I. Introduction

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STT 997 (SS 2025)

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Outline

Generative Model

- The advent of high-dimensional and large-scale data has increased the richness of information within the data, even without human-annotated labels, emphasizing the need for advanced statistical methods.
- Recent advancements have enabled the learning and generation of complex data. These models are now commonly referred to as *Generative AI* or *Generative Models*.

A screenshot of a generated video by OpenAI Sora. More examples can be found at `https://openai.com/sora/`.

Generative Model

- Let $\vec{X} = (X_1, \ldots, X_p)^T$ be observations following $p(\vec{x})$, e.g., $p = 1,024 \times 1,024 \times 3 \approx 3.15$M for color images shown above.
- Generative models learn the joint distribution of all observed variables, $\vec{X}$:

$$p(\vec{x}). \tag{1}$$

With $p(\vec{x})$, we can augment data, investigate cluster structures, and detect anomalies.

Images are from CelebA dataset (Liu et al., 2015).

Generative Model

- In this course, the term 'Generative Model' refers to statistical models that learn the distribution of observations either without human-annotated labels or with auxiliary information.[1]
- Deep generative models have shown remarkable performance as:
  1. simulators by generating realistic data,
  2. dimension reduction tools by extracting low-dimensional representations,
  3. inference tools by translating observations to other domains.

[1] For example, demographic information in medical data or timestamps in temporal data.

Application: Image Generation

- After training, generative models can synthesize realistic data without prior information such as age and race in face generation.
- These models can be used to augment data, generate privacy-free samples, and enhance virtual reality experiences.

The generated image is from `http://thispersondoesnotexist.com/`

Application: Text-to-Image Generation

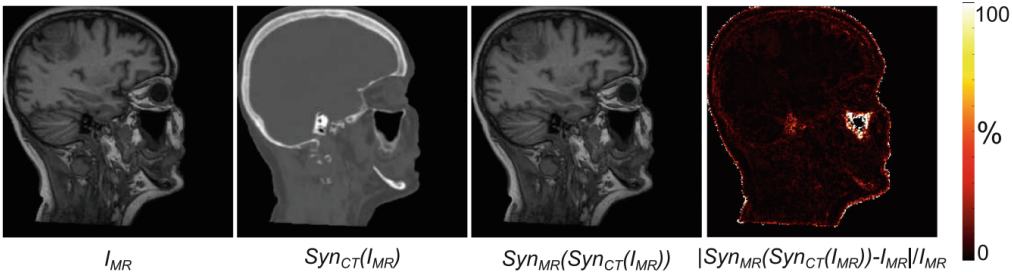
- Images are generated by DALL-E-2 using

  "There is a clean desk in the middle. Outside the window, a whale shark is swimming in the dark night sky above Manhattan."

- Generated images reflect semantic information in text descriptions.

Images are generated with DALL-E-2 (Ramesh et al., 2022).

Application: Cross Modality Transfer

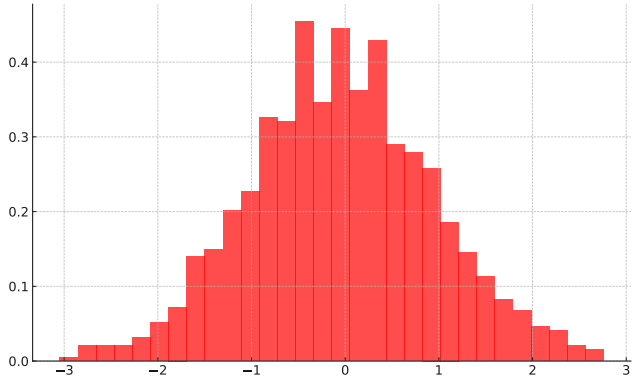


- Generative models are also useful in imputing missing modalities, e.g., MR $\rightarrow$ CT, or enhancing data resolution.

Images are from Wolterink et al. (2017).

How to Learn Distributions: Toy Example

- Let's begin with a basic example. Assume we observed n univariate samples $x_1, \ldots, x_n$ having the following histogram:



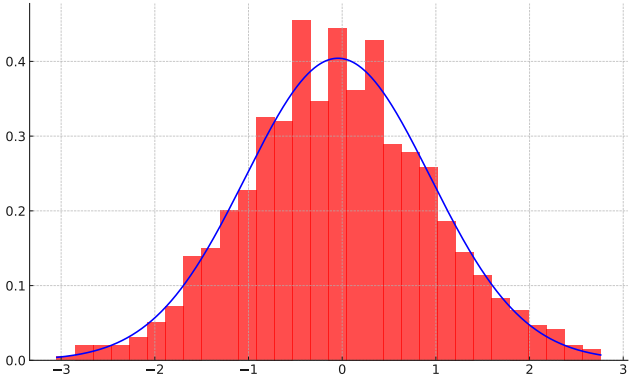
How to Learn Distributions: Toy Example

- How to learn the distribution where x_i comes from?
- One way is to model it as Gaussian and find the optimal mean and std parameters.
- $p_\theta(x) := (2\pi\sigma^2)^{-1/2} \exp\left((x-\mu)^2/(2\sigma^2)\right)$ where $\theta = (\mu, \sigma^2)^T \in \mathbb{R} \times \mathbb{R}^+$.

Q: What are good evaluation criteria for optimality? How do we determine which parameter values are superior?

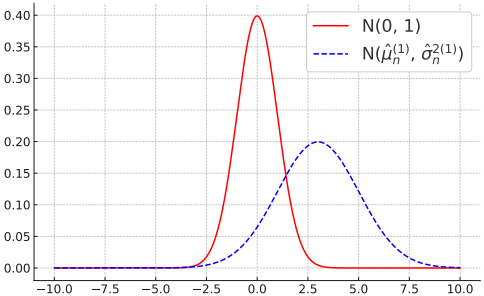
How to Learn Distributions: Toy Example

- $l_n(\theta) := \sum_{i=1}^n \log p_\theta(x_i) = -(n/2)\log\sigma^2 - \sum_{i=1}^n (x_i-\mu)^2/(2\sigma^2) - (n/2)\log 2\pi$
- $\arg\max_\theta l_n(\theta) = (\hat{\mu}_n, \hat{\sigma_n^2})^T = \left(\bar{x}, n^{-1}\sum_{i=1}^n (x_i-\bar{x})^2\right)^T$



How to Learn Distributions: Toy Example

- There is no closed-form expression for the MLEs when addressing complex data and models.
- We usually run iterative algorithms to approximate optimal parameters.

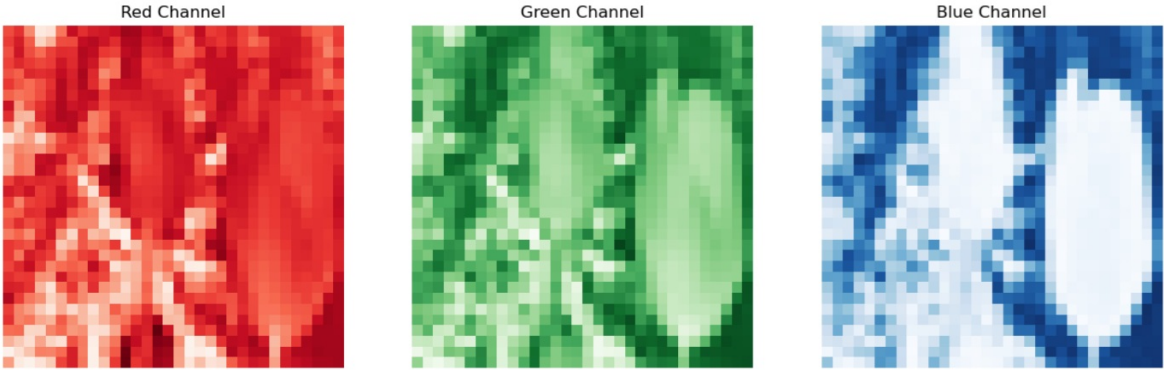


Challenges in Generative Models

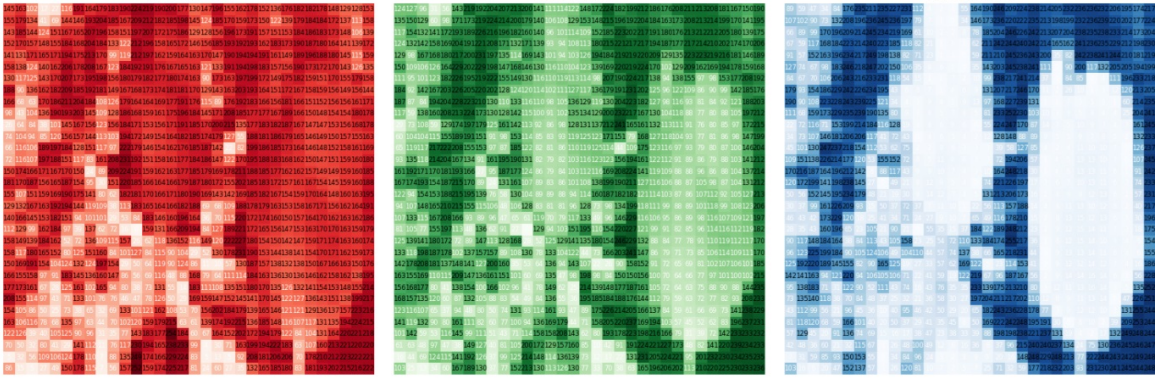
- **High-dimensional Data**: For data like 4K-resolution color images, the dimensionality is $3,840 \times 2,160 \times 3 (\approx 24M)$.
- **Complex Structure**: Image, video, audio, and language data exhibit complex structures.

Challenges in Generative Models

Challenges in Generative Models



Challenges in Generative Models



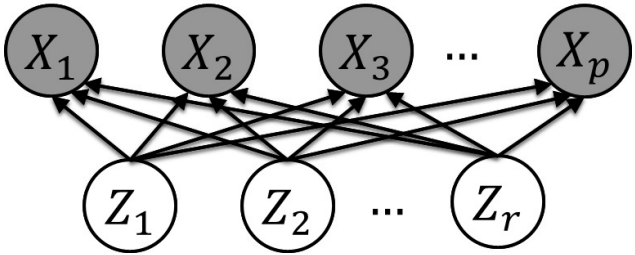
Challenges in Generative Models

- How to model the distribution of high-dimensional data efficiently?
- How to evaluate the generated data and train the model distribution?

Example of generated images, edited from Li et al. (2024)

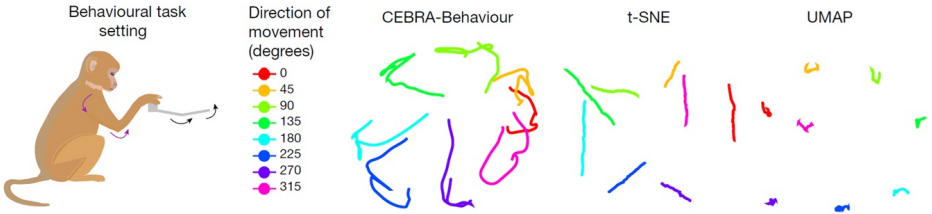
Outline

Latent Variable Model



- Latent variable models are popular approaches in generative models.
- For example, we can mix latent independent components to generate observations:
  1. Latent Factors: $\vec{Z} \sim \prod_{j=1}^{r} p(z_j)$
  2. Observations: $\vec{X}|\vec{Z} = \vec{z} \sim \prod_{j=1}^{p} p(x_j|\vec{Z} = \vec{z})$

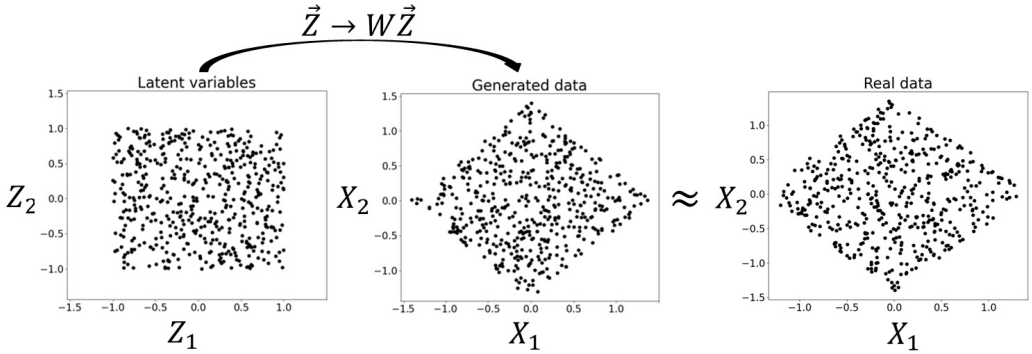
Latent Variable Model



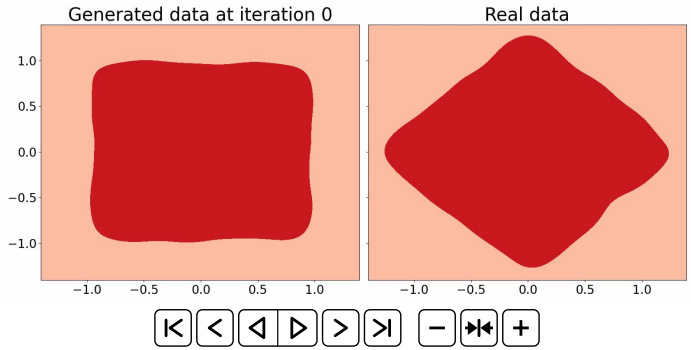
- Generative models can interpret the semantic meanings of factors $\vec{Z}$ and how they affect observations $\vec{X}$.
- The figure shows an analysis of electrophysiology recordings from the somatosensory cortex of monkeys.
- Compared to other (nonlinear) embedding techniques, deep generative models provide more explainable results.

Images are edited from Schneider et al. (2023).

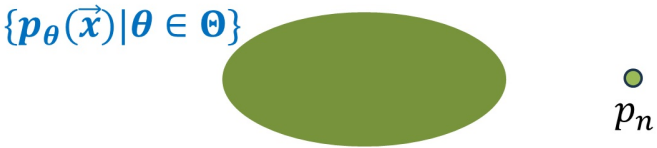
Example: Independent Component Analysis



Example: Independent Component Analysis

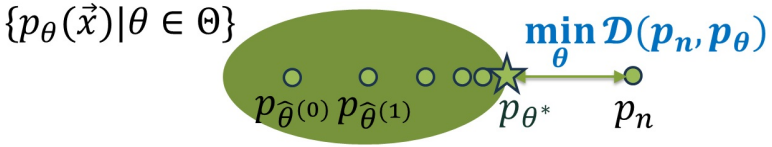


Statistical Reasoning with Generative Model



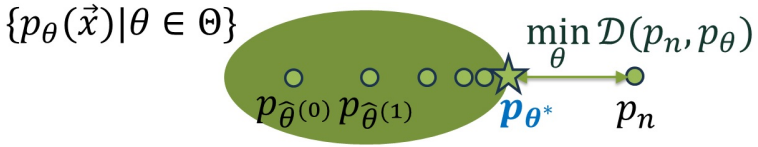
- Key elements to learn generative models include
  1. **Model Class**: A flexible class of $p_\theta(\vec{x})$ reflecting prior knowledge.

Statistical Reasoning with Generative Model



- Key elements to learn generative models include
  1. **Model Class**: A flexible class of $p_\theta(\vec{x})$ reflecting prior knowledge.
  2. **Statistical Distance**: Measure differences between p_n and p_θ.

Statistical Reasoning with Generative Model



- Key elements to learn generative models include
  1. **Model Class**: A flexible class of $p_\theta(\vec{x})$ reflecting prior knowledge.
  2. **Statistical Distance**: Measure differences between p_n and p_θ.
  3. **Representation**: Infer knowledges with $p_{\theta^*}(\vec{z}|\vec{x})$.

Outline

Examples of Statistical Distances

- Deep generative models learn p_n by minimizing $\mathcal{D}(p_n, p_\theta)$, where $\mathcal{D}$ denotes a statistical distance.
- The effectiveness of $\mathcal{D}$ varies depending on the type of data and the specific algorithm implementation. Each $\mathcal{D}$ necessitates different model classes and corresponding loss functions.
- Popular choices of $\mathcal{D}$ include:
  1. f-divergence
  2. Integral Probability Metric
  3. Wasserstein Distance[2]
  4. Fisher Divergence

[2]Named after "Leonid Vaserštein", though "Wasserstein" is more commonly used in English publications.

Examples of Statistical Distances

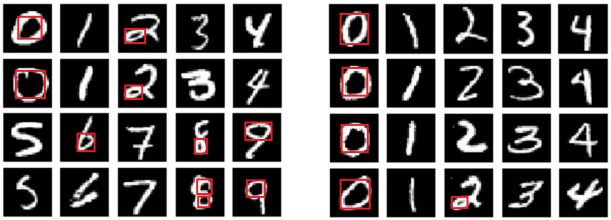
1. f-divergence:

- The f-divergences (Rényi, 1961) are expectations of density ratios mapped by convex functions $f : \mathbb{R}^+ \to \mathbb{R}$, satisfying $f(1) = 0$. They can be expressed as:

$$\mathcal{D}_f(p||q) := \int f\left(\frac{p(\vec{x})}{q(\vec{x})}\right) q(\vec{x})\, d\vec{x} \tag{2}$$

- The $\mathrm{KL}(p_n||p_\theta)$ equals $\mathcal{D}_f(p_n||p_\theta)$ when $f(u) = u \log u$.
  Proof:
  $\mathcal{D}_f(p_n||p_\theta) = \int \Big(p_n(\vec{x})/p_\theta(\vec{x})\Big) \log \Big(p_n(\vec{x})/p_\theta(\vec{x})\Big) p_\theta(\vec{x}) d\vec{x} = \int \log \Big(p_n(\vec{x})/p_\theta(\vec{x})\Big) p_n(\vec{x}) d\vec{x}.$
- Thus, all likelihood maximization methods target minimizing this specific f-divergence.

Examples of Statistical Distances



2. **Integral Probability Metric**: The integral probability metrics (IPMs, Müller, 1997) between distributions are the largest difference between their summary statistics.

- For example, when we use the number of circles in images as summary statistics, the difference is 0.5 (real) − 0.25 (generated) = 0.25.

Image source: MNIST (Deng, 2012)

Examples of Statistical Distances

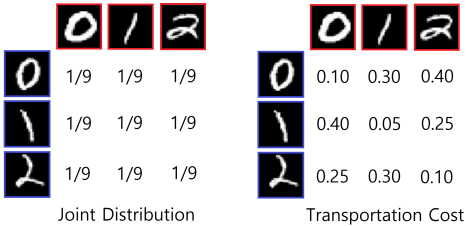
2. **Integral Probability Metric**:

- We can consider many summary statistics together to precisely compare distributions.
- The IPMs can be expressed as:

$$\gamma_{\mathcal{F}}(\mathbb{P}, \mathbb{Q}) := \sup_{f \in \mathcal{F}} \left| \int f(\vec{x})\, d\mathbb{P}(\vec{x}) - \int f(\vec{x})\, d\mathbb{Q}(\vec{x}) \right| \tag{3}$$

  where $\mathcal{F}$ is a class of real-valued functions, and $\mathbb{P}$ and $\mathbb{Q}$ are probability measures.
- Examples of $\mathcal{F}$ include the class of all 1-Lipschitz continuous functions, and functions from reproducing kernel Hilbert space (RKHS).

Examples of Statistical Distances

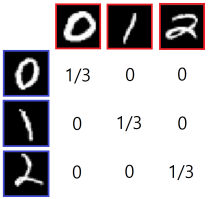


3. **Wasserstein Distance**: Wasserstein distance (Monge, 1781; Kantorovich, 1960) represents the minimum expected transportation cost between two distributions.

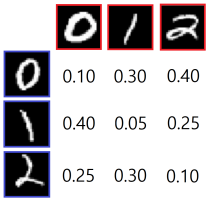
- For example, consider the above joint distribution. The transportation cost is calculated as:

$$
\begin{aligned}
&(1/3) \times \big(0.10 \times (1/3) + 0.30 \times (1/3) + 0.40 \times (1/3)\big) \\
&+ (1/3) \times \big(0.40 \times (1/3) + 0.05 \times (1/3) + 0.25 \times (1/3)\big) \\
&+ (1/3) \times \big(0.25 \times (1/3) + 0.30 \times (1/3) + 0.10 \times (1/3)\big) = 0.24.
\end{aligned}
$$

Examples of Statistical Distances



Joint Distribution



Transportation Cost

3. Wasserstein Distance

- We can consider another joint distribution. The transportation cost is

$$
\begin{aligned}
&(1/3)\big(0.10(1) + 0.30(0) + 0.40(0)\big) \\
&+ (1/3)\big(0.40(0) + 0.05(1) + 0.25(0)\big) \\
&+ (1/3)\big(0.25(0) + 0.30(0) + 0.10(1)\big) = 0.08.
\end{aligned}
$$

Examples of Statistical Distances

3. Wasserstein Distance

- The p-**Wasserstein distance** can be expressed as

$$W_p(\mathbb{P}, \mathbb{Q}; d) := \Big(\inf_{\pi \in \Pi(\mathbb{P}, \mathbb{Q})} \int d^p(\vec{x}, \vec{x}') d\pi(\vec{x}, \vec{x}') \Big)^{1/p} \tag{4}$$

where $p \in [1, \infty)$ and $\Pi(\mathbb{P}, \mathbb{Q})$ is the set of all joint distributions whose marginals are $\mathbb{P}$ and $\mathbb{Q}$.

Examples of Statistical Distances

4. **Fisher Divergence**: Fisher divergence (Johnson, 2004; Hyvärinen, 2005) is the expected difference between the (Stein) scores (Liu et al., 2016)[3] of two distributions. It can be expressed as:

$$\mathrm{FD}(p \parallel q) = \int \left\| \nabla_{\vec{x}} \log p(\vec{x}) - \nabla_{\vec{x}} \log q(\vec{x}) \right\|^2 p(\vec{x})\, d\vec{x}. \tag{5}$$

- It is zero if and only if $p = q$.
  Proof:

$$\nabla_{\vec{x}} \log p(\vec{x}) = \nabla_{\vec{x}} \log q(\vec{x}) \implies p(\vec{x}) = Cq(\vec{x}) \tag{6}$$

  and $C = 1$ because $\int p(\vec{x}) d\vec{x} = \int q(\vec{x}) d\vec{x} = 1$.

[3] The term 'score' here refers to the gradient w.r.t. realizations, which differs from usual terms in parametric family distributions.

Examples of Statistical Distances

4. **Fisher Divergence**: This is a useful measure for learning energy-based models (Teh et al., 2003), such as Boltzmann distributions:

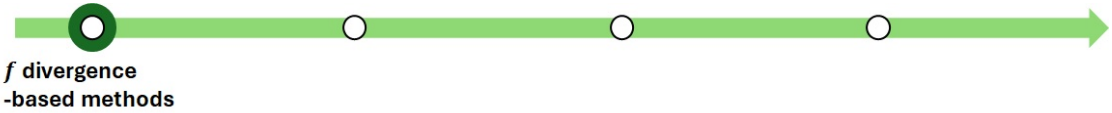
$$p_\theta(\vec{x}) = \frac{1}{C(\theta)} \exp(-E_\theta(\vec{x})) \tag{7}$$

where $C(\theta) := \int \exp(-E_\theta(\vec{x}))\, d\vec{x}$. In this case,

$$\nabla_{\vec{x}} \log p_\theta(\vec{x}) = -\nabla_{\vec{x}} E_\theta(\vec{x}) \tag{8}$$

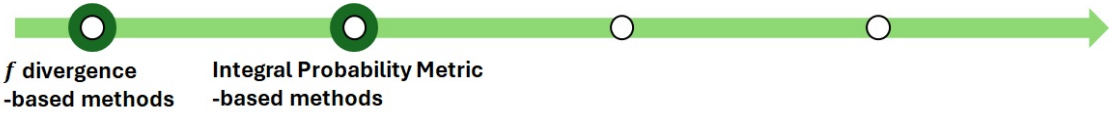
holds, and the normalizing constant disappears.

Chronicle of Deep Generative Model



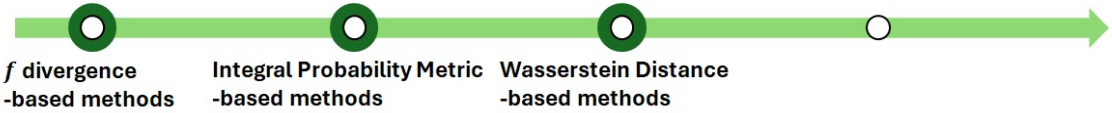
- Variational Autoencoder (VAE, Kingma and Welling, 2014)
- Generative Adversarial Network (GAN, Goodfellow et al., 2014)
- f-GAN (Nowozin et al., 2016)

Chronicle of Deep Generative Model



- Generative Moment Matching Networks (Li et al., 2015)
- Maximum Mean Discrepancy GANs (Li et al., 2017)
- Sobolev GANs (Mroueh et al., 2017)

Chronicle of Deep Generative Model



- Wasserstein GANs (Arjovsky et al., 2017)
- Wasserstein GAN with gradient penalty (Gulrajani et al., 2017)
- Wasserstein Autoencoders (Tolstikhin et al., 2018)

Chronicle of Deep Generative Model

- Noise Conditional Score Networks (Song and Ermon, 2019)
- Denoising Diffusion Probabilistic Models (Ho et al., 2020)

Advanced Topics

- Asymptotic efficiencies according to statistical distances, e.g., minimax convergence rates of IPM-based generative models (Uppal et al., 2019).
- Methods for data domains other than images, e.g., generative pre-trained transformers (GPTs, Radford, 2018) and their variations for language data.
- Advanced graphical models reflecting domain knowledge, e.g., DALL-E (Ramesh et al., 2021) for generating images from text descriptions.

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