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

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

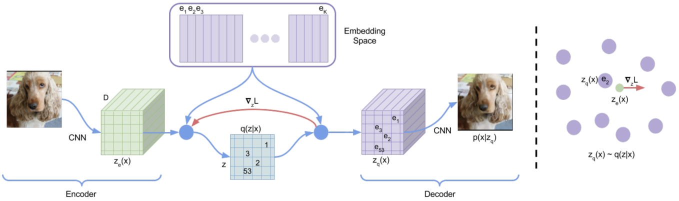
Vector Quantization

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

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

Straight-Through Gradient Estimation

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

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

Recap of Previous Lecture

Theorem

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

ELBO Surgery

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

Optimal Prior

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

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

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

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

ELBO with Learnable VAE Prior

$$\mathcal{L}_{\phi,\boldsymbol{\theta}}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)}\left[\log p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta}) + \log p(\mathbf{z}|\boldsymbol{\lambda}) - \log q(\mathbf{z}|\mathbf{x},\phi)\right]$$

$$= \mathbb{E}_{q(\mathbf{z}|\mathbf{x},\phi)}\Big[\log p(\mathbf{x}|\mathbf{z},\boldsymbol{\theta}) + \underbrace{\Big(\log p(f_{\boldsymbol{\lambda}}(\mathbf{z})) + \log|\det(\mathbf{J}_\mathbf{f})|\Big)}_{\text{flow-based prior}} - \log q(\mathbf{z}|\mathbf{x},\phi)\Big]$$

$$\mathbf{z} = \mathbf{f}_{\boldsymbol{\lambda}}^{-1}(\mathbf{z}^*) = \mathbf{g}_{\boldsymbol{\lambda}}(\mathbf{z}^*), \quad \mathbf{z}^* \sim p(\mathbf{z}^*) = \mathcal{N}(0, \mathbf{I})$$

Chen X. et al. Variational Lossy Autoencoder, 2016

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.

Theis L., Oord A., Bethge M. A Note on the Evaluation of Generative Models, 2015

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High Likelihood
Poor Samples

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

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

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

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

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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.

Theis L., Oord A., Bethge M. A Note on the Evaluation of Generative Models, 2015

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

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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.

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Define a discriminative model (classifier):

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

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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 $p(\mathbf{x}|\boldsymbol{\theta})$.
- Standard classifiers are trained by minimizing cross-entropy loss.

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

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Cross-Entropy for Discriminator

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

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Generative Model

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

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

Generative Adversarial Networks (GAN)

Cross-Entropy for Discriminative Model

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

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

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GAN Objective

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

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

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

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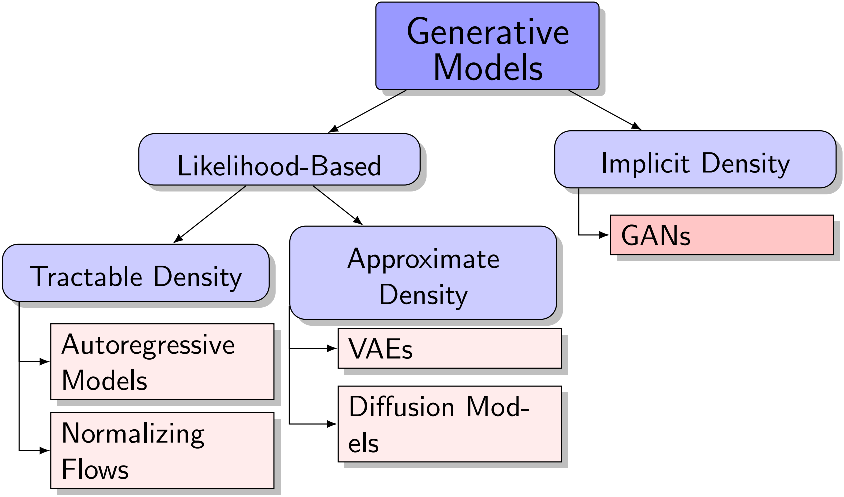
Generative Models Zoo



GAN Optimality

Theorem

The minimax game

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

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

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Proof (Fixed G)

$$V(G, D) = \mathbb{E}_{\pi(\mathbf{x})} \log D(\mathbf{x}) + \mathbb{E}_{p(\mathbf{x}|\boldsymbol{\theta})} \log(1 - D(\mathbf{x}))$$

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

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Proof (Fixed G)

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

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

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

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

GAN Optimality

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

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

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

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$$= \mathrm{KL}\left(\pi(\mathbf{x}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) + \mathrm{KL}\left(p(\mathbf{x}|\boldsymbol{\theta}) \parallel \frac{\pi(\mathbf{x}) + p(\mathbf{x}|\boldsymbol{\theta})}{2} \right) - 2\log 2$$

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

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

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

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

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$$= 2\,\mathrm{JSD}(\pi(\mathbf{x}) \,\|\, p(\mathbf{x}|\boldsymbol{\theta})) - 2\log 2.$$

Jensen-Shannon Divergence (Symmetric KL Divergence)

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

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

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Jensen-Shannon Divergence (Symmetric KL Divergence)

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This can be regarded as a proper distance metric!

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

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

GAN Optimality

Theorem

The following minimax game

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

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.

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Reality

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

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

GAN Training

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

Objective

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

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

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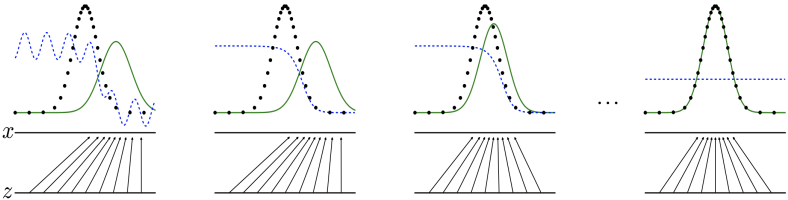

(a) (b) (c) (d)

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

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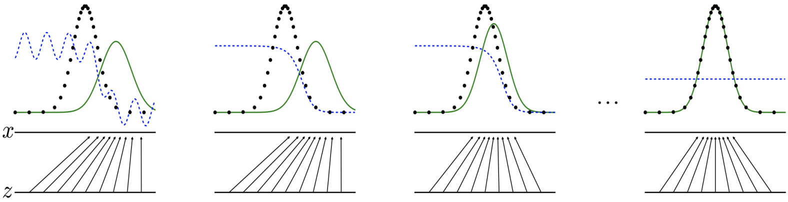


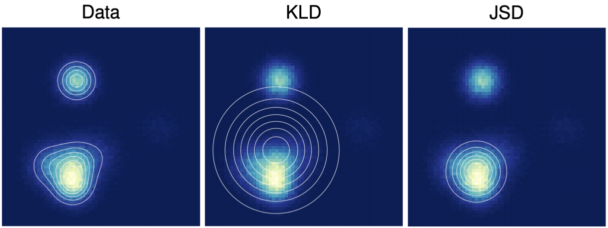
(a) (b) (c) (d)

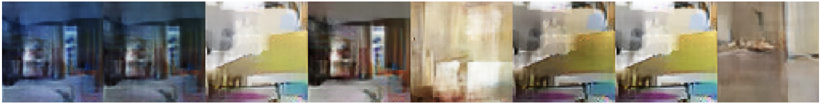
- $\mathbf{z} \sim p(\mathbf{z})$ is a latent variable.
- $p(\mathbf{x}|\mathbf{z}, \theta) = \delta(\mathbf{x} - \mathbf{G}_{\theta}(\mathbf{z}))$ serves as a deterministic decoder (like normalizing flows).
- There is no encoder present.

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

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.





Goodfellow I. J. et al. Generative Adversarial Networks, 2014
Metz L. et al. Unrolled Generative Adversarial Networks, 2016

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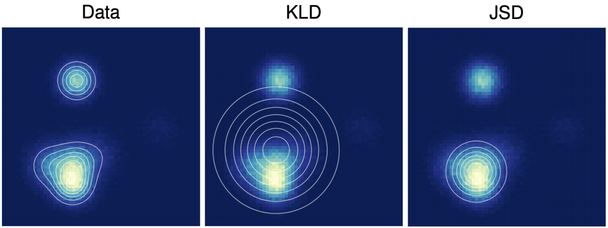

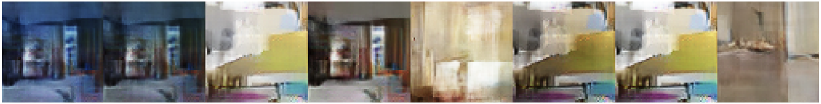

Numerous methods have been proposed to tackle mode collapse: changing architectures, adding regularization terms, injecting noise.

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

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

$$\mathrm{JSD}(\pi \,\|\, p) = \frac{1}{2}\Big[\mathrm{KL}\Big(\pi(\mathbf{x}) \,\|\, \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2}\Big) + \mathrm{KL}\Big(p(\mathbf{x}) \,\|\, \frac{\pi(\mathbf{x}) + p(\mathbf{x})}{2}\Big)\Big]$$

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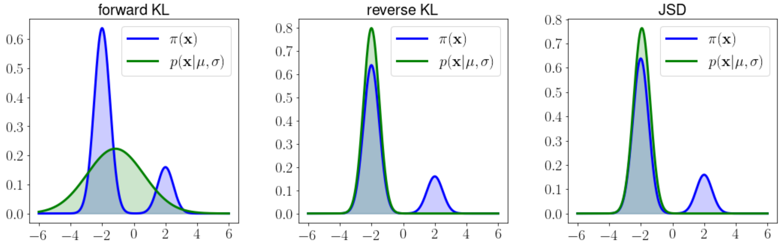

Outline

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

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.

Weng L. From GAN to WGAN, 2019

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

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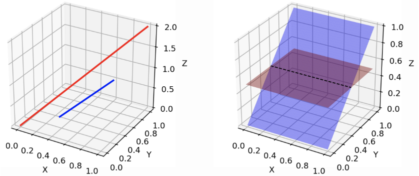

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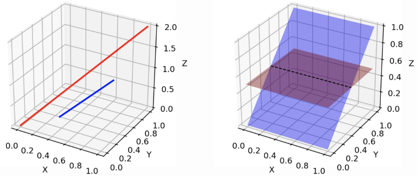

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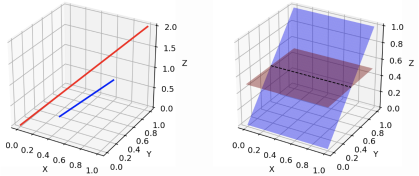


- If $\pi(\mathbf{x})$ and $p(\mathbf{x}|\boldsymbol{\theta})$ are disjoint, a smooth optimal discriminator can exist!
- For such low-dimensional, disjoint manifolds:

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

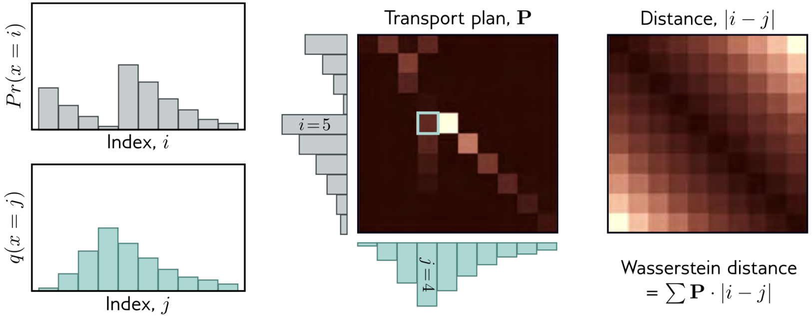
Weng L. From GAN to WGAN, 2019
Arjovsky M., Bottou L. Towards Principled Methods for Training Generative Adversarial Networks, 2017

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.



Simon J.D. Prince. *Understanding Deep Learning, 2023*

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.

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

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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.

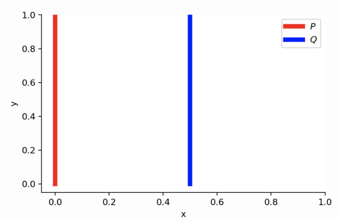
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

Wasserstein Distance vs KL vs JSD

Consider two-dimensional distributions:

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

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



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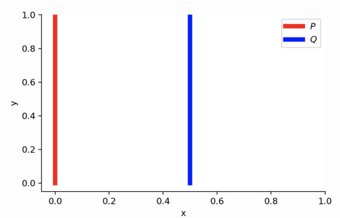

- $\theta = 0$: Both distributions are identical.

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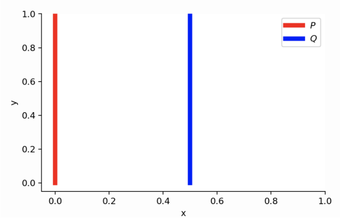

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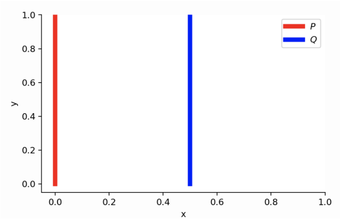

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Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

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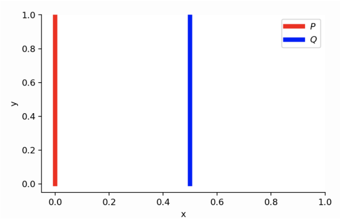

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$$W(\pi, p) = |\theta|$$

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 $\mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z})$ 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.

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

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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 $\mathcal{X}$.

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

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

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

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

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

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

Wasserstein GAN

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

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

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

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

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

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- 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 $\boldsymbol{\Phi}$, then f_ϕ is K-Lipschitz.

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

Wasserstein GAN

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

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

$$\geq \max_{\phi \in \boldsymbol{\Phi}} \Big[\mathbb{E}_{\pi(\mathbf{x})} f_\phi(\mathbf{x}) - \mathbb{E}_{p(\mathbf{x})} f_\phi(\mathbf{x}) \Big]$$

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

Wasserstein GAN

Standard GAN Objective

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

WGAN Objective

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

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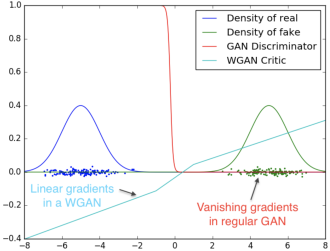
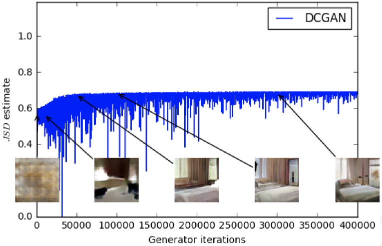
- The discriminator D is replaced by function f: in WGAN, it is known as the **critic**, which is *not* a classifier.
- *"Weight clipping is a clearly terrible way to enforce a Lipschitz constraint."*
  - If c is large, optimizing the critic is hard.
  - If c is small, gradients may vanish.

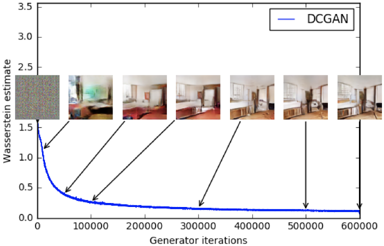
Arjovsky M., Chintala S., Bottou L. Wasserstein GAN, 2017

Wasserstein GAN

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







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

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.