Deep Generative Models

Lecture 10

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Spring, 2022

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

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

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

ELBO objective

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

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

We have to estimate density ratio

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

Adversarial Variational Bayes

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

Mescheder L., Nowozin S., Geiger A. Adversarial variational bayes: Unifying variational autoencoders and generative adversarial networks, 2017

Recap of previous lecture

Standard GAN

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

Main problems

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

Informal theoretical results

Distribution of real images $\pi(\mathbf{x})$ and distribution of generated images $p(\mathbf{x}|\boldsymbol{\theta})$ 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

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 $\mathbf{y}$).
- $\gamma(\mathbf{x}, \mathbf{y})$ – the amount, $\|\mathbf{x} - \mathbf{y}\|$– the distance.

Theorem (Kantorovich-Rubinstein duality)

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

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

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

Outline

1. Wassestein GAN

2. WGAN with Gradient Penalty

3. Spectral Normalization GAN

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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)

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

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

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

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

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

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

$$\geq \max_{\phi \in \mathbf{\Phi}} \left[\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}, \phi) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x}, \phi) \right]$$

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

Wassestein GAN

Vanilla GAN objective

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

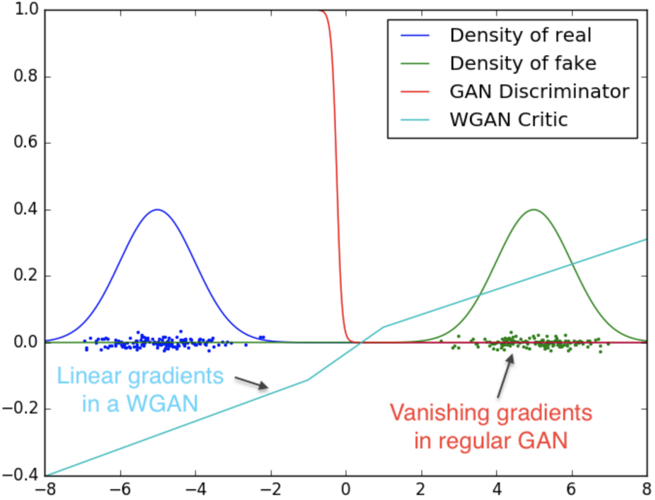
WGAN objective

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

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

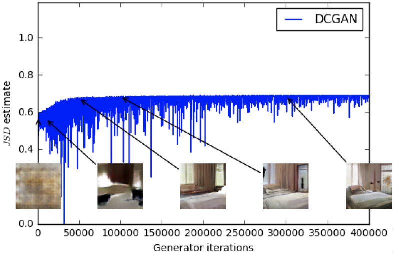
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

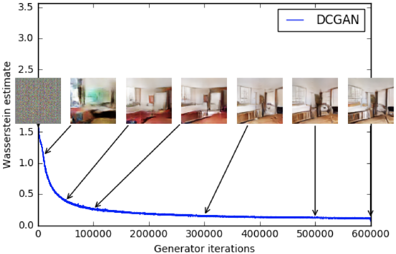
Wasserstein GAN



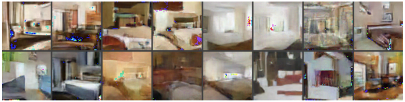
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

Wasserstein GAN





- *JSD* correlates poorly with the sample quality. Stays constast 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."

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

Outline

1. Wassestein GAN

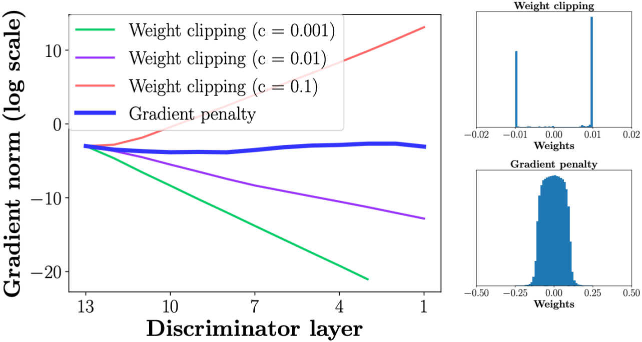
2. WGAN with Gradient Penalty

3. Spectral Normalization GAN

Wasserstein GAN with Gradient Penalty

Weight clipping analysis

- The critic ignores higher moments of the data distribution.
- 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. Then, there is 1-Lipschitz function f^* which is the optimal solution of

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

Let γ be the optimal transportation plan between $\pi(\mathbf{x})$ and $p(\mathbf{x})$. Then, if f^* is differentiable, $\gamma(\mathbf{x} = \mathbf{y}) = 0$ and $\hat{\mathbf{x}}_t = t\mathbf{x} + (1 - t)\mathbf{y}$ with $\mathbf{x} \sim \pi(\mathbf{x})$, $\mathbf{y} \sim p(\mathbf{x}|\boldsymbol{\theta})$, $t \in [0, 1]$ 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 $p(\mathbf{x})$.

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.

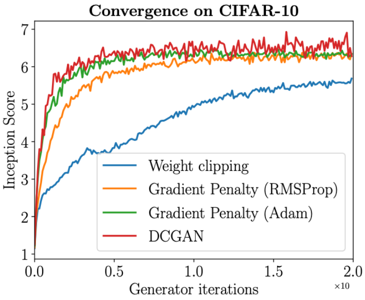
Gradient penalty

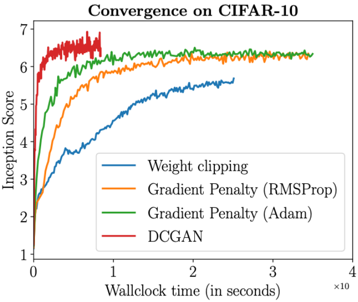
$$W(\pi||p) = \underbrace{\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x})}_{\text{original critic loss}} + \lambda \underbrace{\mathbb{E}_{U[0,1]} \left[(\|\nabla_{\hat{\mathbf{x}}} f(\hat{\mathbf{x}})\|_2 - 1)^2 \right]}_{\text{gradient penalty}},$$

- 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 $p(\mathbf{x}|\boldsymbol{\theta})$.
- 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

Wasserstein GAN with Gradient Penalty





WGAN-GP convergence

Min. score	Only GAN	Only WGAN-GP	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

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

Spectral Normalization GAN

Definition

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

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

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

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

Statement 2

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

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

Miyato T. et al. Spectral Normalization for Generative Adversarial Networks, 2018

Outline

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 $\|f\|_L \leq 1$.

Miyato T. et al. Spectral Normalization for Generative Adversarial Networks, 2018

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 $k = 0, \dots, n-1$: (n is a large enough 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

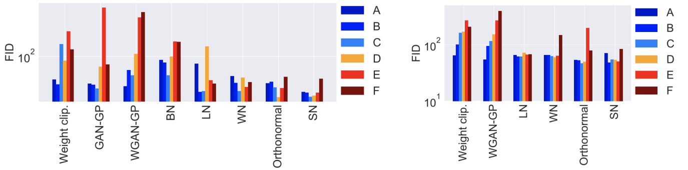
$$\|\mathbf{W}\|_2 = \lambda_{\max}(\mathbf{W}^T\mathbf{W}) \approx \mathbf{u}_n^T\mathbf{W}\mathbf{v}_n.$$

Miyato T. et al. Spectral Normalization for Generative Adversarial Networks, 2018

Spectral Normalization GAN

Algorithm 1 SGD with spectral normalization

- Initialize $\tilde{\boldsymbol{u}}_l \in \mathcal{R}^{d_l}$ for $l = 1, \ldots, L$ 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:
  $$\tilde{\boldsymbol{v}}_l \leftarrow (W^l)^{\mathrm{T}} \tilde{\boldsymbol{u}}_l / \|(W^l)^{\mathrm{T}} \tilde{\boldsymbol{u}}_l\|_2 \quad (20)$$
  $$\tilde{\boldsymbol{u}}_l \leftarrow W^l \tilde{\boldsymbol{v}}_l / \|W^l \tilde{\boldsymbol{v}}_l\|_2 \quad (21)$$
  2. Calculate $\bar{W}_{\mathrm{SN}}$ with the spectral norm:
  $$\bar{W}^l_{\mathrm{SN}}(W^l) = W^l / \sigma(W^l), \text{ where } \sigma(W^l) = \tilde{\boldsymbol{u}}_l^{\mathrm{T}} W^l \tilde{\boldsymbol{v}}_l \quad (22)$$
  3. Update W^l with SGD on mini-batch dataset $\mathcal{D}_M$ with a learning rate α:
  $$W^l \leftarrow W^l - \alpha \nabla_{W^l} \ell(\bar{W}^l_{\mathrm{SN}}(W^l), \mathcal{D}_M) \quad (23)$$



(a) CIFAR-10 (b) STL-10

Miyato T. et al. Spectral Normalization for Generative Adversarial Networks, 2018

Summary

- Wasserstein GAN uses Kantorovich-Rubinstein duality to obtain EM distance.
- 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.