

Deep Generative Models

Lecture 11

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Recap of previous lecture

Standard GAN

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

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

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

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

Recap of previous lecture

WGAN objective

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

- ▶ Function f in WGAN is usually called *critic*.
- ▶ If parameters ϕ lie in a compact set $\Phi \in [-0.01, 0.01]^d$ then $f(\mathbf{x}, \phi)$ will be K -Lipschitz continuous function.

Gradient penalty

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

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

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

Outline

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

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

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

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

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

Spectral Normalization GAN

Algorithm 1 SGD with spectral normalization

- Initialize $\tilde{\mathbf{u}}_l \in \mathcal{R}^{d_l}$ for $l = 1, \dots, L$ 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 :

$$\tilde{\mathbf{v}}_l \leftarrow (W^l)^T \tilde{\mathbf{u}}_l / \|(W^l)^T \tilde{\mathbf{u}}_l\|_2 \quad (20)$$

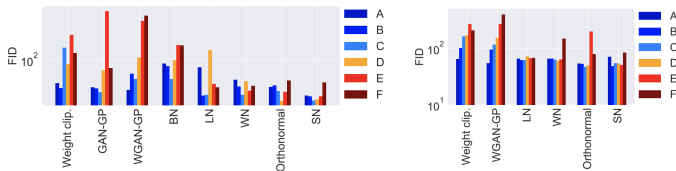
$$\tilde{\mathbf{u}}_l \leftarrow W^l \tilde{\mathbf{v}}_l / \|W^l \tilde{\mathbf{v}}_l\|_2 \quad (21)$$

2. Calculate \bar{W}_{SN}^l with the spectral norm:

$$\bar{W}_{\text{SN}}^l(W^l) = W^l / \sigma(W^l), \text{ where } \sigma(W^l) = \tilde{\mathbf{u}}_l^T W^l \tilde{\mathbf{v}}_l \quad (22)$$

3. Update W^l with SGD on mini-batch dataset \mathcal{D}_M with a learning rate α :

$$W^l \leftarrow W^l - \alpha \nabla_{W^l} \ell(\bar{W}_{\text{SN}}^l(W^l), \mathcal{D}_M) \quad (23)$$



(a) CIFAR-10

(b) STL-10

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 $\pi(\mathbf{x})$!

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 $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ 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	$\int p(x) \log \frac{2p(x)}{p(x)+q(x)} + q(x) \log \frac{2q(x)}{p(x)+q(x)} dx - \log(4)$	$u \log u - (u+1) \log(u+1)$

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

f-divergence family

Fenchel conjugate

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

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

f-divergence

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

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} .

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

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

This is a lower bound because of Jensen-Shannon 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 $T(\mathbf{x}) = \log D(\mathbf{x})$.

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

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.



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

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



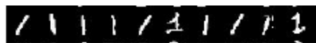
Low sharpness



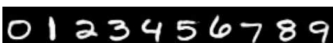
High sharpness

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).

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).

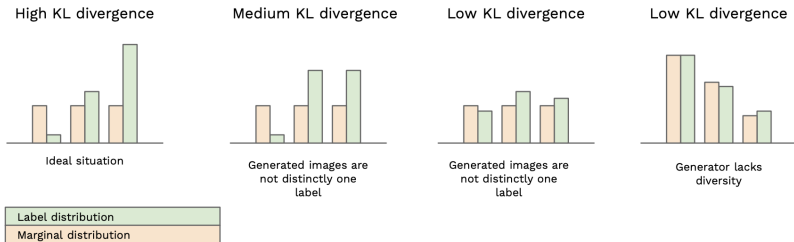


image credit: <https://medium.com/octavian-ai/a-simple-explanation-of-the-inception-score-372dff6a8c7a>

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

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

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.

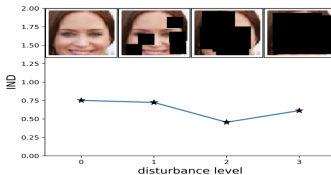
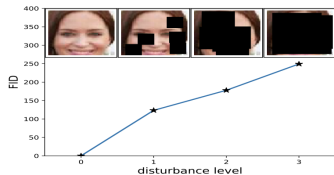
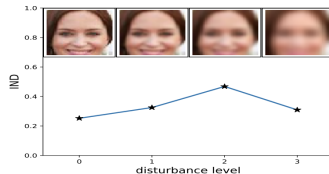
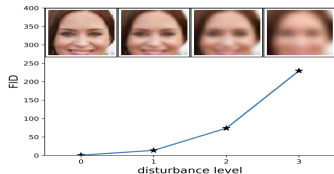
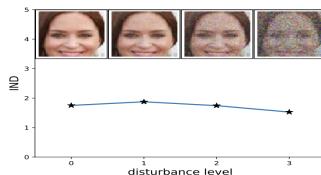
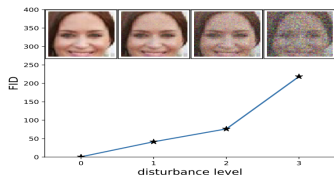
Frechet Inception Distance

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

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

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

- ▶ 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

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

- ▶ 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

Summary

- ▶ Spectral normalization is a weight normalization technique to enforce Lipschitzness, which is helpful for generator and discriminator.
- ▶ f-divergence family is a unified framework for divergence minimization, which uses variational approximation. Standard GAN is a special case of it.
- ▶ Inception Score and Frechet Inception Distance are the common metrics for GAN evaluation, but both of them have drawbacks.