

Deep Generative Models

Lecture 6

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Recap of Previous Lecture

Assumptions

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

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

- ▶ Suppose the VAE employs a discrete latent code c , with prior $p(c) = \text{Uniform}\{1, \dots, K\}$.

ELBO

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

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

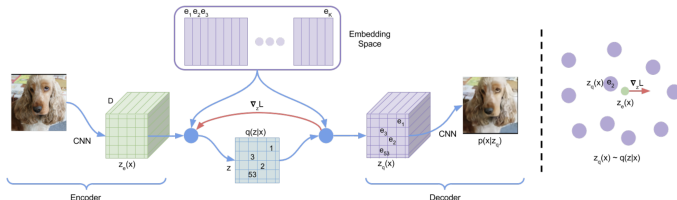
Vector Quantization

Define the codebook $\{\mathbf{e}_k\}_{k=1}^K$, where $\mathbf{e}_k \in \mathbb{R}^L$ and K is the size of the dictionary.

$$\mathbf{z}_q = \mathbf{q}(\mathbf{z}) = \mathbf{e}_{k^*}, \quad \text{where } k^* = \arg \min_k \|\mathbf{z} - \mathbf{e}_k\|.$$

Oord A., Vinyals O., Kavukcuoglu K. Neural Discrete Representation Learning, 2017

Recap of Previous Lecture



Deterministic Variational Posterior

$$q(c_{ij} = k^* | \mathbf{x}, \phi) = \begin{cases} 1, & \text{if } k^* = \arg \min_k ||[\mathbf{z}_e]_{ij} - \mathbf{e}_k||; \\ 0, & \text{otherwise.} \end{cases}$$

ELBO

$$\mathcal{L}_{\phi, \theta}(\mathbf{x}) = \mathbb{E}_{q(c|\mathbf{x}, \phi)} \log p(\mathbf{x} | \mathbf{e}_c, \theta) - \log K = \log p(\mathbf{x} | \mathbf{z}_q, \theta) - \log K.$$

Straight-Through Gradient Estimation

$$\frac{\partial \log p(\mathbf{x} | \mathbf{z}_q, \theta)}{\partial \phi} = \frac{\partial \log p(\mathbf{x} | \mathbf{z}_q, \theta)}{\partial \mathbf{z}_q} \cdot \frac{\partial \mathbf{z}_q}{\partial \phi} \approx \frac{\partial \log p(\mathbf{x} | \mathbf{z}_q, \theta)}{\partial \mathbf{z}_q} \cdot \frac{\partial \mathbf{z}_e}{\partial \phi}$$

Recap of Previous Lecture

Theorem

$$\frac{1}{n} \sum_{i=1}^n \text{KL}(q(\mathbf{z}|\mathbf{x}_i, \phi) \parallel p(\mathbf{z})) = \text{KL}(q_{\text{agg}}(\mathbf{z}|\phi) \parallel p(\mathbf{z})) + \mathbb{I}_q[\mathbf{x}, \mathbf{z}].$$

ELBO Surgery

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \underbrace{\frac{1}{n} \sum_{i=1}^n \mathbb{E}_{q(\mathbf{z}|\mathbf{x}_i, \phi)} \log p(\mathbf{x}_i|\mathbf{z}, \theta)}_{\text{Reconstruction Loss}} - \underbrace{\mathbb{I}_q[\mathbf{x}, \mathbf{z}]}_{\text{MI}} - \underbrace{\text{KL}(q_{\text{agg}}(\mathbf{z}|\phi) \parallel p(\mathbf{z}))}_{\text{Marginal KL}}$$

Optimal Prior

$$\text{KL}(q_{\text{agg}}(\mathbf{z}|\phi) \parallel p(\mathbf{z})) = 0 \Leftrightarrow p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i, \phi).$$

Thus, the optimal prior distribution $p(\mathbf{z})$ is the aggregated variational posterior $q_{\text{agg}}(\mathbf{z}|\phi)$.

Hoffman M. D., Johnson M. J. ELBO surgery: yet another way to carve up the variational evidence lower bound, 2016

Recap of Previous Lecture

- ▶ Standard Gaussian $p(\mathbf{z}) = \mathcal{N}(0, \mathbf{I}) \Rightarrow$ over-regularization.
- ▶ $p(\mathbf{z}) = q_{\text{agg}}(\mathbf{z}|\phi) = \frac{1}{n} \sum_{i=1}^n q(\mathbf{z}|\mathbf{x}_i, \phi) \Rightarrow$ overfitting and extremely high computational cost.

Revisiting ELBO

$$\frac{1}{n} \sum_{i=1}^n \mathcal{L}_{\phi, \theta}(\mathbf{x}_i) = \text{RL} - \text{MI} - \text{KL}(q_{\text{agg}}(\mathbf{z}|\phi) \parallel p(\mathbf{z}|\boldsymbol{\lambda}))$$

This is the forward KL divergence with respect to $p(\mathbf{z}|\boldsymbol{\lambda})$.

ELBO with Learnable VAE Prior

$$\begin{aligned} \mathcal{L}_{\phi, \theta}(\mathbf{x}) &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} [\log p(\mathbf{x}|\mathbf{z}, \theta) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x}, \phi)] \\ &= \mathbb{E}_{q(\mathbf{z}|\mathbf{x}, \phi)} \left[\log p(\mathbf{x}|\mathbf{z}, \theta) + \underbrace{\left(\log p(\mathbf{f}_{\boldsymbol{\lambda}}(\mathbf{z})) + \log |\det(\mathbf{J}_{\mathbf{f}})| \right)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x}, \phi) \right] \\ \mathbf{z} &= \mathbf{f}_{\boldsymbol{\lambda}}^{-1}(\mathbf{z}^*) = \mathbf{g}_{\boldsymbol{\lambda}}(\mathbf{z}^*), \quad \mathbf{z}^* \sim p(\mathbf{z}^*) = \mathcal{N}(0, \mathbf{I}) \end{aligned}$$

Outline

1. Likelihood-Free Learning
2. Generative Adversarial Networks (GAN)
3. Wasserstein Distance
4. Wasserstein GAN

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Likelihood-Based Models

Poor Likelihood
High-Quality Samples

$$p_1(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \mathcal{N}(\mathbf{x} | \mathbf{x}_i, \epsilon \mathbf{I})$$

If ϵ is very small, this model produces excellent, sharp samples but achieves poor likelihoods on test data.

High Likelihood
Poor Samples

$$p_2(\mathbf{x}) = 0.01p(\mathbf{x}) + 0.99p_{\text{noise}}(\mathbf{x})$$

$$\begin{aligned} \log [0.01p(\mathbf{x}) + 0.99p_{\text{noise}}(\mathbf{x})] &\geq \\ &\geq \log [0.01p(\mathbf{x})] = \log p(\mathbf{x}) - \log 100 \end{aligned}$$

This model contains mostly noisy, irrelevant samples; for high dimensions, $\log p(\mathbf{x})$ scales linearly with m .

- ▶ Likelihood isn't always a suitable metric for evaluating generative models.
- ▶ Sometimes, the likelihood function can't even be computed exactly.

Likelihood-Free Learning

Motivation

We're interested in approximating the true data distribution $\pi(\mathbf{x})$. Instead of searching over all distributions, let's learn a model $p(\mathbf{x}|\boldsymbol{\theta}) \approx \pi(\mathbf{x})$.

Suppose we have two sets of samples:

- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ — real data;
- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\boldsymbol{\theta})$ — generated (fake) data.

Define a discriminative model (classifier):

$$p(y = 1|\mathbf{x}) = P(\mathbf{x} \sim \pi(\mathbf{x})); \quad p(y = 0|\mathbf{x}) = P(\mathbf{x} \sim p(\mathbf{x}|\boldsymbol{\theta}))$$

Assumption

The generative model $p(\mathbf{x}|\boldsymbol{\theta})$ matches $\pi(\mathbf{x})$ if a discriminative model $p(y|\mathbf{x})$ can't distinguish between them — that is, if $p(y = 1|\mathbf{x}) = 0.5$ for every \mathbf{x} .

Generative Adversarial Networks (GAN)

- ▶ The more expressive the discriminator, the closer we get to the optimal $p(\mathbf{x}|\theta)$.
- ▶ Standard classifiers are trained by minimizing cross-entropy loss.

Cross-Entropy for Discriminator

$$\min_{p(y|\mathbf{x})} \left[-\mathbb{E}_{\pi(\mathbf{x})} \log p(y=1|\mathbf{x}) - \mathbb{E}_{p(\mathbf{x}|\theta)} \log p(y=0|\mathbf{x}) \right]$$
$$\max_{p(y|\mathbf{x})} \left[\mathbb{E}_{\pi(\mathbf{x})} \log p(y=1|\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\theta)} \log p(y=0|\mathbf{x}) \right]$$

Generative Model

Suppose $p(\mathbf{x}, \mathbf{z}|\theta) = p(\mathbf{x}|\mathbf{z}, \theta)p(\mathbf{z})$, where $p(\mathbf{z})$ is a base distribution, and $p(\mathbf{x}|\mathbf{z}, \theta) = \delta(\mathbf{x} - \mathbf{G}_\theta(\mathbf{z}))$ is deterministic.

Generative Adversarial Networks (GAN)

Cross-Entropy for Discriminative Model

$$\max_{p(y|\mathbf{x})} [\mathbb{E}_{\pi(\mathbf{x})} \log p(y = 1|\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\theta)} \log p(y = 0|\mathbf{x})]$$

- ▶ **Discriminator:** A classifier $p(y = 1|\mathbf{x}, \phi) = D_\phi(\mathbf{x}) \in [0, 1]$, distinguishing real and generated samples. The discriminator aims to **maximize** cross-entropy.
- ▶ **Generator:** The generative model $\mathbf{x} = \mathbf{G}_\theta(\mathbf{z})$, $\mathbf{z} \sim p(\mathbf{z})$, seeks to fool the discriminator. The generator aims to **minimize** cross-entropy.

GAN Objective

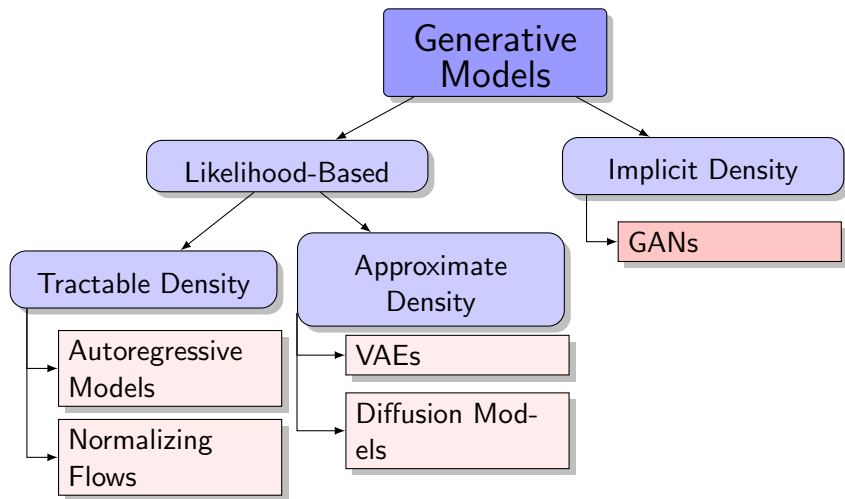
$$\min_G \max_D [\mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\theta)} \log(1 - D(\mathbf{x}))]$$

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

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Generative Models Zoo



GAN Optimality

Theorem

The minimax game

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

achieves its global optimum when $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$, and $D^*(\mathbf{x}) = 0.5$.

Proof (Fixed G)

$$\begin{aligned} V(G, D) &= \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log(1 - D(\mathbf{x})) \\ &= \int \underbrace{[\pi(\mathbf{x}) \log D(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta}) \log(1 - D(\mathbf{x}))]}_{y(D)} d\mathbf{x} \end{aligned}$$

$$\frac{dy(D)}{dD} = \frac{\pi(\mathbf{x})}{D(\mathbf{x})} - \frac{p(\mathbf{x}|\boldsymbol{\theta})}{1 - D(\mathbf{x})} = 0 \quad \Rightarrow \quad D^*(\mathbf{x}) = \frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}$$

GAN Optimality

Proof Continued (Fixed $D = D^*$)

$$\begin{aligned} V(G, D^*) &= \mathbb{E}_{\pi(\mathbf{x})} \log \left(\frac{\pi(\mathbf{x})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})} \right) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log \left(\frac{p(\mathbf{x}|\boldsymbol{\theta})}{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})} \right) \\ &= \text{KL} \left(\pi(\mathbf{x}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) + \text{KL} \left(p(\mathbf{x}|\boldsymbol{\theta}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) - 2 \log 2 \\ &= 2 \text{JSD}(\pi(\mathbf{x}) \parallel p(\mathbf{x}|\boldsymbol{\theta})) - 2 \log 2. \end{aligned}$$

Jensen-Shannon Divergence (Symmetric KL Divergence)

$$\text{JSD}(\pi(\mathbf{x}) \parallel p(\mathbf{x}|\boldsymbol{\theta})) = \frac{1}{2} \left[\text{KL} \left(\pi(\mathbf{x}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) + \text{KL} \left(p(\mathbf{x}|\boldsymbol{\theta}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) \right]$$

This can be regarded as a proper distance metric!

$$V(G^*, D^*) = -2 \log 2, \quad \pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta}), \quad D^*(\mathbf{x}) = 0.5.$$

GAN Optimality

Theorem

The following minimax game

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

achieves its global optimum precisely when $\pi(\mathbf{x}) = p(\mathbf{x}|\boldsymbol{\theta})$, and $D^*(\mathbf{x}) = 0.5$.

Expectations

If the generator can express **any** function and the discriminator is **optimal** at every step, the generator **will converge** to the target distribution.

Reality

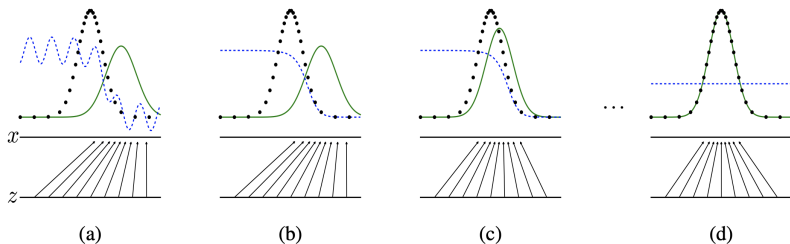
- ▶ Generator updates are performed in parameter space, and the discriminator is often imperfectly optimized.
- ▶ Generator and discriminator losses typically oscillate during GAN training.

GAN Training

Assume both generator and discriminator are parametric models:
 $D_\phi(\mathbf{x})$ and $\mathbf{G}_\theta(\mathbf{z})$.

Objective

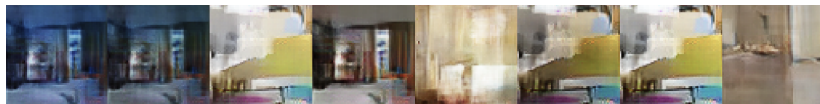
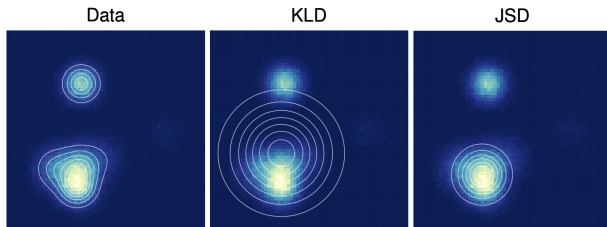
$$\min_{\theta} \max_{\phi} [\mathbb{E}_{\pi(\mathbf{x})} \log D_\phi(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log(1 - D_\phi(\mathbf{G}_\theta(\mathbf{z})))]$$



- ▶ $\mathbf{z} \sim p(\mathbf{z})$ is a latent variable.
- ▶ $p(\mathbf{x}|\mathbf{z}, \theta) = \delta(\mathbf{x} - \mathbf{G}_\theta(\mathbf{z}))$ serves as a deterministic decoder (like normalizing flows).
- ▶ There is no encoder present.

Mode Collapse

Mode collapse refers to the phenomenon where the generator in a GAN produces only one or a few different modes of the distribution.



Numerous methods have been proposed to tackle mode collapse: changing architectures, adding regularization terms, injecting noise.

Goodfellow I. J. et al. Generative Adversarial Networks, 2014

Metz L. et al. Unrolled Generative Adversarial Networks, 2016

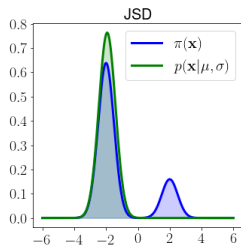
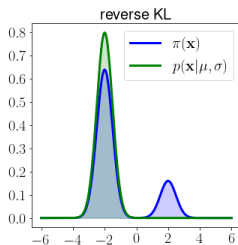
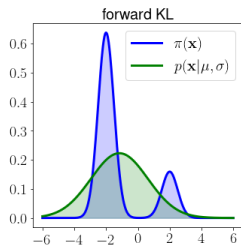
Jensen-Shannon vs Kullback-Leibler Divergences

- ▶ $\pi(\mathbf{x})$ is a fixed mixture of two Gaussians.
- ▶ $p(\mathbf{x}|\mu, \sigma) = \mathcal{N}(\mu, \sigma^2)$.

Mode Covering vs. Mode Seeking

$$\text{KL}(\pi \parallel p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad \text{KL}(p \parallel \pi) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

$$\text{JSD}(\pi \parallel p) = \frac{1}{2} \left[\text{KL} \left(\pi(\mathbf{x}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2} \right) + \text{KL} \left(p(\mathbf{x}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2} \right) \right]$$

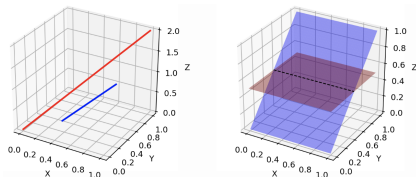


Outline

1. Likelihood-Free Learning
2. Generative Adversarial Networks (GAN)
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Theoretical Results

- ▶ The dimensionality of \mathbf{z} is less than that of \mathbf{x} , so $p(\mathbf{x}|\boldsymbol{\theta})$ with $\mathbf{x} = \mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z})$ lives on a low-dimensional manifold.
- ▶ The true data distribution $\pi(\mathbf{x})$ is also supported on a low-dimensional manifold.



- ▶ If $\pi(\mathbf{x})$ and $p(\mathbf{x}|\boldsymbol{\theta})$ are disjoint, a smooth optimal discriminator can exist!
- ▶ For such low-dimensional, disjoint manifolds:

$$\text{KL}(\pi \parallel p) = \text{KL}(p \parallel \pi) = \infty, \quad \text{JSD}(\pi \parallel p) = \log 2$$

Weng L. *From GAN to WGAN*, 2019

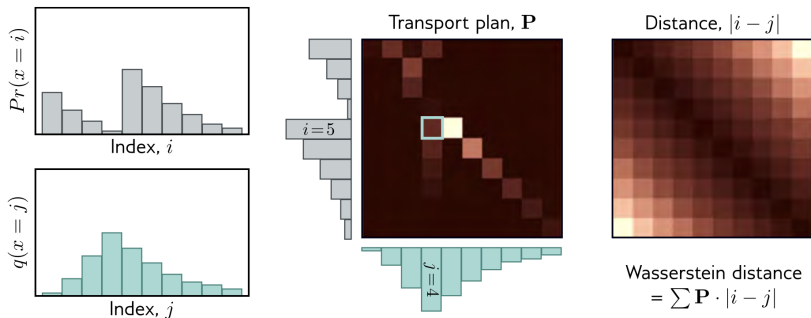
Arjovsky M., Bottou L. *Towards Principled Methods for Training Generative Adversarial Networks*, 2017

Wasserstein Distance (Discrete)

Also known as the **Earth Mover's Distance**.

Optimal Transport Formulation

The minimum cost of moving and transforming a pile of "dirt" shaped like one probability distribution to match another.



Wasserstein Distance (Continuous)

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

- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ is the transport plan: the amount of “dirt” assigned from \mathbf{x} to \mathbf{y} .

$$\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} = p(\mathbf{y}); \quad \int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \pi(\mathbf{x}).$$

- ▶ $\Gamma(\pi, p)$ denotes the set of all joint distributions $\gamma(\mathbf{x}, \mathbf{y})$ with marginals π and p .
- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ is the mass, $\|\mathbf{x} - \mathbf{y}\|$ is the distance.

Wasserstein Metric

$$W_s(\pi, p) = \inf_{\gamma \in \Gamma(\pi, p)} \left(\mathbb{E}_{(\mathbf{x}, \mathbf{y}) \sim \gamma} \|\mathbf{x} - \mathbf{y}\|^s \right)^{1/s}$$

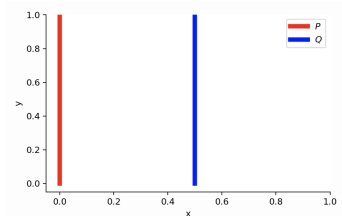
In our setting, $W(\pi, p) = W_1(\pi, p)$, which is the transport cost using the ℓ_1 norm.

Wasserstein Distance vs KL vs JSD

Consider two-dimensional distributions:

$$\pi(x, y) = (0, U[0, 1])$$

$$p(x, y|\theta) = (\theta, U[0, 1])$$



- $\theta = 0$: Both distributions are identical.

$$\text{KL}(\pi \parallel p) = \text{KL}(p \parallel \pi) = \text{JSD}(p \parallel \pi) = W(\pi, p) = 0$$

- $\theta \neq 0$:

$$\text{KL}(\pi \parallel p) = \int_{U[0,1]} 1 \log \frac{1}{0} dy = \infty = \text{KL}(p \parallel \pi)$$

$$\text{JSD}(\pi \parallel p) = \frac{1}{2} \left(\int_{U[0,1]} 1 \log \frac{1}{1/2} dy + \int_{U[0,1]} 1 \log \frac{1}{1/2} dy \right) = \log 2$$

$$W(\pi, p) = |\theta|$$

Weng L. *From GAN to WGAN*, 2019

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

Wasserstein Distance vs KL vs JSD

Theorem 1

Let $\mathbf{G}_\theta(\mathbf{z})$ be (almost) any feedforward neural network, and $p(\mathbf{z})$ a prior over \mathbf{z} such that $\mathbb{E}_{p(\mathbf{z})}\|\mathbf{z}\| < \infty$. Then $W(\pi, p)$ is continuous everywhere and differentiable almost everywhere.

Theorem 2

Let π be a distribution on a compact space \mathcal{X} and let $\{p_t\}_{t=1}^\infty$ be a sequence of distributions on \mathcal{X} .

$$\text{KL}(\pi \parallel p_t) \rightarrow 0 \quad (\text{or } \text{KL}(p_t \parallel \pi) \rightarrow 0) \quad (1)$$

$$\text{JSD}(\pi \parallel p_t) \rightarrow 0 \quad (2)$$

$$W(\pi, p_t) \rightarrow 0 \quad (3)$$

In summary, as $t \rightarrow \infty$, $(1) \Rightarrow (2)$, and $(2) \Rightarrow (3)$.

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Wasserstein GAN

Wasserstein Distance

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

The infimum over all possible $\gamma \in \Gamma(\pi, p)$ is computationally intractable.

Theorem (Kantorovich-Rubinstein Duality)

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

where $f : \mathbb{R}^m \rightarrow \mathbb{R}$ is K -Lipschitz ($\|f\|_L \leq K$):

$$|f(\mathbf{x}_1) - f(\mathbf{x}_2)| \leq K \|\mathbf{x}_1 - \mathbf{x}_2\|, \quad \forall \mathbf{x}_1, \mathbf{x}_2 \in \mathcal{X}.$$

We can thus estimate $W(\pi \parallel p)$ using only samples and a neural function f .

Wasserstein GAN

Theorem (Kantorovich-Rubinstein Duality)

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

- ▶ We must ensure that f is K -Lipschitz continuous.
- ▶ Let $f_\phi(\mathbf{x})$ be a feedforward neural network parameterized by ϕ .
- ▶ If the weights ϕ are restricted to a compact set Φ , then f_ϕ is K -Lipschitz.
- ▶ Clamp weights within the box $\Phi = [-c, c]^d$ (e.g. $c = 0.01$) after each update.

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

Wasserstein GAN

Standard GAN Objective

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

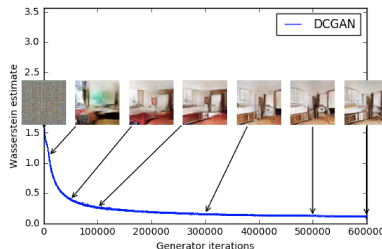
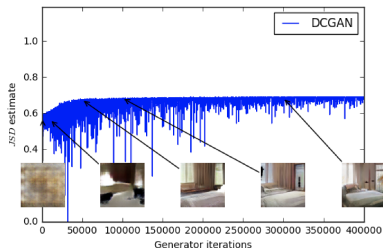
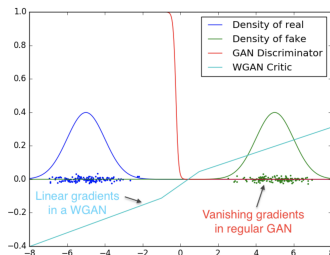
WGAN Objective

$$\min_{\theta} W(\pi \parallel p) \approx \min_{\theta} \max_{\phi \in \Phi} \left[\mathbb{E}_{\pi(\mathbf{x})} f_{\phi}(\mathbf{x}) - \mathbb{E}_{p(\mathbf{z})} f_{\phi}(\mathbf{G}_{\theta}(\mathbf{z})) \right]$$

- ▶ The discriminator D is replaced by function f : in WGAN, it is known as the **critic**, which is *not* a classifier.
- ▶ *"Weight clipping is a clearly terrible way to enforce a Lipschitz constraint."*
 - ▶ If c is large, optimizing the critic is hard.
 - ▶ If c is small, gradients may vanish.

Wasserstein GAN

- ▶ WGAN provides nonzero gradients even if distributions' supports are disjoint.
- ▶ $JSD(\pi \parallel p)$ is poorly correlated with sample quality and remains near its maximum value $\log 2 \approx 0.69$.
- ▶ $W(\pi \parallel p)$ is tightly correlated with quality.



Summary

- ▶ Likelihood is not a reliable metric for generative model evaluation.
- ▶ Adversarial learning casts distribution matching as a minimax game.
- ▶ GANs, in theory, optimize the Jensen-Shannon divergence.
- ▶ KL and JS divergences fail as objectives when the model and data distributions are disjoint.
- ▶ The Earth Mover's (Wasserstein) distance provides a more meaningful loss for distribution matching.
- ▶ Kantorovich-Rubinstein duality allows us to compute the EM distance using only samples.
- ▶ Wasserstein GAN enforces the Lipschitz condition on the critic through weight clipping—although better alternatives exist.