Deep Generative Models

Lecture 9

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Recap of previous lecture

Main problems of standard GAN

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

Standard GAN

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

Informal theoretical results

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

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

- $\gamma(\mathbf{x}, \mathbf{y})$ – 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.

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

Recap of previous lecture

WGAN objective

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

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

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

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

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

Recap of previous lecture

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

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

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

Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017
Gulrajani I. et al. Improved Training of Wasserstein GANs, 2017

Recap of previous lecture

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

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

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

Critic spectral norm

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

Spectral Normalization GAN

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

Power iteration approximates the value of $\|\mathbf{W}\|_2$.

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

Outline

1. f-divergence minimization

2. Evaluation of likelihood-free models
   - Inception score
   - Frechet Inception Distance
   - Precision-Recall

Outline

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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 $D : \mathcal{S} \times \mathcal{S} \to \mathbb{R}$ 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

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

Chalenge

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

f-divergence family

f-divergence

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

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

Name	$D_f(P\|Q)$	Generator $f(u)$
Kullback-Leibler	$\int p(x) \log \frac{p(x)}{q(x)} \, \mathrm{d}x$	$u \log u$
Reverse KL	$\int q(x) \log \frac{q(x)}{p(x)} \, \mathrm{d}x$	$-\log u$
Pearson χ^2	$\int \frac{(q(x)-p(x))^2}{p(x)} \, \mathrm{d}x$	$(u-1)^2$
Squared Hellinger	$\int \left(\sqrt{p(x)} - \sqrt{q(x)}\right)^2 \mathrm{d}x$	$(\sqrt{u}-1)^2$
Jensen-Shannon	$\frac{1}{2} \int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} \, \mathrm{d}x$	$-(u+1)\log \frac{1+u}{2} + u \log u$
GAN	$\int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} \, \mathrm{d}x - \log(4)$	$u \log u - (u+1)\log(u+1)$

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Fenchel conjugate

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

Important property: $f^{**} = f$ for convex f.

f-divergence

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

$$= \int p(\mathbf{x}) \sup_{t \in \text{dom}_{f^*}} \left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})} t - f^*(t) \right) d\mathbf{x} =$$

$$= \int \sup_{t \in \text{dom}_{f^*}} \left(\pi(\mathbf{x}) t - p(\mathbf{x}) f^*(t) \right) d\mathbf{x}.$$

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 $\mathbf{x}$.

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

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

$$D_f(\pi || p) = \int \sup_{t \in \mathrm{dom}_{f^*}} \left(\pi(\mathbf{x}) t - p(\mathbf{x}) f^*(t)\right) d\mathbf{x} \geq$$

$$\geq \sup_{T \in \mathcal{T}} \int \left(\pi(\mathbf{x}) T(\mathbf{x}) - p(\mathbf{x}) f^*(T(\mathbf{x}))\right) d\mathbf{x} =$$

$$= \sup_{T \in \mathcal{T}} \left[\mathbb{E}_\pi T(\mathbf{x}) - \mathbb{E}_p f^*(T(\mathbf{x}))\right]$$

This is a lower bound because of Jensen inequality and restricted class of functions $\mathcal{T} : \mathcal{X} \to \mathbb{R}$.

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Variational divergence estimation

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

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

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

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

f-divergence family

Variational divergence estimation

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

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

Nowozin S., Cseke B., Tomioka R. f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization, 2016

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 take some pretrained image classification model to get the conditional label distribution $p(y|\mathbf{x})$ (e.g. ImageNet classifier).

What do we want from samples?

- **Sharpness**

Low sharpness

High sharpness

The conditional distribution $p(y|\mathbf{x})$ should have low entropy (each image $\mathbf{x}$ should have distinctly recognizable object).

- **Diversity**

Low diversity

High diversity

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

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image credit: https://deepgenerativemodels.github.io

Evaluation of likelihood-free models

What do we want from samples?

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

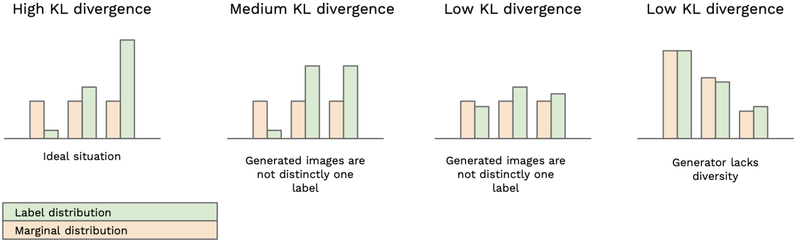


image credit: https://medium.com/octavian-ai/a-simple-explanation-of-the-inception-score-372dff6a8c7a

Outline

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

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

Salimans T. et al. Improved Techniques for Training GANs, 2016

Outline

Evaluation of likelihood-free models

Theorem (informal)

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

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

This is intractable to calculate all moments.

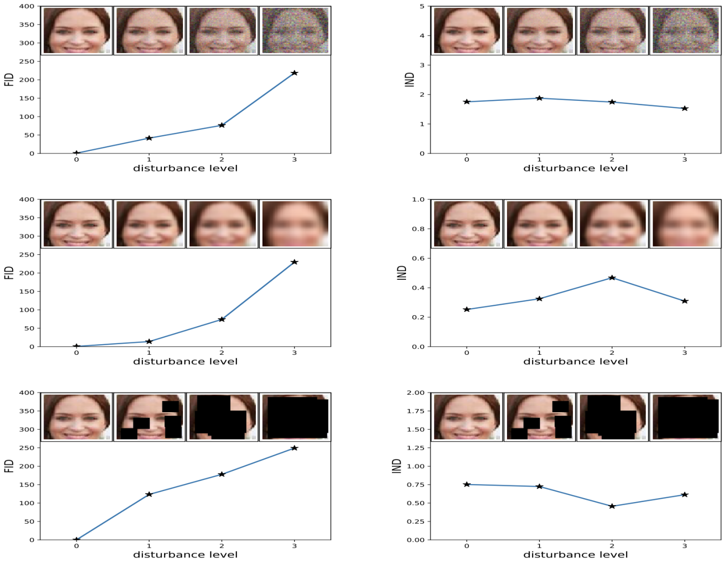
Frechet Inception Distance

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

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

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

Evaluation of likelihood-free models



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

Limitations

Inception Score

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

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

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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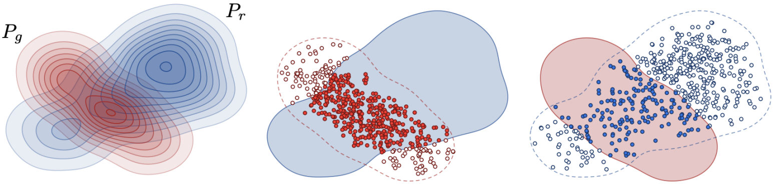
Precision-Recall for Generative Models

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.



(a) Example distributions (b) Precision (c) Recall

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

Kynkäänniemi T. et al. Improved precision and recall metric for assessing generative models, 2019

Precision-Recall for generative models

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

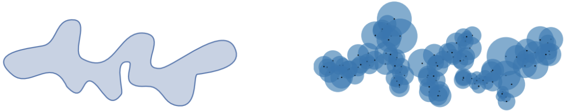
Embed samples using pretrained classifier network (as previously):

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

Define binary function:

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

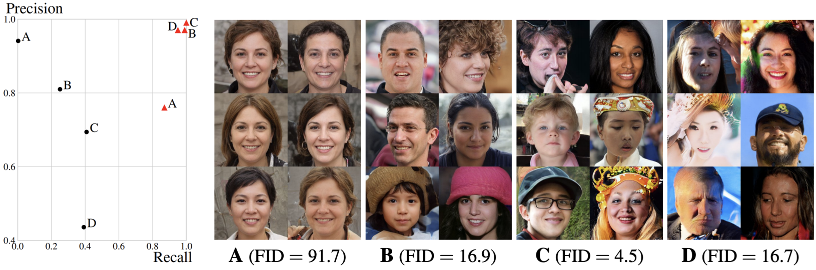
$$\text{Precision}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_p} f(\mathbf{g}, \mathcal{G}_\pi); \;\; \text{Recall}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_\pi} f(\mathbf{g}, \mathcal{G}_p).$$

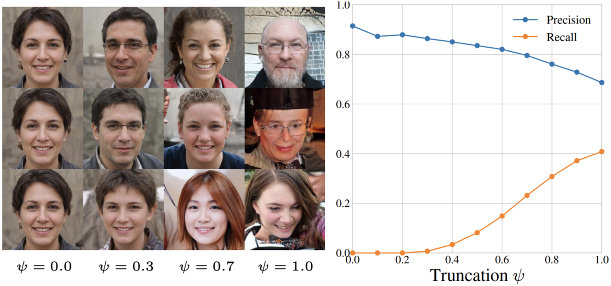


(a) True manifold (b) Approx. manifold

Kynkäänniemi T. et al. Improved precision and recall metric for assessing generative models, 2019

Precision-Recall for generative models





Kynkäänniemi T. et al. Improved precision and recall metric for assessing generative models, 2019

Truncation trick

BigGAN: truncated normal sampling

$$p(\mathbf{z}|\psi) = \mathcal{N}(\mathbf{z}|0, 1) / \int_{-\infty}^{\psi} \mathcal{N}(\mathbf{z}|0, 1) d\mathbf{z}$$

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 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

- 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 allows to select model that compromises the sample quality and the sample diversity.
- Truncation tricks help to select model with compomised samples: diverse and sharp.