

# Deep Generative Models

## Lecture 8

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## 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

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

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

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

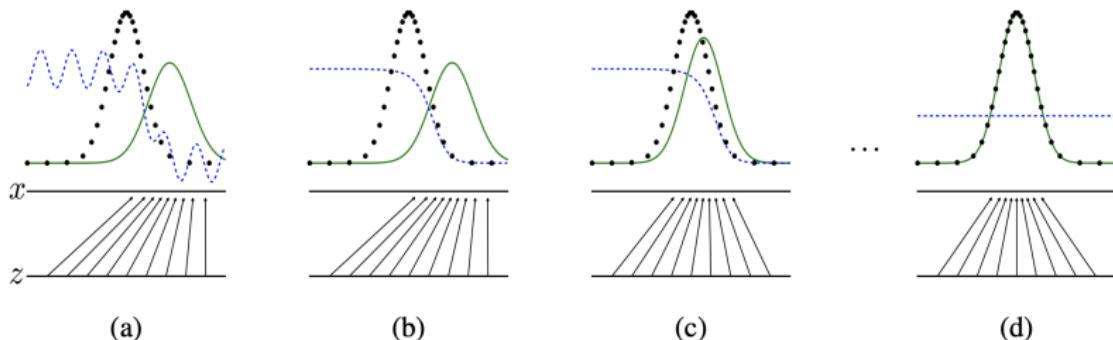
If the generator could be **any** function and the discriminator is **optimal** at every step, then the generator is **guaranteed to converge** to the data distribution.

## 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

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



## Recap of previous lecture

### Main problems of standard GAN

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

### Standard GAN

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

### Informal theoretical results

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

In this case

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

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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

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

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

### Theorem (Kantorovich-Rubinstein duality)

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

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

## Recap of previous lecture

### WGAN objective

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

- ▶ Function  $f$  in WGAN is usually called *critic*.
- ▶ If parameters  $\phi$  lie in a compact set  $\Phi \in [-c, c]^d$  then  $f(x, \phi)$  will be  $K$ -Lipschitz continuous function.

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

"Weight clipping is a clearly terrible way to enforce a Lipschitz constraint"

## Recap of previous lecture

### Theorem

Let  $\pi(\mathbf{x})$  and  $p(\mathbf{x})$  be two distribution in  $\mathcal{X}$ , a compact metric space. Let  $\gamma$  be the optimal transportation plan between  $\pi(\mathbf{x})$  and  $p(\mathbf{x})$ . Then

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

### Gradient penalty

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

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

# Outline

1. f-divergence minimization
2. Evaluation of likelihood-free models
  - Inception score
  - Frechet Inception Distance
  - Precision-Recall

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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 $\chi^2$	$\int \frac{(q(x)-p(x))^2}{p(x)} dx$	$(u-1)^2$
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

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

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

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

# f-divergence family

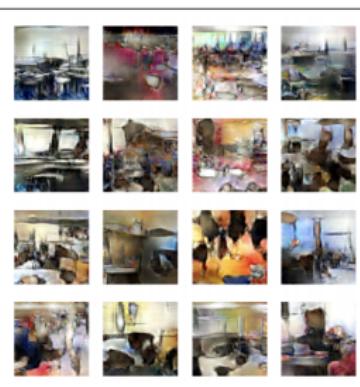
## Variational divergence estimation

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

**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

# Outline

1. f-divergence minimization
2. Evaluation of likelihood-free models
  - Inception score
  - Frechet Inception Distance
  - Precision-Recall

# Evaluation of likelihood-free models

How to evaluate generative models?

## Likelihood-based models

- ▶ Split data to train/val/test.
- ▶ Fit model on the train part.
- ▶ Tune hyperparameters on the validation part.
- ▶ Evaluate generalization by reporting likelihoods on the test set.

Not all models have tractable likelihoods

- ▶ VAE: compare ELBO values.
- ▶ GAN: ???

# 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  $x$  should have distinctly recognizable object).

- ▶ Diversity



The marginal distribution  $p(y) = \int p(y|x)p(x)dx$  should have high entropy (there should be as many classes generated as possible).

# Evaluation of likelihood-free models

## What do we want from samples?

- ▶ **Sharpness.** The conditional distribution  $p(y|x)$  should have low entropy (each image  $x$  should have distinctly recognizable object).
- ▶ **Diversity.** The marginal distribution  $p(y) = \int p(y|x)p(x)dx$  should have high entropy (there should be as many classes generated as possible).

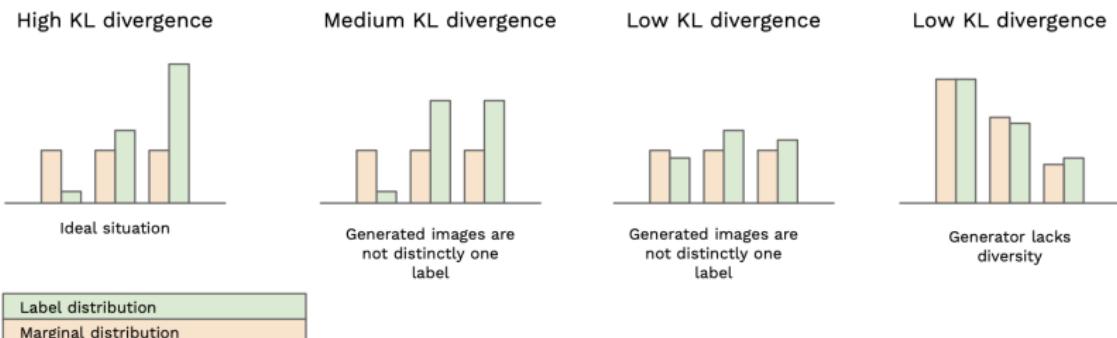


image credit: <https://medium.com/octavian-ai/a-simple-explanation-of-the-inception-score-372dff6a8c7a>

# Outline

1. f-divergence minimization
2. Evaluation of likelihood-free models

Inception score

Frechet Inception Distance

Precision-Recall

# Evaluation of likelihood-free models

What do we want from samples?

- ▶ Sharpness  $\Rightarrow$  low  $H(y|\mathbf{x}) = - \sum_y \int_{\mathbf{x}} p(y, \mathbf{x}) \log p(y|\mathbf{x}) d\mathbf{x}$ .
- ▶ Diversity  $\Rightarrow$  high  $H(y) = - \sum_y p(y) \log p(y)$ .

Inception Score

$$\begin{aligned} IS &= \exp(H(y) - H(y|\mathbf{x})) \\ &= \exp \left( - \sum_y p(y) \log p(y) + \sum_y \int_{\mathbf{x}} p(y, \mathbf{x}) \log p(y|\mathbf{x}) d\mathbf{x} \right) \\ &= \exp \left( \sum_y \int_{\mathbf{x}} p(y, \mathbf{x}) \log \frac{p(y|\mathbf{x})}{p(y)} d\mathbf{x} \right) \\ &= \exp \left( \mathbb{E}_{\mathbf{x}} \sum_y p(y|\mathbf{x}) \log \frac{p(y|\mathbf{x})}{p(y)} \right) = \exp (\mathbb{E}_{\mathbf{x}} KL(p(y|\mathbf{x}) || p(y))) \end{aligned}$$

# Outline

1. f-divergence minimization
2. Evaluation of likelihood-free models

Inception score

**Frechet Inception Distance**

Precision-Recall

# Evaluation of likelihood-free models

## Theorem (informal)

If  $\pi(\mathbf{x})$  and  $p(\mathbf{x}|\theta)$  has moment generation functions then

$$\pi(\mathbf{x}) = p(\mathbf{x}|\theta) \Leftrightarrow \mathbb{E}_\pi \mathbf{x}^k = \mathbb{E}_p \mathbf{x}^k, \quad \forall k \geq 1.$$

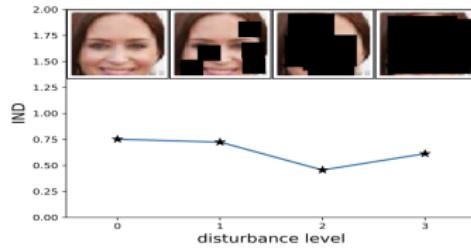
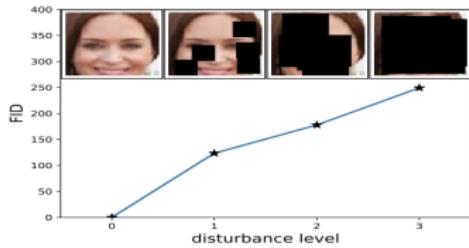
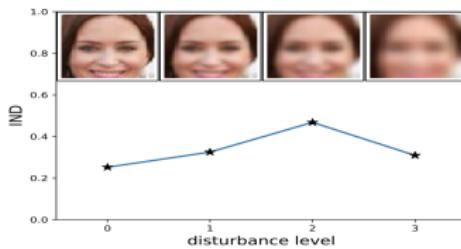
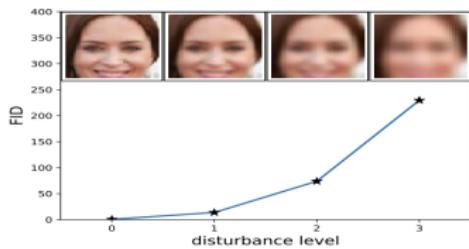
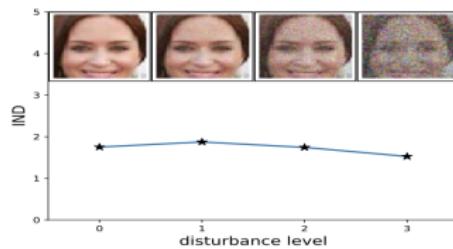
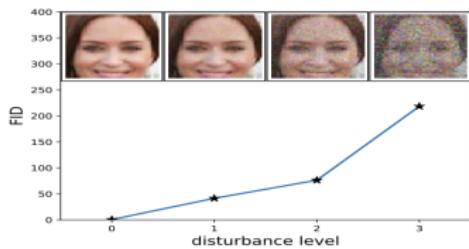
This is intractable to calculate all moments.

## Frechet Inception Distance

$$FID(\pi, p) = \|\mathbf{m}_\pi - \mathbf{m}_p\|_2^2 + \text{Tr} \left( \boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2\sqrt{\boldsymbol{\Sigma}_\pi \boldsymbol{\Sigma}_p} \right)$$

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

# Evaluation of likelihood-free models



# Limitations

## Inception Score

$$IS = \exp(\mathbb{E}_{\mathbf{x}} KL(p(y|\mathbf{x}) || p(y)))$$

- ▶ If generator produces images with a different set of labels from the classifier training set, IS will be low.
- ▶ If generator produces one image per class, the IS will be perfect (there is no measure of intra-class diversity).

## Frechet Inception Distance

$$FID = \|\mathbf{m}_\pi - \mathbf{m}_p\|_2^2 + \text{Tr} \left( \boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2\sqrt{\boldsymbol{\Sigma}_\pi \boldsymbol{\Sigma}_p} \right)$$

- ▶ Needs a large sample size for evaluation.
- ▶ Calculation of FID is slow.
- ▶ Estimates only two sample moments.

Both scores depend on the pretrained classifier  $p(y|\mathbf{x})$ .

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Barratt S., Sharma R. A Note on the Inception Score, 2018

Heusel M. et al. GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium, 2017

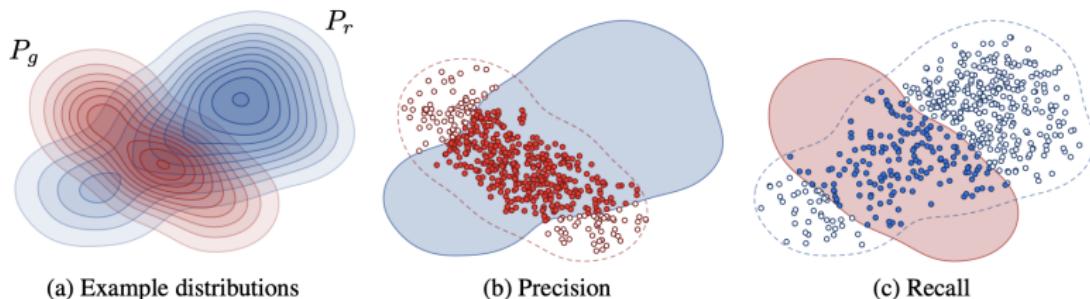
# Outline

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# Precision-Recall for Generative Models

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 for generative models

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

Embed samples using pretrained classifier network (as previously):

$$\mathcal{G}_\pi = \{\mathbf{g}_i\}_{i=1}^n, \quad \mathcal{G}_p = \{\mathbf{g}_i\}_{i=1}^n.$$

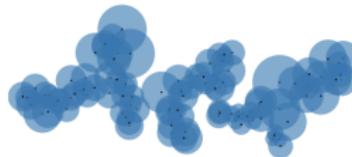
Define binary function:

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

$$\text{Precision}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_p} f(\mathbf{g}, \mathcal{G}_\pi); \quad \text{Recall}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_\pi} f(\mathbf{g}, \mathcal{G}_p).$$

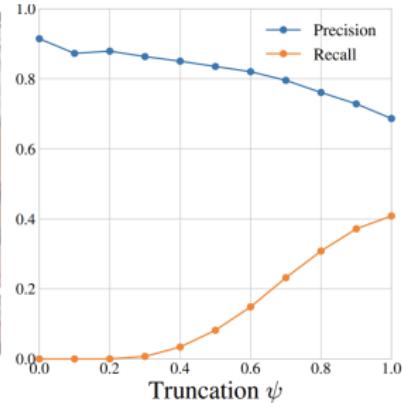
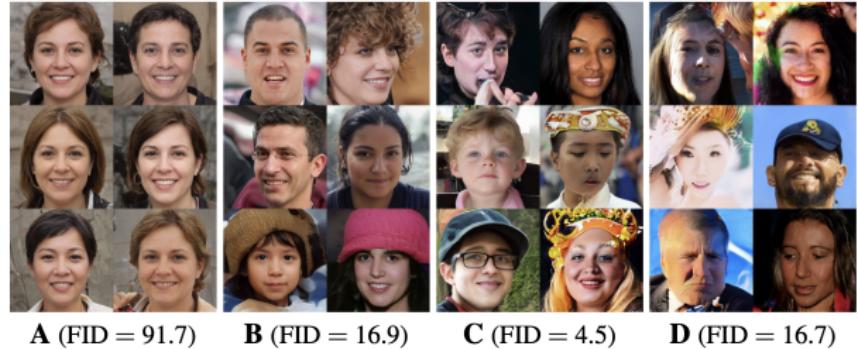
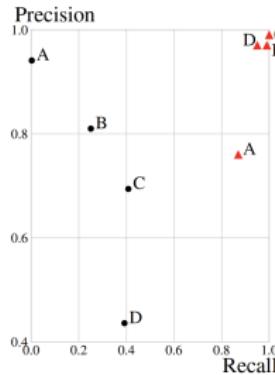


(a) True manifold



(b) Approx. manifold

# Precision-Recall for generative models



## Truncation trick

BigGAN: truncated normal sampling

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

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

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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

- ▶ f-divergence family is a unified framework for divergence minimization, which uses variational approximation. Standard GAN is a special case of it.
- ▶ We need measure of quality for implicit models like GANs. One way is to analyze sharpness and diversity of samples.
- ▶ Inception Score and Frechet Inception Distance are the common metrics for GAN evaluation, but both of them have drawbacks.
- ▶ Precision-recall allow to select model that compromises the sample quality and the sample diversity.
- ▶ Truncation tricks help to select model with compromised samples: diverse and sharp.