

Deep Generative Models

Lecture 8

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AI Masters

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Recap of previous lecture

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}) \Rightarrow$ over-regularization;
- ▶ $p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}|\phi) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i, \phi) \Rightarrow$ overfitting and highly expensive.

ELBO revisiting

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_i(q, \theta) = \text{RL} - \text{MI} - \text{KL}(q_{\text{agg}}(\mathbf{z}|\phi) || p(\mathbf{z}|\lambda))$$

It is Forward KL with respect to $p(\mathbf{z}|\lambda)$.

ELBO with flow-based VAE prior

$$\begin{aligned} \mathcal{L}(\phi, \theta) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} [\log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(\mathbf{z}|\lambda) - \log q(\mathbf{z}|\mathbf{x}, \phi)] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\left(\log p(\mathbf{f}_{\lambda}(\mathbf{z})) + \log |\det(\mathbf{J}_{\mathbf{f}})| \right)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \phi) \right] \\ \mathbf{z} &= \mathbf{f}_{\lambda}^{-1}(\mathbf{z}^*) = \mathbf{g}_{\lambda}(\mathbf{z}^*), \quad \mathbf{z}^* \sim p(\mathbf{z}^*) = \mathcal{N}(0, \mathbf{I}) \end{aligned}$$

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

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

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

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

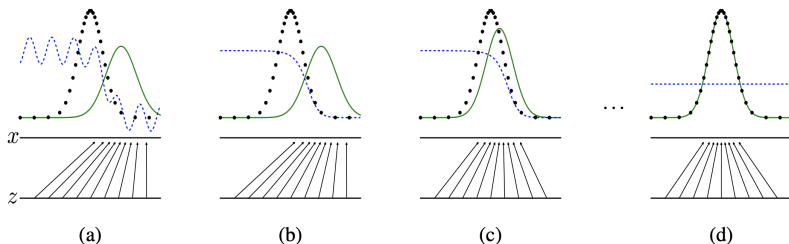
If the generator could be **any** function and the discriminator is **optimal** at every step, then the generator is **guaranteed to converge** to the data distribution.

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

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



Outline

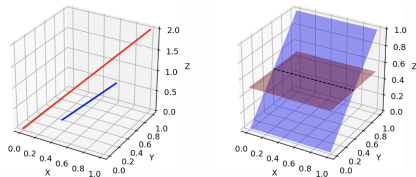
1. Wasserstein distance
2. Lipschitzness of Wasserstein GAN critic
 - Wasserstein GAN
 - WGAN with Gradient Penalty
3. f-divergence minimization

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Informal theoretical results

- ▶ The dimensionality of \mathbf{z} is lower than the dimensionality of \mathbf{x} . Hence, support of $p(\mathbf{x}|\boldsymbol{\theta})$ with $\mathbf{x} = \mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z})$ 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 $p(\mathbf{x}|\boldsymbol{\theta})$ have disjoint supports, then there is a smooth optimal discriminator.
- ▶ For such low-dimensional disjoint manifolds

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

Weng L. From GAN to WGAN, 2019

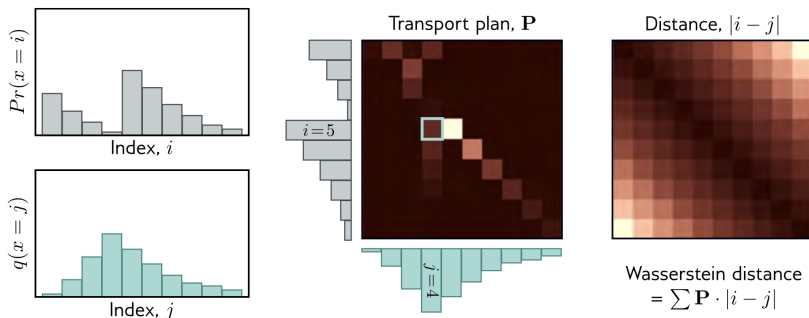
Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

Wasserstein distance (discrete)

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

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.



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

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

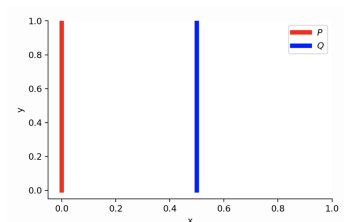
Here we will use $W(\pi, p) = W_1(\pi, p)$ that corresponds to the optimal transport formulation.

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

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

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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

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

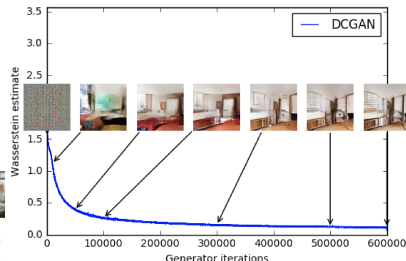
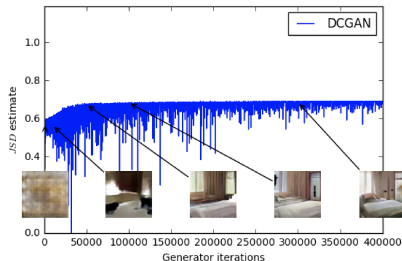
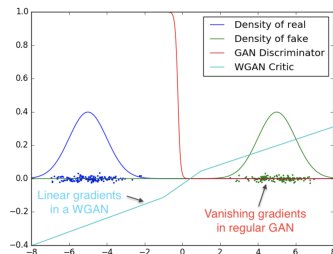
WGAN objective

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

- ▶ 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

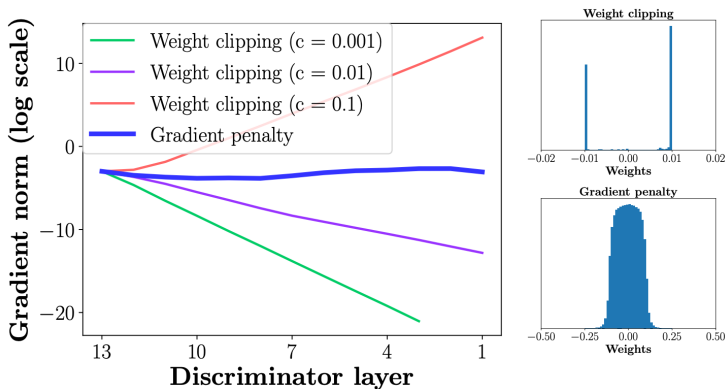
- ▶ WGAN has non-zero gradients for disjoint supports.
- ▶ $JSD(\pi||p)$ correlates poorly with the sample quality. Stays constant nearly maximum value $\log 2 \approx 0.69$.
- ▶ $W(\pi||p)$ is highly correlated with the sample quality.



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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 $\mathbf{y} \sim \pi(\mathbf{x})$, $\mathbf{z} \sim p(\mathbf{x}|\theta)$, $t \in [0, 1]$ 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

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

- ▶ 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 $\mathbf{z} \sim p(\mathbf{x}|\theta)$.
- ▶ 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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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 $D : \mathcal{P} \times \mathcal{P} \rightarrow \mathbb{R}$ 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

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

Challenge

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

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

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

f-divergence family

Fenchel conjugate

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

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

f-divergence

$$\begin{aligned} D_f(\pi || p) &= \mathbb{E}_{p(\mathbf{x})} f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) = \int p(\mathbf{x}) f\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right) d\mathbf{x} = \\ &= \int p(\mathbf{x}) \sup_{t \in \text{dom}_{f^*}} \left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})} t - f^*(t)\right) d\mathbf{x} = \\ &= \int \sup_{t \in \text{dom}_{f^*}} (\pi(\mathbf{x}) t - p(\mathbf{x}) f^*(t)) d\mathbf{x}. \end{aligned}$$

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

$$\begin{aligned} D_f(\pi||p) &= \int \sup_{t \in \text{dom}_{f^*}} (\pi(\mathbf{x})t - p(\mathbf{x})f^*(t)) d\mathbf{x} \geq \\ &\geq \sup_{T \in \mathcal{T}} \int (\pi(\mathbf{x})T(\mathbf{x}) - p(\mathbf{x})f^*(T(\mathbf{x}))) d\mathbf{x} = \\ &= \sup_{T \in \mathcal{T}} [\mathbb{E}_{\pi} T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))] \end{aligned}$$

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

f-divergence family

Variational divergence estimation

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

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

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

f-divergence family

Variational divergence estimation

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

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



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

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