Deep Generative Models

Lecture 6

Roman Isachenko

Moscow Institute of Physics and Technology Yandex School of Data Analysis

2025, Autumn

Assumptions

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

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

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

ELBO

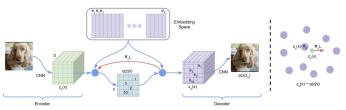
$$\mathcal{L}_{\phi, heta}(\mathbf{x}) = \mathbb{E}_{q_{\phi}(c|\mathbf{x})} \log p_{ heta}(\mathbf{x}|c) - \underbrace{\mathrm{KL}(q_{\phi}(c|\mathbf{x}) \parallel p(c))}_{\phi, heta} o \max_{\phi, heta}.$$

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

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.

$$\mathbf{z}_q = \mathbf{q}(\mathbf{z}) = \mathbf{e}_{k^*}, \quad ext{where} \ \ k^* = rg\min_{\mathbf{z}} \|\mathbf{z} - \mathbf{e}_k\|.$$



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

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

Straight-Through Gradient Estimation

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

Theorem

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

ELBO Surgery

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

Optimal Prior

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

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

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

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

Revisiting ELBO

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

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

ELBO with Learnable VAE Prior

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

Outline

1. Likelihood-Free Learning

2. Generative Adversarial Networks (GAN)

3. Wasserstein Distance

4. Wasserstein GAN

Outline

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

3. Wasserstein Distance

4. Wasserstein GAN

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.

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

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

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

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

 $\log \left[0.01 p(\mathbf{x}) + 0.99 p_{\mathsf{noise}}(\mathbf{x}) \right] \geq$

 $\geq \log [0.01p(x)] = \log p(x) - \log 100$

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

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

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

 $\log [0.01 p(\mathbf{x}) + 0.99 p_{\text{noise}}(\mathbf{x})] \ge$
 $\ge \log [0.01 p(\mathbf{x})] = \log p(\mathbf{x}) - \log 100$

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.

Motivation

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

Motivation

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

Suppose we have two sets of samples:

- $\{\mathbf{x}_i\}_{i=1}^{n_1} \sim p_{\mathsf{data}}(\mathbf{x})$ real data;
- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p_{\theta}(\mathbf{x})$ generated (fake) data.

Motivation

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

Suppose we have two sets of samples:

- $ightharpoonup \{\mathbf{x}_i\}_{i=1}^{n_1} \sim p_{\mathsf{data}}(\mathbf{x})$ real data;
- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p_{\theta}(\mathbf{x})$ generated (fake) data.

Define a discriminative model (classifier):

$$p(y = 1|\mathbf{x}) = P(\mathbf{x} \sim p_{\text{data}}(\mathbf{x})); \quad p(y = 0|\mathbf{x}) = P(\mathbf{x} \sim p_{\theta}(\mathbf{x}))$$

Motivation

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

Suppose we have two sets of samples:

- $\{\mathbf{x}_i\}_{i=1}^{n_1} \sim p_{\mathsf{data}}(\mathbf{x})$ real data;
- $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p_{\theta}(\mathbf{x})$ generated (fake) data.

Define a discriminative model (classifier):

$$p(y = 1|\mathbf{x}) = P(\mathbf{x} \sim p_{\mathsf{data}}(\mathbf{x})); \quad p(y = 0|\mathbf{x}) = P(\mathbf{x} \sim p_{\theta}(\mathbf{x}))$$

Assumption

The generative model $p_{\theta}(\mathbf{x})$ matches $p_{\text{data}}(\mathbf{x})$ 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} .

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

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

Cross-Entropy for Discriminator

$$\min_{p(y|\mathbf{x})} \left[-\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log p(y=1|\mathbf{x}) - \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y=0|\mathbf{x}) \right]$$

$$\max_{p(y|\mathbf{x})} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log p(y = 1|\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y = 0|\mathbf{x}) \right]$$

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

Cross-Entropy for Discriminator

$$\begin{split} & \min_{p(y|\mathbf{x})} \left[-\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log p(y=1|\mathbf{x}) - \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y=0|\mathbf{x}) \right] \\ & \max_{p(y|\mathbf{x})} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log p(y=1|\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y=0|\mathbf{x}) \right] \end{split}$$

Generative Model

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

Cross-Entropy for Discriminative Model

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

Cross-Entropy for Discriminative Model

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

- **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.

Cross-Entropy for Discriminative Model

$$\max_{p(y|\mathbf{x})} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log p(y=1|\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y=0|\mathbf{x}) \right]$$

- **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

$$\min_{G} \max_{D} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log (1 - D(\mathbf{x})) \right]$$

Cross-Entropy for Discriminative Model

$$\max_{p(y|\mathbf{x})} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log p(y=1|\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log p(y=0|\mathbf{x}) \right]$$

- **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

$$\min_{G} \max_{D} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log (1 - D(\mathbf{x})) \right]$$

$$\min_{C} \max_{D} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(\mathbf{G}(\mathbf{z}))) \right]$$

Outline

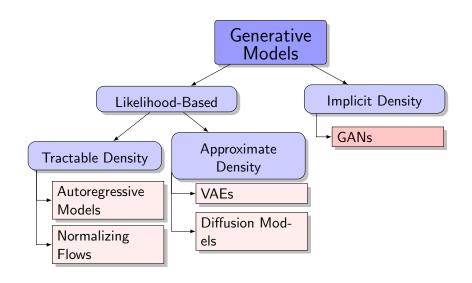
1. Likelihood-Free Learning

2. Generative Adversarial Networks (GAN)

3. Wasserstein Distance

4. Wasserstein GAN

Generative Models Zoo



Theorem

The minimax game

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

achieves its global optimum when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, and $D^*(\mathbf{x}) = 0.5$.

Theorem

The minimax game

$$\min_{G} \max_{D} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(\mathbf{G}(\mathbf{z}))) \right]$$

$$V(G,D)$$

achieves its global optimum when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, and $D^*(\mathbf{x}) = 0.5$.

Proof (Fixed G)

$$V(G, D) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p_{m{ heta}}(\mathbf{x})} \log (1 - D(\mathbf{x}))$$

Theorem

The minimax game

$$\min_{G} \max_{D} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(\mathbf{G}(\mathbf{z}))) \right]$$

$$V(G,D)$$

achieves its global optimum when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, and $D^*(\mathbf{x}) = 0.5$.

Proof (Fixed G)

$$\begin{split} V(G, D) &= \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log (1 - D(\mathbf{x})) \\ &= \int \underbrace{\left[p_{\mathsf{data}}(\mathbf{x}) \log D(\mathbf{x}) + p_{\boldsymbol{\theta}}(\mathbf{x}) \log (1 - D(\mathbf{x}))\right]}_{y(D)} d\mathbf{x} \end{split}$$

Theorem

The minimax game

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

achieves its global optimum when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, and $D^*(\mathbf{x}) = 0.5$.

Proof (Fixed G)

$$\begin{split} V(G, D) &= \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} \log (1 - D(\mathbf{x})) \\ &= \int \underbrace{\left[p_{\mathsf{data}}(\mathbf{x}) \log D(\mathbf{x}) + p_{\boldsymbol{\theta}}(\mathbf{x}) \log (1 - D(\mathbf{x}))\right]}_{y(D)} d\mathbf{x} \end{split}$$

$$\frac{dy(D)}{dD} = \frac{p_{\mathsf{data}}(\mathbf{x})}{D(\mathbf{x})} - \frac{p_{\theta}(\mathbf{x})}{1 - D(\mathbf{x})} = 0 \qquad \Rightarrow \quad D^*(\mathbf{x}) = \frac{p_{\mathsf{data}}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}$$

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

$$V(\textit{G},\textit{D}^*) = \mathbb{E}_{\textit{p}_{\mathsf{data}}(\mathbf{x})} \log \left(\frac{p_{\mathsf{data}}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\boldsymbol{\theta}}(\mathbf{x})} \right) + \mathbb{E}_{\textit{p}_{\boldsymbol{\theta}}(\mathbf{x})} \log \left(\frac{p_{\boldsymbol{\theta}}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\boldsymbol{\theta}}(\mathbf{x})} \right)$$

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

$$V(G, D^*) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log \left(\frac{p_{\text{data}}(\mathbf{x})}{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log \left(\frac{p_{\theta}(\mathbf{x})}{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right)$$

$$= \text{KL} \left(p_{\text{data}}(\mathbf{x}) \parallel \frac{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) + \text{KL} \left(p_{\theta}(\mathbf{x}) \parallel \frac{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) - 2 \log 2$$

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

$$V(G, D^{*}) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log \left(\frac{p_{\text{data}}(\mathbf{x})}{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log \left(\frac{p_{\theta}(\mathbf{x})}{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right)$$

$$= \text{KL} \left(p_{\text{data}}(\mathbf{x}) \parallel \frac{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) + \text{KL} \left(p_{\theta}(\mathbf{x}) \parallel \frac{p_{\text{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) - 2 \log 2$$

$$= 2 \text{JSD}(p_{\text{data}}(\mathbf{x}) \parallel p_{\theta}(\mathbf{x})) - 2 \log 2.$$

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

$$\begin{split} V(G, D^*) &= \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log \left(\frac{p_{\mathsf{data}}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log \left(\frac{p_{\theta}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) \\ &= \mathrm{KL} \left(p_{\mathsf{data}}(\mathbf{x}) \parallel \frac{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) + \mathrm{KL} \left(p_{\theta}(\mathbf{x}) \parallel \frac{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) - 2 \log 2 \\ &= 2 \, \mathrm{JSD}(p_{\mathsf{data}}(\mathbf{x}) \parallel p_{\theta}(\mathbf{x})) - 2 \log 2. \end{split}$$

Jensen-Shannon Divergence (Symmetric KL Divergence)

$$\mathrm{JSD}(p_{\mathsf{data}}(\mathbf{x}) \| p_{\boldsymbol{\theta}}(\mathbf{x})) = \frac{1}{2} \left[\mathrm{KL} \left(p_{\mathsf{data}}(\mathbf{x}) \| \star \right) + \mathrm{KL} \left(p_{\boldsymbol{\theta}}(\mathbf{x}) \| \star \right) \right]$$

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

$$\begin{split} V(G, D^*) &= \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log \left(\frac{p_{\mathsf{data}}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) + \mathbb{E}_{p_{\theta}(\mathbf{x})} \log \left(\frac{p_{\theta}(\mathbf{x})}{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})} \right) \\ &= \mathrm{KL} \left(p_{\mathsf{data}}(\mathbf{x}) \parallel \frac{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) + \mathrm{KL} \left(p_{\theta}(\mathbf{x}) \parallel \frac{p_{\mathsf{data}}(\mathbf{x}) + p_{\theta}(\mathbf{x})}{2} \right) - 2 \log 2 \\ &= 2 \operatorname{JSD}(p_{\mathsf{data}}(\mathbf{x}) \parallel p_{\theta}(\mathbf{x})) - 2 \log 2. \end{split}$$

Jensen-Shannon Divergence (Symmetric KL Divergence)

$$JSD(p_{\mathsf{data}}(\mathbf{x}) \| p_{\theta}(\mathbf{x})) = \frac{1}{2} \left[KL \left(p_{\mathsf{data}}(\mathbf{x}) \| \star \right) + KL \left(p_{\theta}(\mathbf{x}) \| \star \right) \right]$$

This can be regarded as a proper distance metric!

$$V(G^*, D^*) = -2 \log 2$$
, $p_{data}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, $D^*(\mathbf{x}) = 0.5$.

Theorem

The following minimax game

$$\min_{G} \max_{D} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(\mathbf{G}(\mathbf{z}))) \right]$$

achieves its global optimum precisely when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, 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.

Theorem

The following minimax game

$$\min_{G} \max_{D} \Bigl[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D(\mathbf{G}(\mathbf{z}))) \Bigr]$$

achieves its global optimum precisely when $p_{\text{data}}(\mathbf{x}) = p_{\theta}(\mathbf{x})$, 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

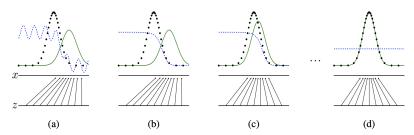
$$\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi}} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D_{\boldsymbol{\phi}}(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D_{\boldsymbol{\phi}}(\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z}))) \right]$$

GAN Training

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

Objective

$$\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi}} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D_{\boldsymbol{\phi}}(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D_{\boldsymbol{\phi}}(\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z}))) \right]$$

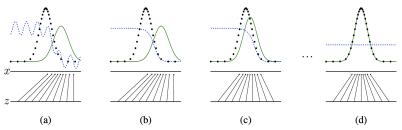


GAN Training

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

Objective

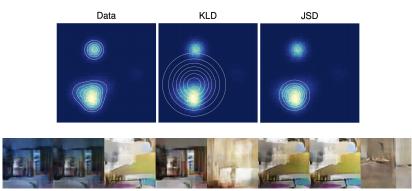
$$\min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi}} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \log D_{\boldsymbol{\phi}}(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D_{\boldsymbol{\phi}}(\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z}))) \right]$$



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

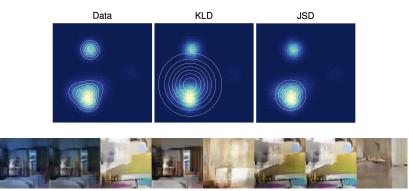
Mode Collapse

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



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

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

Mode Covering vs. Mode Seeking

$$\mathrm{KL}(\pi \parallel p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad \mathrm{KL}(p_{\boldsymbol{\theta}} \parallel p_{\mathsf{data}}) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

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

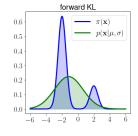
Jensen-Shannon vs Kullback-Leibler Divergences

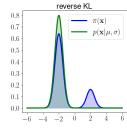
- $ightharpoonup p_{data}(\mathbf{x})$ is a fixed mixture of two Gaussians.
- \triangleright $p(\mathbf{x}|\mu,\sigma) = \mathcal{N}(\mu,\sigma^2).$

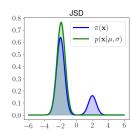
Mode Covering vs. Mode Seeking

$$\mathrm{KL}(\pi \parallel p) = \int \pi(\mathbf{x}) \log \frac{\pi(\mathbf{x})}{p(\mathbf{x})} d\mathbf{x}, \quad \mathrm{KL}(p_{\boldsymbol{\theta}} \parallel p_{\mathsf{data}}) = \int p(\mathbf{x}) \log \frac{p(\mathbf{x})}{\pi(\mathbf{x})} d\mathbf{x}$$

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







Outline

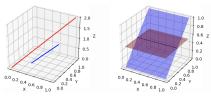
1. Likelihood-Free Learning

- 2. Generative Adversarial Networks (GAN)
- 3. Wasserstein Distance

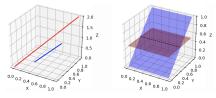
4. Wasserstein GAN

The dimensionality of z is less than that of x, so $p_{\theta}(x)$ with $x = G_{\theta}(z)$ lives on a low-dimensional manifold.

- The dimensionality of z is less than that of x, so $p_{\theta}(x)$ with $x = G_{\theta}(z)$ lives on a low-dimensional manifold.
- The true data distribution $p_{data}(\mathbf{x})$ is also supported on a low-dimensional manifold.

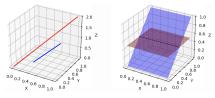


- The dimensionality of z is less than that of x, so $p_{\theta}(x)$ with $x = G_{\theta}(z)$ lives on a low-dimensional manifold.
- The true data distribution $p_{data}(\mathbf{x})$ is also supported on a low-dimensional manifold.



▶ If $p_{\text{data}}(\mathbf{x})$ and $p_{\theta}(\mathbf{x})$ are disjoint, a smooth optimal discriminator can exist!

- The dimensionality of z is less than that of x, so $p_{\theta}(x)$ with $x = G_{\theta}(z)$ lives on a low-dimensional manifold.
- The true data distribution $p_{data}(\mathbf{x})$ is also supported on a low-dimensional manifold.



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

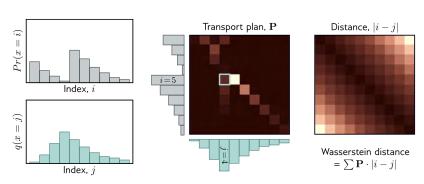
$$\mathrm{KL}(p_{\mathsf{data}} \parallel p_{\theta}) = \mathrm{KL}(p_{\theta} \parallel p_{\mathsf{data}}) = \infty, \quad \mathrm{JSD}(p_{\mathsf{data}} \parallel p_{\theta}) = \log 2$$

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)

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \frac{\gamma(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2}{\gamma(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2}$$

 $\gamma(\mathbf{x}_1, \mathbf{x}_2)$ is the transport plan: the amount of "dirt" assigned from \mathbf{x}_1 to \mathbf{x}_2 .

$$\int \gamma(\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x} = p(\mathbf{x}_2); \quad \int \gamma(\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x}_2 = \pi(\mathbf{x}_1).$$

- ▶ $\Gamma(\pi, p)$ denotes the set of all joint distributions $\gamma(\mathbf{x}_1, \mathbf{x}_2)$ with marginals π and p.
- $ightharpoonup \gamma(\mathbf{x}_1,\mathbf{x}_2)$ is the mass, $\|\mathbf{x}_1-\mathbf{x}_2\|$ is the distance.

Wasserstein Distance (Continuous)

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \frac{\gamma(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2}{\gamma(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2}$$

 $ightharpoonup \gamma(\mathbf{x}_1, \mathbf{x}_2)$ is the transport plan: the amount of "dirt" assigned from \mathbf{x}_1 to \mathbf{x}_2 .

$$\int \gamma(\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x} = p(\mathbf{x}_2); \quad \int \gamma(\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x}_2 = \pi(\mathbf{x}_1).$$

- $ightharpoonup \Gamma(\pi, p)$ denotes the set of all joint distributions $\gamma(\mathbf{x}_1, \mathbf{x}_2)$ with marginals π and p.
- $ightharpoonup \gamma(\mathbf{x}_1,\mathbf{x}_2)$ is the mass, $\|\mathbf{x}_1-\mathbf{x}_2\|$ is the distance.

Wasserstein Metric

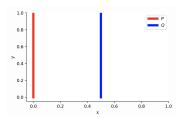
$$W_s(\pi, p) = \inf_{\gamma \in \Gamma(\pi, p)} \left(\mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \|\mathbf{x}_1 - \mathbf{x}_2\|^s \right)^{1/s}$$

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

Consider two-dimensional distributions:

$$p_{\text{data}}(x, y) = (0, U[0, 1])$$

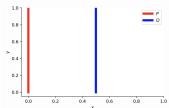
$$p_{\theta}(x,y) = (\theta, U[0,1])$$



Consider two-dimensional distributions:

$$p_{\mathsf{data}}(x,y) = (0, U[0,1])$$

$$p_{\theta}(x,y) = (\theta, U[0,1])$$



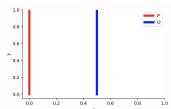
 $\theta = 0$: Both distributions are identical.

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}}) = \mathrm{JSD}(p_{\theta} \| p_{\mathsf{data}}) = W(p_{\mathsf{data}} \| p_{\theta}) = 0$$

Consider two-dimensional distributions:

$$p_{\text{data}}(x,y) = (0, U[0,1])$$

$$p_{\theta}(x,y) = (\theta, U[0,1])$$



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

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}}) = \mathrm{JSD}(p_{\theta} \| p_{\mathsf{data}}) = W(p_{\mathsf{data}} \| p_{\theta}) = 0$$

 $\theta \neq 0$:

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\boldsymbol{ heta}}) = \int_{U[0.1]} 1 \log \frac{1}{0} \, dy = \infty = \mathrm{KL}(p_{\boldsymbol{ heta}} \| p_{\mathsf{data}})$$

Consider two-dimensional distributions:

$$p_{\text{data}}(x, y) = (0, U[0, 1])$$

 $p_{\theta}(x, y) = (\theta, U[0, 1])$

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

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}}) = \mathrm{JSD}(p_{\theta} \| p_{\mathsf{data}}) = W(p_{\mathsf{data}} \| p_{\theta}) = 0$$

 $\theta \neq 0$:

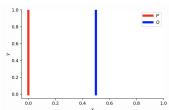
$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \int_{U[0.1]} 1 \log \frac{1}{0} \, dy = \infty = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}})$$

$$\mathrm{JSD}(p_{\mathsf{data}} \| p_{\theta}) = \frac{1}{2} \left(\int_{U[0,1]} 1 \log \frac{1}{1/2} dy + \int_{U[0,1]} 1 \log \frac{1}{1/2} dy \right) = \log 2$$

Consider two-dimensional distributions:

$$p_{\text{data}}(x, y) = (0, U[0, 1])$$

 $p_{\theta}(x, y) = (\theta, U[0, 1])$



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

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}}) = \mathrm{JSD}(p_{\theta} \| p_{\mathsf{data}}) = W(p_{\mathsf{data}} \| p_{\theta}) = 0$$

 $\theta \neq 0$:

$$\mathrm{KL}(p_{\mathsf{data}} \| p_{\theta}) = \int_{U[0,1]} 1 \log \frac{1}{0} \, dy = \infty = \mathrm{KL}(p_{\theta} \| p_{\mathsf{data}})$$

$$\mathrm{JSD}(p_{\mathsf{data}} \| p_{\theta}) = \frac{1}{2} \left(\int_{\mathit{U}[0,1]} 1 \log \frac{1}{1/2} dy + \int_{\mathit{U}[0,1]} 1 \log \frac{1}{1/2} dy \right) = \log 2$$

$$W(p_{\text{data}}||p_{\theta}) = |\theta|$$

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 $W(p_{\text{data}}\|p_{\theta})$ is continuous everywhere and differentiable almost everywhere.

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 $W(p_{\text{data}}\|p_{\theta})$ 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} .

$$\mathrm{KL}(\pi \| p_t) \to 0 \quad (\text{or } \mathrm{KL}(p_t \| \pi) \to 0)$$
 (1)

$$JSD(\pi || p_t) \to 0 \tag{2}$$

$$W(\pi \| p_t) \to 0 \tag{3}$$

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

Outline

1. Likelihood-Free Learning

Generative Adversarial Networks (GAN)

3. Wasserstein Distance

4. Wasserstein GAN

Wasserstein Distance

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x} \, d\mathbf{x}_1 \| \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x} \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \mathbf{x}_1 -$$

Wasserstein Distance

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x} \, d\mathbf{x}$$

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

Wasserstein Distance

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x} \, d\mathbf{x}_1 \| \mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) \, d\mathbf{x}_2 \| \mathbf{x}_1 - \mathbf{x}_2 \| \mathbf{x}_1 - \mathbf$$

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

Theorem (Kantorovich-Rubinstein Duality)

$$W(\pi \| p) = rac{1}{K} \max_{\|f\|_{L} \le K} \left[\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x}) \right]$$

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

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

Wasserstein Distance

$$W(\pi \| p) = \inf_{\gamma \in \Gamma(\pi, p)} \mathbb{E}_{(\mathbf{x}_1, \mathbf{x}_2) \sim \gamma} \| \mathbf{x}_1 - \mathbf{x}_2 \| = \inf_{\gamma \in \Gamma(\pi, p)} \int \| \mathbf{x}_1 - \mathbf{x}_2 \| \gamma(\mathbf{x}_1, \mathbf{x}_2) d\mathbf{x} d\mathbf{x}$$

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

Theorem (Kantorovich-Rubinstein Duality)

$$W(\pi \| p) = rac{1}{K} \max_{\|f\|_{\infty} < K} \left[\mathbb{E}_{\pi(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f(\mathbf{x})
ight]$$

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

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

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

Theorem (Kantorovich-Rubinstein Duality)

$$W(p_{\mathsf{data}} \| p_{m{ heta}}) = rac{1}{K} \max_{\|f\|_{L} \leq K} \Bigl[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p_{m{ heta}}(\mathbf{x})} f(\mathbf{x}) \Bigr]$$

- ▶ 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.

Theorem (Kantorovich-Rubinstein Duality)

$$W(p_{\mathsf{data}} \| p_{\boldsymbol{\theta}}) = \frac{1}{K} \max_{\|f\|_{\boldsymbol{t}} \leq K} \left[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} f(\mathbf{x}) \right]$$

- ▶ 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.

$$\begin{split} K \cdot W(p_{\mathsf{data}} \| p_{\boldsymbol{\theta}}) &= \max_{\|f\|_L \leq K} \Bigl[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} f(\mathbf{x}) - \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} f(\mathbf{x}) \Bigr] \geq \\ &\geq \max_{\boldsymbol{\phi} \in \boldsymbol{\Phi}} \Bigl[\mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} f_{\boldsymbol{\phi}}(\mathbf{x}) - \mathbb{E}_{p_{\boldsymbol{\theta}}(\mathbf{x})} f_{\boldsymbol{\phi}}(\mathbf{x}) \Bigr] \end{split}$$

Standard GAN Objective

$$\min_{m{ heta}} \max_{m{\phi}} \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D_{m{\phi}}(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D_{m{\phi}}(\mathbf{G}_{m{ heta}}(\mathbf{z})))$$

WGAN Objective

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

Standard GAN Objective

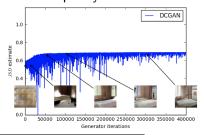
$$\min_{m{ heta}} \max_{m{\phi}} \mathbb{E}_{p_{\mathsf{data}}(\mathbf{x})} \log D_{m{\phi}}(\mathbf{x}) + \mathbb{E}_{p(\mathbf{z})} \log (1 - D_{m{\phi}}(\mathbf{G}_{m{ heta}}(\mathbf{z})))$$

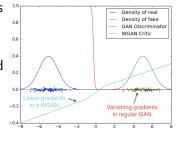
WGAN Objective

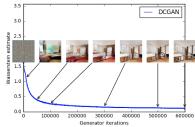
$$\min_{\boldsymbol{\theta}} W(p_{\text{data}} \| p_{\boldsymbol{\theta}}) \approx \min_{\boldsymbol{\theta}} \max_{\boldsymbol{\phi} \in \boldsymbol{\Phi}} \left[\mathbb{E}_{p_{\text{data}}(\mathbf{x})} f_{\boldsymbol{\phi}}(\mathbf{x}) - \mathbb{E}_{p(\mathbf{z})} f_{\boldsymbol{\phi}}(\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z}))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

- ► 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.

- WGAN provides nonzero gradients even if distributions' supports are disjoint.
- ▶ JSD($p_{\text{data}} || p_{\theta}$) is poorly correlated with sample quality and remains near its maximum value $\log 2 \approx 0.69$.
- $W(p_{\text{data}}||p_{\theta})$ 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.