

Deep Generative Models

Lecture 7

Roman Isachenko

Moscow Institute of Physics and Technology
Yandex School of Data Analysis

2024, Autumn

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

- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ – real samples;
- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\theta)$ – generated (or fake) samples.

Let define discriminative model (classifier):

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

Assumption

Generative distribution $p(\mathbf{x}|\theta)$ 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

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

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

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

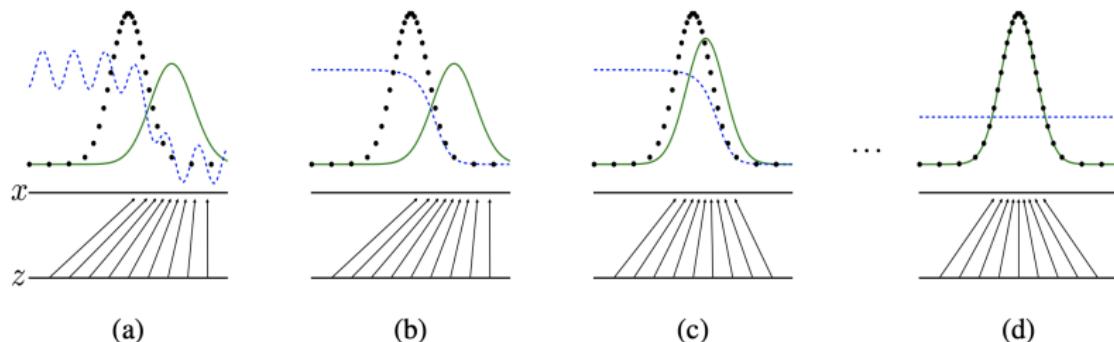
If the generator could be **any** function and the discriminator is **optimal** at every step, then the generator is **guaranteed to converge** to the data distribution.

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

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



Recap of previous lecture

Main problems of standard GAN

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

Standard GAN

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

Informal theoretical results

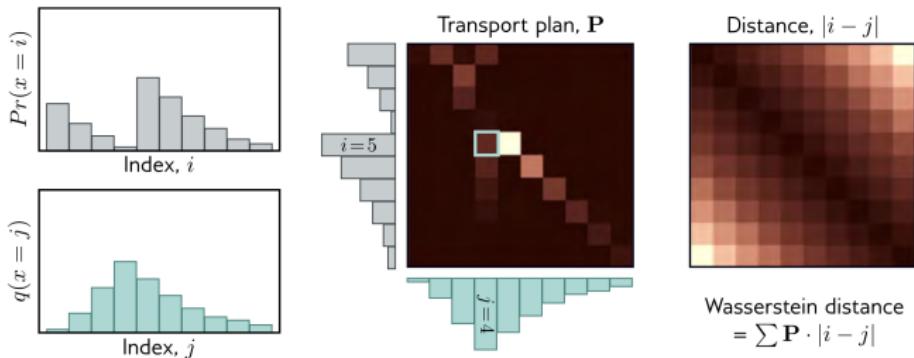
The real images distribution $\pi(\mathbf{x})$ and the generated images distribution $p(\mathbf{x}|\theta)$ are low-dimensional and have disjoint supports.
In this case

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

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

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

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

Outline

1. Wasserstein GAN
2. f-divergence minimization
3. Evaluation of likelihood-free models
 - Frechet Inception Distance (FID)
 - Precision-Recall

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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)

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

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

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

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

Wasserstein GAN

Standard GAN objective

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

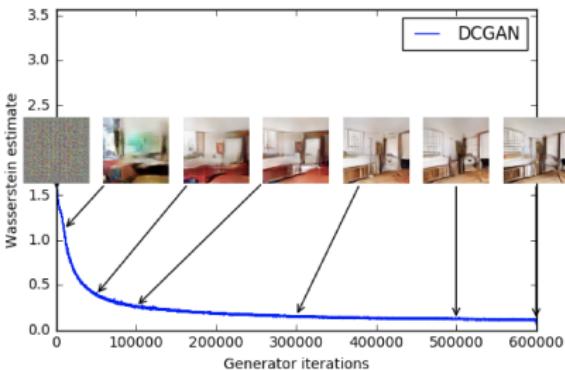
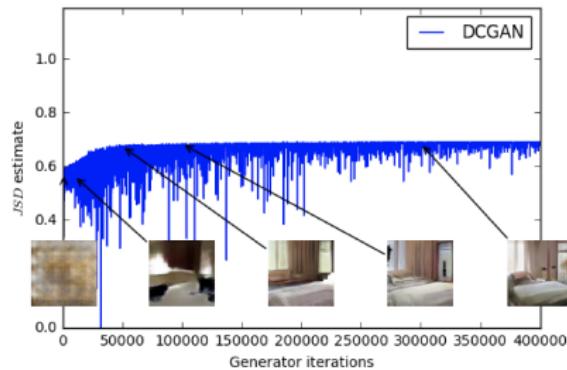
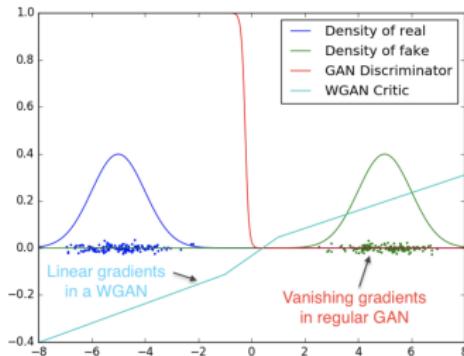
WGAN objective

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

- ▶ Discriminator D is similar to the function f , but 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.



Outline

1. Wasserstein GAN
2. f-divergence minimization
3. Evaluation of likelihood-free models
 - Frechet Inception Distance (FID)
 - Precision-Recall

Divergences

- ▶ Forward KL divergence in the maximum likelihood estimation.
- ▶ Reverse KL in the variational inference (KL term in ELBO).
- ▶ JS divergence in the 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 $\pi(x)$!

f-divergence family

f-divergence

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

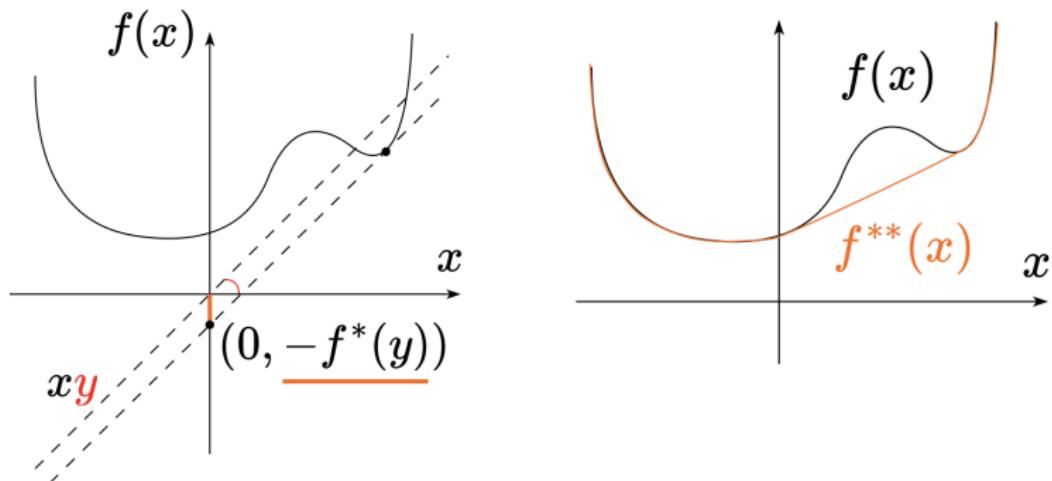
Here $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is a convex, lower semicontinuous function satisfying $f(1) = 0$.

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 family

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

Variational f-divergence estimation

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

f-divergence family

Variational divergence estimation

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

- ▶ Here \mathcal{T} is a predefined class of functions.
- ▶ 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 $T(\mathbf{x}) = \log D(\mathbf{x})$ ($D(\mathbf{x}) \in [0, 1]$).

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

f-divergence family

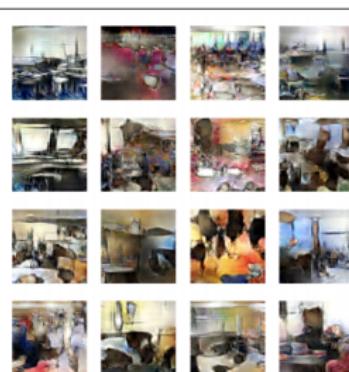
Variational divergence estimation

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

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



(a) GAN



(b) KL



(c) Squared Hellinger

Outline

1. Wasserstein GAN
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3. Evaluation of likelihood-free models
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Evaluation of likelihood-free models

Likelihood-based models

- ▶ **train part:** fit the model.
- ▶ **validation part:** tune the hyperparameters.
- ▶ **test part:** evaluate generalization by reporting the likelihood.

Not all models have tractable likelihood
(VAE: compare ELBO values; GAN: ???).

What do we want from samples?

- ▶ Sharpness



- ▶ Diversity



Evaluation of likelihood-free models

Let's take some pretrained image classification model to get the conditional label distribution $p(y|x)$ (e.g. ImageNet classifier).

What do we want from samples?

- ▶ **Sharpness.** The **conditional** distribution $p(y|x)$ should have low entropy (each image x depicts distinctly recognizable object).
- ▶ **Diversity.** The **marginal** distribution $p(y) = \int p(y|x)p(x)dx$ should have high entropy (we generate all classes uniformly).

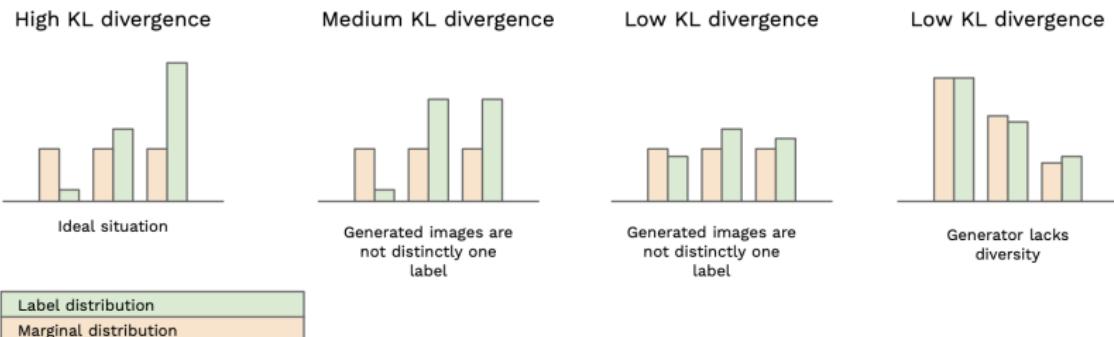


image credit: <https://medium.com/octavian-ai/a-simple-explanation-of-the-inception-score-372dff6a8c7a>

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Frechet Inception Distance (FID)

Wasserstein metric

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

Theorem

If $\pi(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi)$, $p(\mathbf{y}) = \mathcal{N}(\boldsymbol{\mu}_p, \boldsymbol{\Sigma}_p)$, then

$$W_2^2(\pi, p) = \|\boldsymbol{\mu}_\pi - \boldsymbol{\mu}_p\|^2 + \text{tr} \left[\boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2 \left(\boldsymbol{\Sigma}_\pi^{1/2} \boldsymbol{\Sigma}_p \boldsymbol{\Sigma}_\pi^{1/2} \right)^{1/2} \right]$$

Frechet Inception Distance

$$\text{FID}(\pi, p) = W_2^2(\pi, p)$$

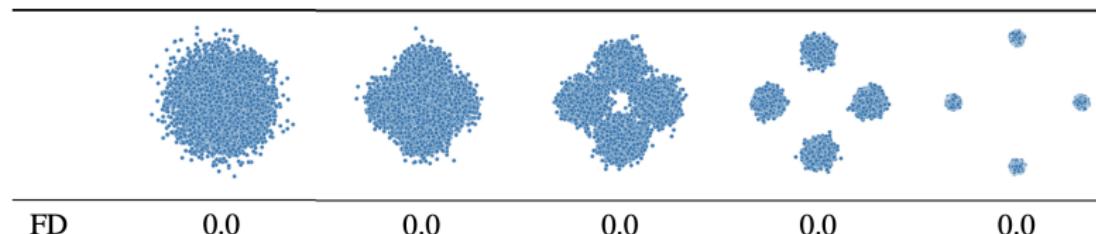
- ▶ Representations are the outputs of the intermediate layer from the pretrained classification model.
- ▶ $\boldsymbol{\mu}_\pi$, $\boldsymbol{\Sigma}_\pi$ and $\boldsymbol{\mu}_p$, $\boldsymbol{\Sigma}_p$ are the statistics of the feature representations for the samples from $\pi(\mathbf{x})$ and $p(\mathbf{x}|\theta)$.

Frechet Inception Distance (FID)

$$\text{FID}(\pi, p) = \|\boldsymbol{\mu}_\pi - \boldsymbol{\mu}_p\|^2 + \text{tr} \left[\boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2 \left(\boldsymbol{\Sigma}_\pi^{1/2} \boldsymbol{\Sigma}_p \boldsymbol{\Sigma}_\pi^{1/2} \right)^{1/2} \right]$$

- ▶ Needs a large sample size for evaluation.
- ▶ Calculation of FID is slow.
- ▶ High dependence on the pretrained classification model.
- ▶ Uses the normality assumption!

$$FID(p(\mathbf{x}), \mathcal{N}(0, \mathbf{I}))$$



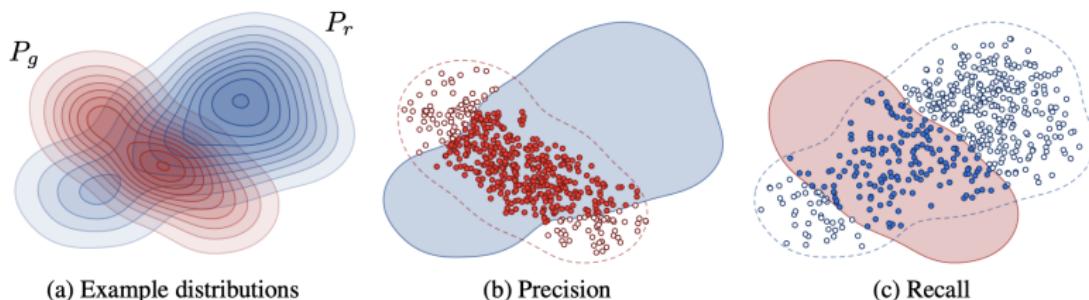
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Precision-Recall

What do we want from samples

- ▶ **Sharpness:** generated samples should be of high quality.
- ▶ **Diversity:** their variation should match that observed in the training set.



- ▶ **Precision** denotes the fraction of generated images that are realistic.
- ▶ **Recall** measures the fraction of the training data manifold covered by the generator.

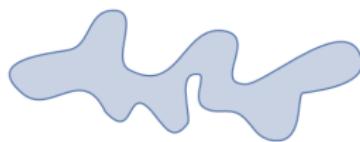
Precision-Recall

- ▶ $\mathcal{S}_\pi = \{\mathbf{x}_i\}_{i=1}^n \sim \pi(\mathbf{x})$ – real samples;
- ▶ $\mathcal{S}_p = \{\mathbf{x}_i\}_{i=1}^n \sim p(\mathbf{x}|\theta)$ – generated samples.

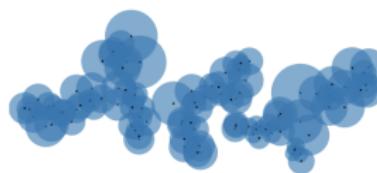
Define binary function:

$$\mathbb{I}(\mathbf{x}, \mathcal{S}) = \begin{cases} 1, & \text{if exists } \mathbf{x}' \in \mathcal{S} : \|\mathbf{x} - \mathbf{x}'\|_2 \leq \|\mathbf{x}' - \text{NN}_k(\mathbf{x}', \mathcal{S})\|_2; \\ 0, & \text{otherwise.} \end{cases}$$

$$\text{Precision}(\mathcal{S}_\pi, \mathcal{S}_p) = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{S}_p} \mathbb{I}(\mathbf{x}, \mathcal{S}_\pi); \quad \text{Recall}(\mathcal{S}_\pi, \mathcal{S}_p) = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{S}_\pi} \mathbb{I}(\mathbf{x}, \mathcal{S}_p).$$



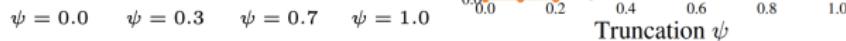
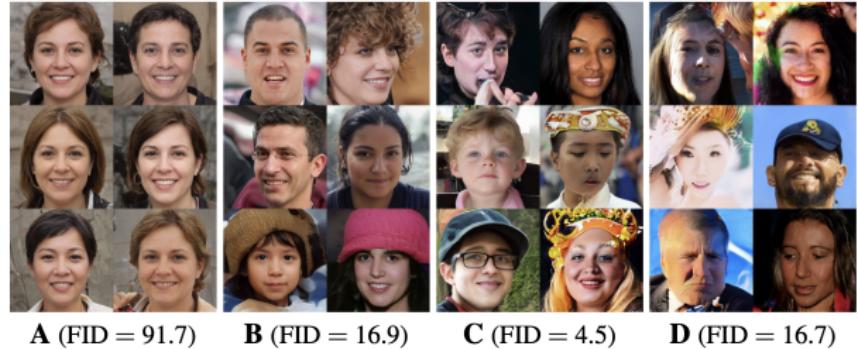
(a) True manifold



(b) Approx. manifold

Embed the samples using the pretrained network (as for FID).

Precision-Recall



Truncation trick

BigGAN: truncated normal sampling

$$p(\mathbf{z}|\psi) = \frac{\mathcal{N}(\mathbf{z}|0, \mathbf{I})}{\int_{-\infty}^{\psi} \mathcal{N}(\mathbf{z}'|0, \mathbf{I}) d\mathbf{z}'}$$

Elements of $\mathbf{z} \sim \mathcal{N}(0, \mathbf{I})$ which fall outside a predefined range are resampled.

StyleGAN

$$\mathbf{z}' = \hat{\mathbf{z}} + \psi \cdot (\mathbf{z} - \hat{\mathbf{z}}), \quad \hat{\mathbf{z}} = \mathbb{E}_{\mathbf{z}} \mathbf{z}$$

- ▶ Constant ψ is a tradeoff between diversity and fidelity.
- ▶ $\psi = 0.7$ is used for most of the results.

Brock A., Donahue J., Simonyan K. Large Scale GAN Training for High Fidelity Natural Image Synthesis, 2018

Karras T., Laine S., Aila T. A Style-Based Generator Architecture for Generative Adversarial Networks, 2018

Summary

- ▶ Kantorovich-Rubinstein duality gives the way to calculate the EM distance using only samples.
- ▶ Wasserstein GAN uses the weight clipping to ensure the Lipschitness of the critic.
- ▶ f-divergence family is a unified framework for divergence minimization, which uses variational approximation. Standard GAN is a special case of it.
- ▶ Frechet Inception Distance is the most popular metric for the implicit models evaluation.
- ▶ Precision-recall allow to select model that compromises the sample quality and the sample diversity.
- ▶ Truncation tricks help to select model with the compromised samples: diverse and sharp.