(\mathbf{x})$ and $p(\mathbf{x})$. Hence, we could fit implicit generative model.

(a) GAN (b) KL (c) Squared Hellinger

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

Summary

- 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 neccessary conditions for optimal critic.
- f-divergence family is a unified framework for divergence minimization, which uses variational approximation. Standard GAN is a special case of it.