

Deep Generative Models

Lecture 7

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Recap of Previous Lecture

Likelihood-Free Learning

- ▶ Likelihood isn't a perfect metric for generative models.
- ▶ Likelihood may be intractable.

Imagine we have two sets of samples:

- ▶ $\{\mathbf{x}_i\}_{i=1}^{n_1} \sim \pi(\mathbf{x})$ – real samples;
 - ▶ $\{\mathbf{x}_i\}_{i=1}^{n_2} \sim p(\mathbf{x}|\theta)$ – generated (fake) samples.
- $$p(y = 1|\mathbf{x}) = P(\mathbf{x} \sim \pi(\mathbf{x})); \quad p(y = 0|\mathbf{x}) = P(\mathbf{x} \sim p(\mathbf{x}|\theta))$$

Assumption

The generative distribution $p(\mathbf{x}|\theta)$ matches the true distribution $\pi(\mathbf{x})$ if we can't distinguish between them using a discriminative model $p(y|\mathbf{x})$.

- ▶ **Generator:** a generative model $\mathbf{x} = \mathbf{G}(\mathbf{z})$ that produces more realistic samples.
- ▶ **Discriminator:** a classifier $D(\mathbf{x}) \in [0, 1]$ distinguishing real from generated samples.

Recap of Previous Lecture

GAN Optimality Theorem

The minimax game

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

has a global optimum at $\pi(\mathbf{x}) = p(\mathbf{x}|\theta)$, and then $D^*(\mathbf{x}) = 0.5$.

$$\min_G V(G, D^*) = \min_G [2\text{JSD}(\pi \| p) - \log 4] = -\log 4, \quad \pi(\mathbf{x}) = p(\mathbf{x}|\theta).$$

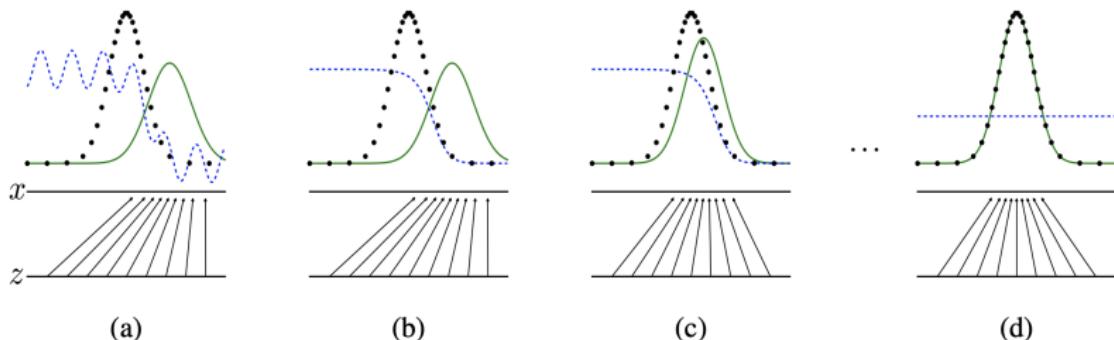
If the generator can be **any** function and the discriminator is **optimal** at each step, then the generator is **guaranteed to converge** to the data distribution.

Recap of Previous Lecture

- ▶ The generator is updated in the parameter space; the discriminator isn't optimal at every iteration.
- ▶ Both generator and discriminator loss typically oscillate during GAN training.

Objective

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



Recap of Previous Lecture

Main Issues With Standard GANs

- ▶ Vanishing gradients (solution: non-saturating GAN).
- ▶ Mode collapse (arises from Jensen-Shannon divergence).

Standard GAN

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

Informal Theoretical Results

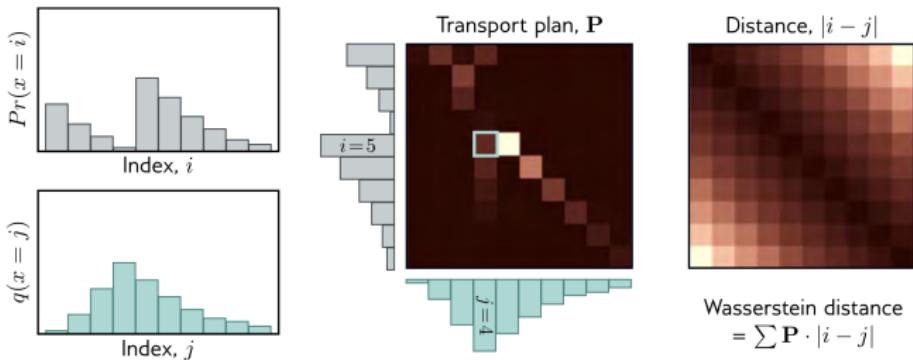
Both the data distribution $\pi(\mathbf{x})$ and the generative distribution $p(\mathbf{x}|\theta)$ are low-dimensional with disjoint supports. In such cases,

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

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

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

Recap of Previous Lecture



Wasserstein Distance

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

- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ – transportation plan (amount of "dirt" to transport from \mathbf{x} to \mathbf{y}).
- ▶ $\Gamma(\pi, p)$ – set of all joint distributions $\gamma(\mathbf{x}, \mathbf{y})$ with marginals π and p ($\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{x} = p(\mathbf{y})$, $\int \gamma(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \pi(\mathbf{x})$).
- ▶ $\gamma(\mathbf{x}, \mathbf{y})$ – the amount; $\|\mathbf{x} - \mathbf{y}\|$ – the distance.

Recap of Previous Lecture

Theorem (Kantorovich-Rubinstein Duality)

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

where $\|f\|_L \leq K$ denotes K -Lipschitz continuous functions.

WGAN Objective

$$\min_{\theta} W(\pi \| p) = \min_{\theta} \max_{\phi \in \Phi} [\mathbb{E}_{\pi(x)} f_{\phi}(x) - \mathbb{E}_{p(z)} f_{\phi}(\mathbf{G}_{\theta}(z))].$$

- ▶ The function f in WGAN is called the *critic*.
- ▶ If parameters ϕ lie in a compact set $\Phi \in [-c, c]^d$, then $f(x, \phi)$ is K -Lipschitz continuous.

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

Outline

1. Evaluation of Likelihood-Free Models

Frechet Inception Distance (FID)

Precision-Recall

CLIP Score

Human Evaluation

2. Langevin Dynamics

3. Score Matching

4. Denoising Score Matching

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Evaluation of Likelihood-Free Models

Likelihood-Based Models

- ▶ **Train:** fit the model.
- ▶ **Validation:** tune hyperparameters.
- ▶ **Test:** assess generalization by reporting likelihood.

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Desirable Properties for Samples

- ▶ Sharpness



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- ▶ Diversity



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Wasserstein Metric

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

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Wasserstein GAN (Optimal Transport)

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

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Theorem

If $\pi(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}_\pi, \boldsymbol{\Sigma}_\pi)$, $p(\mathbf{y}) = \mathcal{N}(\boldsymbol{\mu}_p, \boldsymbol{\Sigma}_p)$, then

$$W_2^2(\pi, p) = \|\boldsymbol{\mu}_\pi - \boldsymbol{\mu}_p\|^2 + \text{tr} \left[\boldsymbol{\Sigma}_\pi + \boldsymbol{\Sigma}_p - 2 \left(\boldsymbol{\Sigma}_\pi^{1/2} \boldsymbol{\Sigma}_p \boldsymbol{\Sigma}_\pi^{1/2} \right)^{1/2} \right]$$

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Frechet Inception Distance

$$\text{FID}(\pi, p) = W_2^2(\pi, p)$$

Frechet Inception Distance (FID)

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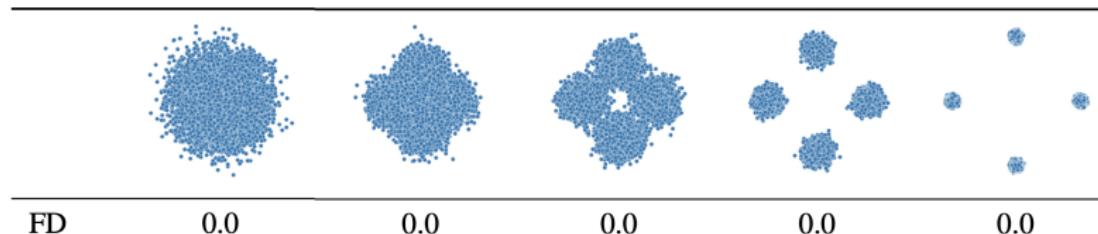
- ▶ FID is computed in the latent space \mathbf{z} .
- ▶ We use a pretrained image embedder to get latent representations $\mathbf{z} = \mathbf{f}(\mathbf{x})$.
- ▶ $\boldsymbol{\mu}_\pi$, $\boldsymbol{\Sigma}_\pi$ and $\boldsymbol{\mu}_p$, $\boldsymbol{\Sigma}_p$ are statistics of latent representations for samples from $\pi(\mathbf{x})$ and $p(\mathbf{x}|\theta)$.

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$FID(p(\mathbf{x}), \mathcal{N}(0, \mathbf{I}))$



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Drawbacks

- ▶ Depends on the pretrained classification network.
- ▶ Uses the normality assumption.
- ▶ May not correlate with human evaluation.

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Model	Model-A	Model-B
FID	21.40	18.42
FID_∞	20.16	17.19
Human rater preference	92.5%	6.9%

Outline

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Precision-Recall

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Precision-Recall

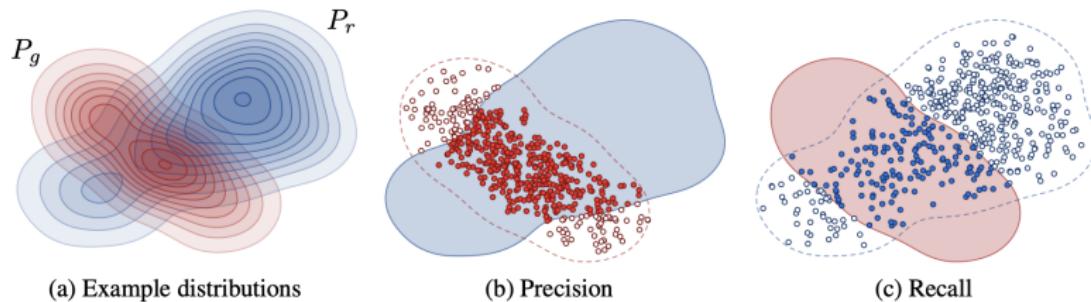
Desirable Properties for Generated Samples

- ▶ **Sharpness:** generated samples should possess high visual quality.
- ▶ **Diversity:** their variation should match that in the training data.

Precision-Recall

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- ▶ **Precision** denotes the fraction of generated images that look realistic.
- ▶ **Recall** measures how well the generator covers the training data manifold.

Precision-Recall

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

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Define a binary function:

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

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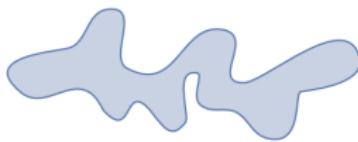
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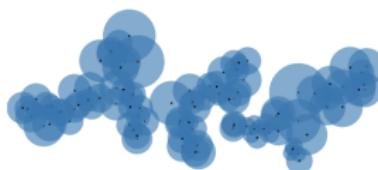
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(a) True manifold



(b) Approx. manifold

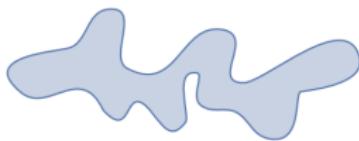
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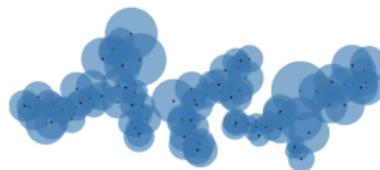
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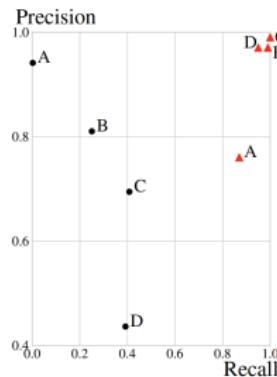
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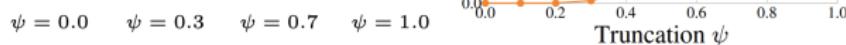
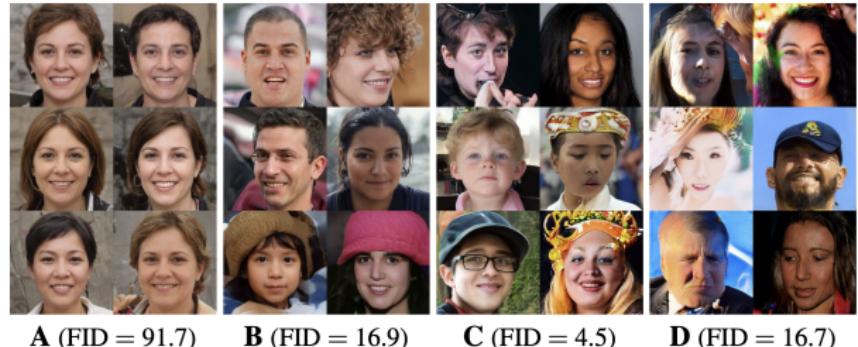
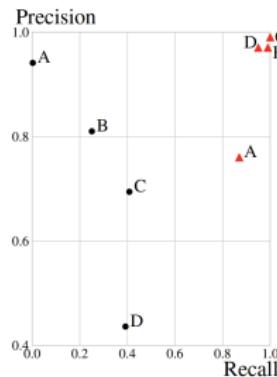
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Embed the samples using a pretrained network (as in FID).

Precision-Recall



Precision-Recall



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

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Human Evaluation

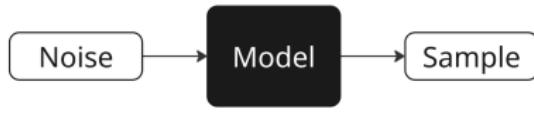
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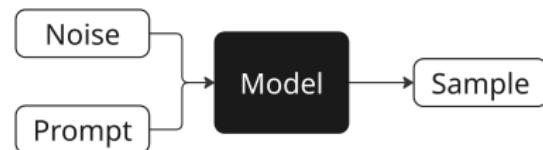
4. Denoising Score Matching

CLIP Score

Unconditional Model

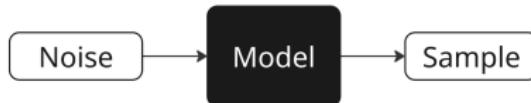


Conditional Model

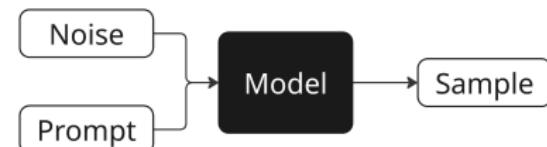


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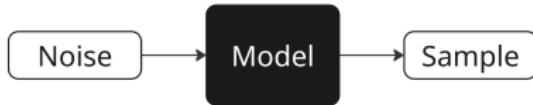
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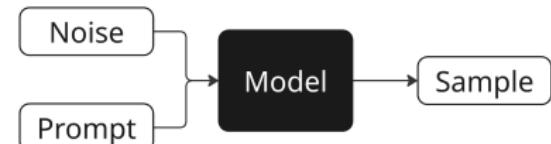
We need a way to measure not only the quality of the generated image, but also how well it's aligned with the prompt.

CLIP Score

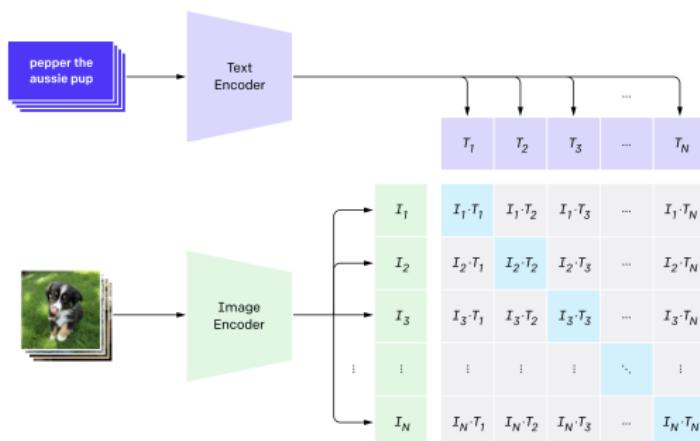
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Аспект	Yandex ART 2.0	Mj 6.1	Mj 6	Ideogram	Recraft	Google Imagen3	Dall-E 3	FLUX	SBER Kandi3.1
Релевантность	0,59	0,58	0,63	0,45	0,51	0,50	0,50	0,54	0,75
Эстетика	0,49	0,55	0,55	0,51	0,51	0,61	0,61	0,54	0,59
Комплексность	0,44	0,73	0,70	0,68	0,76	0,75	0,75	0,71	0,74
Дефектность	0,69	0,57	0,68	0,55	0,59	0,63	0,63	0,50	0,75
Предпочтение	0,66	0,60	0,69	0,49	0,54	0,63	0,63	0,51	0,84

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- ▶ If we reparameterize as $\hat{p}(\mathbf{x}|\theta) = \exp(-f_\theta(\mathbf{x}))$, we eliminate the non-negativity constraint.

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Unnormalized Density

The gradient of the normalized log-density equals that of the unnormalized log-density:

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta) = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\theta) - \nabla_{\mathbf{x}} \log Z_\theta$$

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The gradient of the normalized log-density equals that of the unnormalized log-density:

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta) = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\theta) - \nabla_{\mathbf{x}} \log Z_\theta = \nabla_{\mathbf{x}} \log \hat{p}(\mathbf{x}|\theta)$$

Energy-Based Models

Unnormalized Density

$$p(\mathbf{x}|\theta) = \frac{\hat{p}(\mathbf{x}|\theta)}{Z_\theta}, \quad \text{where } Z_\theta = \int \hat{p}(\mathbf{x}|\theta) d\mathbf{x}$$

- ▶ $\hat{p}(\mathbf{x}|\theta)$ can be any non-negative function.
- ▶ If we reparameterize as $\hat{p}(\mathbf{x}|\theta) = \exp(-f_\theta(\mathbf{x}))$, we eliminate the non-negativity constraint.

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- ▶ Suppose we already have this density (normalized or not) $p(\mathbf{x}|\theta)$.
- ▶ How can we sample from the model?

Langevin Dynamics

Theorem (Informal)

Let \mathbf{x}_0 be a random vector. Under mild regularity conditions, samples from the following dynamics will eventually follow $p(\mathbf{x}|\theta)$ (for sufficiently small η and large I):

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p(\mathbf{x}_I | \theta) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I, \quad \boldsymbol{\epsilon}_I \sim \mathcal{N}(0, \mathbf{I}).$$

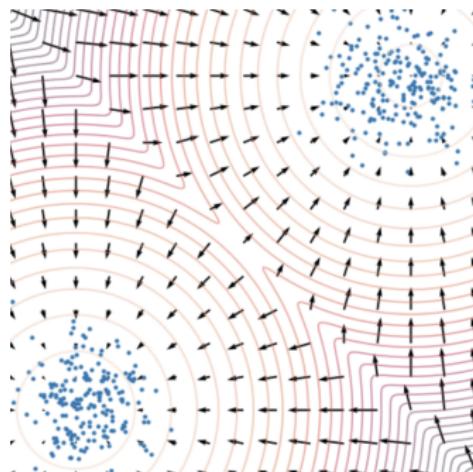
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- ▶ What if $\boldsymbol{\epsilon}_I = \mathbf{0}$?
- ▶ The density $p(\mathbf{x}|\theta)$ is the **stationary** distribution of the Markov chain.
- ▶ The gradient is taken with respect to \mathbf{x} , not θ .
- ▶ $\nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$ defines a vector field.



Outline

1. Evaluation of Likelihood-Free Models

Frechet Inception Distance (FID)

Precision-Recall

CLIP Score

Human Evaluation

2. Langevin Dynamics

3. Score Matching

4. Denoising Score Matching

Score Matching

Score Function

$$s_{\theta}(x) = \nabla_x \log p(x|\theta)$$

Score Matching

Score Function

$$\mathbf{s}_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$$

Langevin Dynamics

If we know the score function $\mathbf{s}_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta)$, we can generate samples from the model using Langevin dynamics:

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \nabla_{\mathbf{x}_I} \log p(\mathbf{x}_I|\theta) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_\theta(\mathbf{x}_I) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I.$$

Score Matching

Score Function

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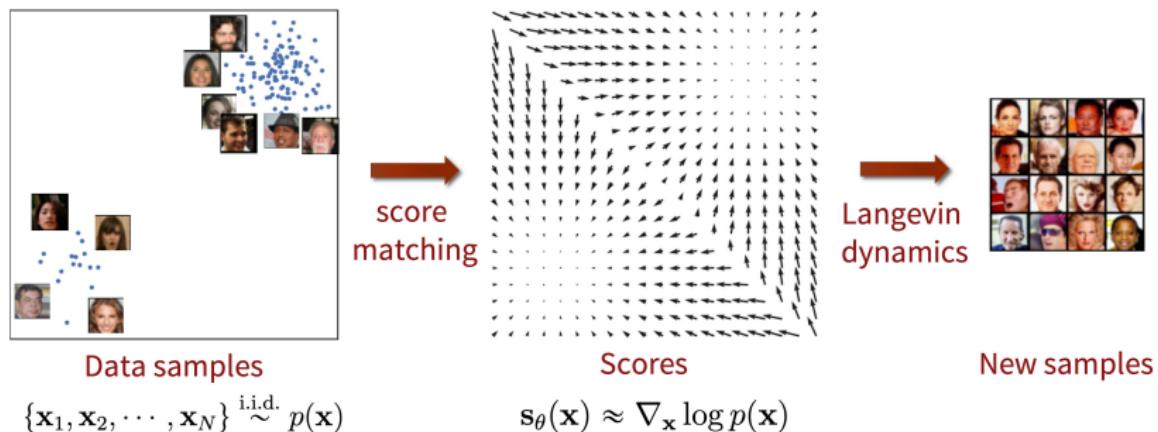
Fisher Divergence

$$\begin{aligned} D_F(\pi, p) &= \frac{1}{2} \mathbb{E}_\pi \| \nabla_{\mathbf{x}} \log p(\mathbf{x}|\theta) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 = \\ &= \frac{1}{2} \mathbb{E}_\pi \| \mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 \rightarrow \min_\theta \end{aligned}$$

Score Matching

Fisher Divergence

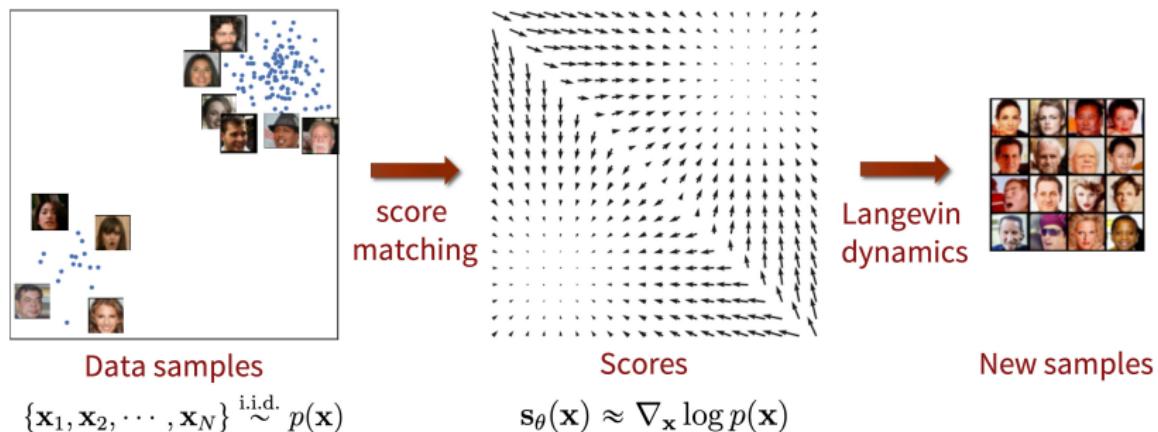
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Score Matching

Fisher Divergence

$$D_F(\pi, p) = \frac{1}{2} \mathbb{E}_\pi \| \mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \|_2^2 \rightarrow \min_{\theta}$$



Problem: We don't know $\nabla_{\mathbf{x}} \log \pi(\mathbf{x})$.

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Denoising Score Matching

Let us perturb the original data $\mathbf{x} \sim \pi(\mathbf{x})$ with Gaussian noise:

$$\mathbf{x}_\sigma = \mathbf{x} + \sigma \cdot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I}), \quad q(\mathbf{x}_\sigma | \mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma^2 \cdot \mathbf{I})$$

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$$q(\mathbf{x}_\sigma) = \int q(\mathbf{x}_\sigma | \mathbf{x}) \pi(\mathbf{x}) d\mathbf{x}.$$

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Assumption

The solution to

$$\frac{1}{2} \mathbb{E}_{q(\mathbf{x}_\sigma)} \| \mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma) \|_2^2 \rightarrow \min_{\theta}$$

satisfies $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma) \approx \mathbf{s}_{\theta, 0}(\mathbf{x}_0) = \mathbf{s}_\theta(\mathbf{x})$ if σ is sufficiently small.

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The solution to

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- ▶ The score function of the noised data nearly matches the score function of the original data.
- ▶ The score function $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$ is parameterized by σ .
- ▶ **Note:** We don't know $q(\mathbf{x}_\sigma)$, just as we don't know $\pi(\mathbf{x})$.

Denoising Score Matching

Theorem

$$\begin{aligned}\mathbb{E}_{q(\mathbf{x}_\sigma)} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)\|_2^2 &= \\ &= \mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{q(\mathbf{x}_\sigma|\mathbf{x})} \|\mathbf{s}_{\theta,\sigma}(\mathbf{x}_\sigma) - \nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma|\mathbf{x})\|_2^2 + \text{const}(\theta)\end{aligned}$$

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Gradient of the Noise Kernel

$$\mathbf{x}_\sigma = \mathbf{x} + \sigma \cdot \epsilon, \quad q(\mathbf{x}_\sigma|\mathbf{x}) = \mathcal{N}(\mathbf{x}, \sigma^2 \cdot \mathbf{I})$$

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- ▶ The right-hand side doesn't require computing $\nabla_{\mathbf{x}_\sigma} \log q(\mathbf{x}_\sigma)$ or even $\nabla_{\mathbf{x}_\sigma} \log \pi(\mathbf{x}_\sigma)$.
- ▶ $\mathbf{s}_{\theta, \sigma}(\mathbf{x}_\sigma)$ is trained to **denoise** the noised samples \mathbf{x}_σ .

Denoising Score Matching

Initial objective:

$$\mathbb{E}_{\pi(\mathbf{x})} \left\| \mathbf{s}_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} \log \pi(\mathbf{x}) \right\|_2^2 \rightarrow \min_{\theta}$$

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This is equivalent to a denoising task:

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$$\mathbb{E}_{\pi(\mathbf{x})} \mathbb{E}_{\mathcal{N}(0, \mathbf{I})} \left\| \mathbf{s}_{\theta,\sigma}(\mathbf{x} + \sigma \cdot \boldsymbol{\epsilon}) + \frac{\boldsymbol{\epsilon}}{\sigma} \right\|_2^2 \rightarrow \min_{\theta}$$

Langevin Dynamics

$$\mathbf{x}_{I+1} = \mathbf{x}_I + \frac{\eta}{2} \cdot \mathbf{s}_{\theta,\sigma}(\mathbf{x}_I) + \sqrt{\eta} \cdot \boldsymbol{\epsilon}_I, \quad \boldsymbol{\epsilon}_I \sim \mathcal{N}(0, \mathbf{I}).$$

Summary

- ▶ Frechet Inception Distance is the most popular metric for evaluating implicit generative models.
- ▶ Precision-recall allows for choosing a model that balances sample quality and diversity.
- ▶ The CLIP score is widely used to measure text-to-image alignment.
- ▶ The gold standard for evaluating generated image quality is human assessment.
- ▶ Langevin dynamics enable sampling from generative models using gradients of the log-likelihood.
- ▶ Score matching proposes minimizing Fisher divergence to estimate the score function.
- ▶ Denoising score matching optimizes Fisher divergence on noisy data, making it estimable with samples.