Deep Generative Models

Lecture 11

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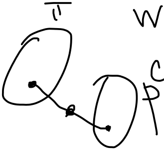
Recap of previous lecture

$W(\pi \| p) \rightarrow$ KRD $\rightarrow$ 1-Lip

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

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



weight clip.

Gradient penalty

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

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 $\mathbf{W}_k^{SN} = \mathbf{W}_k / \underbrace{\|\mathbf{W}_k\|_2}$, 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

Recap of previous lecture

f-divergence minimization

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

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

Variational divergence estimation

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

Fenchel conjugate

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

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

Recap of previous lecture

How to evaluate likelihood-free models?

$p(y|\mathbf{x})$ - pretrained image classification model (e.g. ImageNet classifier).

X

What do we want from samples?

- **Sharpness**

X_1 X_2 X_3

Low sharpness

High sharpness

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

- **Diversity**

Low diversity

High diversity

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

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

Outline

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

2. Discrete VAE latent representations

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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

1. Evaluation of likelihood-free models
    - Inception score
    - Frechet Inception Distance
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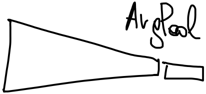
Evaluation of likelihood-free models

$p(y|x)$



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

W_2

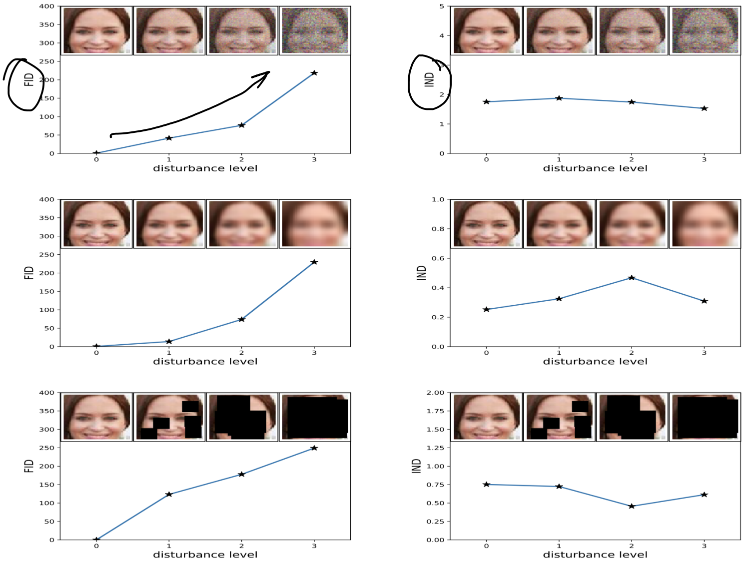
$\|\sigma_\pi - \sigma_p\|^2$

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

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

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

p(y|x)

p(y|x)

Inception Score

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

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

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

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

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

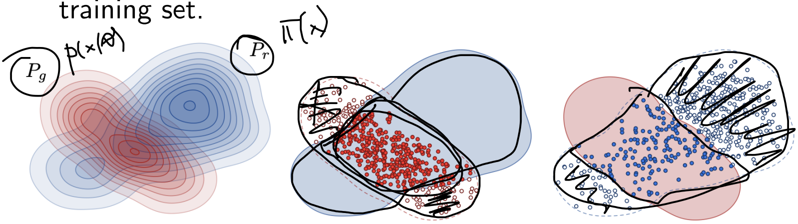
Barratt S., Sharma R. A Note on the Inception Score, 2018
Heusel M. et al. GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium, 2017

Outline

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

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

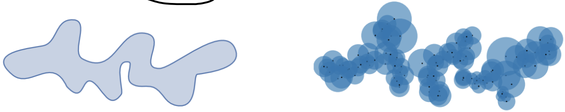
Embed samples using pretrained classifier network (as previously):

$$\mathcal{G}_\pi = \{\mathbf{g}_i\}_{i=1}^{n_1}, \quad \mathcal{G}_p = \{\mathbf{g}_i\}_{i=1}^{n_2}.$$

Define binary function:

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

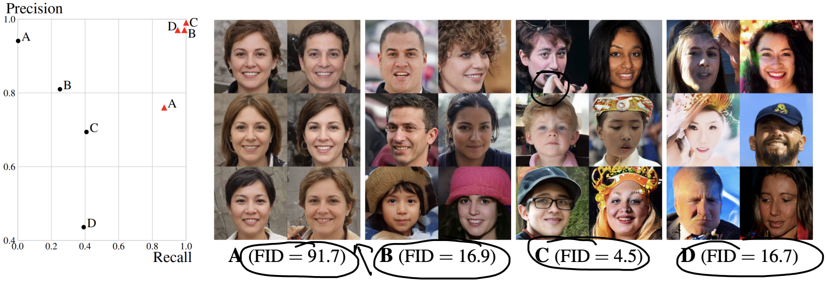
$$\text{Precision}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_p} f(\mathbf{g}, \mathcal{G}_\pi); \;\; \text{Recall}(\mathcal{G}_\pi, \mathcal{G}_p) = \frac{1}{n} \sum_{\mathbf{g} \in \mathcal{G}_\pi} f(\mathbf{g}, \mathcal{G}_p).$$

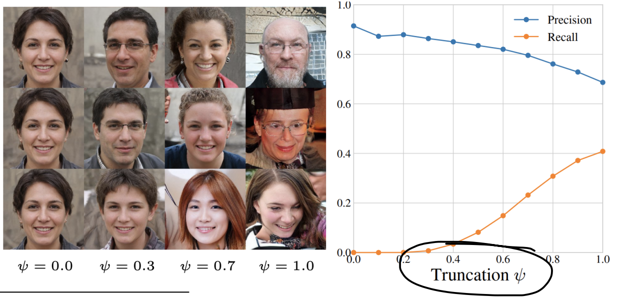


(a) True manifold (b) Approx. manifold

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

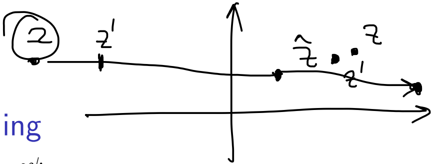
Precision-Recall for generative models





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

Truncation trick



BigGAN: truncated normal sampling

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

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

Outline

$z \sim \mathrm{Cat}(\pi)$

1. Evaluation of likelihood-free models
   - Inception score
   - Frechet Inception Distance
   - Precision-Recall
2. Discrete VAE latent representations

Discrete VAE latents

Motivation

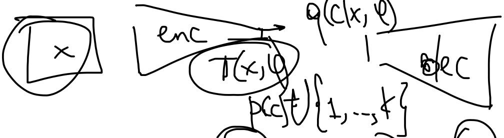
- Previous VAE models had **continuous** latent variables $\mathbf{z}$.
- **Discrete** representations $\mathbf{z}$ are potentially a more natural fit for many of the modalities.
- Powerful autoregressive models (like PixelCNN) have been developed for modelling distributions over discrete variables.
- All cool transformer-like models work with discrete tokens.

ELBO

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \overset{\text{RL}}{\mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)} \log p(\mathbf{x}|\mathbf{z}, \boldsymbol{\theta})} - \overbrace{KL(q(\mathbf{z}|\mathbf{x}, \phi)||p(\mathbf{z}))}^{\text{KL}} \to \max_{\phi, \boldsymbol{\theta}}.$$

- Reparametrization trick to get unbiased gradients.
- Normal assumptions for $q(\mathbf{z}|\mathbf{x}, \phi)$ and $p(\mathbf{z})$ to compute KL analytically.

Discrete VAE latents



Assumptions

- Define dictionary (word book) space $\{\mathbf{e}_k\}_{k=1}^{K}$, where $\mathbf{e}_k \in \mathbb{R}^C$, K is the size of the dictionary.

  μ, σ

- Let $c \sim \text{Categorical}(\boldsymbol{\pi})$, where

$$\boldsymbol{\pi} = (\pi_1, \dots, \pi_K), \quad \pi_k = P(c = k), \quad \sum_{k=1}^{K} \pi_k = 1.$$

- Let VAE model has discrete latent representation c with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

How it should work?

- Our variational posterior $q(c|\mathbf{x}, \phi) = \text{Categorical}(\boldsymbol{\pi}(\mathbf{x}, \phi))$ (encoder) outputs discrete probabilities vector.
- We sample c^* from $q(c|\mathbf{x}, \phi)$ (reparametrization trick analogue).
- Our generative distribution $p(\mathbf{x}|\mathbf{e}_{c^*}, \boldsymbol{\theta})$ (decoder).

Discrete VAE latents

ELBO

DL z , C $\nabla_\phi = \nabla_\phi KL + \nabla_\phi H$

$$\mathcal{L}(\phi, \boldsymbol{\theta}) = \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x}|c, \boldsymbol{\theta}) - \underbrace{KL(q(c|\mathbf{x}, \phi)||p(c))} \to \max_{\phi, \boldsymbol{\theta}}.$$

KL term

$$KL(q(c|\mathbf{x}, \phi)||p(c)) = \sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log \frac{q(k|\mathbf{x}, \phi)}{p(k)} =$$

$$= \underbrace{\sum_{k=1}^{K} \underbrace{q(k|\mathbf{x}, \phi)} \log q(k|\mathbf{x}, \phi)} - \underbrace{\sum_{k=1}^{K} q(k|\mathbf{x}, \phi) \log p(k)} =$$

$$= \underbrace{-H(q(c|\mathbf{x}, \phi))} + \log K.$$

- Is it possible to make reparametrization trick? (we sample from discrete distribution now!).
- Entropy term should be estimated.

Summary

1) $x \rightarrow \text{Resize}(224) = \hat{x}$

2) $\hat{x} \longrightarrow \text{InceptionV3}$

- 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.

- Discrete VAE latents is a natural idea, but we have to avoid non-differentiable sampling operation.