Deep Generative Models
Lecture 10

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Recap of previous lecture

Likelihood-free learning

- Likelihood is not a perfect measure 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.

Two sample test

$$H_0 : \pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta}), \quad H_1 : \pi(\mathbf{x}) \neq p(\mathbf{x}|\boldsymbol{\theta})$$

If test statistic $T(\mathcal{S}_1, \mathcal{S}_2) < \alpha$, then accept H_0, else reject it.

- $p(\mathbf{x}|\boldsymbol{\theta})$ minimizes the value of test statistic $T(\mathcal{S}_1, \mathcal{S}_2)$.
- It is hard to find an appropriate test statistic in high dimensions. $T(\mathcal{S}_1, \mathcal{S}_2)$ could be learnable.

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

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

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

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

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.

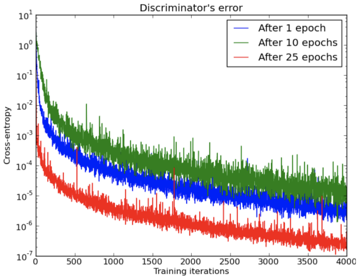
Goodfellow I. J. et al. Generative Adversarial Networks, 2014

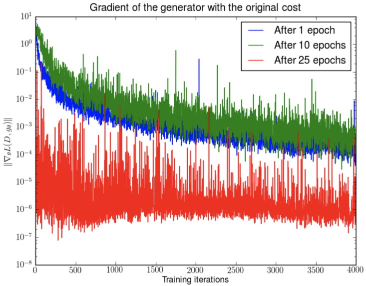
Vanishing gradients

Objective

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

Early in learning, G is poor, D can reject samples with high confidence. In this case, $\log(1 - D(G(\mathbf{z})))$ saturates.





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

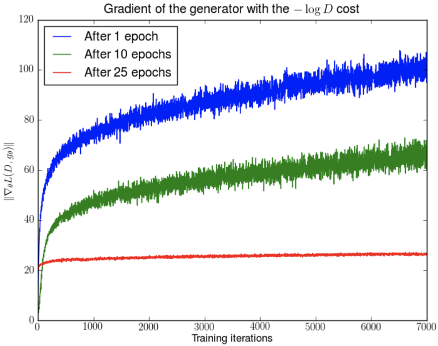
Vanishing gradients

Objective

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

Non-saturating GAN

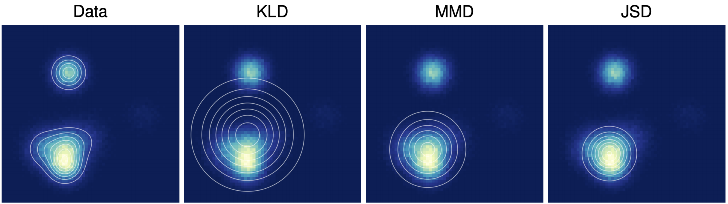
- Maximize $\log D(G(z))$ instead of minimizing $\log(1 - D(G(\mathbf{z})))$.
- Gradients are getting much stronger, but the training is unstable (with increasing mean and variance).

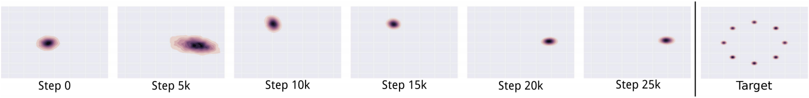


Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

Mode collapse

The phenomena where the generator of a GAN collapses to one or few distribution modes.





Alternate architectures, adding regularization terms, injecting small noise perturbations and other millions bags and tricks are used to avoid the mode collapse.

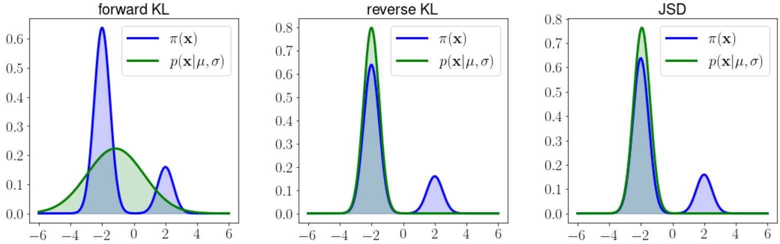
Goodfellow I. J. et al. Generative Adversarial Networks, 2014
Metz L. et al. Unrolled Generative Adversarial Networks, 2016

Jensen-Shannon vs Kullback-Leibler

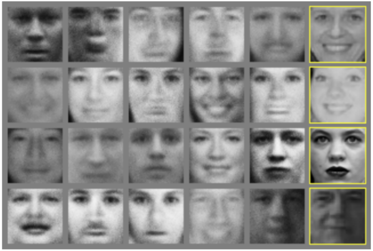
Mode covering vs mode seeking

$$KL(\pi||p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad KL(p||\pi) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

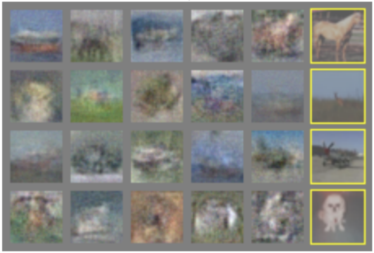
$$JSD(\pi||p) = \frac{1}{2} \left[KL\left(\pi(\mathbf{x}) || \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2}\right) + KL\left(p(\mathbf{x}) || \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2}\right)\right]$$

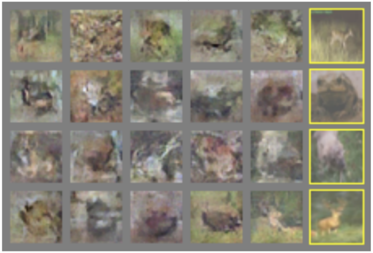


Vanilla GAN results



a) b)



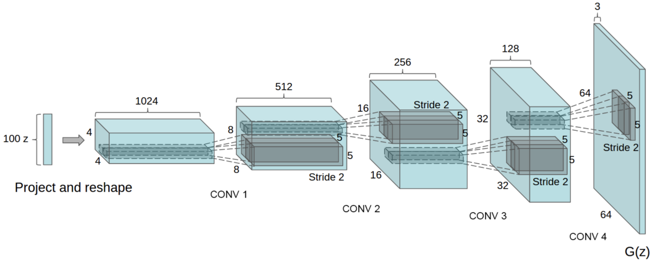


c) d)

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

Deep Convolutional GAN

Architecture



- Mean-pooling instead of max-pooling.
- Transposed convolutions in the generator for upsampling.
- Downsample with strided convolutions and average pooling.
- ReLU for generator, Leaky-ReLU (0.2) for discriminator.
- Output nonlinearity: tanh for Generator, sigmoid for discriminator.
- Batch Normalization used to prevent mode collapse (not applied at the output of G and input of D).
- Adam: small LR $= 2e\text{-}4$; small momentum: 0.5, batch-size: 128.

Radford A., Metz L., Chintala S. Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, 2015

Deep Convolutional GAN

ImageNet samples

Radford A., Metz L., Chintala S. Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, 2015

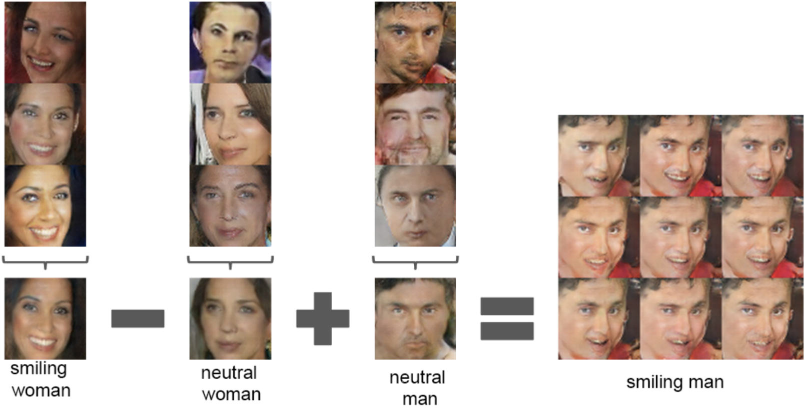
Deep Convolutional GAN

Smooth interpolations

Radford A., Metz L., Chintala S. Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, 2015

Deep Convolutional GAN

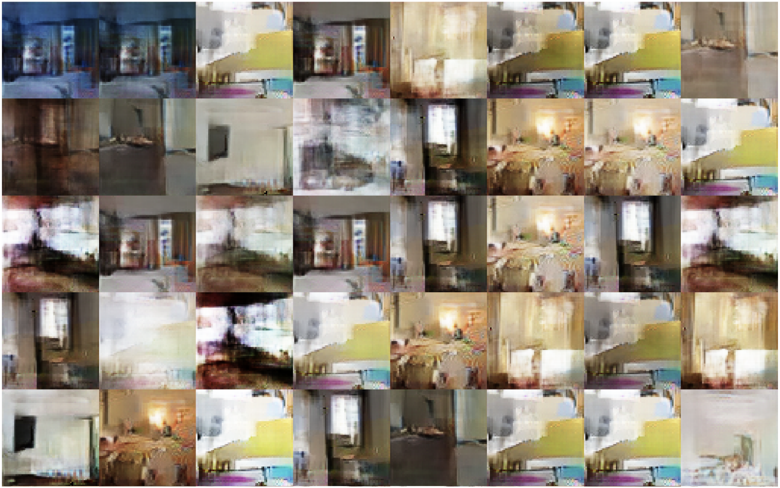
Vector arithmetic



Radford A., Metz L., Chintala S. *Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks, 2015*

Deep Convolutional GAN

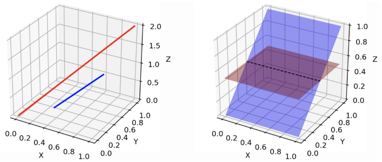
Mode collapse



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

Informal theoretical results

- Since $\mathbf{z}$ usually has lower dimensionality compared to $\mathbf{x}$, manifold $G(\mathbf{z})$ has a measure 0 in $\mathbf{x}$ space. Hence, support of $p(\mathbf{x}|\boldsymbol{\theta})$ 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 $p(\mathbf{x}|\boldsymbol{\theta})$ have disjoint supports, then there is a smooth optimal discrimator. We are not able to learn anything by backproping through it.
- For such low-dimensional disjoint manifolds

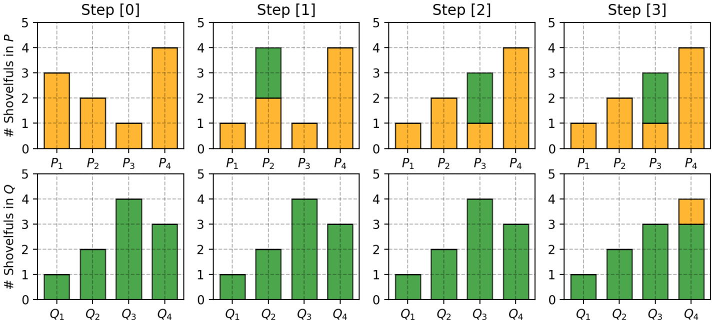
$$KL(\pi||p) = KL(p||\pi) = \infty, \quad JSD(\pi||p) = \log 2$$

- 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)

Also called 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.



$$W(P, Q) = 2(\text{step }1) + 2(\text{step }2) + 1(\text{step }3) = 5$$

Weng L. From GAN to WGAN, 2019

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.

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

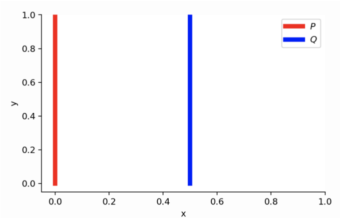
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

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

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

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

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

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

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

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.

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

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

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

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

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

- 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

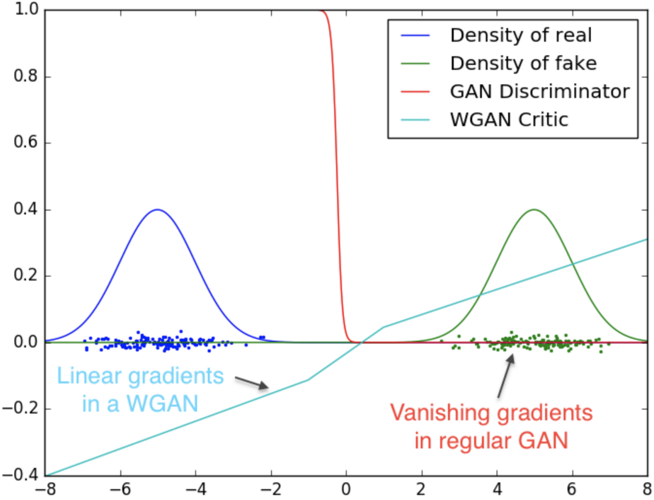
Algorithm 1 WGAN, our proposed algorithm. All experiments in the paper used the default values $\alpha = 0.00005$, $c = 0.01$, $m = 64$, $n_{\text{critic}} = 5$.

Require: : α, the learning rate. c, the clipping parameter. m, the batch size. n_{critic}, the number of iterations of the critic per generator iteration.
Require: : w_0, initial critic parameters. θ_0, initial generator's parameters.

while θ has not converged **do**
    for $t = 0, ..., n_{\text{critic}}$ **do**
        Sample $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$ a batch from the real data.
        Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.
        $g_w \leftarrow \nabla_w \left[\frac{1}{m}\sum_{i=1}^m f_w(x^{(i)}) - \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))\right]$
        $w \leftarrow w + \alpha \cdot \text{RMSProp}(w, g_w)$
        $w \leftarrow \text{clip}(w, -c, c)$
    end for
    Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.
    $g_\theta \leftarrow -\nabla_\theta \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))$
    $\theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, g_\theta)$
end while

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

Wasserstein GAN



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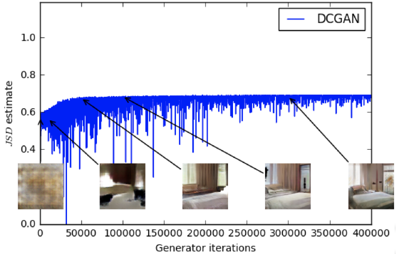
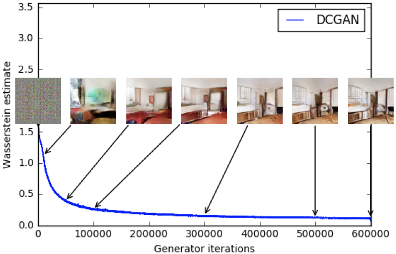
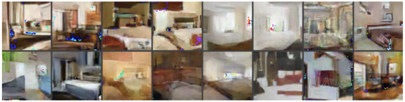
Wasserstein GAN





- *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

Summary

- Mode collapse and vanishing gradients are the two main problems of vanilla GAN. Lots of tips and tricks has to be used to make the GAN training is stable and scalable.
- DCGAN is the first GAN with deep convolutional architecture.
- 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.
- Wasserstein GAN uses Kantorovich-Rubinstein duality to obtain EM distance.
- Weight clipping is a way to enforce Lipschitzness of the critic.