

Deep Generative Models

Lecture 10

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Recap of previous lecture

ELBO objective

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

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

We have to estimate density ratio

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

Adversarial Variational Bayes

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

Recap of previous lecture

Standard GAN

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

Main problems

- ▶ Vanishing gradients (non-saturating GAN does not suffer of it);
- ▶ Mode collapse (caused by behaviour of Jensen-Shannon divergence).

Informal theoretical results

The real images distribution $\pi(\mathbf{x})$ and the generated images distribution $p(\mathbf{x}|\theta)$ 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

Recap of previous lecture

Wasserstein distance

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

- ▶ $\Gamma(\pi, p)$ – the set of all joint distributions $\gamma(\mathbf{x}, \mathbf{y})$ with marginals π and p ($\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} = p(\mathbf{y})$, $\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \pi(\mathbf{x})$)
- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ – transportation plan (the amount of "dirt" that should be transported from point \mathbf{x} to point \mathbf{y}).
- ▶ $\|\mathbf{x} - \mathbf{y}\|$ – the amount, $\|\mathbf{x} - \mathbf{y}\|$ – the distance.

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 $(f : \mathcal{X} \rightarrow \mathbb{R})$.

Outline

1. Wasserstein GAN
2. WGAN with Gradient Penalty
3. Spectral Normalization GAN
4. f-divergence minimization

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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

Standard GAN objective

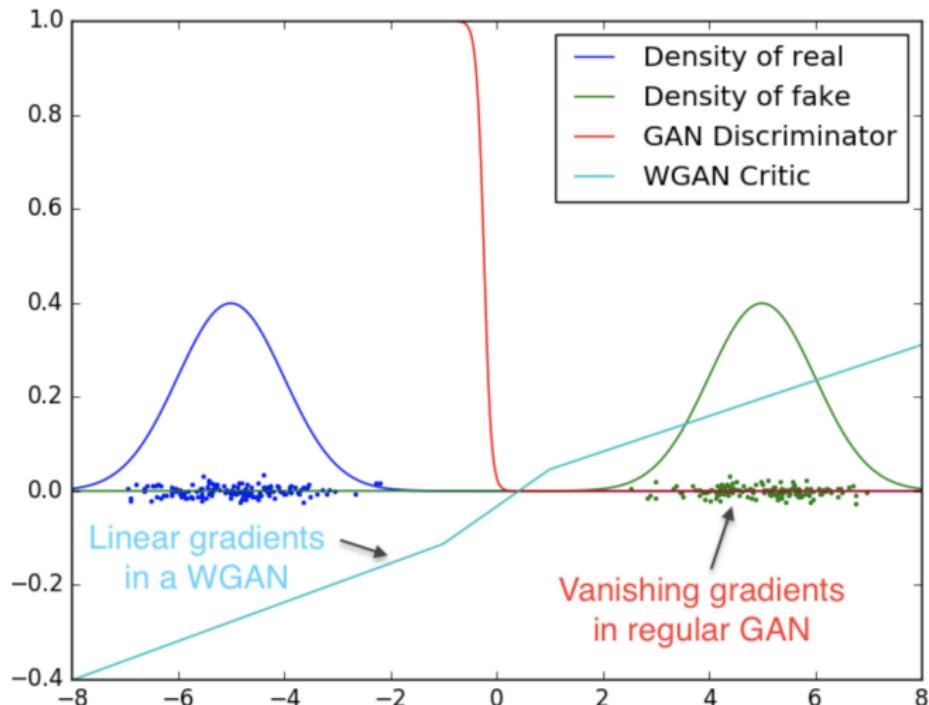
$$\min_{\theta} \max_{\phi} \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}, \phi) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D(G(\mathbf{z}, \theta), \phi))$$

WGAN objective

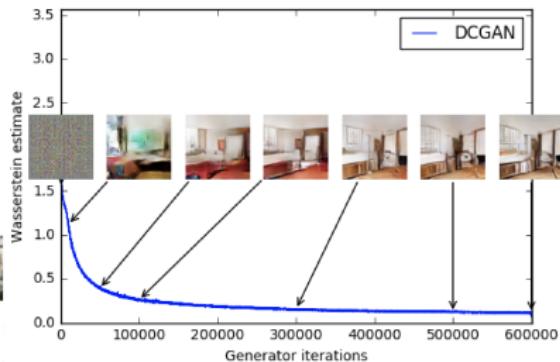
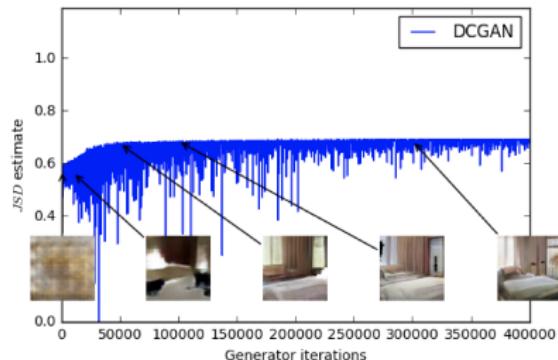
$$\min_{\theta} W(\pi || p) \approx \min_{\theta} \max_{\phi \in \Phi} [\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}, \phi) - \mathbb{E}_{p(\mathbf{z})} f(G(\mathbf{z}, \theta), \phi)] .$$

- ▶ 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.

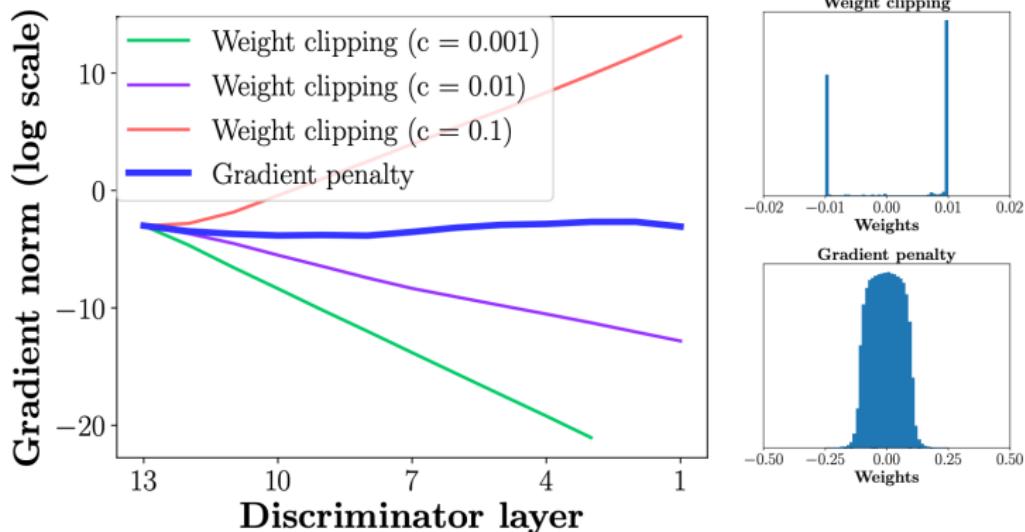


"In no experiment did we see evidence of mode collapse for the WGAN algorithm."

Outline

1. Wasserstein GAN
2. WGAN with Gradient Penalty
3. Spectral Normalization GAN
4. f-divergence minimization

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 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

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

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

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

Corollary

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

Wasserstein GAN with Gradient Penalty

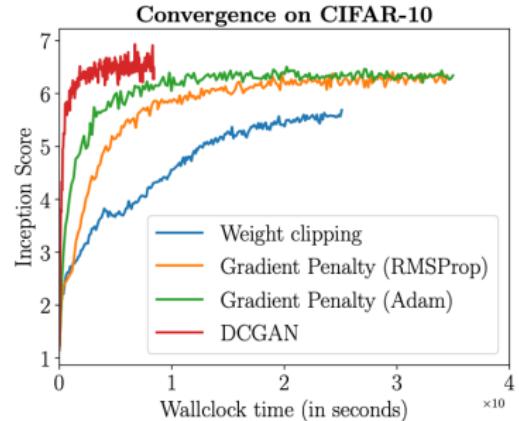
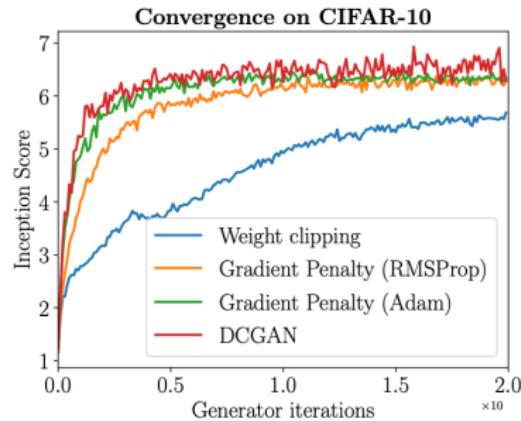
A differentiable function is 1-Lipschitz if and only if it has gradients with norm at most 1 everywhere.

Gradient penalty

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

- ▶ Samples $\hat{\mathbf{x}}_t = t\mathbf{x} + (1 - t)\mathbf{y}$ with $t \in [0, 1]$ are uniformly sampled along straight lines between pairs of points: \mathbf{x} from the data distribution $\pi(\mathbf{x})$ and \mathbf{y} 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.

Wasserstein GAN with Gradient Penalty



WGANGP convergence

Min. score	Only GAN	Only WGANGP	Both succeeded	Both failed
1.0	0	8	192	0
3.0	1	88	110	1
5.0	0	147	42	11
7.0	1	104	5	90
9.0	0	0	0	200

Outline

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3. Spectral Normalization GAN
4. f-divergence minimization

Spectral Normalization GAN

Definition

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

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

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

Statement 1

if g is a K-Lipschitz function then

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

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 $f(\mathbf{x}, \phi)$ of the following form:

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

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).
- ▶ $\mathbf{g}(\mathbf{x}) = \mathbf{W}\mathbf{x}$ 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

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

If we replace the weights in the critic $f(\mathbf{x}, \phi)$ 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 $\|\mathbf{W}\|_2 = \lambda_{\max}(\mathbf{W}^T \mathbf{W})$?

If we apply SVD to compute the $\|\mathbf{W}\|_2$ at each iteration, the algorithm becomes intractable.

Power iteration method

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

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

- ▶ approximate the spectral norm

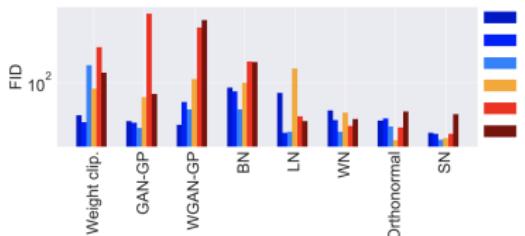
$$\|\mathbf{W}\|_2 = \lambda_{\max}(\mathbf{W}^T \mathbf{W}) \approx \mathbf{u}_K^T \mathbf{W} \mathbf{v}_K.$$

Spectral Normalization GAN

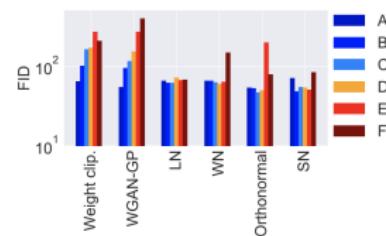
Algorithm 1 SGD with spectral normalization

- Initialize $\tilde{\mathbf{u}}_l \in \mathcal{R}^{d_l}$ for $l = 1, \dots, L$ with a random vector (sampled from isotropic distribution).
- For each update and each layer l :
 1. Apply power iteration method to a unnormalized weight W^l :
$$\tilde{\mathbf{v}}_l \leftarrow (W^l)^T \tilde{\mathbf{u}}_l / \| (W^l)^T \tilde{\mathbf{u}}_l \|_2 \quad (20)$$
$$\tilde{\mathbf{u}}_l \leftarrow W^l \tilde{\mathbf{v}}_l / \| W^l \tilde{\mathbf{v}}_l \|_2 \quad (21)$$
 2. Calculate \bar{W}_{SN} with the spectral norm:
$$\bar{W}_{\text{SN}}^l(W^l) = W^l / \sigma(W^l), \text{ where } \sigma(W^l) = \tilde{\mathbf{u}}_l^T W^l \tilde{\mathbf{v}}_l \quad (22)$$
 3. Update W^l with SGD on mini-batch dataset \mathcal{D}_M with a learning rate α :

$$W^l \leftarrow W^l - \alpha \nabla_{W^l} \ell(\bar{W}_{\text{SN}}^l(W^l), \mathcal{D}_M) \quad (23)$$



(a) CIFAR-10



(b) STL-10

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

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

General divergence minimization task

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

Challenge

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

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	$\int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx - \log(4)$	$u \log u - (u+1) \log(u+1)$

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} .

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

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

f-divergence family

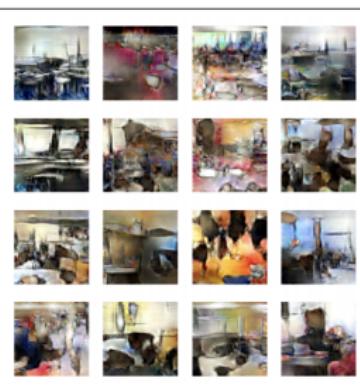
Variational divergence estimation

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

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



(a) GAN



(b) KL



(c) Squared Hellinger

Summary

- ▶ 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 works better.
- ▶ Spectral normalization is a weight normalization technique to enforce Lipshitzness, which is helpful for generator and discriminator.
- ▶ f-divergence family is a unified framework for divergence minimization, which uses variational approximation. Standard GAN is a special case of it.