Deep Generative Models

Lecture 11

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Recap of previous lecture

Vanilla GAN

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

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

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

- $\Gamma(\pi, p)$ – 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.

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

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

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

- 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

Spectral Normalization GAN

How else could we enforce Lipschitzness?

Fact 1

Let denote by $\sigma(\mathbf{A})$ a spectral norm of matrix $\mathbf{A}$.

$$\sigma(\mathbf{A}) = \max_{\mathbf{h} \neq 0} \frac{\|\mathbf{A}\mathbf{h}\|_2}{\|\mathbf{h}\|_2} = \max_{\|\mathbf{h}\|_2 \leq 1} \|\mathbf{A}\mathbf{h}\|_2 = \lambda_{\max}(\mathbf{A}),$$

where $\lambda_{\max}(\mathbf{A})$ is the largest singular value of $\mathbf{A}$.
By definition, Lipschitz norm is

$$\|\mathbf{g}\|_L = \sup_{\mathbf{x}} \sigma(\nabla \mathbf{g}(\mathbf{x}))$$

Fact 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:

$$f(\mathbf{x}, \phi) = \mathbf{W}_{K+1} a_K(\mathbf{W}_K a_{K-1}(\dots a_1(\mathbf{W}_1 \mathbf{x}) \dots)).$$

This feedforward network is a superposition of simple functions.

- a_k is a pointwise nonlinearities. We assume that $\|a_k\|_L = 1$ (it holds for ReLU).
- $\mathbf{g}(\mathbf{x}) = \mathbf{W}\mathbf{x}$ is a linear transformation ($\nabla \mathbf{g}(\mathbf{x}) = \mathbf{W}$).

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

Critic spectral norm

$$\|f\|_L \leq \|\mathbf{W}_{K+1}\| \cdot \prod_{k=1}^{K} \|a_k\|_L \cdot \|\mathbf{W}_k\| = \prod_{k=1}^{K+1} \sigma(\mathbf{W}_k).$$

If we replace the weights in the critic $f(\mathbf{x}, \phi)$ by $\mathbf{W}_k^{SN} = \mathbf{W}_k / \sigma(\mathbf{W}_k)$, we will get $\|f\|_L \leq 1$.

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

Spectral Normalization GAN

How to compute $\sigma(\mathbf{W})$?
If we apply singular value decomposition to compute the $\sigma(\mathbf{W})$ at each round of the algorithm, the algorithm becomes intractable.

Power iteration

- $\mathbf{u}_0$ – 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

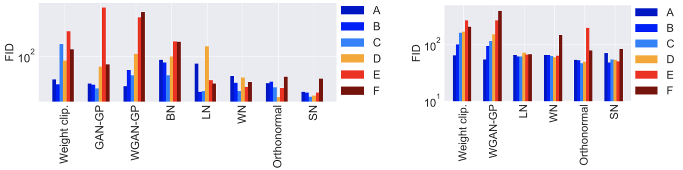
$$\sigma(\mathbf{W}) \approx \mathbf{u}_n^T \mathbf{W} \mathbf{v}_n.$$

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

Spectral Normalization GAN

Algorithm 1 SGD with spectral normalization

- Initialize $\tilde{\boldsymbol{u}}_l \in \mathcal{R}^{d_l}$ for $l = 1, \ldots, L$ 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:
$$\tilde{\boldsymbol{v}}_l \leftarrow (W^l)^{\mathrm{T}} \tilde{\boldsymbol{u}}_l / \|(W^l)^{\mathrm{T}} \tilde{\boldsymbol{u}}_l\|_2 \tag{20}$$
$$\tilde{\boldsymbol{u}}_l \leftarrow W^l \tilde{\boldsymbol{v}}_l / \|W^l \tilde{\boldsymbol{v}}_l\|_2 \tag{21}$$
  2. Calculate $\bar{W}_{\mathrm{SN}}$ with the spectral norm:
$$\bar{W}^l_{\mathrm{SN}}(W^l) = W^l / \sigma(W^l), \text{ where } \sigma(W^l) = \tilde{\boldsymbol{u}}_l^{\mathrm{T}} W^l \tilde{\boldsymbol{v}}_l \tag{22}$$
  3. Update W^l with SGD on mini-batch dataset $\mathcal{D}_M$ with a learning rate α:
$$W^l \leftarrow W^l - \alpha \nabla_{W^l} \ell(\bar{W}^l_{\mathrm{SN}}(W^l), \mathcal{D}_M) \tag{23}$$



(a) CIFAR-10

(b) STL-10

Divergences

What do we have?

- Forward KL divergence in maximum likelihood estimation
- Reverse KL in variational inference
- JS divergence in vanilla 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

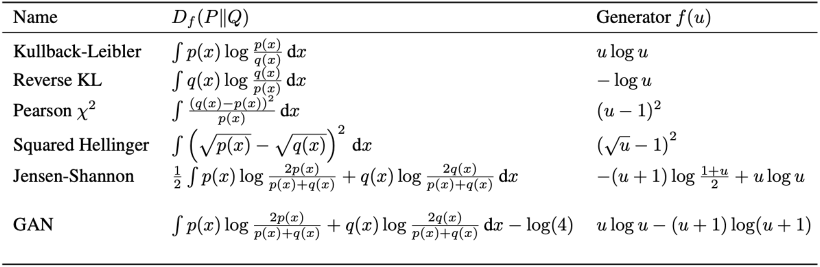
$$\min_{p} D(\pi || p)$$

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	$\int p(x) \log \frac{p(x)}{q(x)} \, dx$	$u \log u$
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

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

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

f-divergence

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

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-GA
Variational Divergence Minimization, 20

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

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

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

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

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

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
Variational Divergen

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 $T^*(\mathbf{x}) = f'\left(\frac{\pi(\mathbf{x})}{p(\mathbf{x})}\right)$.

(a) GAN (b) KL (c) Squared Hellinger

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

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

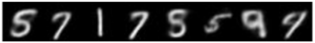
- VAE: compare ELBO values.
- GAN: ???

Evaluation of likelihood-free models

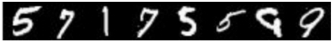
Let take some pretrained image classification model to get the conditional label distribution $p(y|\mathbf{x})$ (e.g. ImageNet classifier).

What do we want from samples?

- **Sharpness**



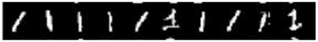
Low sharpness



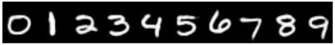
High sharpness

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).

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).

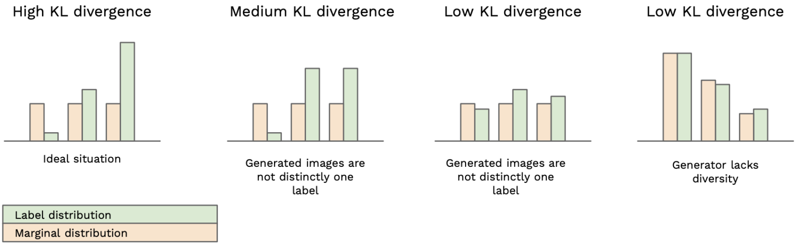


image credit: https://medium.com/octavian-ai/a-simple-explanation-of-the-inception-score-372dff6a8c7a

Evaluation of likelihood-free models

What do we want from samples?

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

Inception Score

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

Evaluation of likelihood-free models

Inception Score

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

IS limitations

- Inception score depends on the quality of the pretrained classifier $p(y|\mathbf{x})$.
- If generator produces images with a different set of labels from the classifier training set, IS will be low.
- If the generator produces one image per class, the IS will be perfect (there is no measure of intra-class diversity).
- IS only require samples from the generator and do not take into account the desired data distribution $\pi(\mathbf{x})$ directly (only implicitly via a classifier).

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.

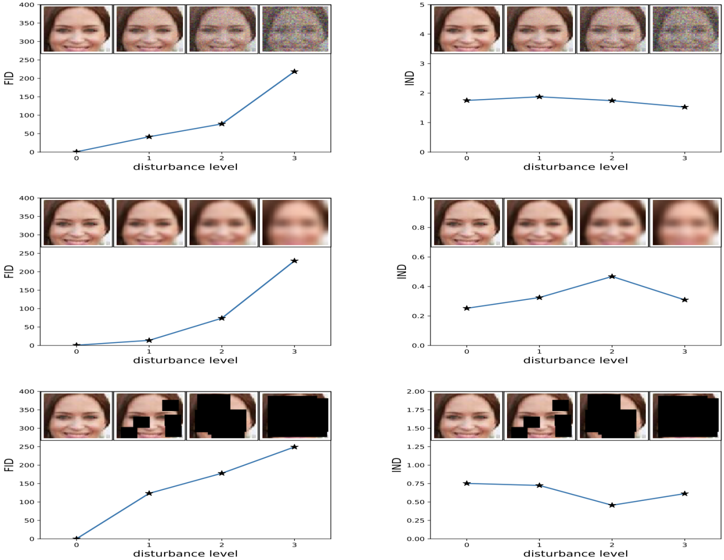
Frechet Inception Distance

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

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



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Evaluation of likelihood-free models

Frechet Inception Distance

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

FID limitations

- FID depends on the pretrained classification model.
- FID needs a large samples size for evaluation.
- Calculation of FID is slow.
- FID estimates only two sample moments.

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

Summary

- Weight clipping is a terrible way to enforce Lipschitzness. Gradient Penalty works better.
- Spectral normalization is a weight normalization technique to enforce Lipshitzness, which is helpful for generator and discriminator.
- f-divergence family is a unified framework for divergence minimization, which uses variational approximation.
- Inception Score and Frechet Inception Distance are the common metrics for GAN evaluation, but both of them have drawbacks.