Generative AI

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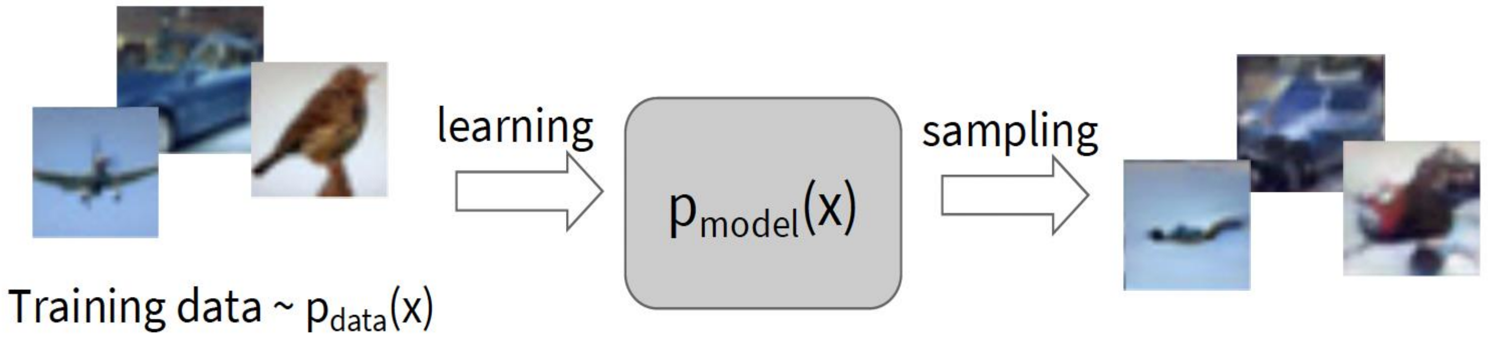
Content

Content

What are Generative Models?

Definition: Generative models learn to generate new data samples resembling a given dataset.



Objectives:

1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
2. Sampling new x from $p_{model}(x)$

Major Generative Models:

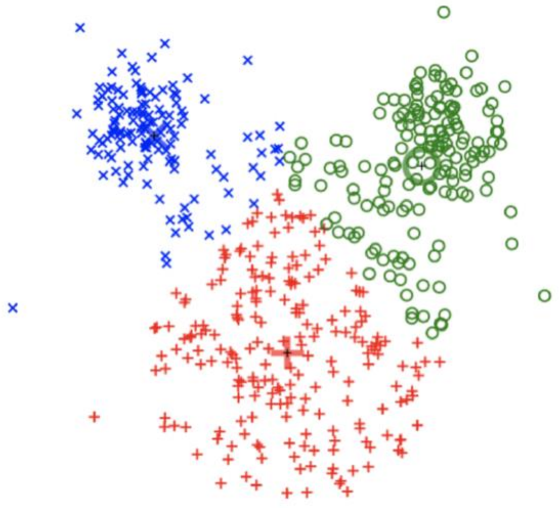
▶ **Explicit Density Models:** Estimate probability distributions (e.g., Gaussian Mixture Models, VAEs).

▶ **Implicit Density Models:** Generate samples without explicit density estimation (e.g., Generative Adversarial Network (GAN)s, Diffusion Models).

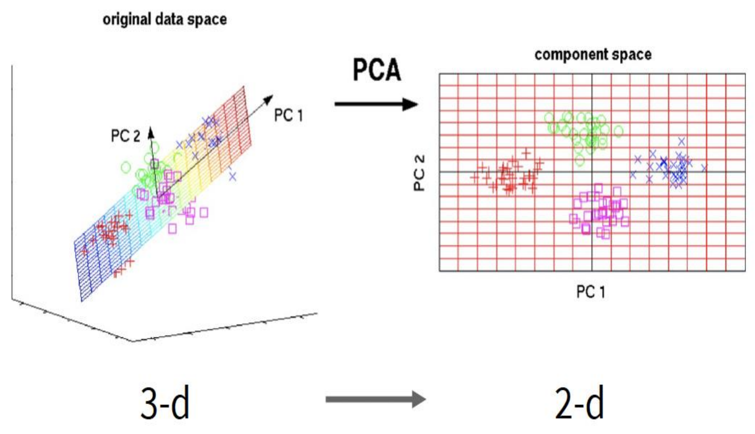
Unsupervised Learning

- **Data:** X — Just data, no labels
- **Goal:** Learn some underlying hidden structure or distribution of the data
- **Examples:** clustering, dimension reduction, feature learning, density estimation, etc.

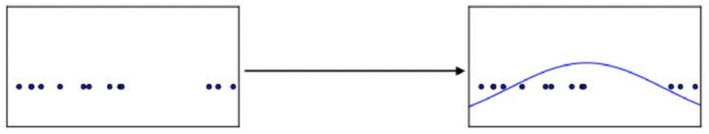
- **Generative models are a subset of unsupervised learning, but not all unsupervised learning techniques are generative (e.g., k-means, PCA)**



K-means clustering



PCA



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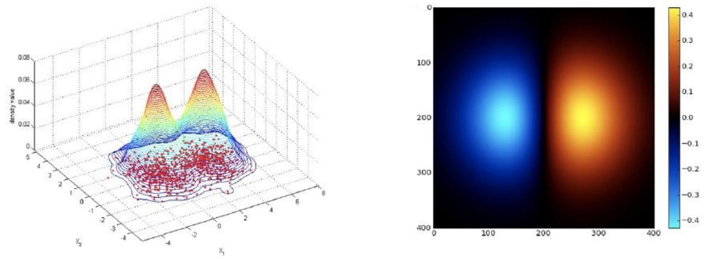
1-d density estimation



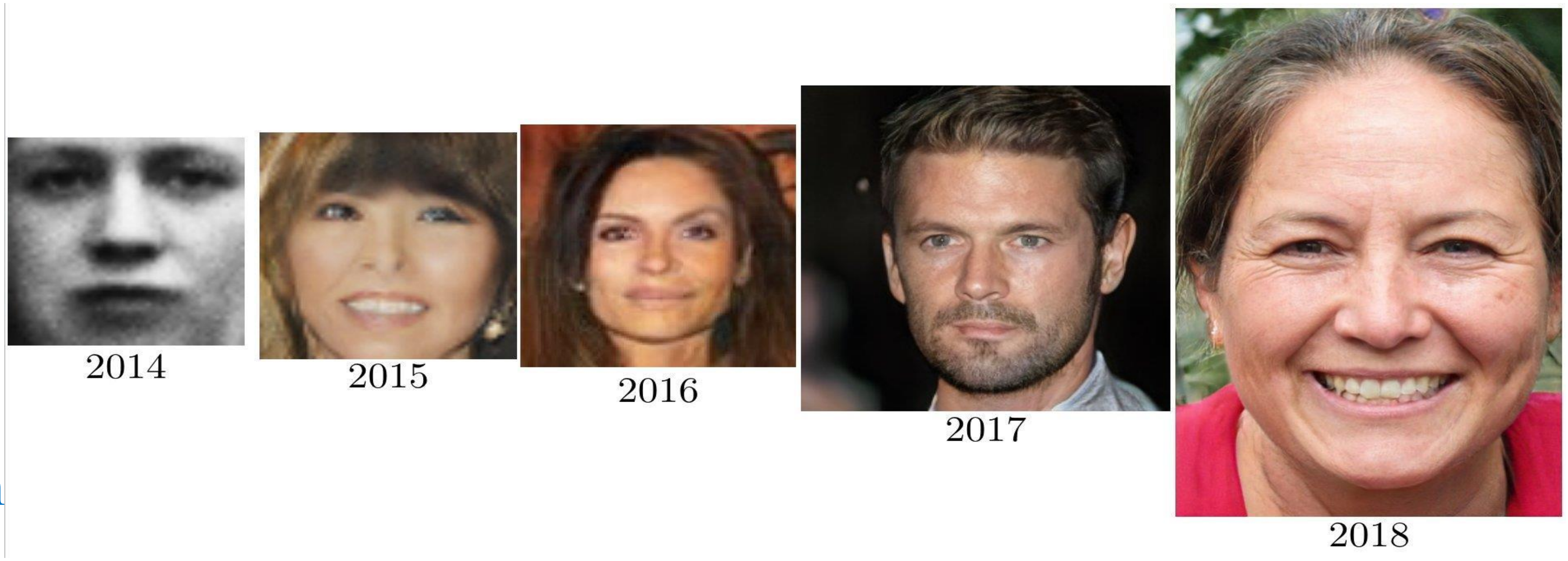
2-d density estimation

Modeling p(x)

2-d density images left and right are CC0 public domain

GenAI on Face Generation

- Better Quality
- High Resolution



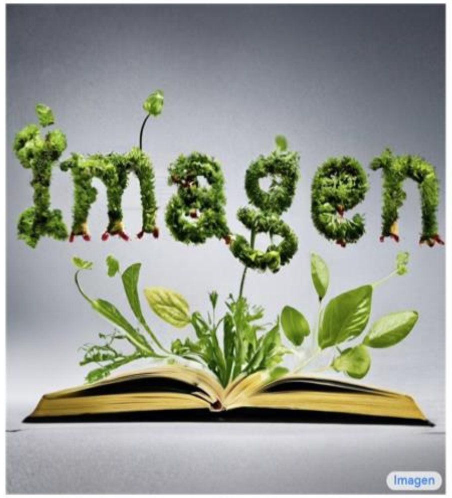
(source)

1024*1024 Images generated by a GAN created by NVIDIA. (source, 2018)

AI Art

Midjourney v5

Emerging Generative Models in 2022-



alphacode
it solutions

Parti
Pathways Autoregressive Text-to-Image Model

DESIGNS.AI

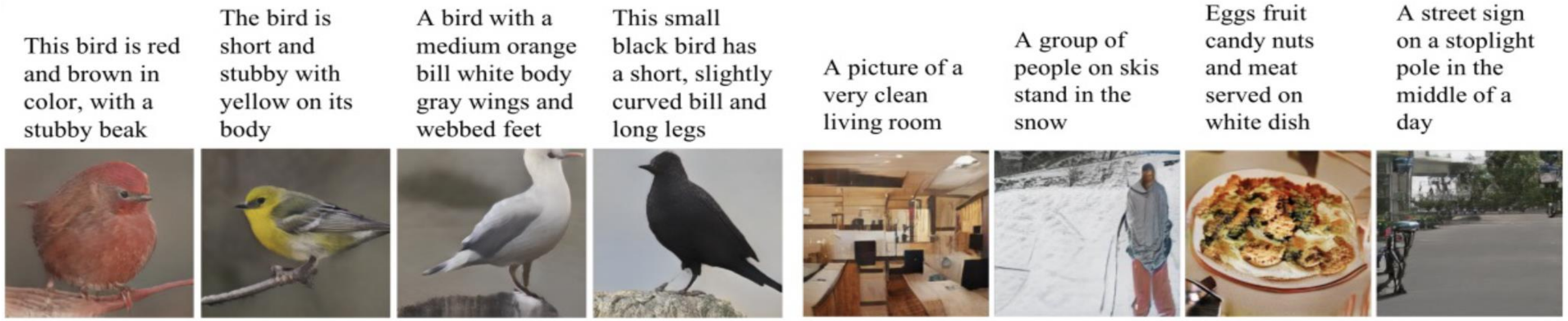
OpenAI
ChatGPT

DALL·E 2

Stable Diffusion

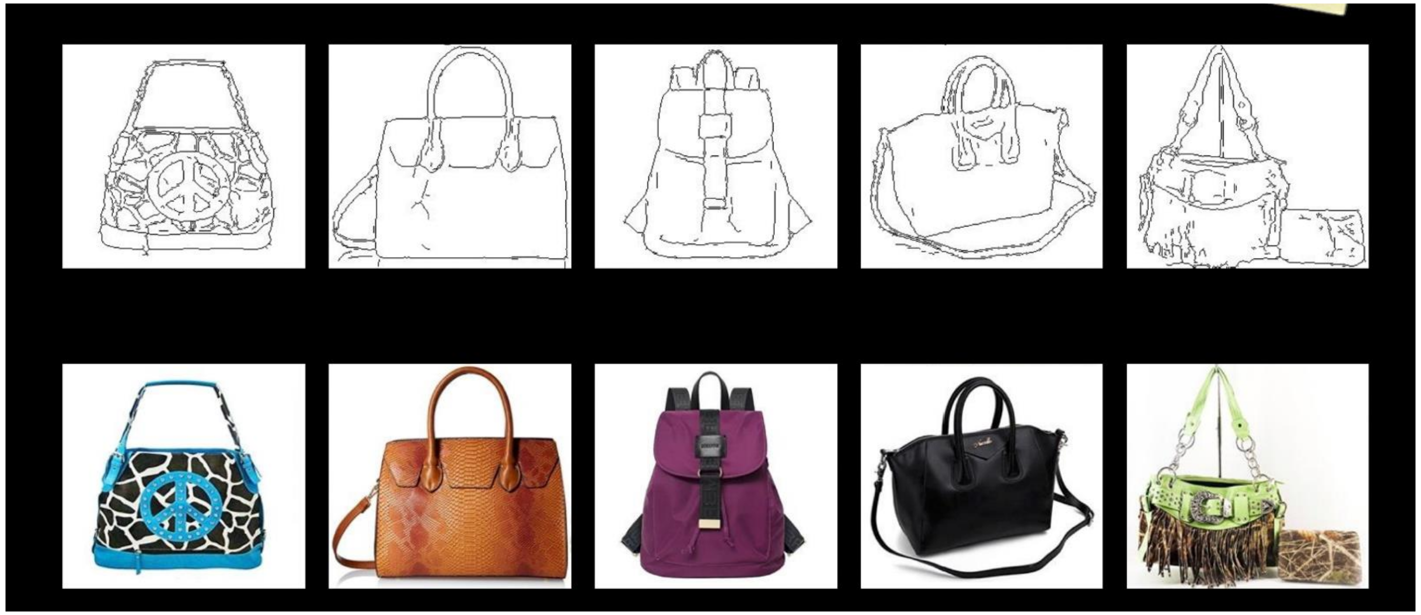
Additional Applications

Text to Image



This bird is red and brown in color, with a stubby beak
The bird is short and stubby with yellow on its body
A bird with a medium orange bill white body gray wings and webbed feet
This small black bird has a short, slightly curved bill and long legs
A picture of a very clean living room
A group of people on skis stand in the snow
Eggs fruit candy nuts and meat served on white dish
A street sign on a stoplight pole in the middle of a day

Fashion Design



Deep Generative Models

Deep generative models are neural network-based models designed to learn complex data distributions and generate realistic synthetic samples that resemble the original training data. These models leverage deep learning to approximate the true underlying data distribution.

Let $X \sim P_X$, where P_X is the distribution of X. Let its density function be p_X.
There are two ways to learn the distribution of X:

- The explicit modeling approach assumes $p_X \in \mathcal{P}_\Theta$, or estimates p_X directly nonparamtrically.
- Generative models learn a generator function $G : \mathbb{R}^m \to \mathbb{R}^p$ such that $G(\eta) \sim P_X$, where $\eta \sim P_\eta$, a known reference distribution.
  - If a generator function G is known, then we know everything about P_X, since we can first sample $\eta \sim P_\eta$, then $G(\eta) \sim P_X$.
  - We usually take the reference distribution to be $N(\mathbf{0}, \mathbf{I}_m)$ or uniform distribution on $[0, 1]^m$.

Taxonomy of Deep Generative Models

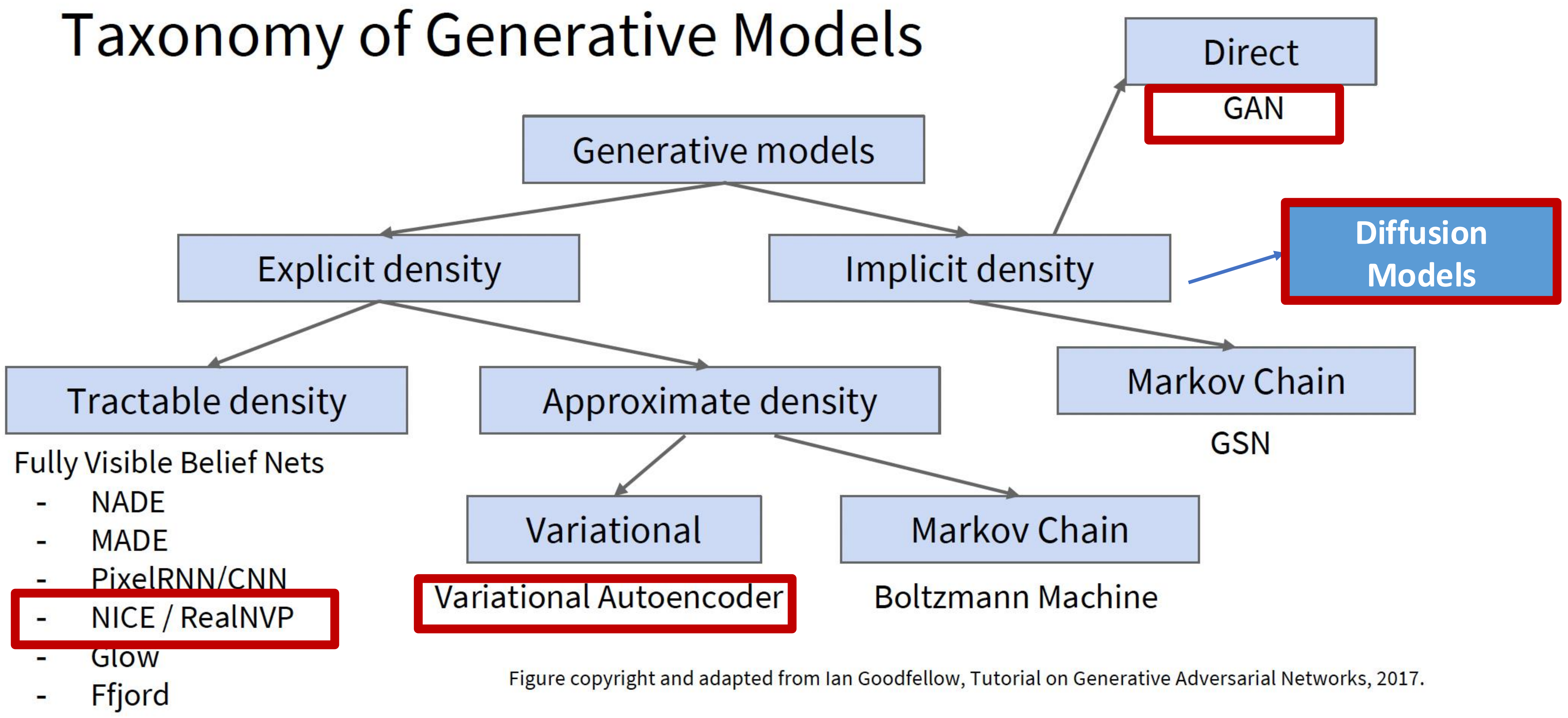


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

The Landscape of Deep Generative Models

Stanford cs231n

Evaluation Metrics

Metric	Measures	Best for	Limitations
Inception Score (IS)	Quality & diversity	Image GANs	Doesn't compare to real data
Fréchet Inception Distance (FID)	Realism & diversity	Image GANs	Requires feature extraction
Precision & Recall	Fidelity & coverage	Any model	Computationally expensive
Log-Likelihood	Probability assignment	VAEs, Flows	Doesn't match human perception
Human Evaluation	Subjective quality	Any model	Expensive and subjective
Downstream Task Performance	Utility in real tasks	Task-driven models	Domain-dependent

Applications of Generative Models in AI

- **Understanding Probability Distributions**
  - Generative models help represent and manipulate high-dimensional probability distributions across various fields.
- **Role in Reinforcement Learning (RL)**
  - Used in model-based RL to simulate possible futures for planning & decision-making.
  - Enables learning in imaginary environments, reducing risks of real-world errors.
  - Guides exploration by tracking visited states & attempted actions.
  - Supports inverse RL for learning from expert demonstrations.
- **Handling Missing Data & Semi-Supervised Learning**
  - Can train with missing data and predict missing inputs.
  - Enables semi-supervised learning, reducing the need for labeled data.
- **Multi-Modal Learning & Sample Generation**
  - Allows multiple correct outputs for a single input (e.g., video frame prediction).
  - GANs excel in generating realistic samples for various AI applications.

Content

What are Autoencoders?

Autoencoders are neural networks designed for dimensionality reduction and feature extraction by compressing and reconstructing data.

They consist of two main components:

❖ **Encoder (e)**: Maps input x to a **low-dimensional latent space** z, where similar inputs have similar latent representations.

$$e: X \rightarrow Z, \quad z = e(x) \quad \text{with } \dim(X) \gg \dim(Z)$$

❖ **Decoder (d)**: Reconstructs x from its latent representation z, mapping back to the original input space.

$$d: Z \rightarrow X \text{ and } \hat{x} = d(z) = d(e(x)).$$

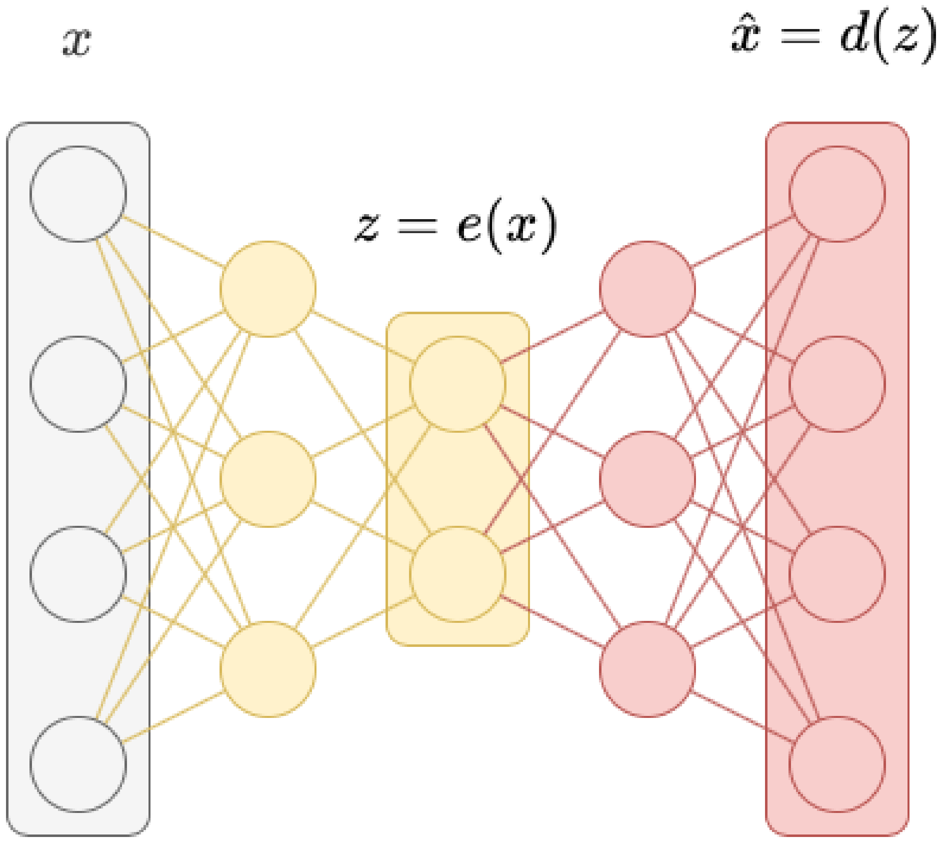
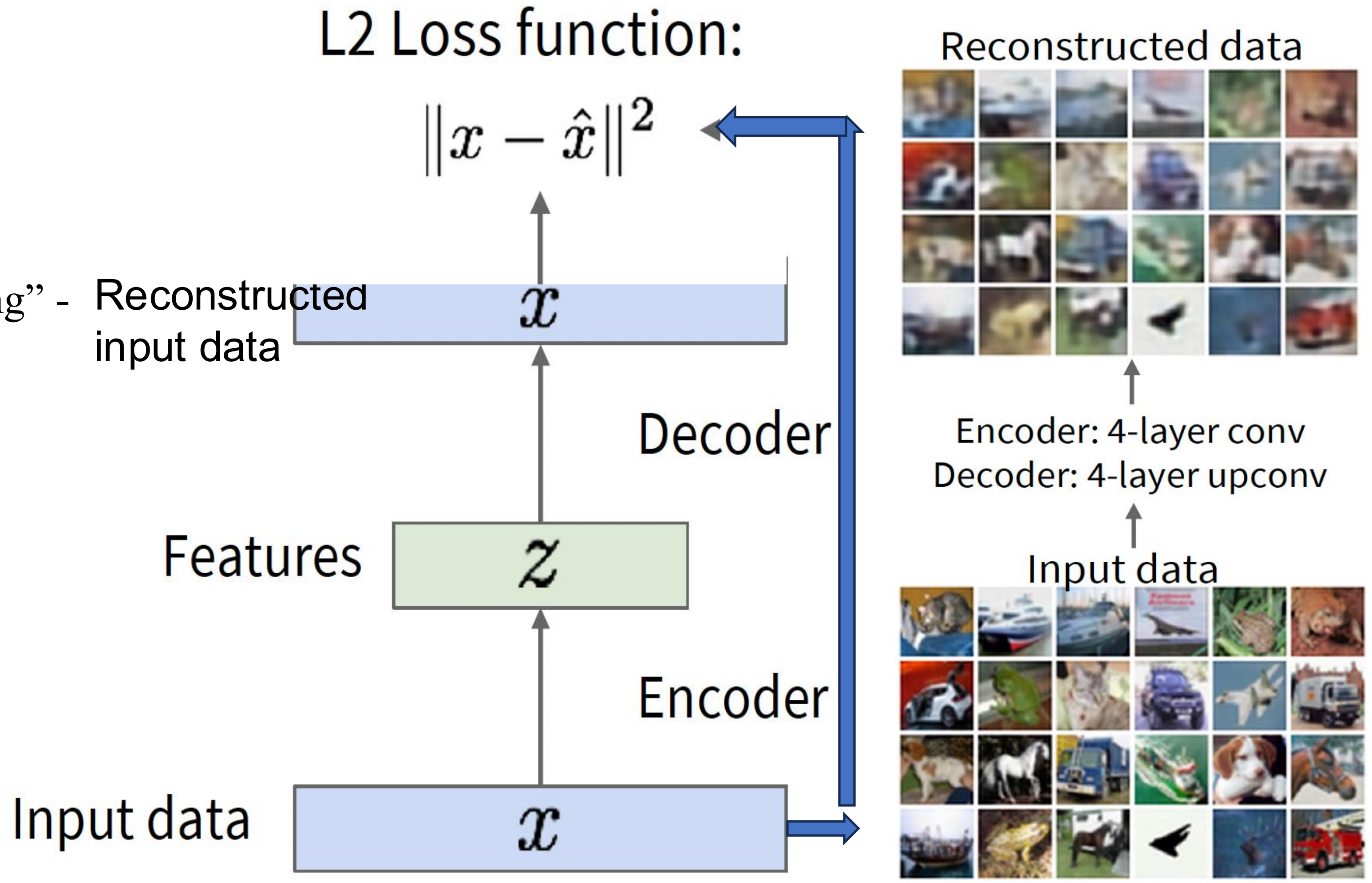


Illustration of autoencoder (source)

What are Autoencoders?

Train such that features can be used to reconstruct original data "Autoencoding" - encoding input itself

Want features to capture meaningful factors of variation in data



Autoencoder Latent Space and Its Limitations

•**Trained on MNIST**, the autoencoder clusters similar digits in the **latent space**.
•**Decoder can reconstruct images** from latent vectors, but gaps in the latent space cause issues.
•**Generative models** aim to produce new samples, but **disjoint latent spaces** in autoencoders make some sampled latent vectors meaningless.
•**Illustration:** In the **top-left corner of the latent space**, unseen regions result in unrealistic reconstructions.
•**Solution: Variational Autoencoders (VAEs)** introduce structured latent spaces to ensure continuity and improve generative performance.
📌 **Key Issue:** Autoencoders are great for representation learning but struggle as generative models due to fragmented latent spaces.

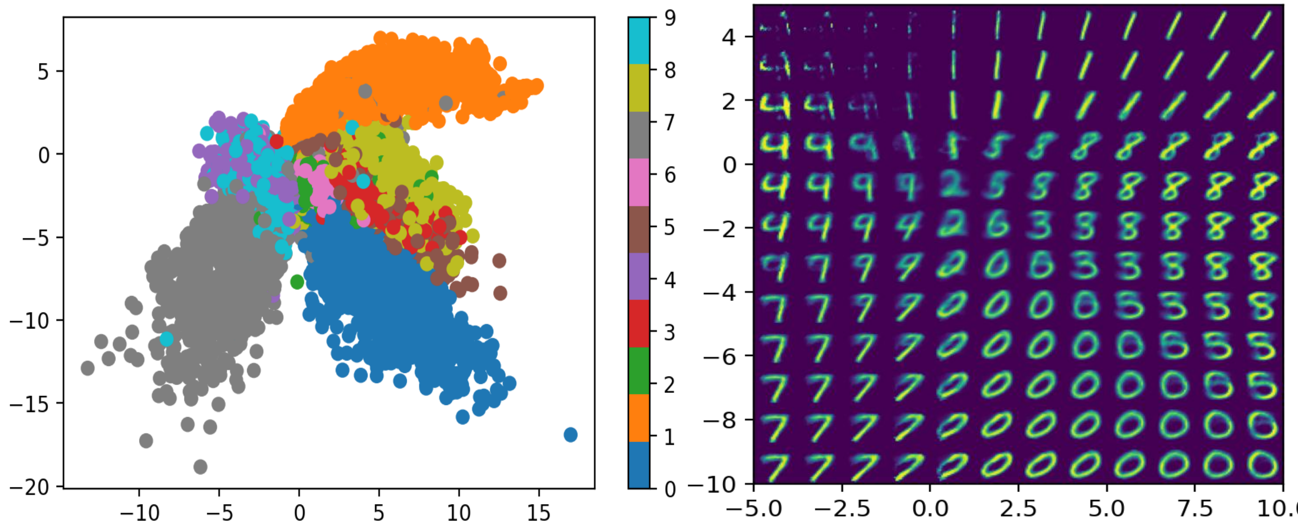


Illustration of example latent vectors using the MNIST dataset (source)

What is a Variational Autoencoder?

📌 **VAE = Autoencoder + Generative Modeling**

- **Same structure as a traditional autoencoder:**
  - ❖ **Encoder:** Compresses input into a latent space representation, but instead of a single point, outputs a probability distribution (Gaussian).
  - ❖ **Decoder:** Samples from this distribution and reconstructs the input.

📌 **Key Difference from Traditional Autoencoders**

❖ Traditional autoencoders map inputs deterministically to a single latent vector z=e(x).

❖ VAEs introduce probabilistic encoding, ensuring smooth and structured latent spaces for better generative performance.

✨ Benefit: Enables meaningful interpolation and sampling for generating new data! 🚀

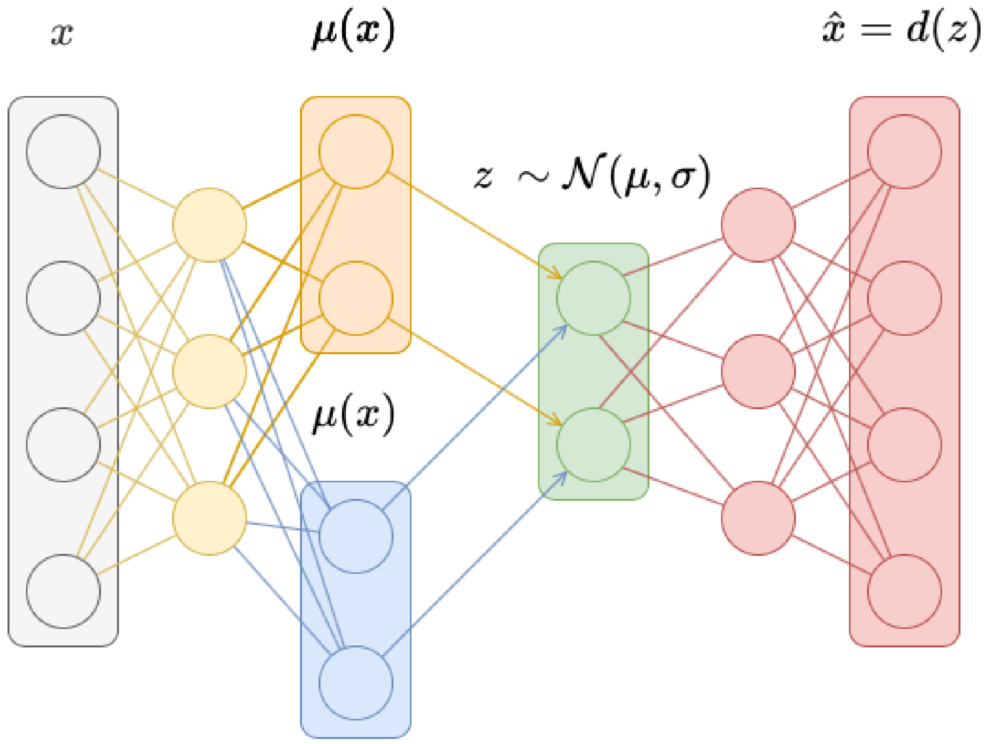


Illustration of VAE (source)

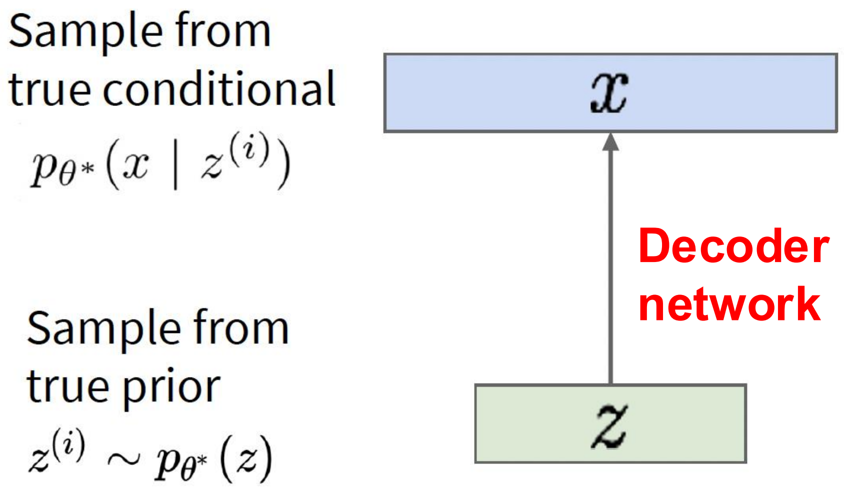
Variational Autoencoder as a DGM

VAEs define an intractable density function with latent

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

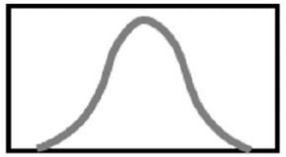
Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation z



Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$
x
Decoder network
Sample from true prior $z^{(i)} \sim p_{\theta^*}(z)$
z

Conditional p(x|z) is complex (generates image) => represent with neural network



Choose prior p(z) to be simple, e.g. Gaussian.

How to train VGE?

Learn model parameters to maximize likelihood of training data

We want to estimate the true parameters of this generative model given training data $\{x^{(i)}\}_{i=1}^{N}$

Q: What is the problem with this?
Intractable!

Data Likelihood

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

$$\log p(x) \approx \log \frac{1}{k} \sum_{i=1}^{k} p(x|z^{(i)}), \text{where } z^{(i)} \sim p(z)$$

Intractable to compute p(x|z) for every z!

Monte Carlo estimation is too high variance

Posterior distribution

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network

$$q_\theta(z|x) \approx p_\theta(z|x)$$

Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

How to approximate VGE?

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Logarithms)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))$$

$\Uparrow$ Decoder network gives pθ(x|z), can compute estimate of this term through sampling (need some trick to differentiate through sampling).

$\Uparrow$ This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$\Uparrow$ pθ(z|x) intractable (saw earlier), can't compute this KL term. But we know KL divergence always >= 0.

How to approximate VGE?

Decoder: reconstruct the input data

Encoder: make approximate posterior distribution. close to prior

$$\log p_\theta(x^{(i)}) = \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}$$

We want to maximize the data likelihood.

Tractable lower bound which we can take gradient of and optimize! (pθ(x|z) differentiable, KL term differentiable)

Variational evidence lower bound (ELBO):

$$\mathcal{L}(x,\theta,\phi) \leq \log p_\theta(x)$$

Training: Maximize lower bound

$$\hat{\theta}, \hat{\phi} = \arg\max_{\theta,\phi} \sum_{i=1}^{n} \mathcal{L}(x_i,\theta,\phi)$$

Stochastic Optimization of ELBO

Algorithm 1: Stochastic optimization of the ELBO. Since noise originates from both the minibatch sampling and sampling of $p(\boldsymbol{\epsilon})$, this is a doubly stochastic optimization procedure. We also refer to this procedure as the *Auto-Encoding Variational Bayes* (AEVB) algorithm.

```
Data:
    $\mathcal{D}$: Dataset
    $q_\phi(\mathbf{z}|\mathbf{x})$: Inference model
    $p_\theta(\mathbf{x}, \mathbf{z})$: Generative model
Result:
    $\theta, \phi$: Learned parameters
$(\theta, \phi) \leftarrow$ Initialize parameters
while SGD not converged do
    $\mathcal{M} \sim \mathcal{D}$ (Random minibatch of data)
    $\boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon})$ (Random noise for every datapoint in $\mathcal{M}$)
    Compute $\tilde{\mathcal{L}}_{\theta,\phi}(\mathcal{M}, \boldsymbol{\epsilon})$ and its gradients $\nabla_{\theta,\phi}\tilde{\mathcal{L}}_{\theta,\phi}(\mathcal{M}, \boldsymbol{\epsilon})$
    Update $\theta$ and $\phi$ using SGD optimizer
end
```

$$\mathcal{L}_{\theta,\phi}(\mathbf{x}) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})\right]$$

$$\nabla_\theta \mathcal{L}_{\theta,\phi}(\mathbf{x}) = \nabla_\theta \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})\right]$$

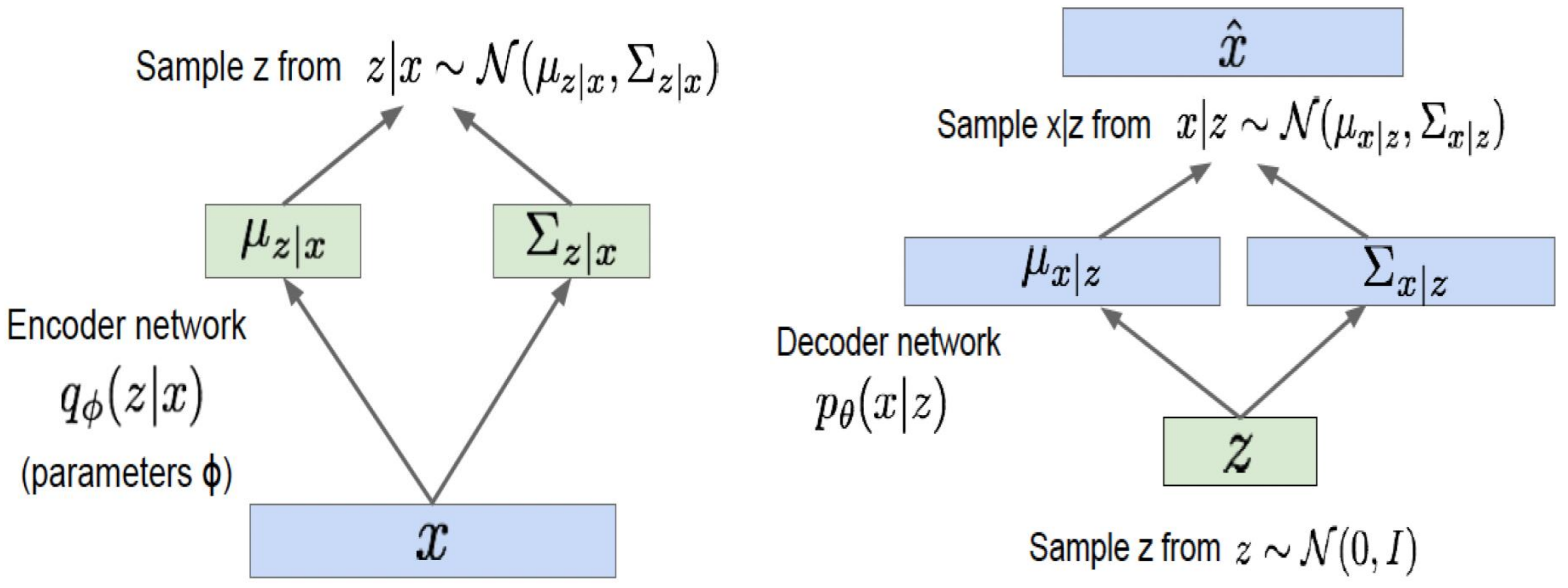
$$\nabla_\phi \mathcal{L}_{\theta,\phi}(\mathbf{x}) = \nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}, \mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})\right]$$

Reparametrization Trick: $\mathbf{z} = \mathbf{g}(\boldsymbol{\epsilon}, \phi, \mathbf{x})$

$$\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[f(\mathbf{z})\right] = \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[f(\mathbf{z})\right]$$

$$\begin{aligned}\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[f(\mathbf{z})\right] &= \nabla_\phi \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[f(\mathbf{z})\right] \\ &= \mathbb{E}_{p(\boldsymbol{\epsilon})}\left[\nabla_\phi f(\mathbf{z})\right] \\ &\simeq \nabla_\phi f(\mathbf{z})\end{aligned}$$

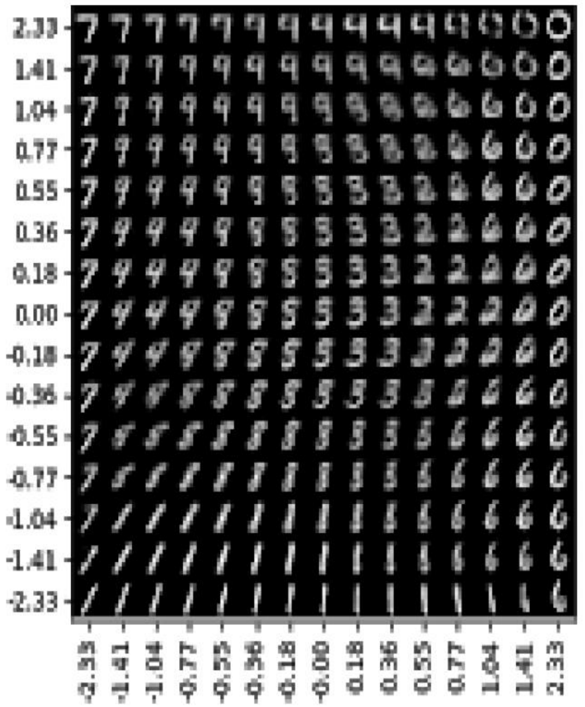
A Theoretical Example

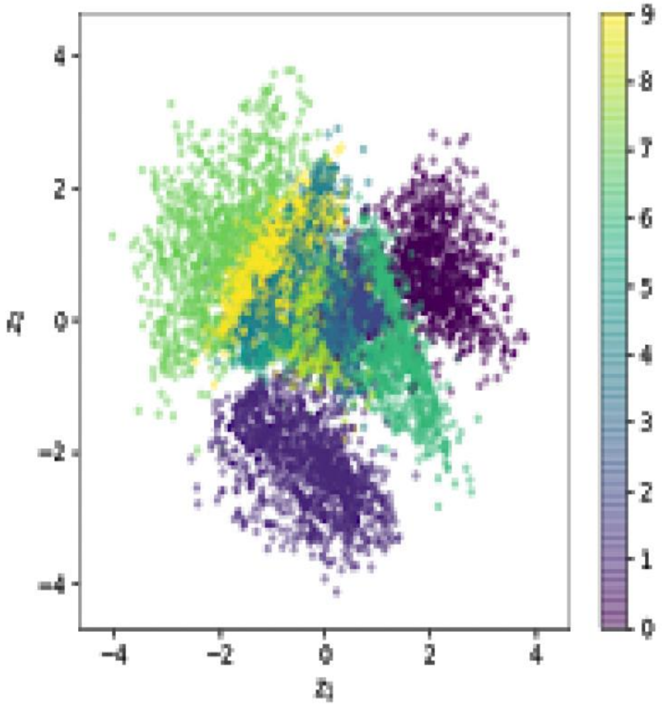

Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$
$\mu_{z|x}$
$\Sigma_{z|x}$
Encoder network
$q_\phi(z|x)$
(parameters ϕ)
x
$\hat{x}$
Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$
$\mu_{x|z}$
$\Sigma_{x|z}$
Decoder network
$p_\theta(x|z)$
z
Sample z from $z \sim \mathcal{N}(0, I)$

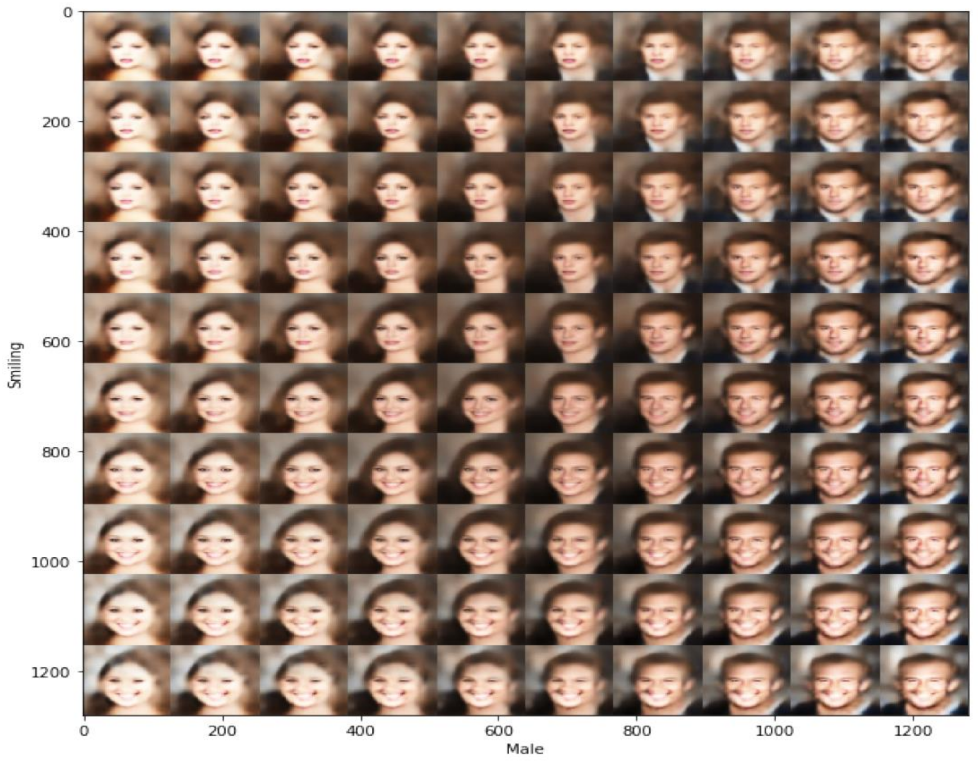
$$\int q_{\boldsymbol{\theta}}(\mathbf{z}) \log p(\mathbf{z})\, d\mathbf{z} = \int \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2) \log \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})\, d\mathbf{z}$$
$$= -\frac{J}{2}\log(2\pi) - \frac{1}{2}\sum_{j=1}^{J}(\mu_j^2 + \sigma_j^2)$$

$$\log p(\mathbf{x}|\mathbf{z}) = \log \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2\mathbf{I})$$
$$\text{where } \boldsymbol{\mu} = \mathbf{W}_4\mathbf{h} + \mathbf{b}_4$$
$$\log \boldsymbol{\sigma}^2 = \mathbf{W}_5\mathbf{h} + \mathbf{b}_5$$
$$\mathbf{h} = \tanh(\mathbf{W}_3\mathbf{z} + \mathbf{b}_3)$$

Real Examples







Strengths & Limitations

📌 **Key Idea:**

- ➢ Adds a probabilistic spin to traditional autoencoders, enabling data generation.
- ➢ Defines an intractable density, requiring variational inference to derive and optimize a lower bound (ELBO).

📌 **Pros:**

✓ Principled generative approach based on probabilistic modeling.

✓ Interpretable latent space enables meaningful structure in representations.

✓ Inference of q(z|x) allows feature extraction for other tasks.

📌 **Cons:**

❌ Optimizes a lower bound on likelihood, which may not be an ideal evaluation metric.

❌ Lower sample quality compared to PixelRNN/PixelCNN.

❌ Blurry reconstructions compared to GANs, which generate sharper images.

📌 **Active Research Areas:**

🔷 Flexible Approximate Posteriors: Moving beyond diagonal Gaussian assumptions to richer models like Gaussian Mixture Models (GMMs) or Categorical Distributions.

🔷 Disentangled Representations: Learning independent latent factors for better interpretability.

🔷 Improving Training Objectives: Hybrid models incorporating adversarial learning (VAE-GANs).

🚀 **Future Directions**: Enhancing sample quality while retaining VAE’s structured latent space!

Content

“This (GANS), and the variations that are now being proposed is the most interesting idea in the last 10 years in ML, in my opinion”

–Yann LeCun

What is GAN?

Problem:

❖ We want to sample from a complex, high-dimensional training distribution.

❖ There is no direct way to explicitly learn or model the data distribution.

Solution:

➢ Instead of learning the distribution explicitly, GANs learn a transformation.

➢ Start by sampling from a simple distribution (e.g., Gaussian noise).

➢ Train a neural network to transform the simple distribution into the training data distribution.

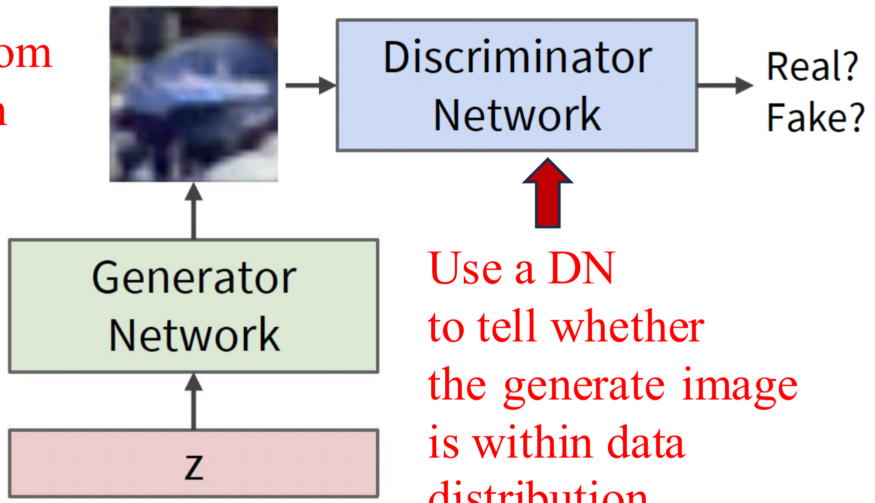
Key Idea:

✓ GANs learn to generate new samples indirectly through adversarial training.

✓ The model never explicitly estimates the probability density function of the data.

Objective: generated images should look "real"

Output: Sample from training distribution



Use a DN to tell whether the generate image is within data distribution ("real") or not

Input: Random noise

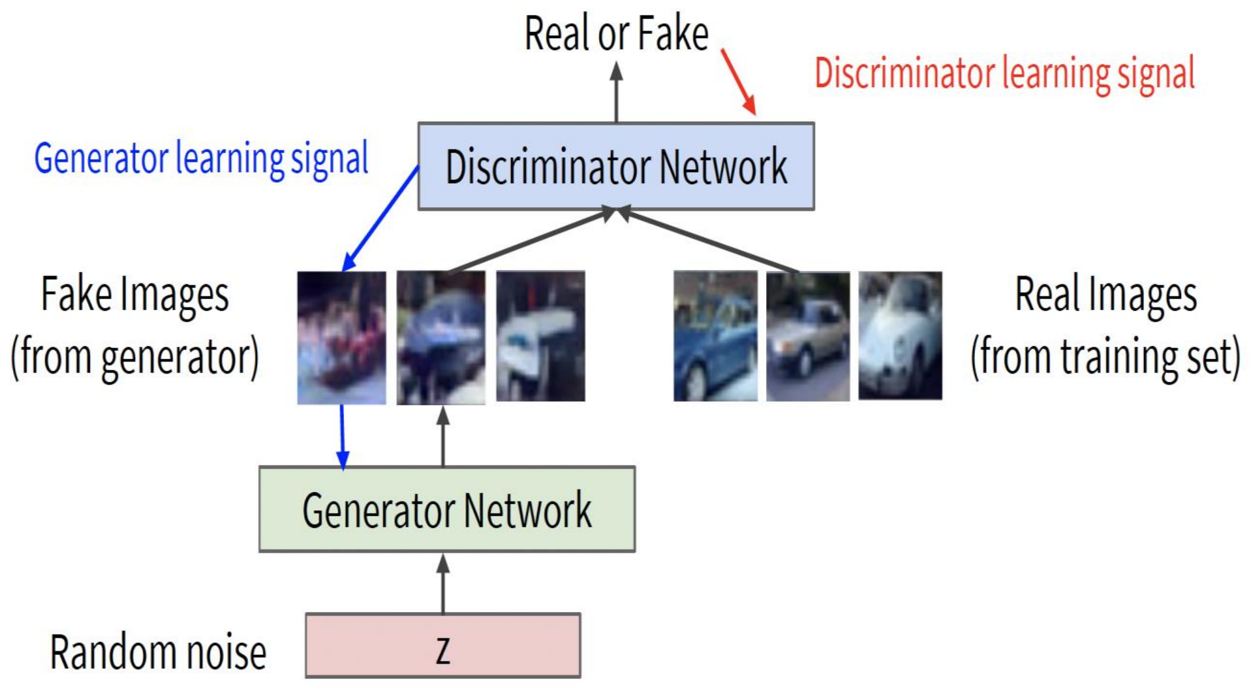
Generative Vs Discriminative Models

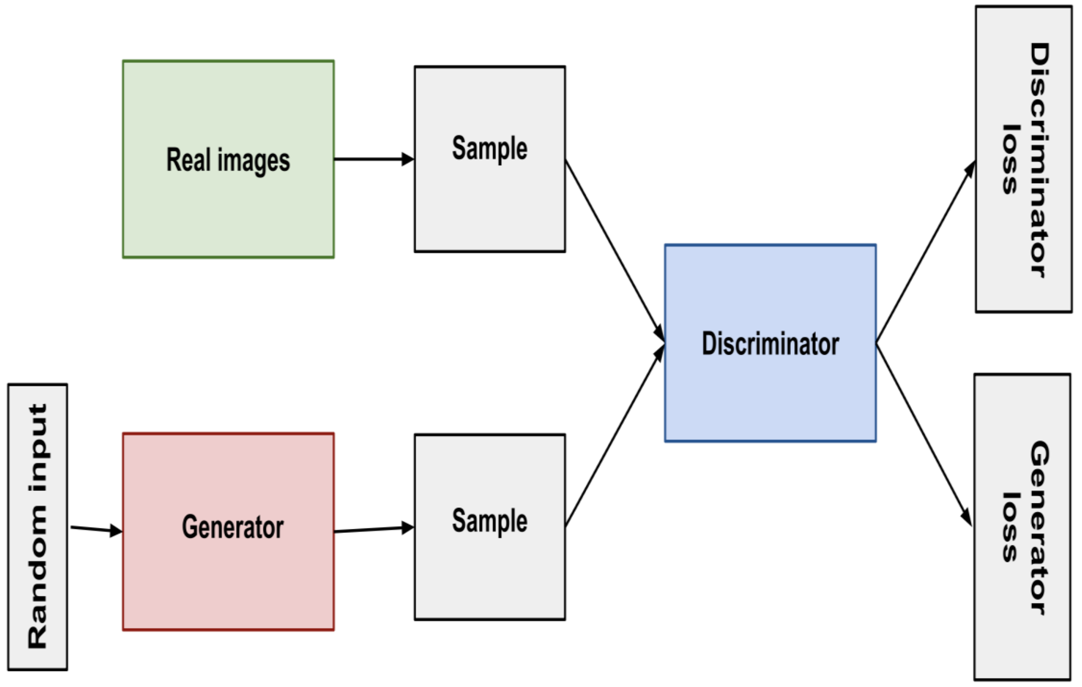
Generative Models:

- Can generate new data samples resembling real data.
- Example: GANs generate realistic images that resemble real ones.

Discriminative Models:

- Focus on classification by distinguishing between different categories.
- Example: A decision tree can classify dogs and cats but cannot generate them.


Real or Fake
Discriminator learning signal
Generator learning signal
Discriminator Network
Fake Images (from generator)
Real Images (from training set)
Generator Network
Random noise
z



Overview of GAN Training

Discriminator Network: Tries to distinguish between real and fake images.
Generator Network: Tries to fool the discriminator by generating real-looking images.
Training Process: Both networks are trained jointly in a minimax game.

Minimax objective function:

$$\underset{\substack{\uparrow \\ \text{Generator objective}}}{\min_{\theta_g}} \ \underset{\substack{\uparrow \\ \text{Discriminator objective}}}{\max_{\theta_d}} \left[\mathbb{E}_{x\sim p_{data}} \log \underbrace{D_{\theta_d}(x)}_{\text{Discriminator output for real data x}} + \mathbb{E}_{z\sim p(z)} \log(1 - \underbrace{D_{\theta_d}(G_{\theta_g}(z))}_{\text{Discriminator output for generated fake data G(z)}})\right]$$

- **Discriminator** (θ_d) wants to maximize the objective such that $D(x) \approx 1$ (real) and $D(G(z)) \approx 0$ (fake).
- **Generator** (θ_g) wants to minimize the objective such that $D(G(z)) \approx 1$ (fooling the discriminator).

GAN Training

Alternate between:

1. Gradient ascent on discriminator

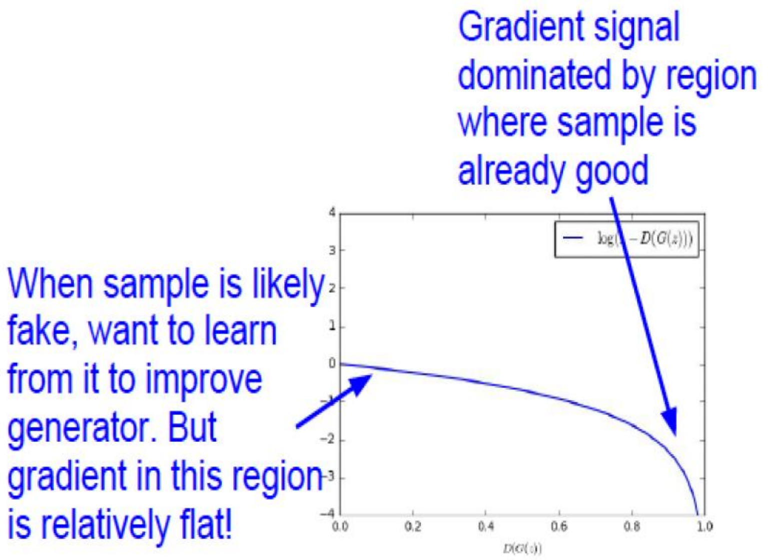
$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

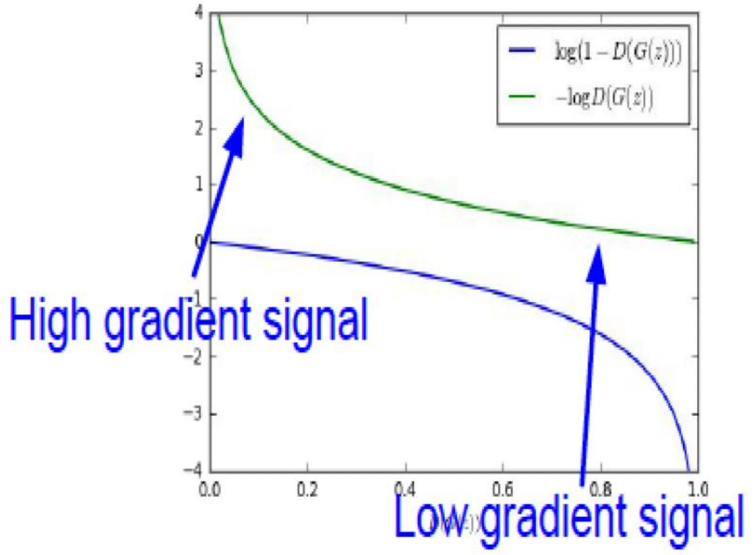
2. Gradient descent on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

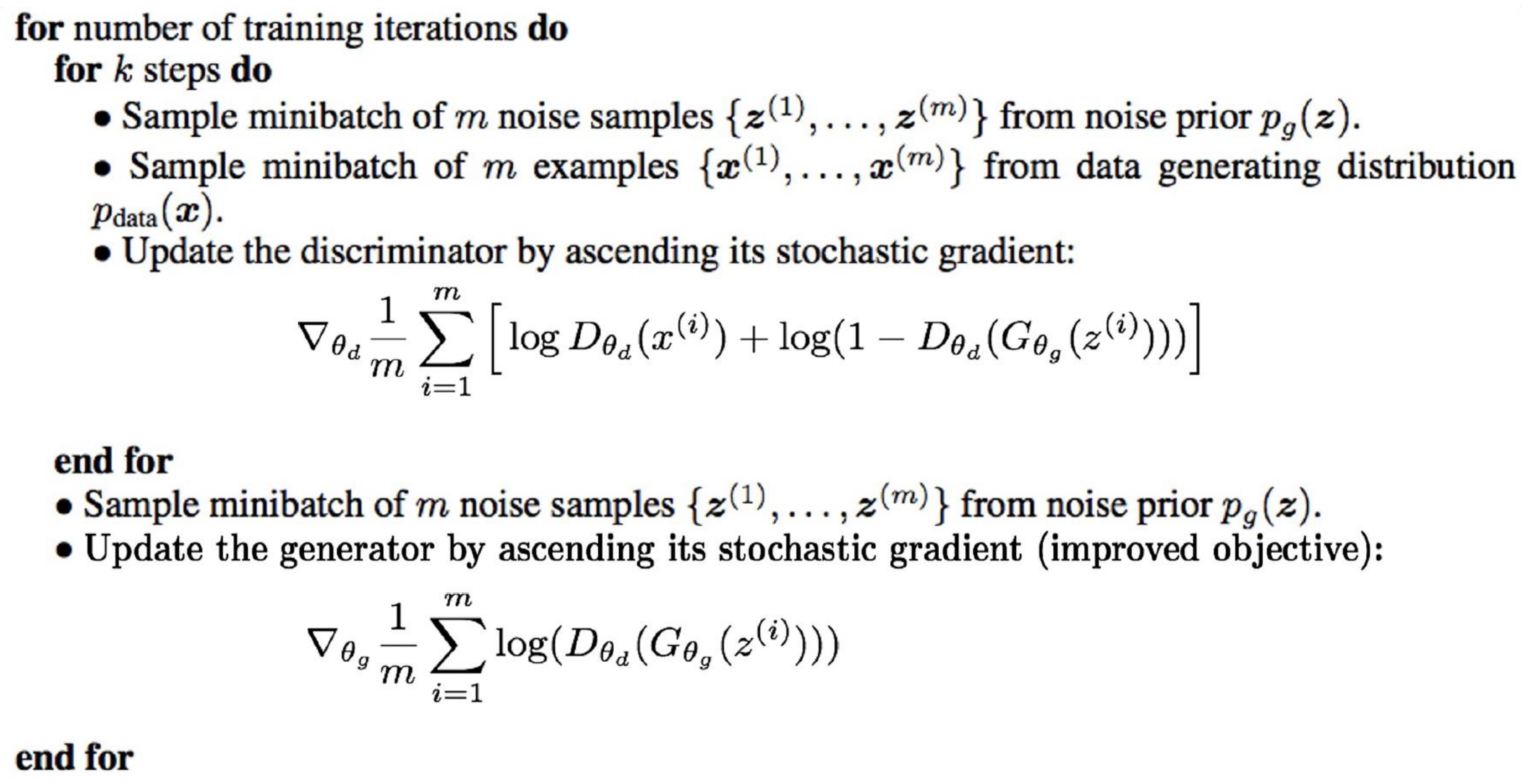
Instead: Consider a different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$





GAN Algorithms



```
for number of training iterations do
    for $k$ steps do
        • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
        • Sample minibatch of $m$ examples $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ from data generating distribution
        $p_{\text{data}}(\boldsymbol{x})$.
        • Update the discriminator by ascending its stochastic gradient:
            $\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[ \log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$
    end for
    • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
    • Update the generator by ascending its stochastic gradient (improved objective):
        $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$
end for
```

Alternating Training for GANs

GAN Training Process (Alternating Phases):

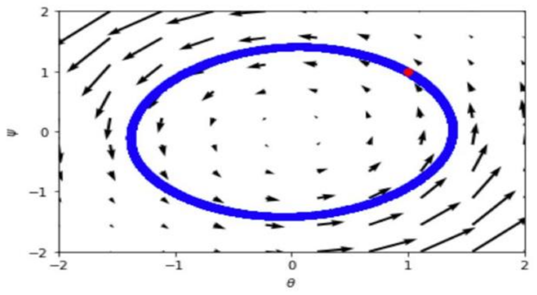
1. Discriminator Training: Trains for one or more epochs while the generator remains unchanged. It learns to differentiate real from generated data, adapting to the generator’s flaws.
2. Generator Training: Trains for one or more epochs while the discriminator remains unchanged. This prevents the generator from chasing a moving target.

Training Dynamics:

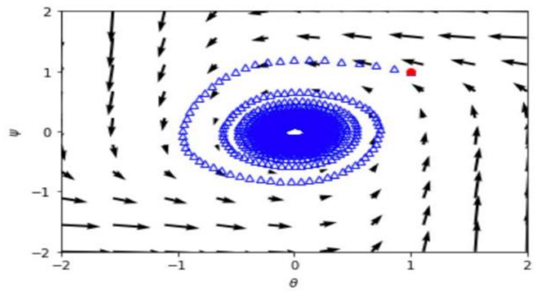
- ❖ As the generator improves, the discriminator struggles to distinguish real from fake data.
- ❖ A perfect generator results in a discriminator with 50% accuracy (random guessing).
- ❖ Overtraining can degrade performance, leading to unstable convergence where the generator receives meaningless feedback.

Challenges in GAN Training

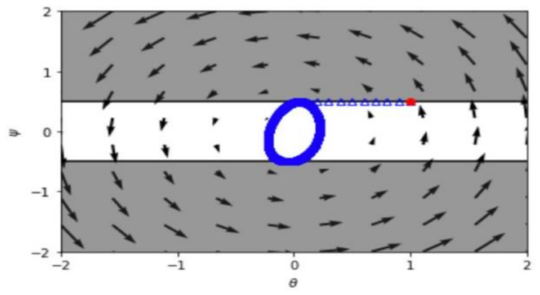
- **Hyperparameter Sensitivity:** GANs are sensitive to learning rates, batch sizes, and architectural choices.
- **Mode Collapse:** The generator produces limited diversity.
- **Training Instability:** The minimax optimization is difficult to balance.
- **Vanishing/Exploding Gradients:** The discriminator can become too strong or weak, leading to poor gradients.
- **Non-Convergence:** The model oscillates instead of converging.



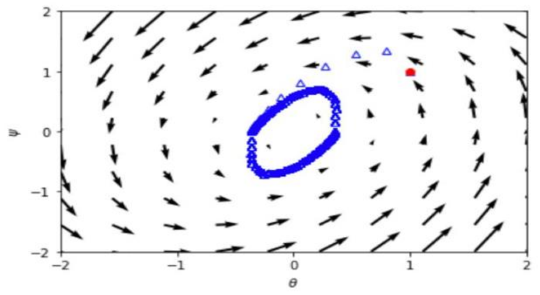
(a) Standard GAN



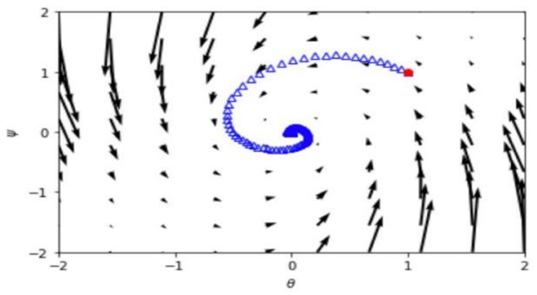
(b) Non-saturating GAN



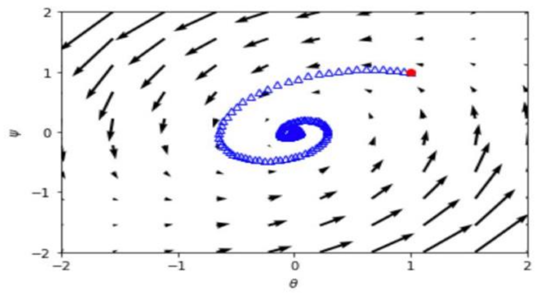
(c) WGAN ($n_d = 5$)



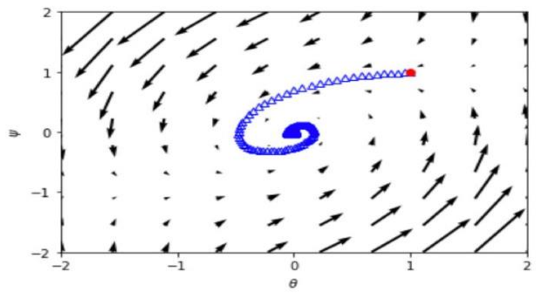
(d) WGAN-GP ($n_d = 5$)



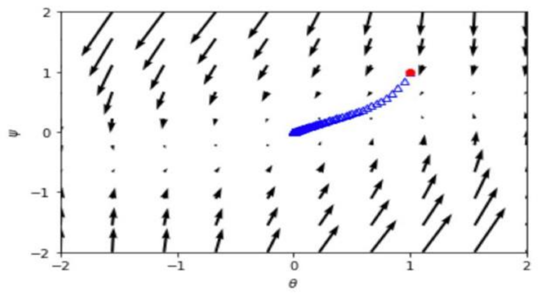
(e) Consensus optimization



(f) Instance noise



(g) Gradient penalty



(h) Gradient penalty (CR)

Hyperparameter Sensitivity

1. Adjust Learning Rates Carefully

- ❖ **Learning Rate (α)**: Too high → instability, Too low → slow convergence.
- ❖ **Two-Timescale Update Rule (TTUR)**: Use a smaller learning rate for the generator than the discriminator to balance training.

2. Tune Adam Hyperparameters

- ➢ Standard settings **(β1=0.9, β2=0.999)** can lead to oscillations.
- ➢ For **GANs**, reducing β1 to **0.5** improves stability.

3. Normalize Inputs and Use Spectral Normalization

- ✓ Normalize training images between **[−1,1]** instead of [0,1] (for Tanh activation).
- ✓ Use **Spectral Normalization** on the discriminator to control weight magnitudes.

4. Improve Loss Functions

- o **Wasserstein Loss (WGAN)**: Uses Earth-Mover distance for better gradient behavior.
- o **Gradient Penalty (WGAN-GP)**: Adds stability and prevents exploding gradients:

5. Use Progressive Training

- ❑ **Start with low-resolution images**, gradually increasing resolution (used in **Progressive Growing GANs**).
- ❑ Helps GAN **learn simple features first** before complex details.

Hyperparameter Sensitivity

6. Apply Regularization Techniques

•**Batch Normalization**: Helps control variance, but can cause mode collapse in GANs.
•**Instance Normalization**: Often more stable than batch normalization.
•**Dropout in Discriminator**: Helps prevent overfitting.

7. Monitor Convergence and Use Early Stopping

•**Track GAN metrics** (FID, Inception Score) instead of just loss values.
•**Avoid overtraining**: If the discriminator gets too strong, **freeze it temporarily**.

8. Use Larger Batch Sizes

•GANs often benefit from **larger batch sizes** (e.g., 128–512) to stabilize updates.
•**Gradient accumulation** can be used if GPU memory is limited.

9. Data Augmentation

•**Apply transformations (rotation, flipping, color jitter)** to make training more robust.
•Prevents the discriminator from memorizing training data.

10. Experiment with Alternative Architectures

•**Self-Attention GANs (SAGAN)**: Improves global structure modeling.
•**BigGAN**: Uses **larger batch sizes** and **orthogonal regularization** for stability.

Mode Collapse

Mode Collapse in GANs refers to a common failure mode where the **generator** fails to capture the full diversity of the data distribution and produces **limited variations** of samples. Instead of generating a wide range of outputs, it collapses to generating a few or even a single type of sample repeatedly.

Why Does Mode Collapse Occur?

- ❖ **Imbalanced Generator-Discriminator Learning**
- ❖ **Training Instability**
- ❖ **Lack of Diversity-Promoting Mechanisms**

1.

Effects of Mode Collapse

- ❖ **Reduced Sample Diversity** → Poor representation of the real dataset.
- ❖ **Low-Quality Generation** → Outputs look repetitive and lack variety.
- ❖ **Unreliable Model** → The generator fails to generalize.

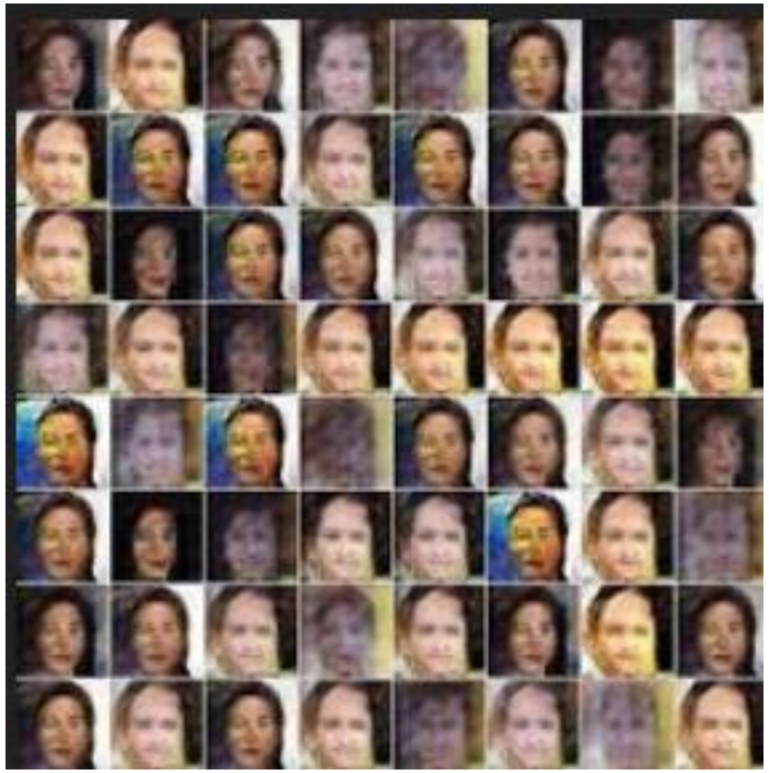


Illustration of example monotonous output. (source)

Techniques to Mitigate Mode Collapse

1. **Minibatch Discrimination**

   Encourages diversity by comparing samples in each batch.

2. **Feature Matching**

   Instead of just fooling the discriminator, the generator learns to match feature statistics of real data.

3. **Wasserstein GAN (WGAN)**

   Uses the Earth Mover (Wasserstein) distance to **stabilize training** and avoid collapsing to few modes.

4. **Unrolled GANs**

   Allows the generator to anticipate discriminator updates, preventing it from getting stuck in mode collapse.

5. **Mutual Information Regularization**

   Forcing the generator to learn **meaningful latent representations** that generate diverse outputs.

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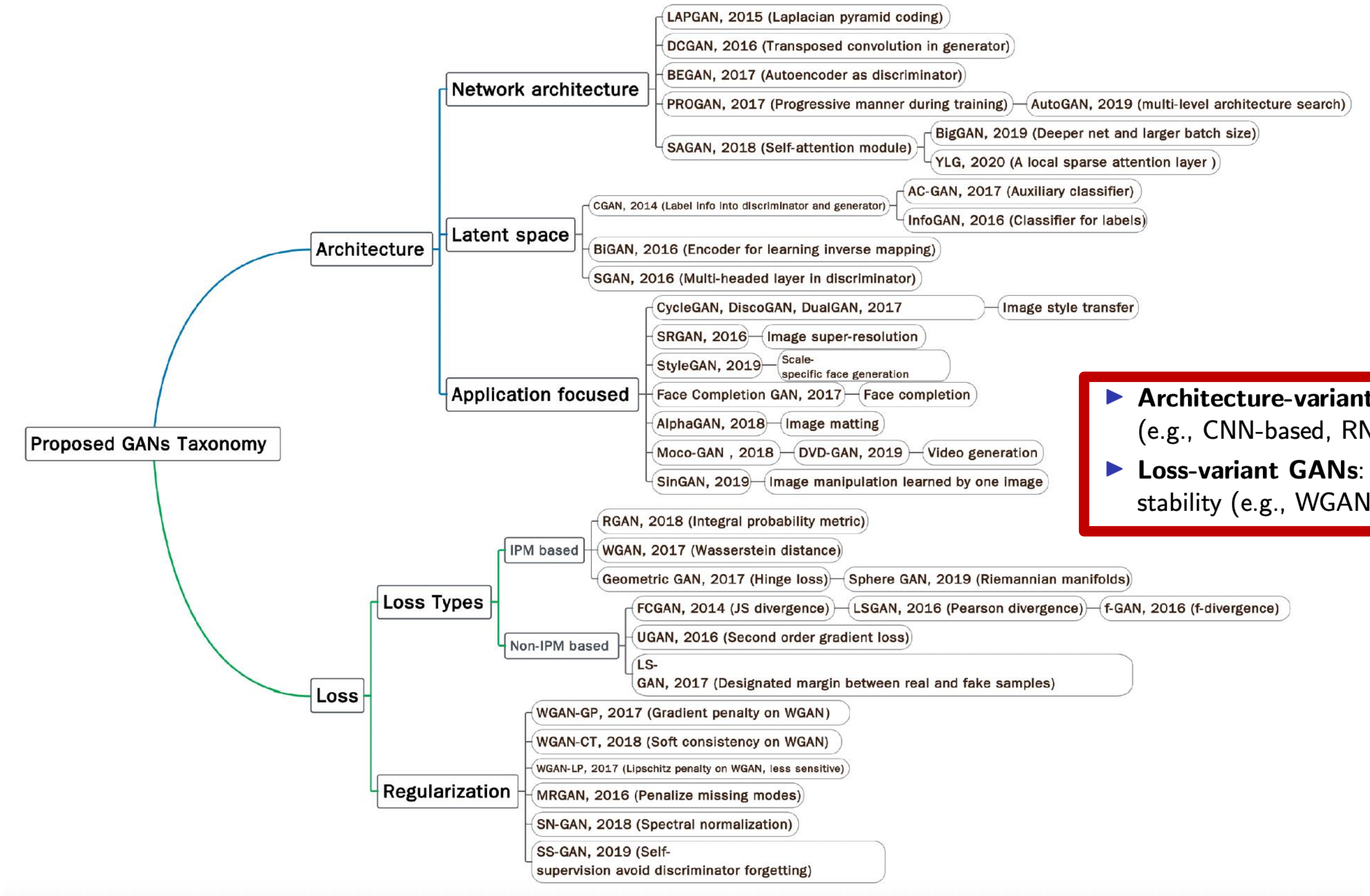
More details of example GAN suffering mode collapse: https://neptune.ai/blog/gan-failure-modes

The taxonomy of the recent GANs

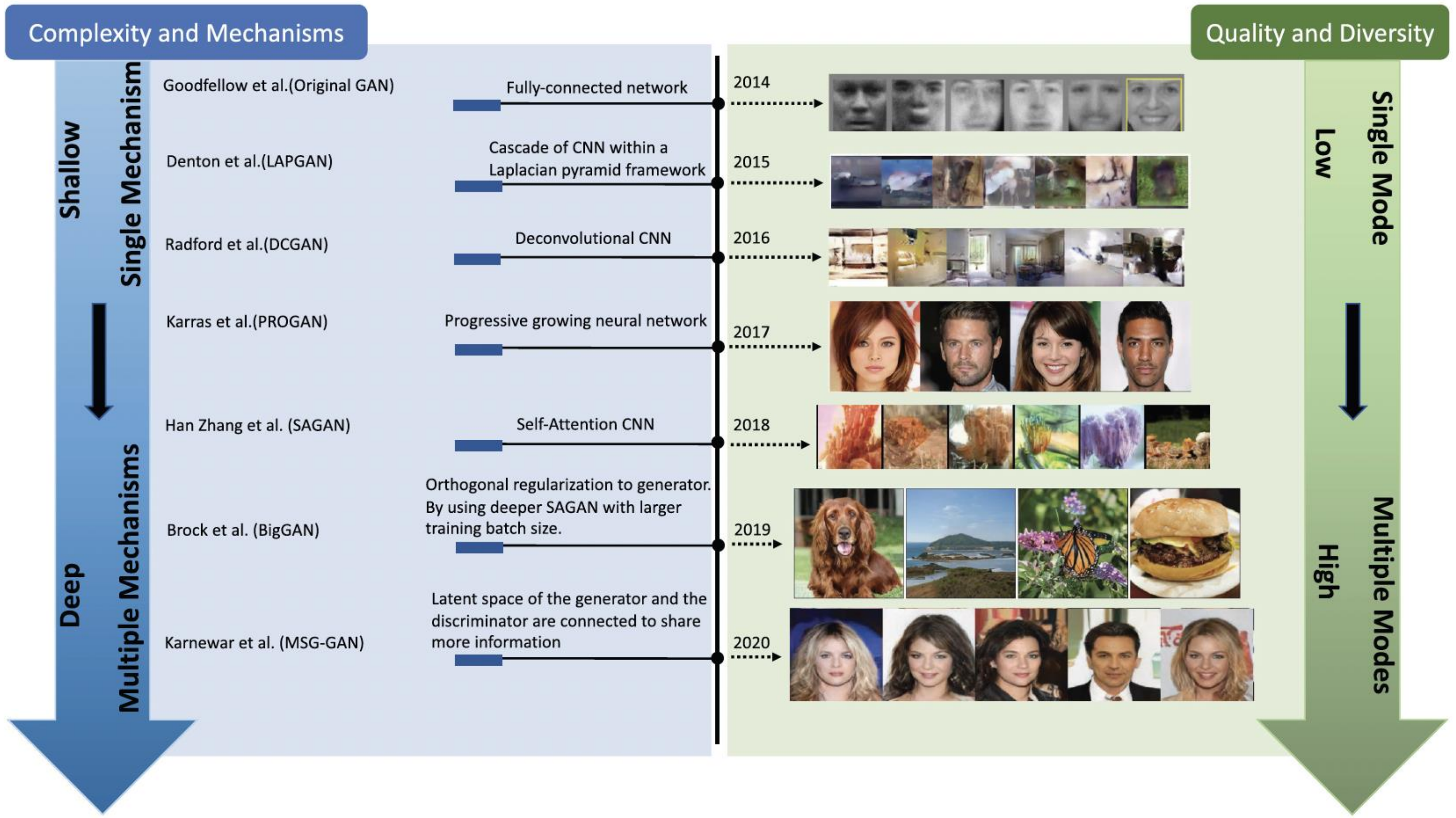

Proposed GANs Taxonomy
Architecture
Network architecture
LAPGAN, 2015 (Laplacian pyramid coding)
DCGAN, 2016 (Transposed convolution in generator)
BEGAN, 2017 (Autoencoder as discriminator)
PROGAN, 2017 (Progressive manner during training)
AutoGAN, 2019 (multi-level architecture search)
SAGAN, 2018 (Self-attention module)
BigGAN, 2019 (Deeper net and larger batch size)
YLG, 2020 (A local sparse attention layer)
Latent space
CGAN, 2014 (Label info into discriminator and generator)
AC-GAN, 2017 (Auxiliary classifier)
InfoGAN, 2016 (Classifier for labels)
BiGAN, 2016 (Encoder for learning inverse mapping)
SGAN, 2016 (Multi-headed layer in discriminator)
Application focused
CycleGAN, DiscoGAN, DualGAN, 2017
Image style transfer
SRGAN, 2016
Image super-resolution
StyleGAN, 2019
Scale-specific face generation
Face Completion GAN, 2017
Face completion
AlphaGAN, 2018
Image matting
Moco-GAN , 2018
DVD-GAN, 2019
Video generation
SinGAN, 2019
Image manipulation learned by one image
Loss
Loss Types
IPM based
RGAN, 2018 (Integral probability metric)
WGAN, 2017 (Wasserstein distance)
Geometric GAN, 2017 (Hinge loss)
Sphere GAN, 2019 (Riemannian manifolds)
Non-IPM based
FCGAN, 2014 (JS divergence)
LSGAN, 2016 (Pearson divergence)
f-GAN, 2016 (f-divergence)
UGAN, 2016 (Second order gradient loss)
LS-GAN, 2017 (Designated margin between real and fake samples)
Regularization
WGAN-GP, 2017 (Gradient penalty on WGAN)
WGAN-CT, 2018 (Soft consistency on WGAN)
WGAN-LP, 2017 (Lipschitz penalty on WGAN, less sensitive)
MRGAN, 2016 (Penalize missing modes)
SN-GAN, 2018 (Spectral normalization)
SS-GAN, 2019 (Self-supervision avoid discriminator forgetting)

- **Architecture-variant GANs**: Modify network structures (e.g., CNN-based, RNN-based models).
- **Loss-variant GANs**: Modify loss functions to improve stability (e.g., WGAN, LSGAN, f-GAN).

Different GANs

Model	Stability	Mode Collapse	Convergence	Sample Quality	Special Features
GAN	Low	High	Unstable	Medium	Baseline
LSGAN	Medium	Medium	More stable	Medium	Least squares loss
WGAN	High	Low	More stable	High	Wasserstein distance
WGAN-GP	Very High	Very Low	Very stable	Very High	Gradient Penalty
cGAN	Medium	Medium	Stable	High	Class conditioning
StyleGAN	High	Low	Stable	Very High	Style control

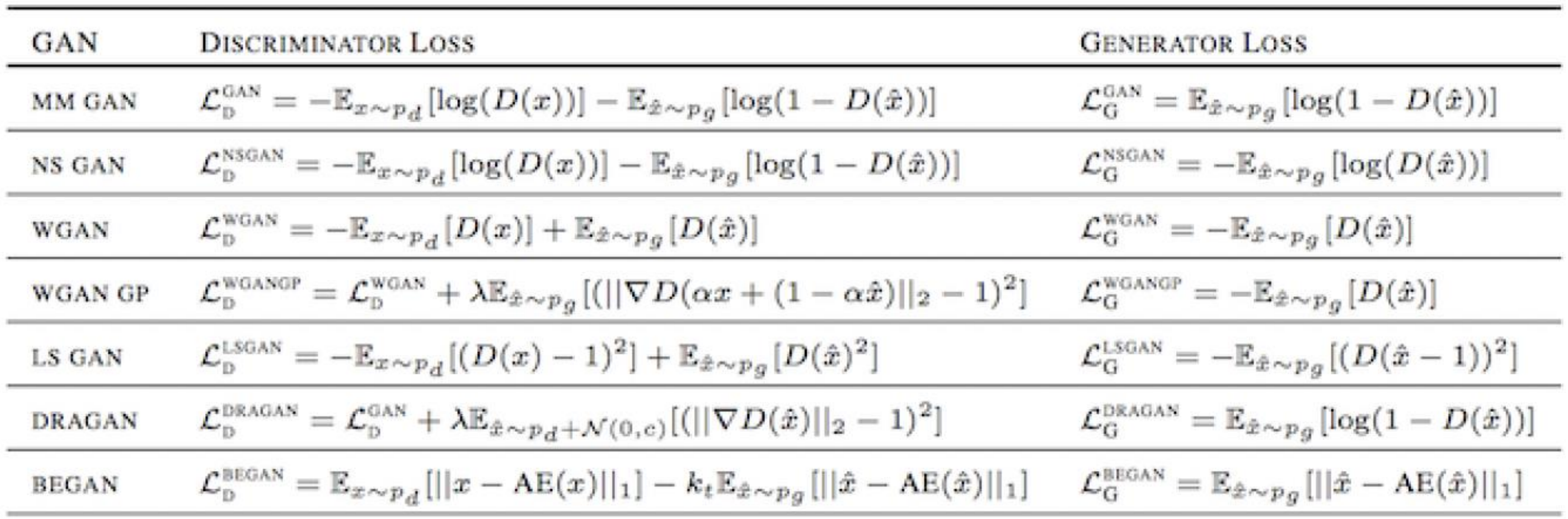
Timeline of GAN architectures


Complexity and Mechanisms
Quality and Diversity
Shallow
Single Mechanism
Deep
Multiple Mechanisms
Goodfellow et al.(Original GAN)
Fully-connected network
2014
Denton et al.(LAPGAN)
Cascade of CNN within a Laplacian pyramid framework
2015
Radford et al.(DCGAN)
Deconvolutional CNN
2016
Karras et al.(PROGAN)
Progressive growing neural network
2017
Han Zhang et al. (SAGAN)
Self-Attention CNN
2018
Brock et al. (BigGAN)
Orthogonal regularization to generator. By using deeper SAGAN with larger training batch size.
2019
Karnewar et al. (MSG-GAN)
Latent space of the generator and the discriminator are connected to share more information
2020
Single Mode
Low
High
Multiple Modes

Complexity in blue stream refers to size of the architecture and computational cost such as batch size. Mechanisms refer to the number of types of operations (e.g., convolution, deconvolution, self-attention) used in the architecture (e.g., FCGAN uses fully connected layers for both discriminator and generator. In this case, the value for mechanisms is 1).

Loss-variant GANs

- Jointly training two networks is challenging, can be unstable. Choosing objectives with better loss landscapes helps training, and is an active area of research.
- $X \sim P_X$ vs. $G(Z) \sim P_G$ with $Z \sim N(0, I)$.
- Training GAN is equivalent to minimizing Jensen-Shannon divergence between generator and data distributions.
- $D(P_X, P_G) = \sup_{f \in \mathcal{F}} \left\{ \mathbb{E}_{X \sim P_X} \phi_1(f(X)) - \mathbb{E}_{Y \sim P_G} \phi_2(f(Y)) \right\}$



GAN	Discriminator Loss	Generator Loss
MM GAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{GAN}} = -\mathbb{E}_{x\sim p_d}[\log(D(x))] - \mathbb{E}_{\hat{x}\sim p_g}[\log(1 - D(\hat{x}))]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{GAN}} = \mathbb{E}_{\hat{x}\sim p_g}[\log(1 - D(\hat{x}))]$
NS GAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{NSGAN}} = -\mathbb{E}_{x\sim p_d}[\log(D(x))] - \mathbb{E}_{\hat{x}\sim p_g}[\log(1 - D(\hat{x}))]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{NSGAN}} = -\mathbb{E}_{\hat{x}\sim p_g}[\log(D(\hat{x}))]$
WGAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{WGAN}} = -\mathbb{E}_{x\sim p_d}[D(x)] + \mathbb{E}_{\hat{x}\sim p_g}[D(\hat{x})]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{WGAN}} = -\mathbb{E}_{\hat{x}\sim p_g}[D(\hat{x})]$
WGAN GP	$\mathcal{L}_{\mathrm{D}}^{\mathrm{WGANGP}} = \mathcal{L}_{\mathrm{D}}^{\mathrm{WGAN}} + \lambda\mathbb{E}_{\hat{x}\sim p_g}[(\|\|\nabla D(\alpha x + (1-\alpha\hat{x})\|\|_2 - 1)^2]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{WGANGP}} = -\mathbb{E}_{\hat{x}\sim p_g}[D(\hat{x})]$
LS GAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{LSGAN}} = -\mathbb{E}_{x\sim p_d}[(D(x) - 1)^2] + \mathbb{E}_{\hat{x}\sim p_g}[D(\hat{x})^2]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{LSGAN}} = -\mathbb{E}_{\hat{x}\sim p_g}[(D(\hat{x} - 1))^2]$
DRAGAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{DRAGAN}} = \mathcal{L}_{\mathrm{D}}^{\mathrm{GAN}} + \lambda\mathbb{E}_{\hat{x}\sim p_d + \mathcal{N}(0,c)}[(\|\|\nabla D(\hat{x})\|\|_2 - 1)^2]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{DRAGAN}} = \mathbb{E}_{\hat{x}\sim p_g}[\log(1 - D(\hat{x}))]$
BEGAN	$\mathcal{L}_{\mathrm{D}}^{\mathrm{BEGAN}} = \mathbb{E}_{x\sim p_d}[\|\|x - \mathrm{AE}(x)\|\|_1] - k_t\mathbb{E}_{\hat{x}\sim p_g}[\|\|\hat{x} - \mathrm{AE}(\hat{x})\|\|_1]$	$\mathcal{L}_{\mathrm{G}}^{\mathrm{BEGAN}} = \mathbb{E}_{\hat{x}\sim p_g}[\|\|\hat{x} - \mathrm{AE}(\hat{x})\|\|_1]$

GAN-related Loss Functions

GANs aim to approximate the real data distribution $p_{data}(x)$ using a generator network $G(\eta)$, where $\eta \sim p_z(\eta)$ is drawn from a simple prior distribution.

- ▶ The training process is driven by a discriminator D(x), which distinguishes real from generated samples.
- ▶ The loss function should measure **the divergence** between $p_{data}(x)$ and $p_g(x)$ where $p_g(x)$ is the distribution of generated samples

Minimax Loss: In the original GANs, the generator tries to minimize the following function while the discriminator tries to maximize it:

$$\min_G \max_D V(D,G) = E_x[\log(D(x))] + E_z[\log(1 - D(G(z)))]$$

The formula derives from the cross-entropy between the real and generated distributions.

$$\max_D V(D,G) = \max_D \{\mathbb{E}_{x\sim P_{\text{data}}}[\log D(x)] + \mathbb{E}_{x\sim P_g}[\log(1 - D(x))]\}$$

For a given x, the optimal discriminator is given by

$$D^*(x) = \frac{P_{\text{data}}(x)}{P_{\text{data}}(x) + P_g(x)}$$

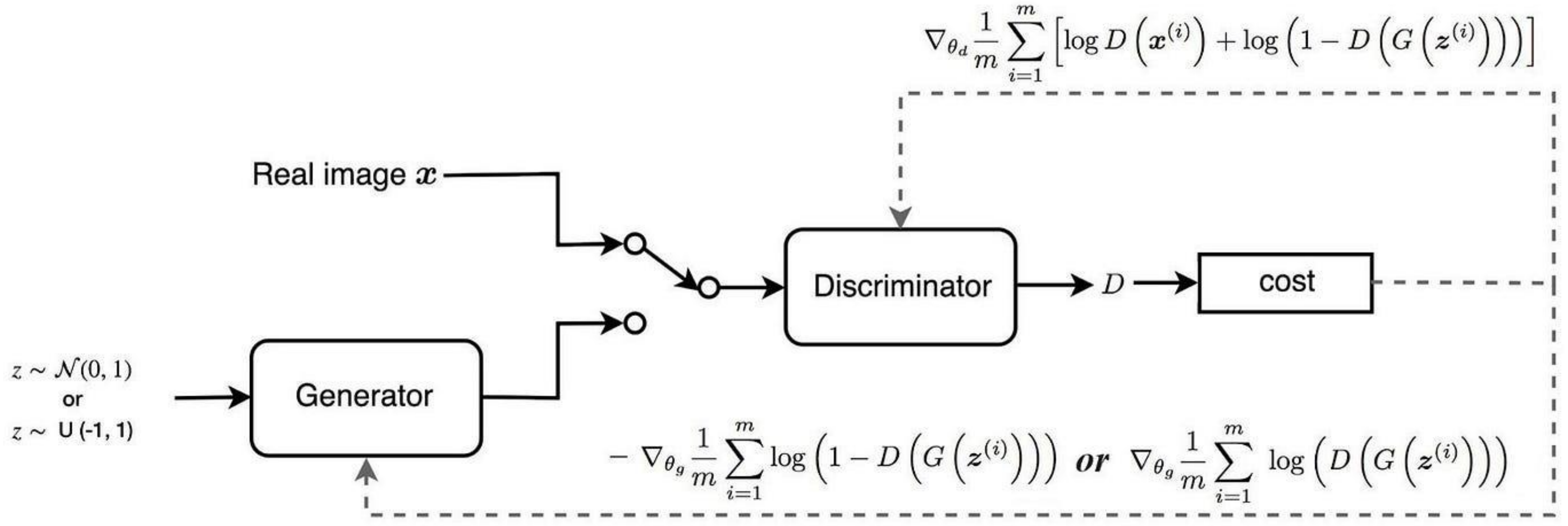
Thus, minimizing the GAN objective is equivalent to minimizing the Jensen-Shannon divergence as follows:

$$\min_G V(G,D^*) = \min_G JS(P_{\text{data}} \| P_g) + \log 4 = \min_G KL(P_{\text{data}} \| M) + KL(P_g \| M)$$

$$M(x) = \tfrac{1}{2}(P_{\text{data}}(x) + P_g(x))$$

Minimax Loss

The Standard GAN loss function can further be categorized into two parts: Discriminator loss and Generator loss. The diagram below summarizes how we train the discriminator and the generator using the corresponding gradient.



$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)\right]$
Real image $\boldsymbol{x}$
Discriminator
D
cost
$z \sim \mathcal{N}(0, 1)$
or
$z \sim$ U (-1, 1)
Generator
$-\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)$ *or* $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)$

Non-Saturating GAN Loss

Wasserstein GAN (WGAN)

Let Ω be a subset of $\mathbb{R}^d$. Let $\mathcal{B}_p(\Omega)$ be the set of Borel probability measures on Ω with finite pth moment. The p-Wasserstein metric is defined as

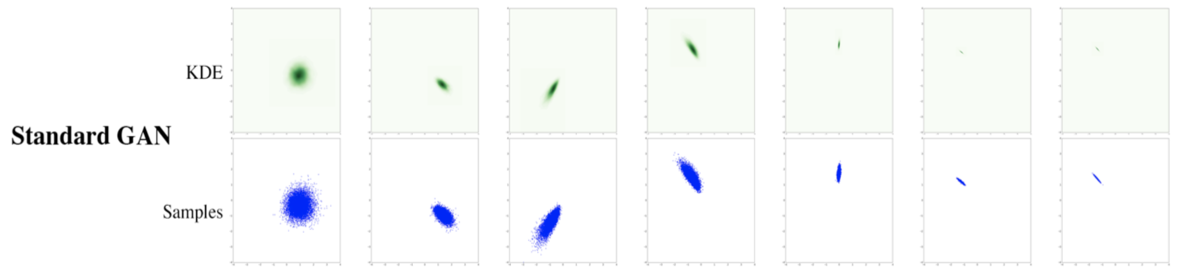
$$W_p(\mu,\nu) = \left(\inf_{\gamma \in \Gamma(\mu,\nu)} \int |x-y|^p d\gamma(x,y) \right)^{1/p}, \quad \mu \text{ and } \nu \in \mathcal{B}_p(\Omega).$$

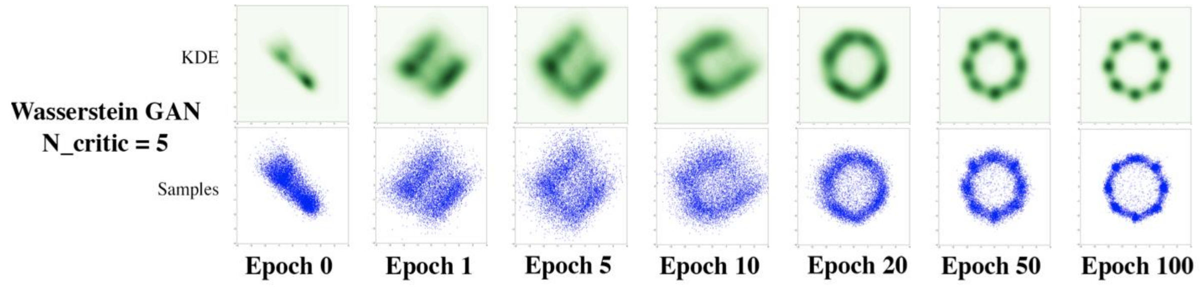
For the special case of p = 1, the p-Wasserstein metric is also known as the Monge-Rubinstein metric, or the earth mover distance.

The 1-Wasserstein metric can be expressed as (Villani, 2008),

$$W_1(\mu,\nu) = \sup_{f \in \mathcal{F}_1} \left\{ \int f(x)d\mu(x) - \int f(x)d\nu(x) \right\},$$

This expression of 1-Wasserstein metric is computationally convenient, which is used in the construction of Wasserstein generative adversarial networks (WGAN) (Arjovsky et al., 2017).





Training WGAN

Critic (Discriminator) Loss:

$$L_D = \mathbb{E}_{x\sim P_{\text{data}}}[D(x)] - \mathbb{E}_{z\sim P_z}[D(G(z))]$$

Methods to Enforce Lipschitz Constraint:

Weight Clipping (Original WGAN):

$$-c \leq w \leq c$$

Generator Loss:

$$L_G = -\mathbb{E}_{z\sim P_z}[D(G(z))]$$

Training Process:

1. Update the critic D multiple times per generator update.
2. Compute Wasserstein distance using the critic's output.
3. Update generator G to minimize the critic's output.

$$\nabla_{\theta_D} L_D = \nabla_{\theta_D} \left(\mathbb{E}_{x\sim P_{\text{data}}}[D(x)] - \mathbb{E}_{z\sim P_z}[D(G(z))]\right)$$

$$\theta_D \leftarrow \theta_D + \eta_D \nabla_{\theta_D} L_D$$

Gradient Penalty (WGAN-GP):

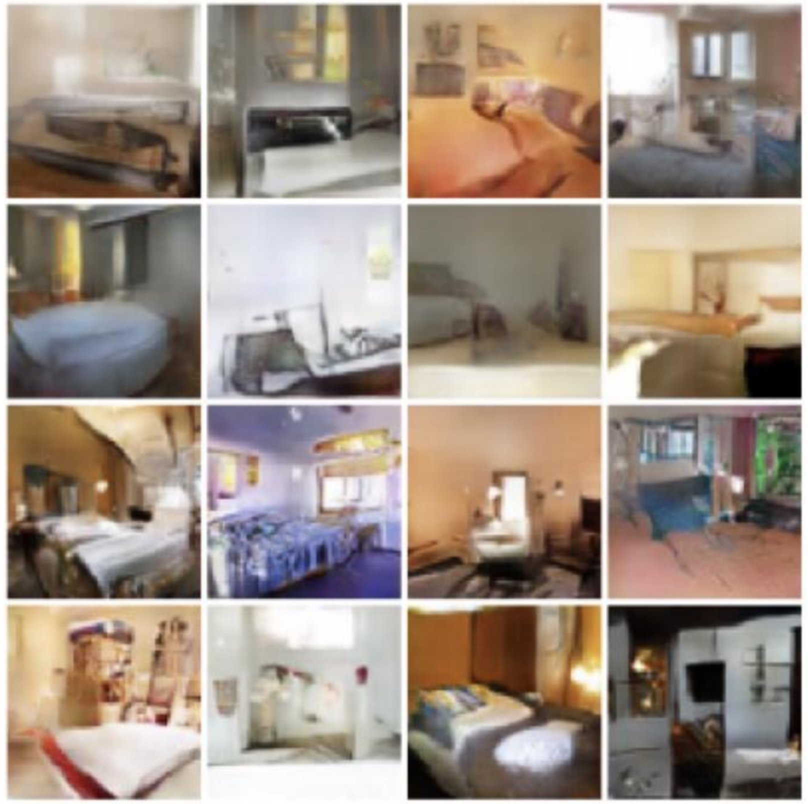
$$L_{\text{GP}} = \lambda \mathbb{E}_{\hat{x}\sim P_{\hat{x}}}[(\|\nabla_{\hat{x}} D(\hat{x})\|_2 - 1)^2]$$

$$\nabla_{\theta_G} L_G = -\nabla_{\theta_G} \mathbb{E}_{z\sim P_z}[D(G(z))]$$

$$\theta_G \leftarrow \theta_G + \eta_G \nabla_{\theta_G} L_G$$

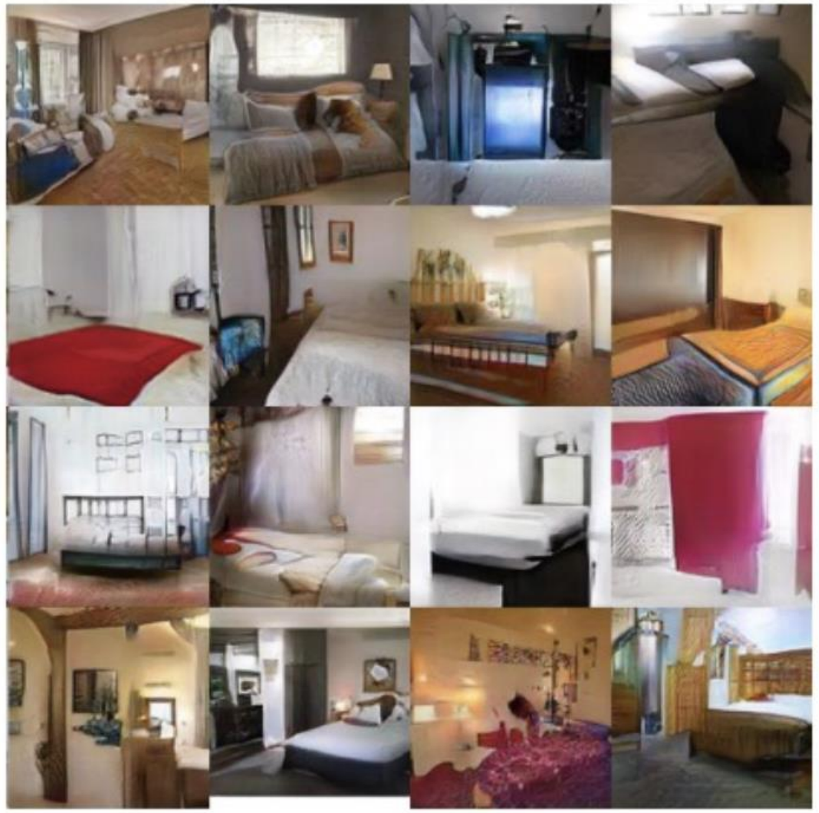
WGAN vs WGAN-NP

Wasserstein GAN (WGAN)



Arjovsky, Chintala, and Bouttou, “Wasserstein GAN”, 2017

WGAN with Gradient Penalty (WGAN-GP)



Gulrajani et al, “Improved Training of Wasserstein GANs”, NeurIPS 2017

Tips to improve GAN performance

- Change the cost function for a better optimization goal.
- Add additional penalties to the cost function to enforce constraints.
- Avoid overconfidence and overfitting.
- Better ways of optimizing the model.
- Add labels (Conditional GAN).
- More details and other implementation tips: https://towardsdatascience.com/gan-ways-to-improve-gan-performance-acf37f9f59b

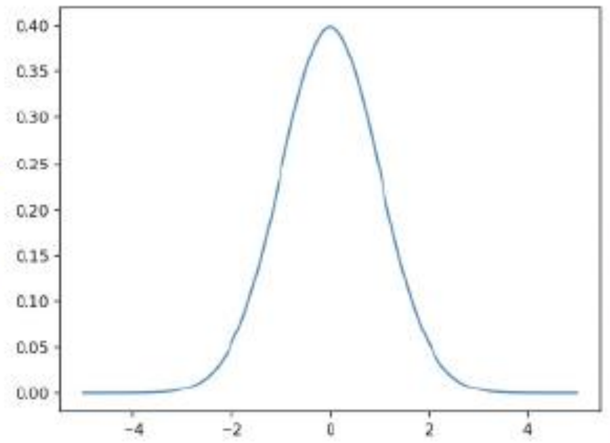
Content

General Goal

- Fit a density model $p_\theta(x)$ for a continuous random variable $X \in \mathbb{R}^D$
  - Good fit to the training data (really, the underlying distribution!)
  - For new x, ability to evaluate $p_\theta(x)$
  - Ability to sample from $p_\theta(x)$
  - And, ideally, a latent representation that's meaningful

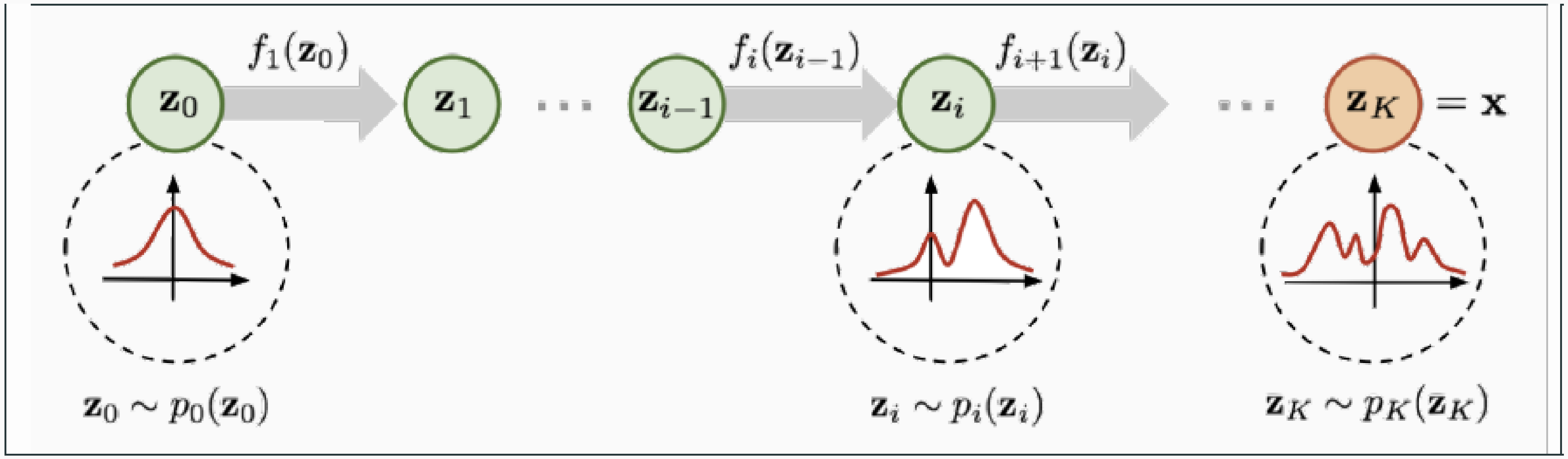
High Dimensional Data

$$\begin{tikzcd} x \arrow[r, shift left, "f\ (\text{inference})"] & z \arrow[l, shift left, "f^{-1}\ (\text{sampling})"] \end{tikzcd}$$



x and z must have the same dimension

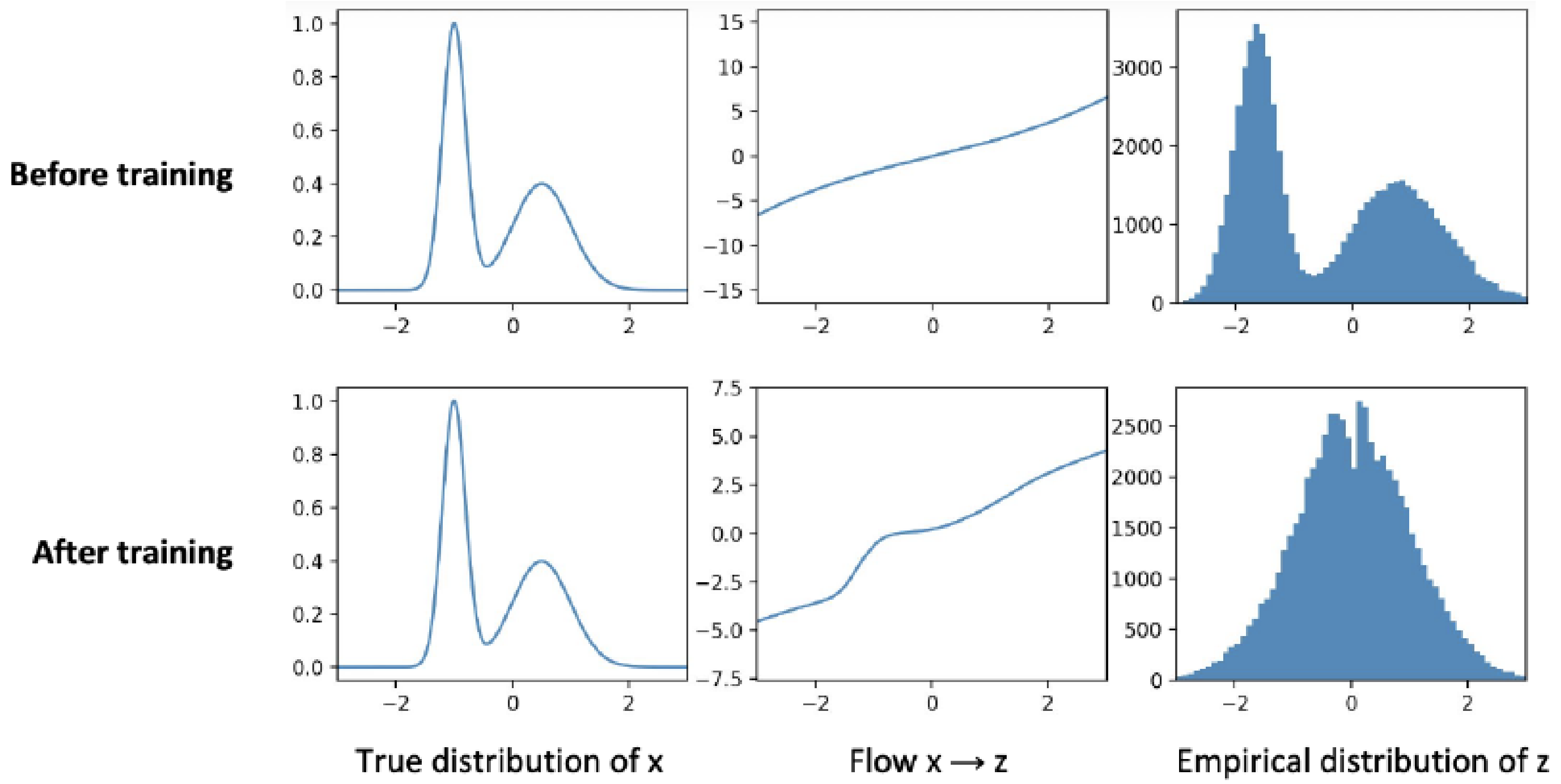
Normalizing Flow



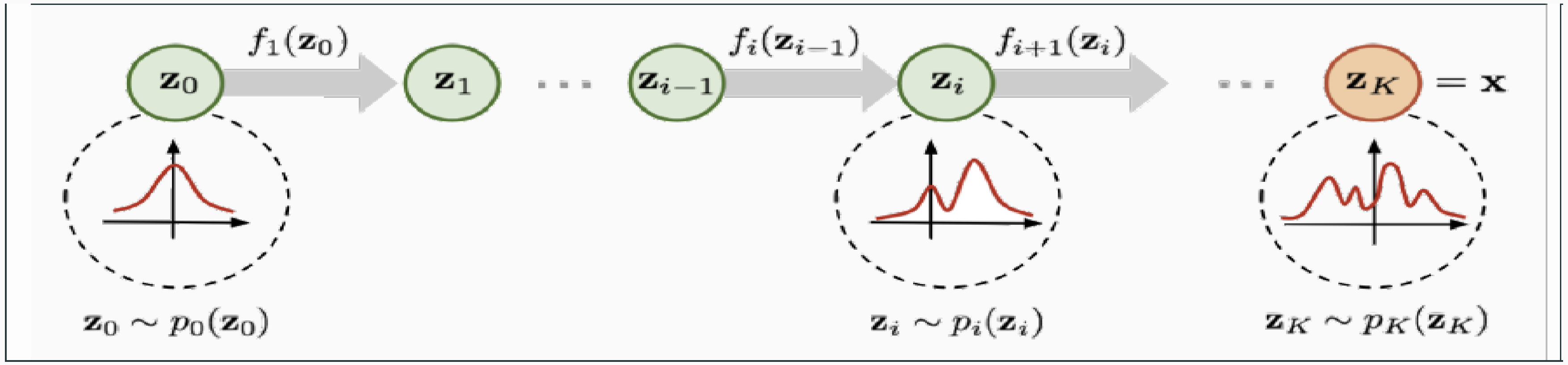
$f_1(\mathbf{z}_0)$
$f_i(\mathbf{z}_{i-1})$
$f_{i+1}(\mathbf{z}_i)$
$\mathbf{z}_0$
$\mathbf{z}_1$
$\mathbf{z}_{i-1}$
$\mathbf{z}_i$
$\mathbf{z}_K = \mathbf{x}$
$\mathbf{z}_0 \sim p_0(\mathbf{z}_0)$
$\mathbf{z}_i \sim p_i(\mathbf{z}_i)$
$\mathbf{z}_K \sim p_K(\mathbf{z}_K)$

- **Normalizing Flow (NF)**: a flow of invertible transformations that takes $z_0 \sim \mathcal{N}(0, I)$ and outputs x following a complex distribution

A Simple Illustration: X->N(0, 1)



Normalizing Flow


$f_1(\mathbf{z}_0)$
$f_i(\mathbf{z}_{i-1})$
$f_{i+1}(\mathbf{z}_i)$
$\mathbf{z}_0$
$\mathbf{z}_1$
$\mathbf{z}_{i-1}$
$\mathbf{z}_i$
$\mathbf{z}_K = \mathbf{x}$
$\mathbf{z}_0 \sim p_0(\mathbf{z}_0)$
$\mathbf{z}_i \sim p_i(\mathbf{z}_i)$
$\mathbf{z}_K \sim p_K(\mathbf{z}_K)$

- **A flow-based generative model** takes samples of x and learns $f_1^{-1}, f_2^{-1}, \cdots f_k^{-1}$ such that

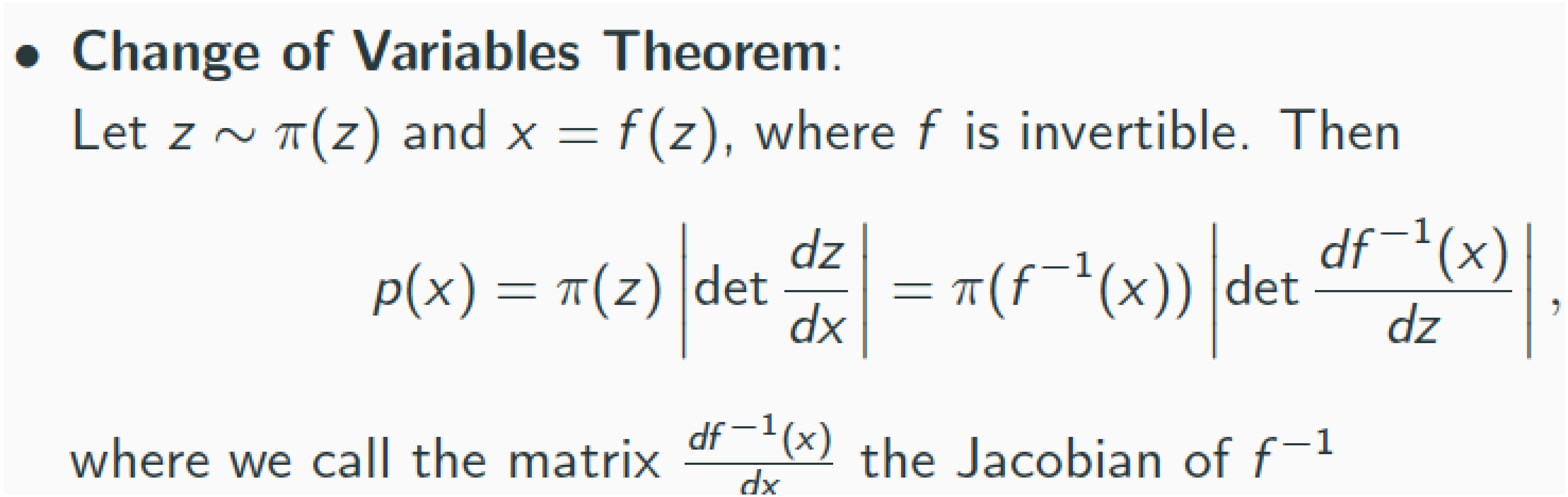
$$z_0 = f_1^{-1} \circ f_2^{-1} \circ \cdots \circ f_K^{-1}(x)$$

- Once the functions are learned, it uses

$$x = f_k \circ f_{k-1} \circ \cdots \circ f_1(z_0)$$

to approximate the distribution of x

NF – Deriving p(x) Explicitly



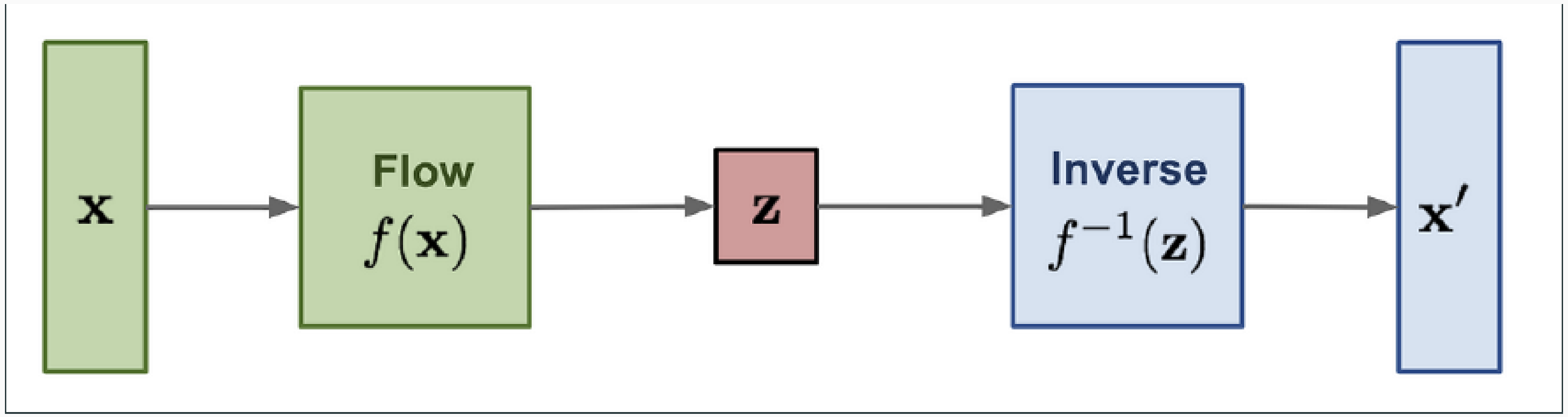
- **Change of Variables Theorem**:

  Let $z \sim \pi(z)$ and $x = f(z)$, where f is invertible. Then

$$p(x) = \pi(z) \left| \det \frac{dz}{dx} \right| = \pi(f^{-1}(x)) \left| \det \frac{df^{-1}(x)}{dz} \right| ,$$

where we call the matrix $\frac{df^{-1}(x)}{dx}$ the Jacobian of f^{-1}

NF – Deriving p(x) Explicitly



- Applying the change of variables theorem recursively and taking the log, we obtain the log-likelihood:

$$\log p(x) = \log \pi_0(z_0) - \sum_{i=1}^{K} \log \left| \det \frac{df_i}{dz_{i-1}} \right|$$

NF – Remarks

- With NF architecture, the objective function arises naturally. For samples $x^{(1)}, x^{(2)}, \cdots, x^{(N)}$,

$$\mathcal{L}(x^{(1)}, x^{(2)}, \cdots, x^{(N)}) = -\frac{1}{N}\sum_{i=1}^{N} \log p(x^{(i)})$$

- The key is in finding a suitable class of the transformations f_i.
- Challenges: Ideally, the transformations are
  — capable of growing arbitrarily complex
  —- yet their inverse and Jacobian are easy to compute

RealNVP

- Short for "Real-valued non-volume preserving" model
- Each transformation $f_i : \mathbb{R}^D \rightarrow \mathbb{R}^D$ for some $i \in \{1, 2, \cdots K\}$ used in this model is termed an **affine coupling layer**

RealNVP – affine coupling layers

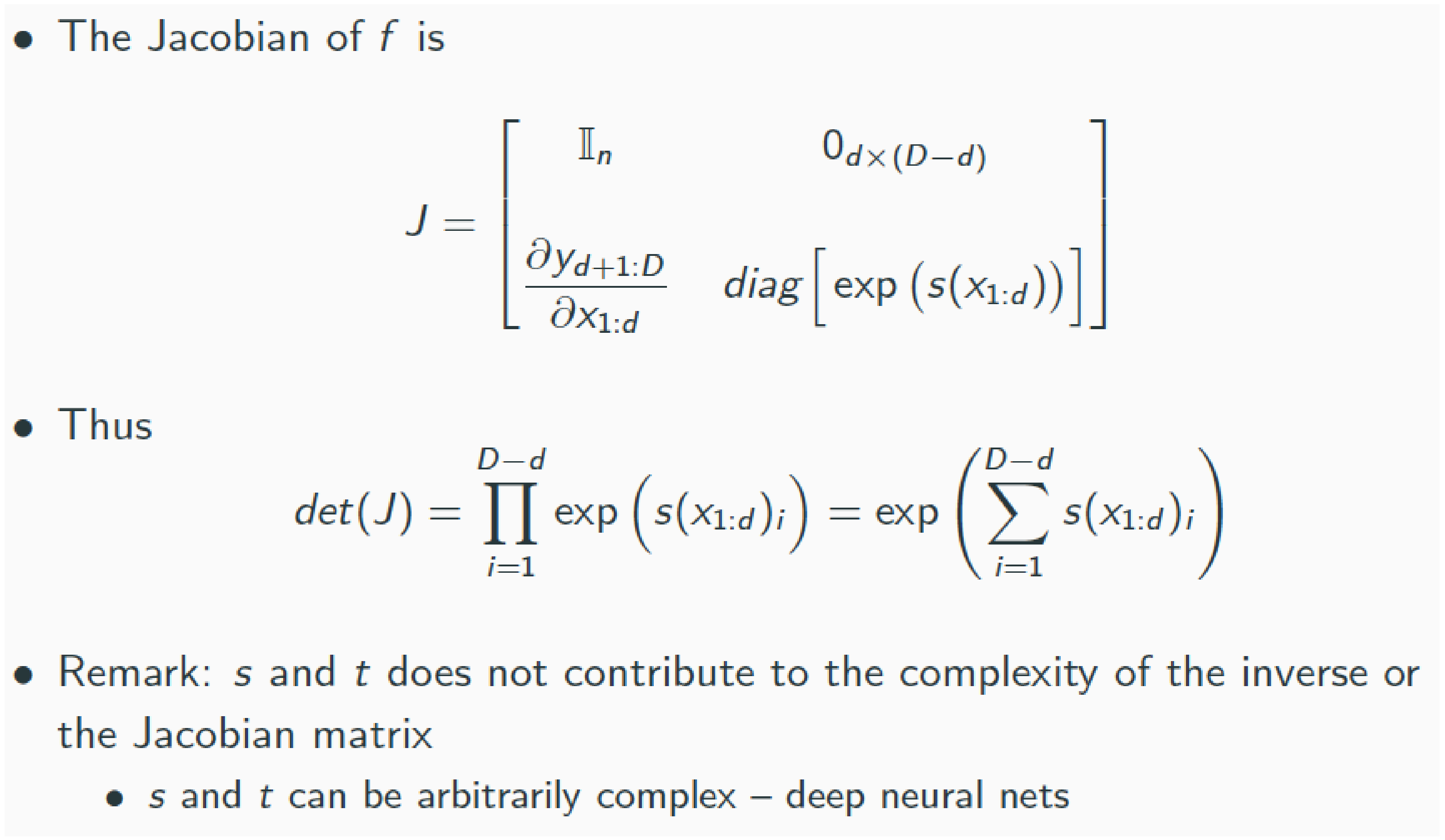
Say $f(x) = y$ is an affine coupling layer. Then for some $d < D$ and some functions $s : \mathbb{R}^d \to \mathbb{R}^{D-d}$ and $t : \mathbb{R}^d \to \mathbb{R}^{D-d}$,

$$\begin{aligned} y_{1:d} &= x_{1:d} \\ y_{d+1:D} &= x_{d+1:D} \odot \exp(s(x_{1:d})) + t(x_{1:d}). \end{aligned}$$

The inverse is

$$\begin{aligned} x_{1:d} &= y_{1:d} \\ x_{d+1:D} &= (y_{d+1:D} - t(y_{1:d})) \odot \exp(-s(y_{1:d})). \end{aligned}$$

RealNVP – affine coupling layers



- The Jacobian of f is

$$J = \begin{bmatrix} \mathbb{I}_n & 0_{d\times(D-d)} \\ \frac{\partial y_{d+1:D}}{\partial x_{1:d}} & diag\left[\exp\left(s(x_{1:d})\right)\right] \end{bmatrix}$$

- Thus

$$det(J) = \prod_{i=1}^{D-d} \exp\left(s(x_{1:d})_i\right) = \exp\left(\sum_{i=1}^{D-d} s(x_{1:d})_i\right)$$

- Remark: s and t does not contribute to the complexity of the inverse or the Jacobian matrix
  - s and t can be arbitrarily complex – deep neural nets

RealNVP – important of good masking

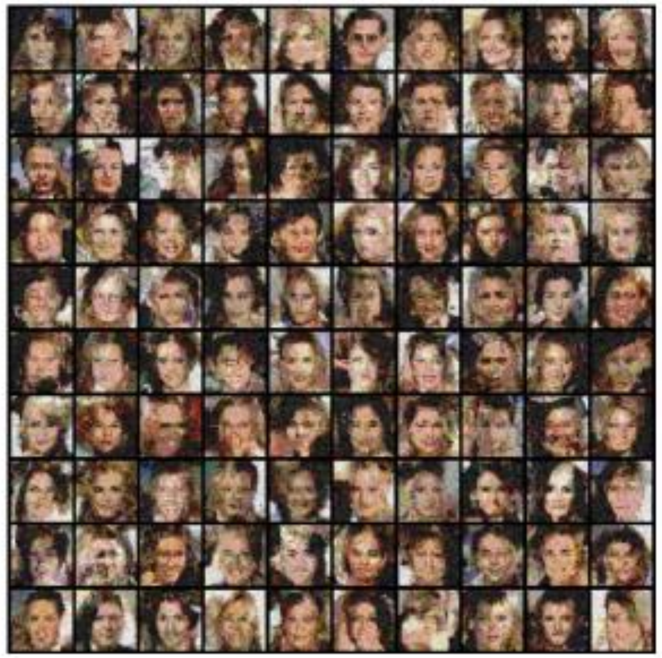
- Each affine flow involves partitioning the elements of the input vector into two groups
    - Termed *masking* by the original paper

- Let b be a *binary mask*, a vector with d ones and $D - d$ zeros. Then we can rewrite y as

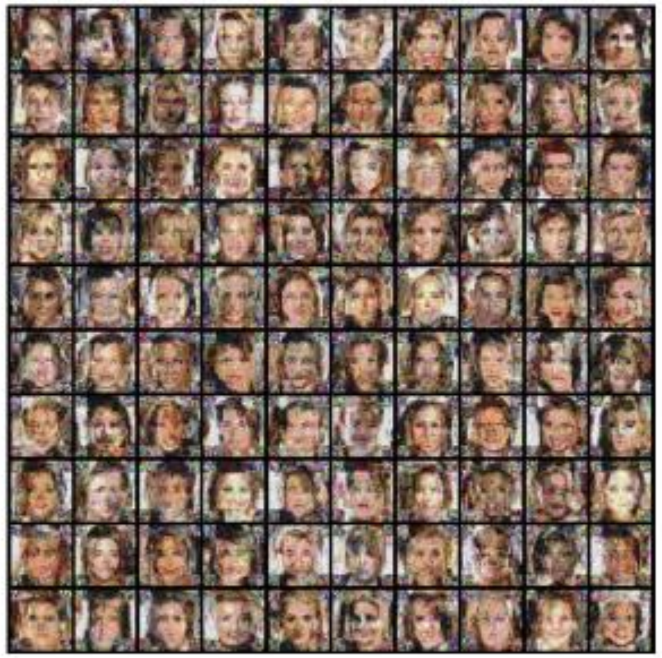
$$y = b \odot x + (1 - b) \odot (x \odot \exp(s(b \odot x)) + t(b \odot x))$$

RealNVP – important of good masking

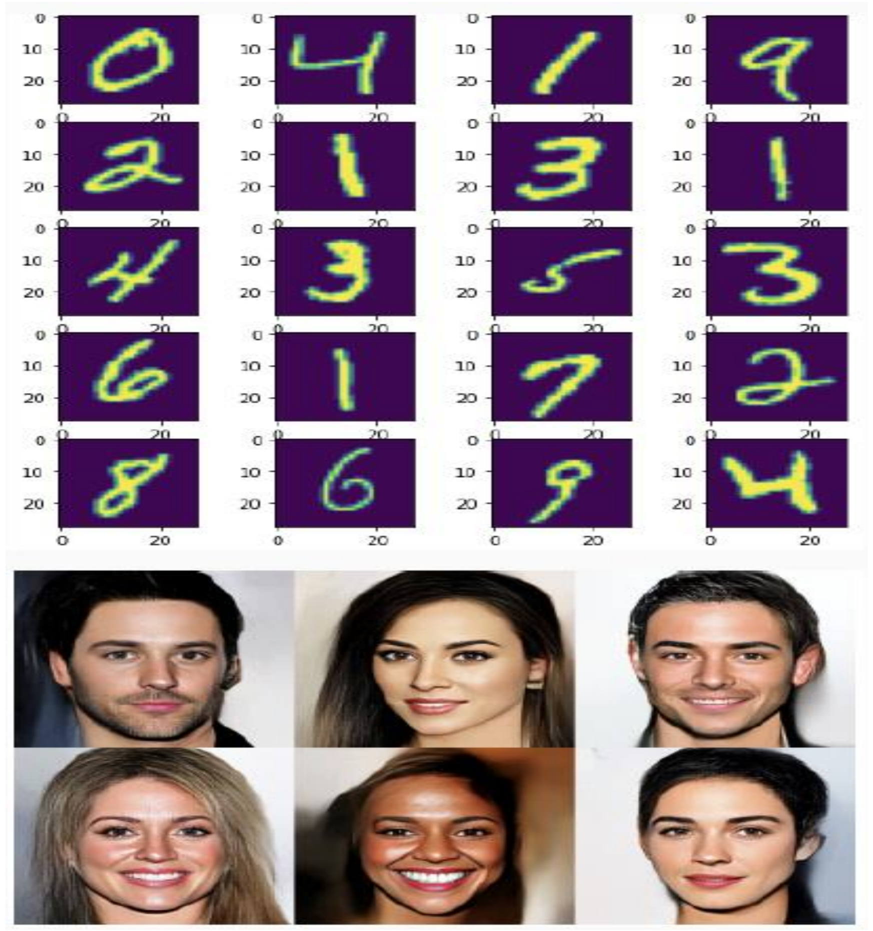
Checkerboard x4; channel squeeze; channel x3; channel unsqueeze; checkerboard x3



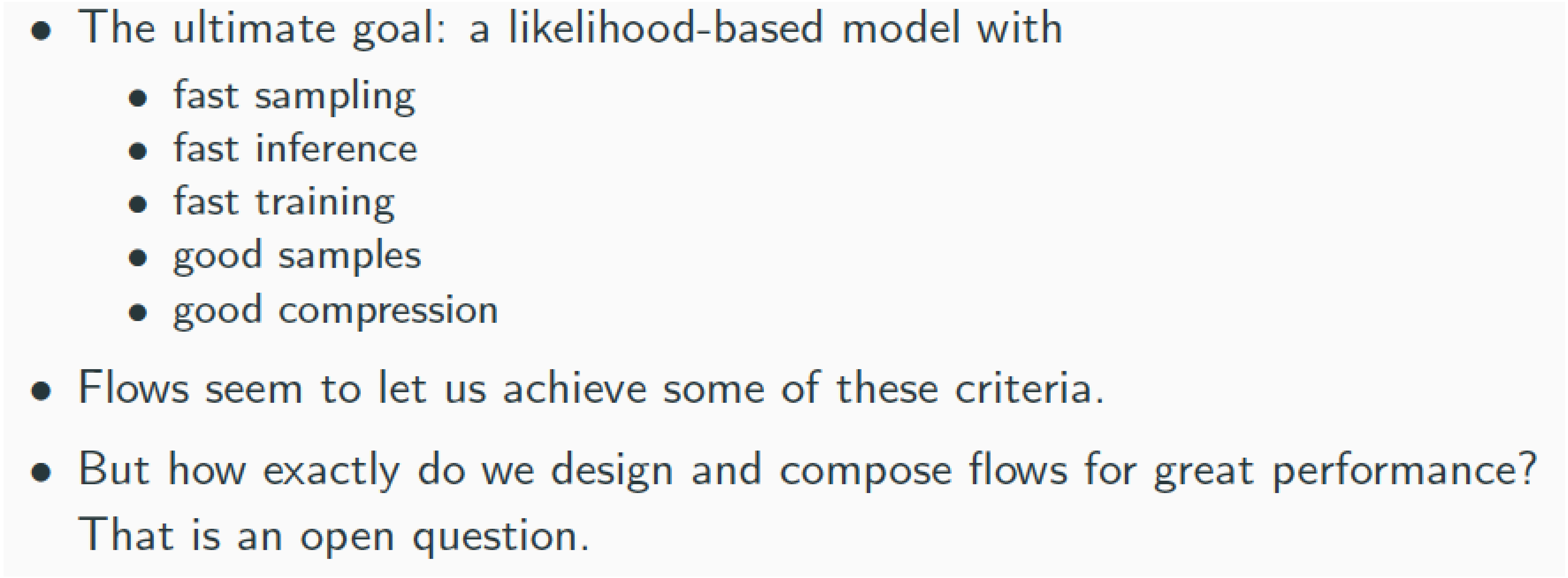
(Mask top half; mask bottom half; mask left half; mask right half) x2



Generative Images



Flow-Based Models Summary



- The ultimate goal: a likelihood-based model with
  - fast sampling
  - fast inference
  - fast training
  - good samples
  - good compression
- Flows seem to let us achieve some of these criteria.
- But how exactly do we design and compose flows for great performance? That is an open question.

Content

EFFICIENT MULTI-MODAL SAMPLING VIA TEMPERED DISTRIBUTION FLOW

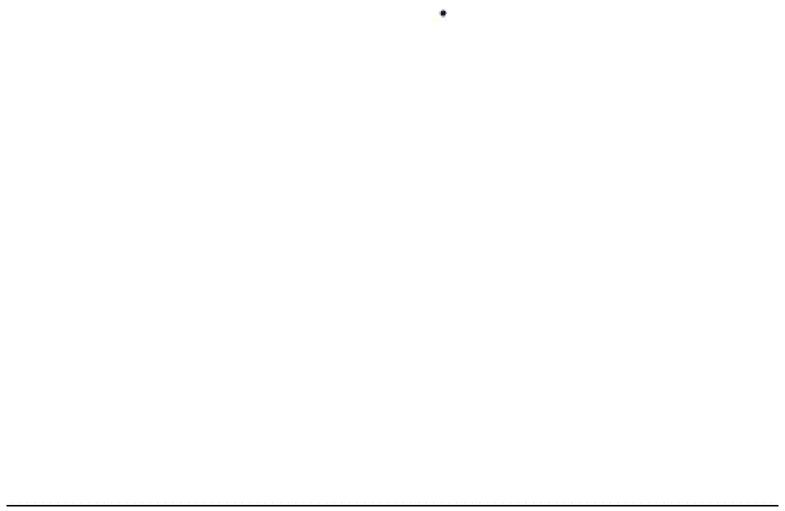
Reference:

Qiu, Y. and Wang, X. (2024). Efficient Multimodal Sampling via Tempered Distribution Flow. *JASA*, 119, 1446-1460.

❑ Tempered Distribution Flow

A Familiar Problem

- Given an unnormalized density function $p(x) \propto \exp\{-E(x)\}$
- Generate a random sample $X_1, X_2, \dots, X_n \sim p(x)$



Video: https://colindcarroll.com/2018/11/24/animated-mcmc-with-matplotlib

Department of Statistics

Why Sampling?

- Question 1: Why do we care about it?
  - It lies at the heart of statistics and machine learning
    - Bayesian models
    - Monte Carlo methods
    - Numerical integration
    - Deep generative models, e.g., energy-based models

Textbook Solution and Challenges

- Question 2: Is it a trivial task?
  - Existing methods face great challenges for complicated distributions
    - Inverse c.d.f. method → Only for univariate distribution
    - Rejection sampling → Hard to find upper bound
    - Importance sampling → Variance control in high dimensions
    - MCMC → Hard to test convergence, computational efficiency

Sampling and simulation is a fundamental yet challenging task

Different but Similar to GenAI

- Given training data, generate new samples from the same distribution
- Training data $\sim P_{data}(x)$, generated samples $\sim P_{model}(x)$; Want to learning $P_{model}(x)$ similar to $P_{data}(x)$.

1024X1024 images generated using the CELEBA-HQ dataset.

❑ Tempered Distribution Flow

- Background
- Sampling via Measure Transport
- Tempered Distribution Flow
- Experiments and Summary

The Framework

- Marzouk et al. (2016) proposed sampling based on measure transport
- Essentially it means "transformation of random variables"
- Suppose $X = T(Z), Z \sim N(0, I_d)$
- Use the distribution of X to approximate the target distribution $p(x)$

Recap

- Let $Z \sim p_z(z)$ be a d-dimensional random vector
- $T: \mathrm{R}^d \to \mathrm{R}^d$ is an invertible and differentiable mapping
- Set $X = T(Z)$, and then X has the density function

$$p_x(x) = p_Z(T^{-1}(x)) \left|\det \frac{\partial T^{-1}}{\partial x}\right|$$

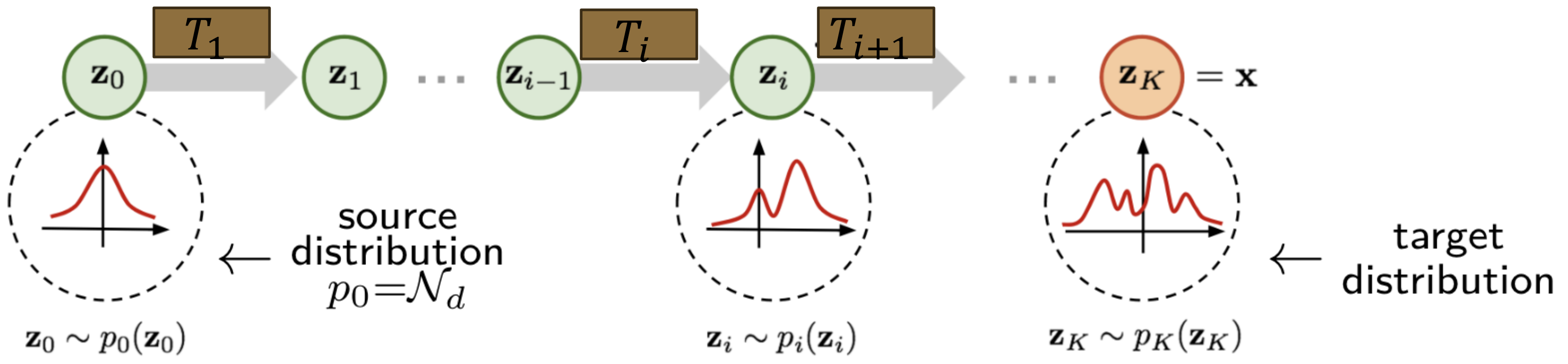
Transport Map

- But the transport map T needs to satisfy some conditions
  1. Invertible and differentiable
  2. T^{-1} and $\det(\partial T^{-1}/\partial x)$ are easy to compute
  3. T is flexible enough to characterize sophisticated nonlinear mappings
- Is it easy, or even possible, to construct such a T?
- E.g., Marzouk et al. (2016) uses polynomials

But not very flexible; computation is hard

Normalizing Flows

- The normalizing flow framework (Rezende & Mohamed, 2015) is one possible solution
- It constructs T via composition $T = T_K \circ T_{K-1} \circ \cdots \circ T_1$
- Each T_i is relatively simple, but satisfies the requirements



T_1
T_i
T_{i+1}
$\mathbf{z}_0$
$\mathbf{z}_1$
$\mathbf{z}_{i-1}$
$\mathbf{z}_i$
$\mathbf{z}_K = \mathbf{x}$
source distribution $p_0 = \mathcal{N}_d$
target distribution
$\mathbf{z}_0 \sim p_0(\mathbf{z}_0)$
$\mathbf{z}_i \sim p_i(\mathbf{z}_i)$
$\mathbf{z}_K \sim p_K(\mathbf{z}_K)$

Example: Real NVP

- One popular class of T is called Real NVP (Dinh et al., 2016)

$$\begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{pmatrix} \overset{T_1}{\Rightarrow} \begin{pmatrix} Y_1 = Z_1 \\ Y_2 = Z_2 \\ Y_3 = \mu_{Y_3}(Z_{1:2}) + \sigma_{Y_3}(Z_{1:2}) \cdot Z_3 \\ Y_4 = \mu_{Y_4}(Z_{1:2}) + \sigma_{Y_4}(Z_{1:2}) \cdot Z_4 \end{pmatrix}$$

$$\begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix} \overset{T_2}{\Rightarrow} \begin{pmatrix} X_1 = \mu_{X_1}(Y_{3:4}) + \sigma_{X_1}(Y_{3:4}) \cdot Y_1 \\ X_2 = \mu_{X_2}(Y_{3:4}) + \sigma_{X_2}(Y_{3:4}) \cdot Y_2 \\ X_3 = Y_3 \\ X_4 = Y_4 \end{pmatrix}$$

- Some elements are unchanged, e.g.,
$$Y_{1:r} = Z_{1:r}$$
- Remaining components are modified with
$$Y_{(r+1):d} = \mu(Z_{1:r}) + \sigma(Z_{1:r}) \odot Z_{(r+1):d}$$
- μ and σ are neural networks

Why Real NVP Works

- T can be easily inverted

$$\begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{pmatrix} \overset{T}{\Rightarrow} \begin{pmatrix} X_1 = Z_1 \\ X_2 = Z_2 \\ X_3 = \mu_{X_3}(Z_{1:2}) + \sigma_{X_3}(Z_{1:2}) \cdot Z_3 \\ X_4 = \mu_{X_4}(Z_{1:2}) + \sigma_{X_4}(Z_{1:2}) \cdot Z_4 \end{pmatrix}$$

$$\begin{pmatrix} Z_1 = X_1 \\ Z_2 = X_2 \\ Z_3 = \left[X_3 - \mu_{X_3}(X_{1:2})\right] / \sigma_{X_3}(X_{1:2}) \\ Z_4 = \left[X_4 - \mu_{X_4}(X_{1:2})\right] / \sigma_{X_4}(X_{1:2}) \end{pmatrix} \overset{T^{-1}}{\Leftarrow} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{pmatrix}$$

Why Real NVP Works

- $\partial T / \partial z$ is lower triangular

$$\begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Z_4 \end{pmatrix} \overset{T}{\Rightarrow} \begin{pmatrix} X_1 = Z_1 \\ X_2 = Z_2 \\ X_3 = \mu_{X_3}(Z_{1:2}) + \sigma_{X_3}(Z_{1:2}) \cdot Z_3 \\ X_4 = \mu_{X_4}(Z_{1:2}) + \sigma_{X_4}(Z_{1:2}) \cdot Z_4 \end{pmatrix}$$

$$J = \frac{\partial T(z)}{\partial z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ * & * & \sigma_{X_3}(z_{1:2}) & 0 \\ * & * & 0 & \sigma_{X_4}(z_{1:2}) \end{pmatrix}$$

- $\det(\partial T / \partial z)$ is the product of diagonal elements
- Some recent theoretical works such as Teshima et al. (2020) show that Real NVP flows are universal approximators for invertible functions
- **All three requirements are satisfied**

Summary

- Overall, normalizing flows are distributional models that
  1. Have a computable density function
  2. Easily generate random samples
  3. Can approximate virtually all continuous distributions

- If we can estimate T accurately, sampling is trivial

Simulate $Z_1, \dots, Z_n \sim N(0, I_d)$, and set $X_i = T(Z_i)$

Measure Transport vs MCMC

	Measure Transport	MCMC
Training	Required	No training
Generation	Extremely fast	Requires many density/gradient evaluations
Convergence test	Easy	Hard
Parallelization	Trivial	Nontrivial
Resulting data points	Independent	Correlated (unless running multiple independent chains)

- In practice, they **complement** each other

❑ Tempered Distribution Flow

The First Try

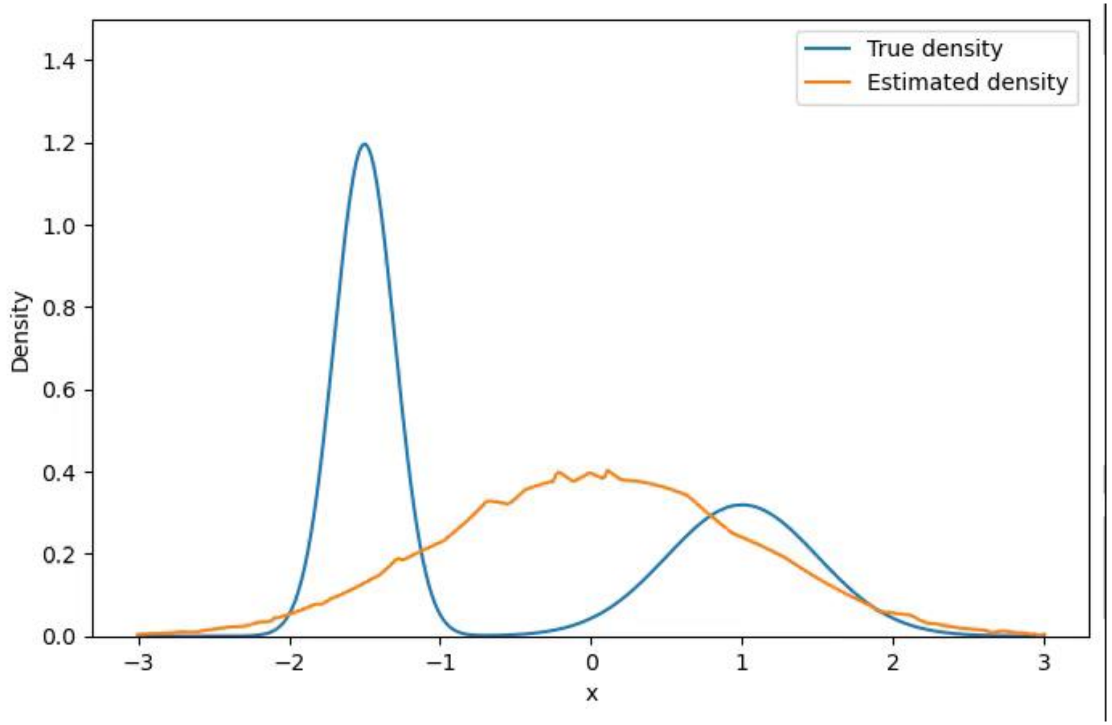
- Assume $T = T_\theta$ is characterized by neural network parameters θ
- Then X has an explicit density function $p_\theta(x)$
- We minimize some "distance" between $p(x)$ and $p_\theta(x)$, e.g.,

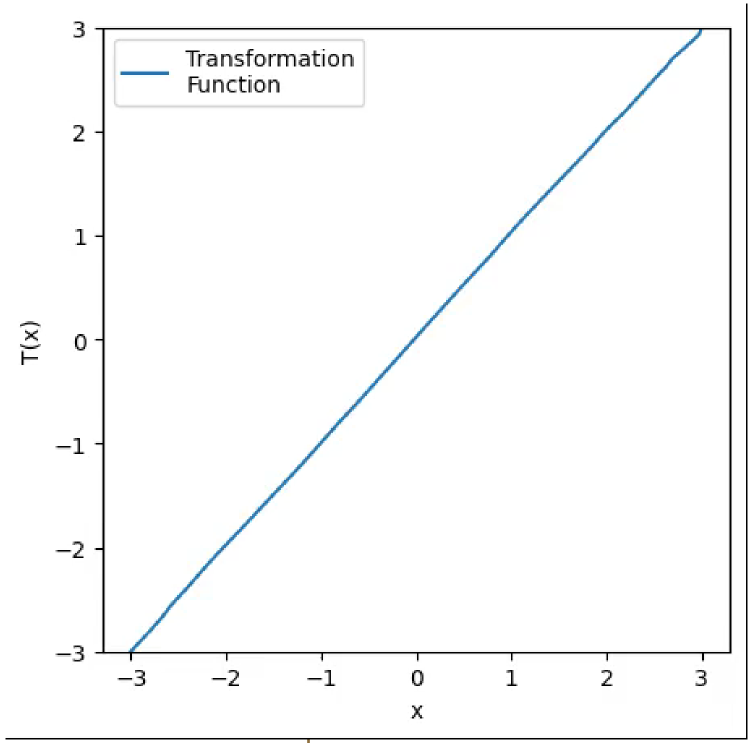
$$\min_\theta \ \mathrm{KL}(p_\theta \| p) = \min_\theta \ \mathrm{E}_{p_\theta} \log p_\theta(x) - \mathrm{E}_{p_\theta} \log p(x)$$

- Expectations can be approximated by Monte Carlo estimators
- θ is optimized using stochastic gradient descent

Demo

- Left: evolution of estimated density. Right: transformation function.



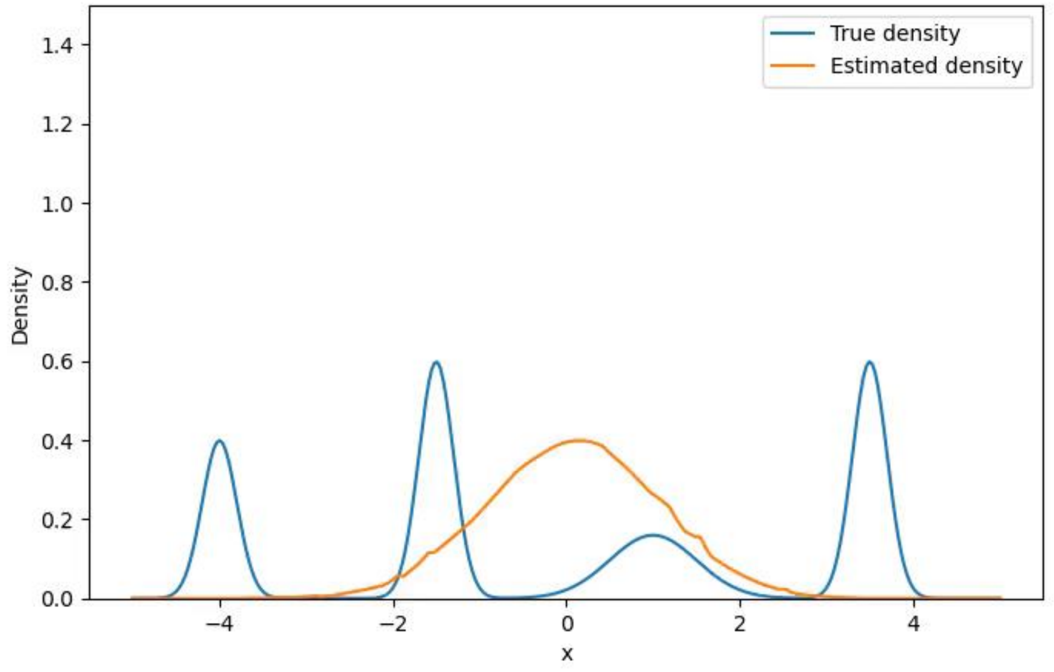


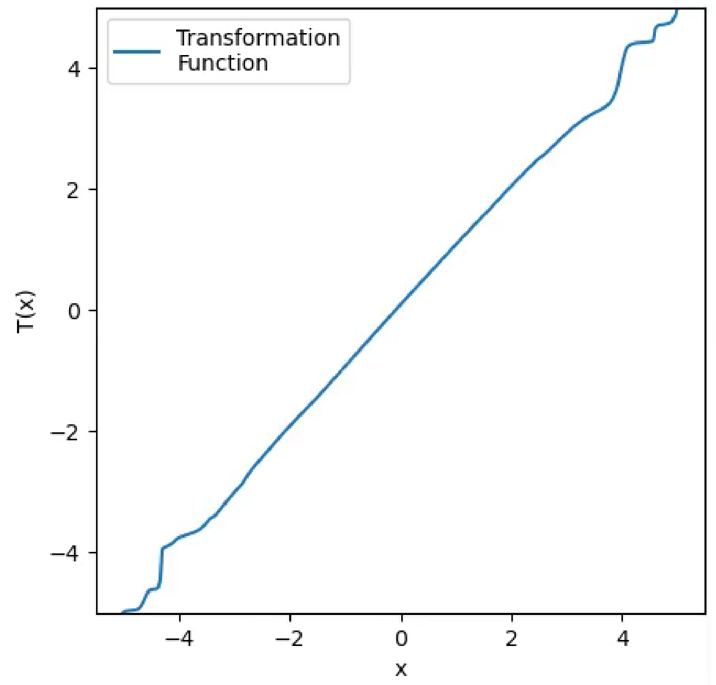
Problem

- The previous demo looks not bad, but…
- What about distributions with many isolated modes?

Multi-modal Distribution

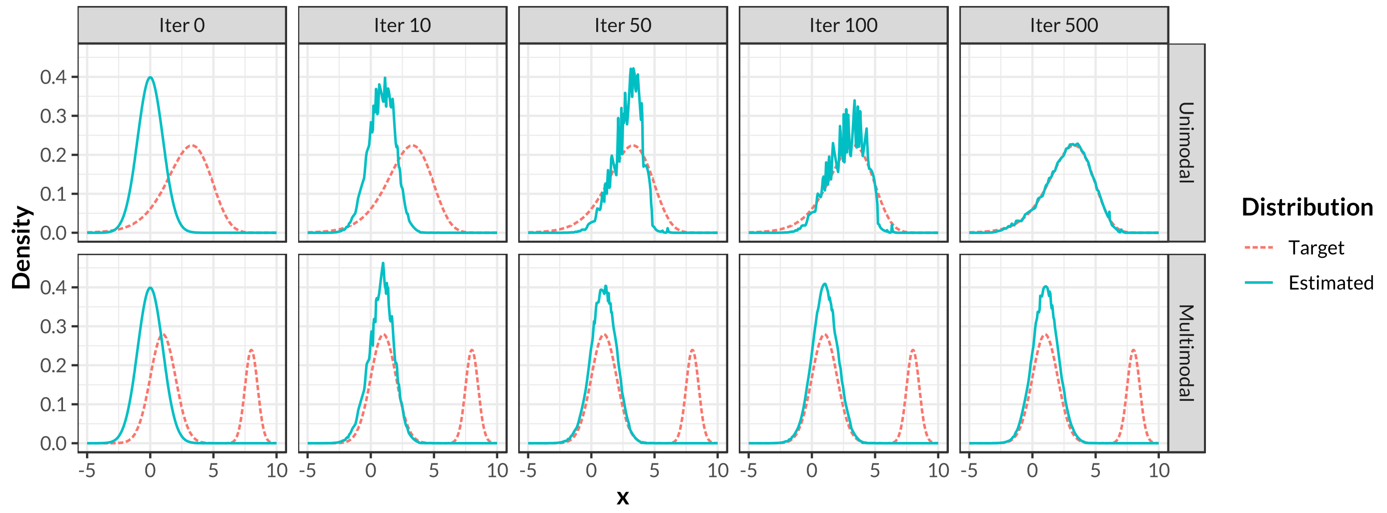
- Left: evolution of estimated density. Right: transformation function.





Issues and Challenges

- For unimodal densities, the method converges very fast and approximates the target density well.
- For multimodal distributions, the method has little progress after certain iterations.
- We need to carefully analyze the dynamics of the optimization process to uncover the reason of failure.



Explanation

- The evolution of $p_\theta(x)$ approximates a continuous-time differential equation (a.k.a. the continuity equation, Ambrosio et al., 2018)

$$\frac{\partial}{\partial t} p_t + \nabla \cdot (\mathrm{v}_t p_t) = 0$$

- v_t is the vector field determined by a function $\mathcal{F}$
- The time-indexed distribution p_t is called a Wasserstein gradient flow, which decreases the functional $\mathcal{F}(\cdot) = \mathrm{KL}(\cdot \,\|p)$ through time, i.e., $\mathrm{d}\mathcal{F}(p_t)/\mathrm{d}t \leq 0$
- But the convergence speed can vary a lot for different target densities p

Theoretical Analysis

Theorem (informal)

If $p(x)$ is log-concave, then

1. $\mathcal{F}(p_t)$ decreases to 0 exponentially fast
2. $H^2(p_t, p) \leq C \cdot |\mathrm{d}\mathcal{F}(p_t)/\mathrm{d}t|$, $H^2(\cdot,\cdot)$ is the squared Hellinger distance

- For log-concave densities, the difference between the sampler distribution and the target distribution decays exponentially fast along the gradient flow
- Gradient does not vanish unless p_t is already close to p, which we call the nonvanishing gradient property

Theoretical Analysis

Theorem (informal)

If $p(x) = \alpha h(x) + (1-\alpha)h(x-\mu)$ is a mixture of two log-concave distributions, then there exists some p_{t^*} such that

$$\lim_{\|\mu\|\to\infty} \mathcal{F}(p_{t^*}) > 0, \qquad \lim_{\|\mu\|\to\infty} |\mathrm{d}\mathcal{F}(p_t)/\mathrm{d}t|_{t=t^*} = 0$$

- There exists a configuration of p_{t^*} such that it is different from the target distribution, but meanwhile the gradient vanishes.
- The vanishing gradient implies an extremely slow convergence speed.

The Proposed Method

Two core ideas:

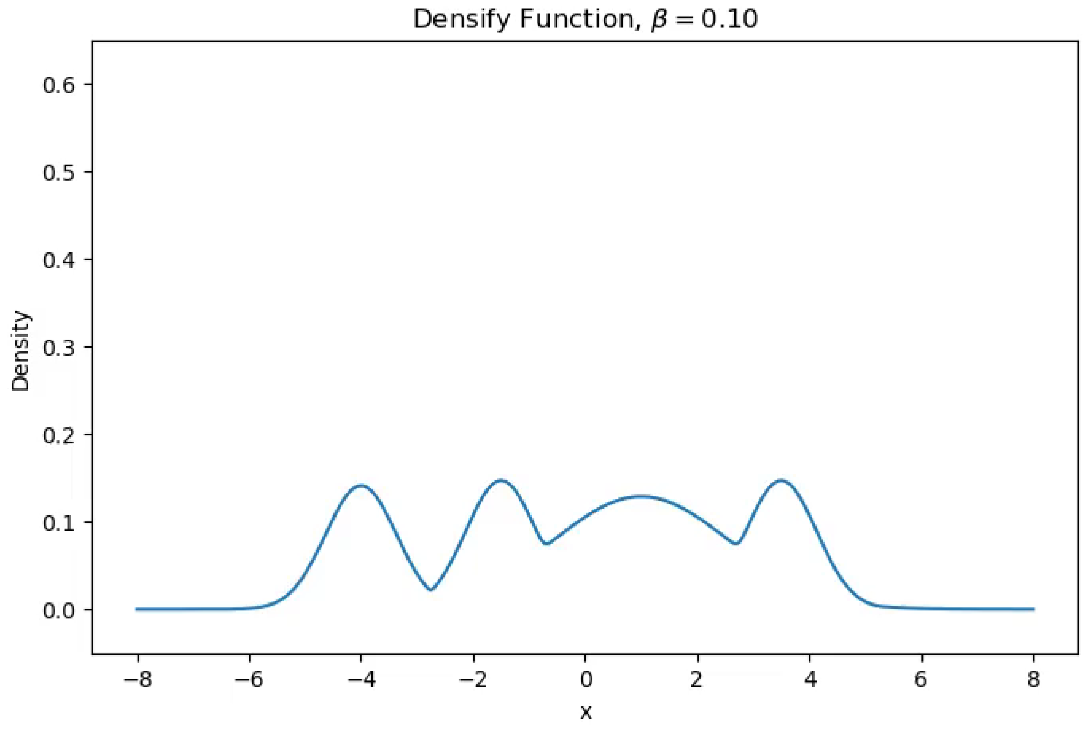
1. Evolve the distribution flow p_t through the tempering curve
2. Replace the KL functional with the L^2 distance

The Tempering Curve

- Instead of directly minimizing the KL divergence, let p_t move along the tempering curve
$$p_{\beta_t}(x) = \frac{1}{Z(\beta_t)} e^{-\beta_t E(x)}$$
- β_t is an increasing function of t, $\beta_0 > 0$, $\beta_t \to 1$
- $p_{\beta_t}(x)$ reduces to the target density $p(x)$ when $\beta_t = 1$
- In practice, discretize the curve into a sequence of distributions p_{β_k}
- $0 < \beta_1 < \beta_2 < \cdots < \beta_T = 1$

The Tempering Curve

- $p_{\beta_t}(x)$ has the same modes as $p(x)$, but they are more connected



Theoretical Analysis

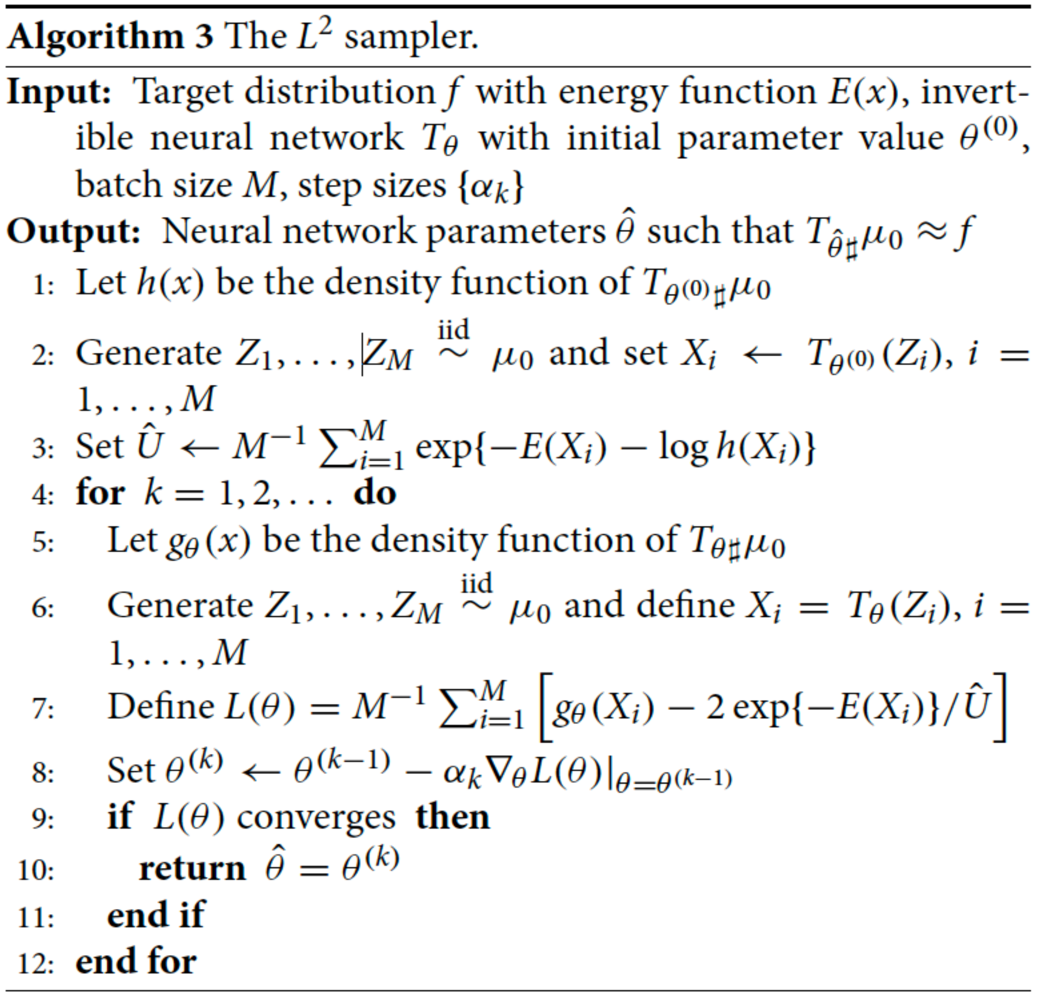
- To transport p_{β_k} to $p_{\beta_{k+1}}$, we solve a Wasserstein gradient flow with respect to the (squared) L^2 distance,

$$\mathcal{G}(\cdot) = \int (\cdot - p(x))^2 \mathrm{d}x$$

- $min_g \, \mathcal{L}(g) = \int g dg \, - 2 \int f dg + \int f^2 d\lambda = E_{X \sim g(x)}[g(X) - 2f(X)] + C$
- Here, the target distribution is $f = p_{\beta_{k+1}}$ and the source distribution is p_{β_k}
- The normalizing constant U in $f(x) = e^{-E(x)}/U$ can be efficiently estimated by importance sampling

$$U = \int e^{-E(x)} \, dx = E_{X \sim h(x)} exp[-E(x) - \log h(X)]$$

The L^2 Flow Sampler



Algorithm 3 The L^2 sampler.

Input: Target distribution f with energy function $E(x)$, invertible neural network T_θ with initial parameter value $\theta^{(0)}$, batch size M, step sizes $\{\alpha_k\}$

Output: Neural network parameters $\hat{\theta}$ such that $T_{\hat{\theta}\sharp}\mu_0 \approx f$

```
1:  Let $h(x)$ be the density function of $T_{\theta^{(0)}\sharp}\mu_0$
2:  Generate $Z_1, \dots, Z_M \overset{\text{iid}}{\sim} \mu_0$ and set $X_i \leftarrow T_{\theta^{(0)}}(Z_i)$, $i = 1, \dots, M$
3:  Set $\hat{U} \leftarrow M^{-1} \sum_{i=1}^{M} \exp\{-E(X_i) - \log h(X_i)\}$
4:  for $k = 1, 2, \dots$ do
5:      Let $g_\theta(x)$ be the density function of $T_{\theta\sharp}\mu_0$
6:      Generate $Z_1, \dots, Z_M \overset{\text{iid}}{\sim} \mu_0$ and define $X_i = T_\theta(Z_i)$, $i = 1, \dots, M$
7:      Define $L(\theta) = M^{-1} \sum_{i=1}^{M} \left[ g_\theta(X_i) - 2\exp\{-E(X_i)\}/\hat{U} \right]$
8:      Set $\theta^{(k)} \leftarrow \theta^{(k-1)} - \alpha_k \nabla_\theta L(\theta)|_{\theta=\theta^{(k-1)}}$
9:      if $L(\theta)$ converges then
10:         return $\hat{\theta} = \theta^{(k)}$
11:     end if
12: end for
```

Theoretical Analysis

- To transport p_{β_k} to $p_{\beta_{k+1}}$, we solve a Wasserstein gradient flow with respect to the (squared) L^2 distance,

$$\mathcal{G}(\cdot) = \int (\cdot - p(x))^2 \mathrm{d}x$$

Theorem (informal)

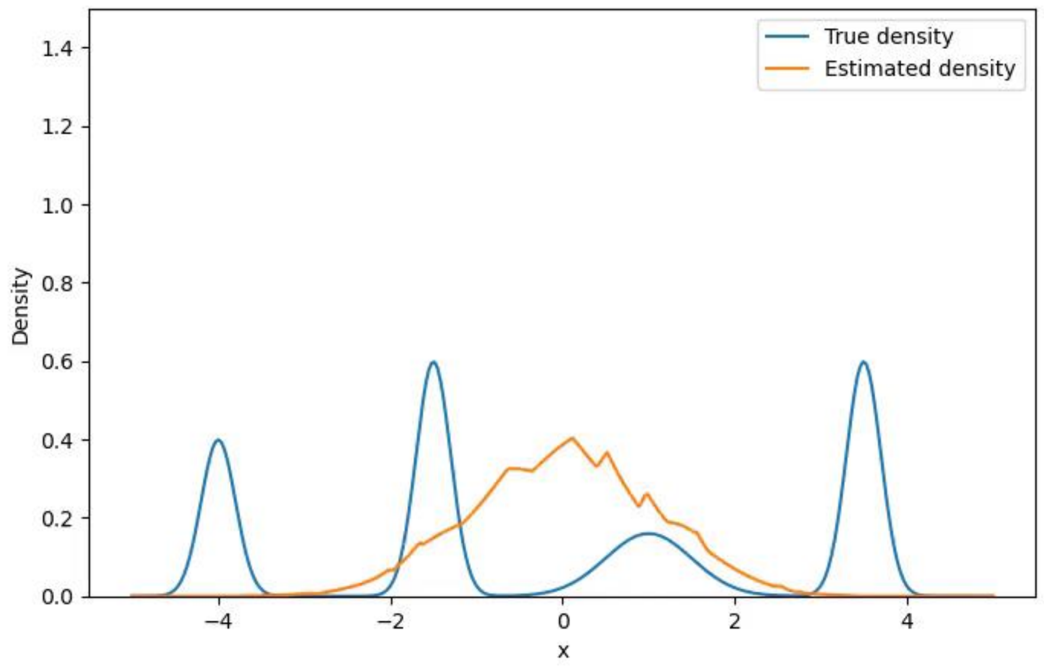
Under some regularity conditions on $p(x)$,

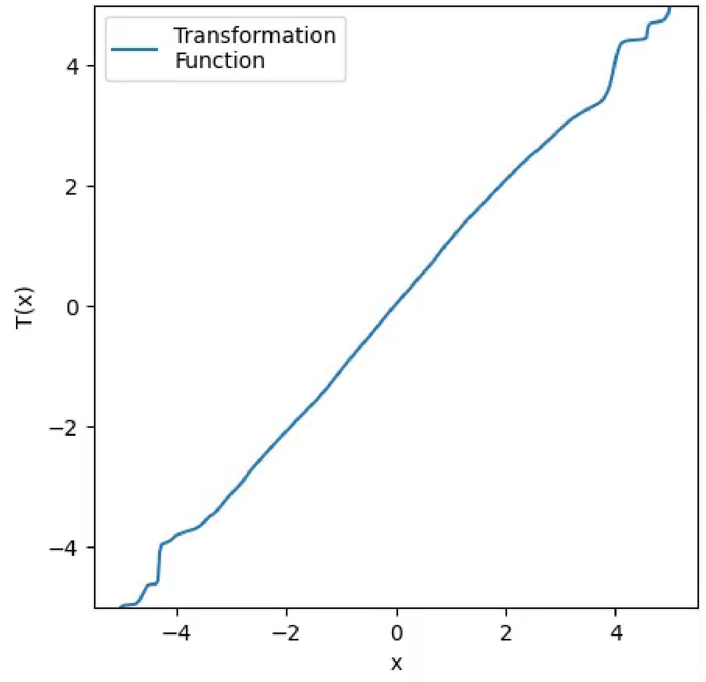
$$\mathcal{G}(p_t) \leq C \cdot |\mathrm{d}\mathcal{G}(p_t)/\mathrm{d}t|^{1/2}$$

- The gradient does not vanish as in the KL case

Tempered Distribution Flow

- Left: evolution of estimated density. Right: transformation function.



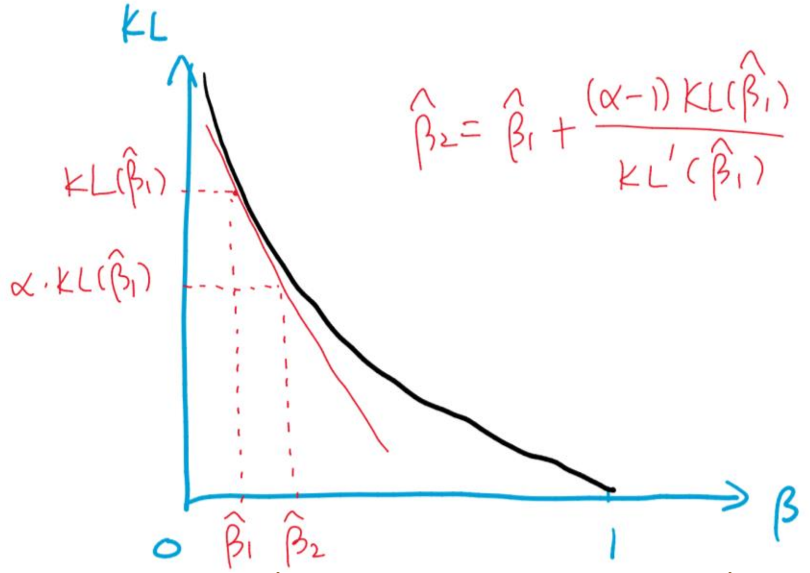


Adaptive Selection of β_t

Theorem

$p_{\beta_t}(x)$ decreases the KL divergence $\mathcal{F}(\cdot) = \mathrm{KL}(\cdot\,\|p)$ along the tempering curve, i.e., $\mathrm{d}\mathcal{F}(p_{\beta_t})/\mathrm{d}t \le 0$.

- Select $\beta_1, \beta_2, \ldots$ to smoothly reduce $\mathcal{F}(p_{\beta_k})$
- For example, pick β_{k+1} based on β_k such that $\mathcal{F}(p_{\beta_{k+1}}) \approx 0.8 \cdot \mathcal{F}(p_{\beta_k})$


KL
$KL(\hat\beta_1)$
$\alpha \cdot KL(\hat\beta_1)$
$\hat\beta_2 = \hat\beta_1 + \frac{(\alpha-1)KL(\hat\beta_1)}{KL'(\hat\beta_1)}$
0
$\hat\beta_1$
$\hat\beta_2$
1
β

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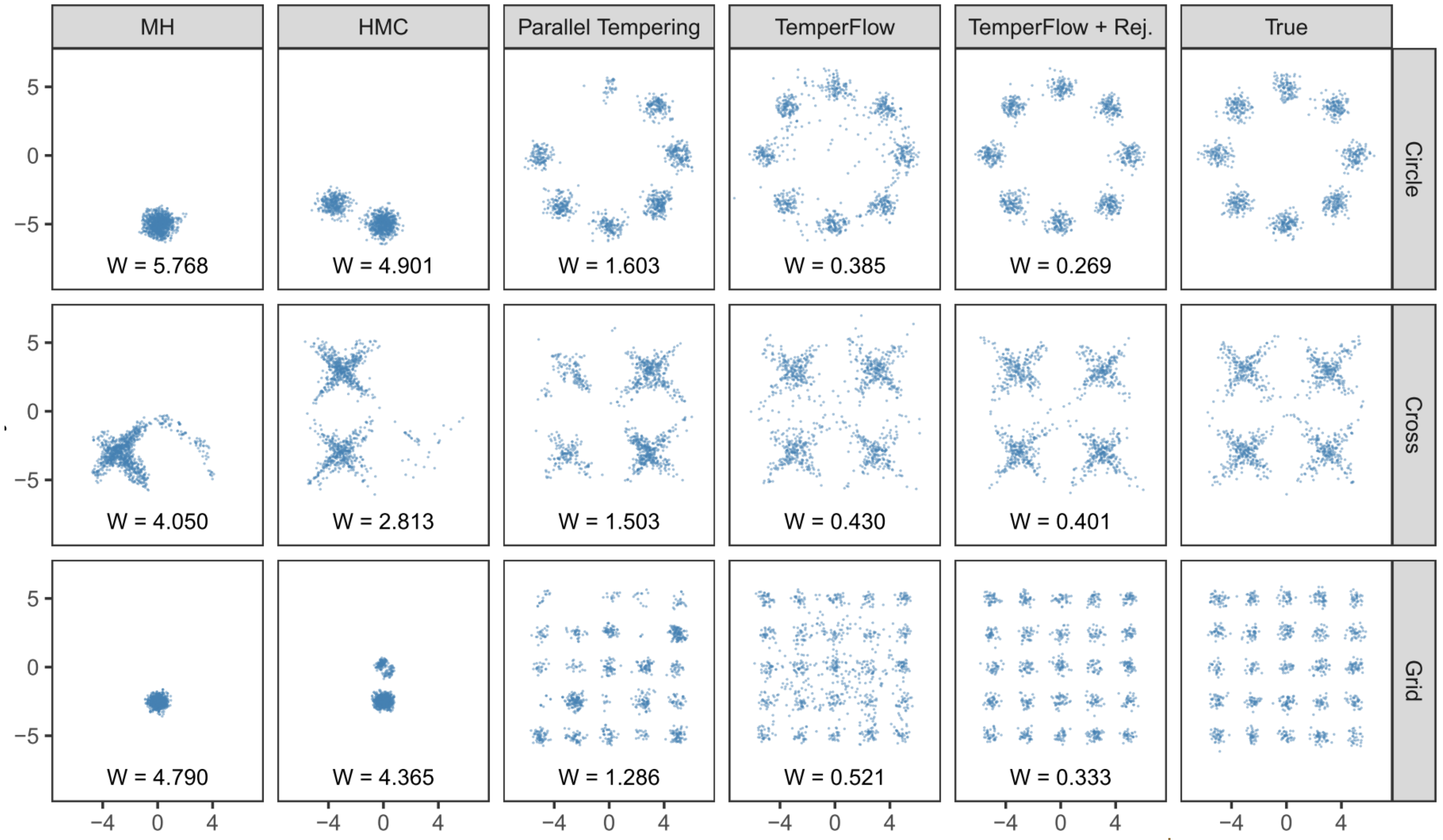
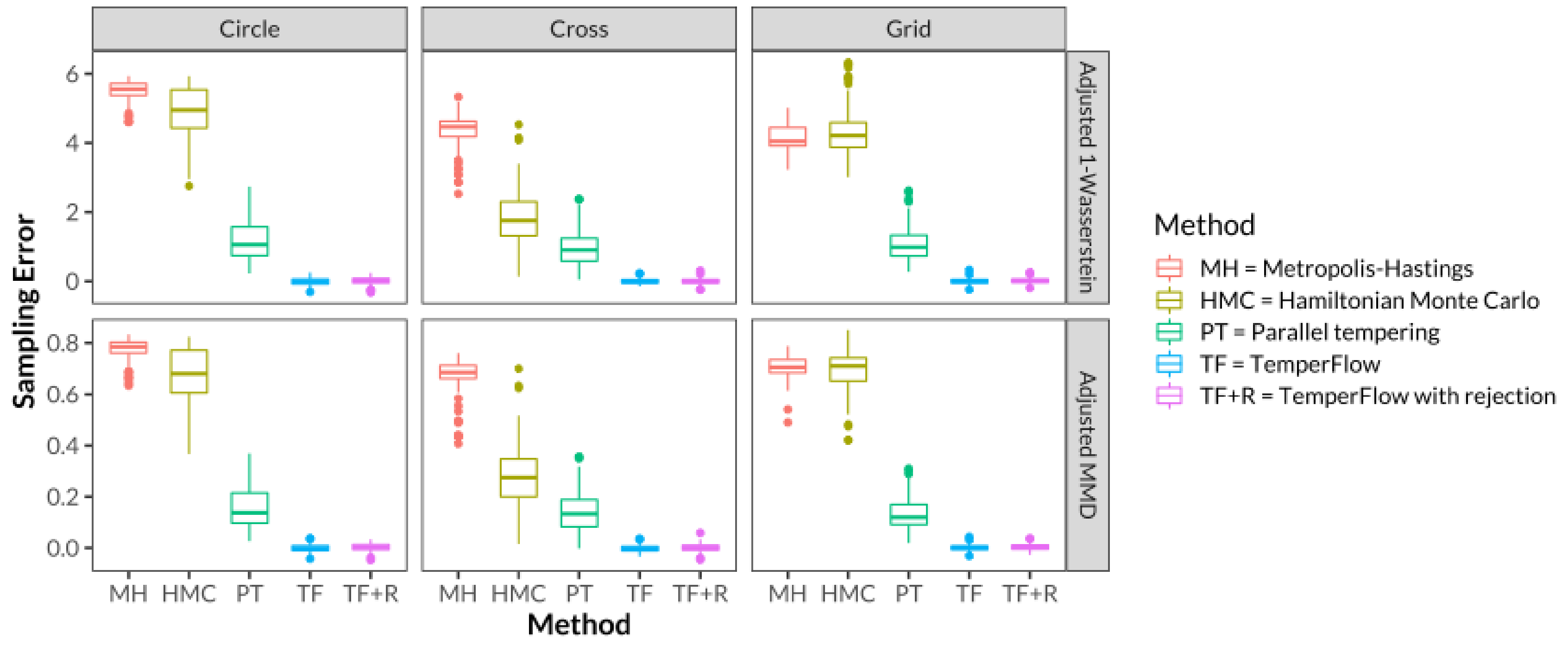
❑ Tempered Distribution Flow

- Background
- Sampling via Measure Transport
- Tempered Distribution Flow
- Experiments and Summary

Gaussian Mixture



Gaussian Mixture



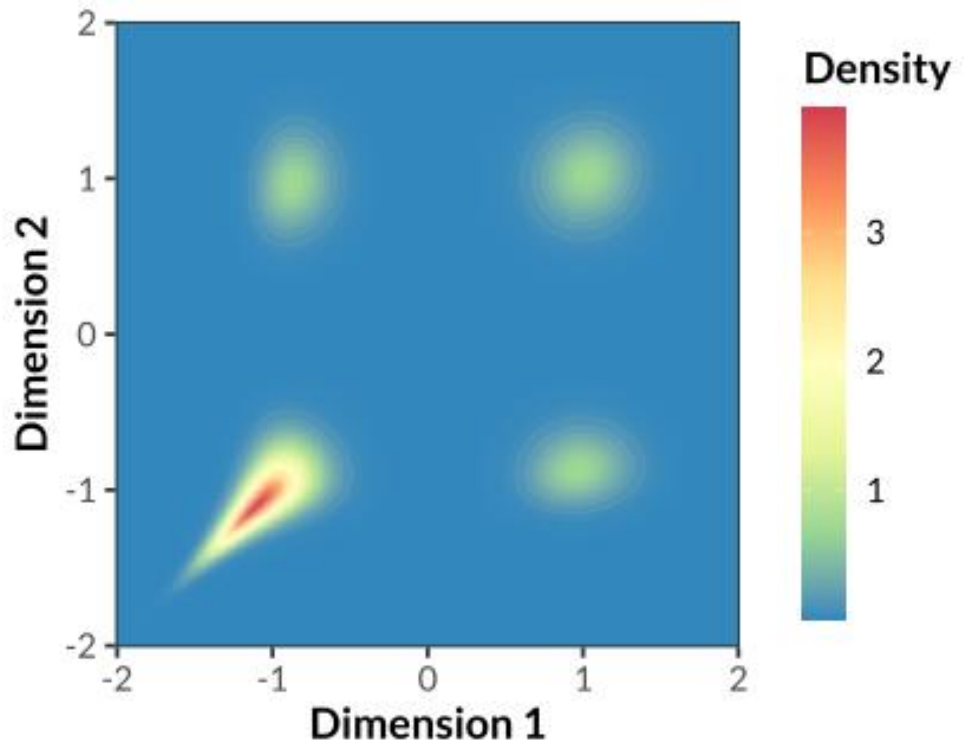
Copula-Generated Distribution

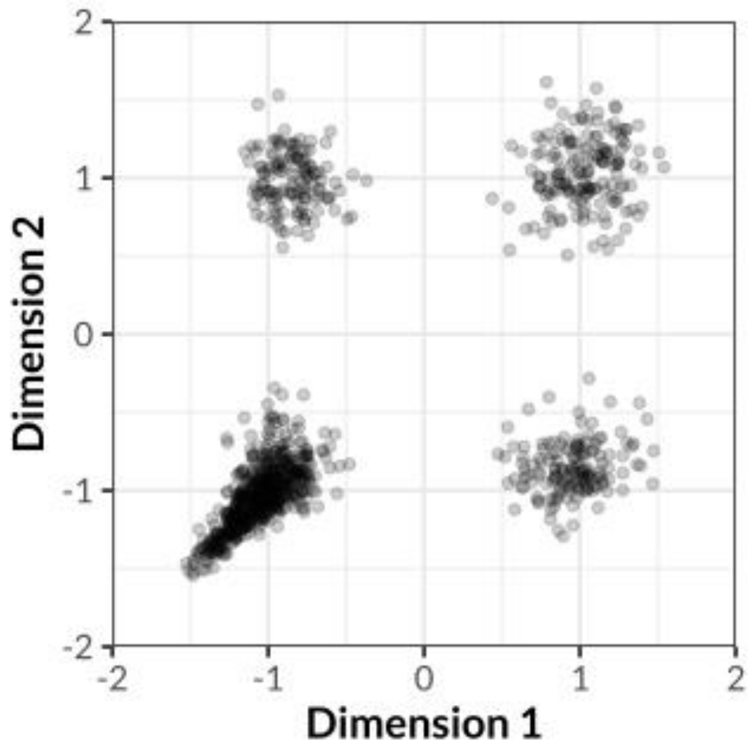
- The target distribution is

$$F(x_1, \dots, x_d) = C(F_1(x_1), \dots, F_d(x_d))$$

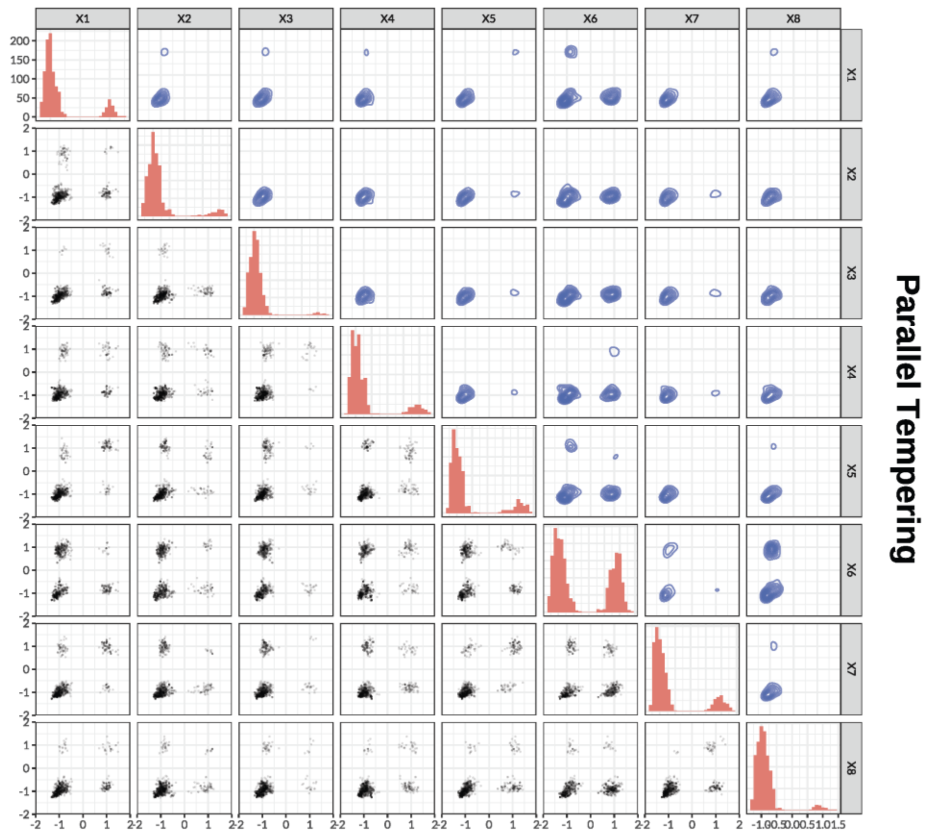
- The first s marginals are Gaussian mixtures; the remaining are normal distributions
- C is the Clayton copula
- The target distribution has 2^s modes; every pair (X_i, X_j) is correlated

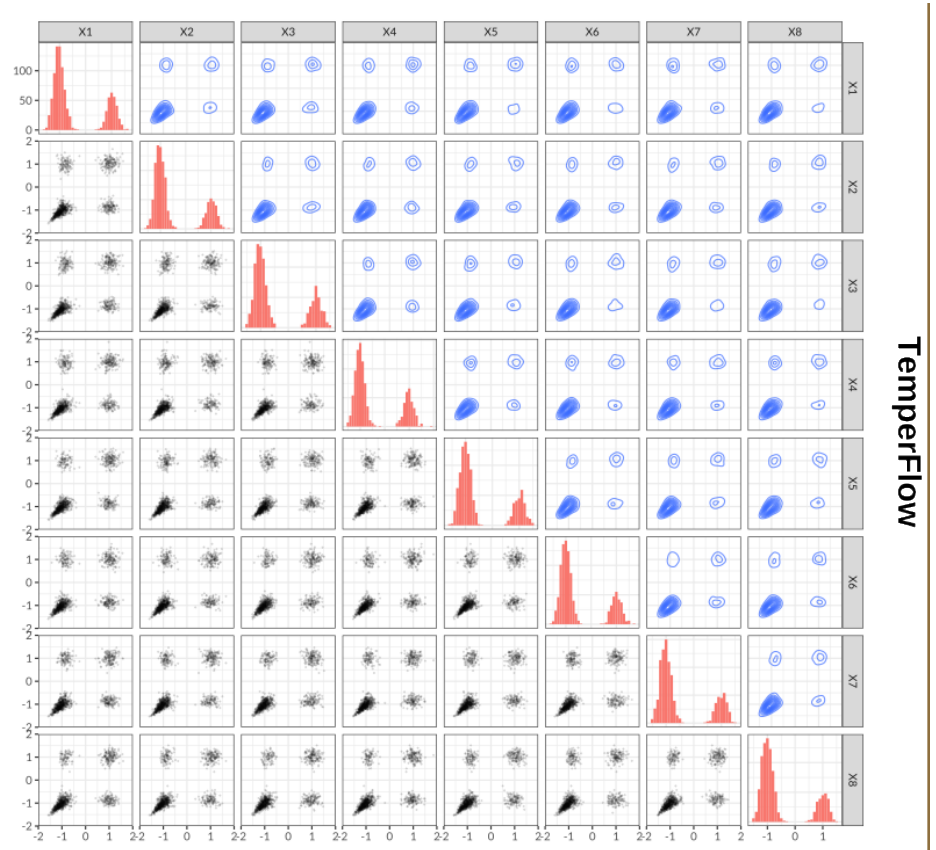
Copula-Generated Distribution





Copula-Generated Distribution





Copula-Generated Distribution

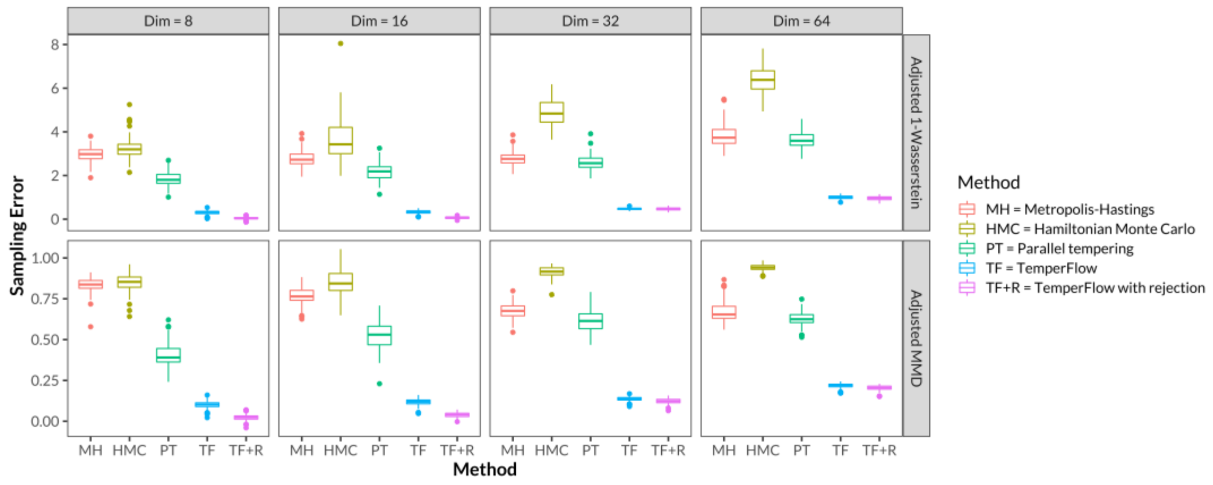


Table S1: Computing time for different sampling methods and dimensions. The first row shows the training time of TemperFlow, and the number in the paranthesis is the number of adaptive β's used in Algorithm 2. Remaining rows show the time to generate 10,000 points by each algorithm. All timing values are in seconds.

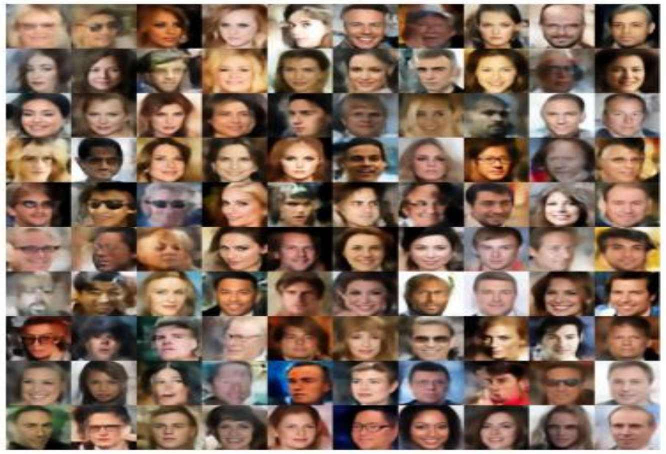
	$p = 8$	$p = 16$	$p = 32$	$p = 64$
(TemperFlow Training)	133.7 (17)	309.9 (21)	598.6 (22)	1475.5 (30)
TemperFlow/10^4	0.00206	0.00449	0.00899	0.0169
TemperFlow+Rej./10^4	0.0148	0.0263	0.0547	0.0928
MH/10^4	11.8	16.0	15.8	15.6
HMC/10^4	80.9	133.0	131.0	130.0
Parallel tempering/10^4	24.9	32.2	32.5	31.9

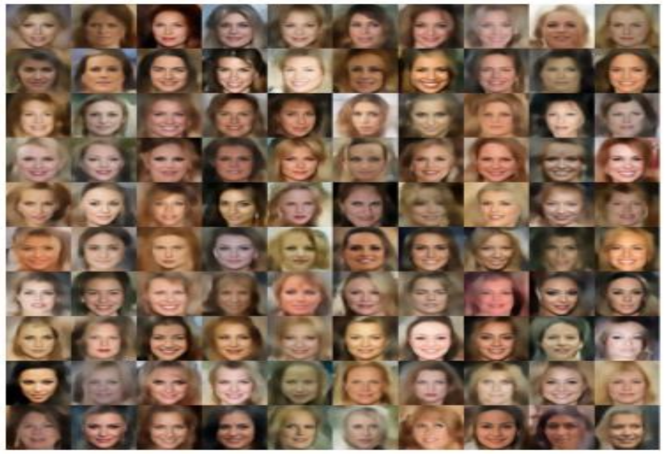
CelebA Data

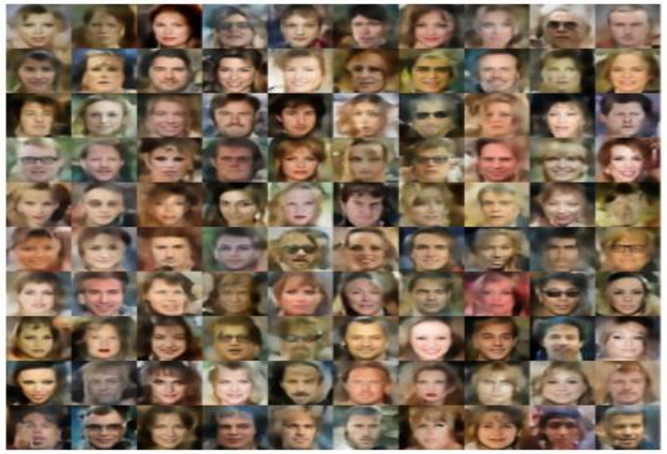
- Colored face images 64X64X3
- We take a subset: female wearing glasses (2677 images), female without gasses (20000 images), male wearing glasses (10346 images), and male without glasses (20000 images)
- A Deep Generative Model:

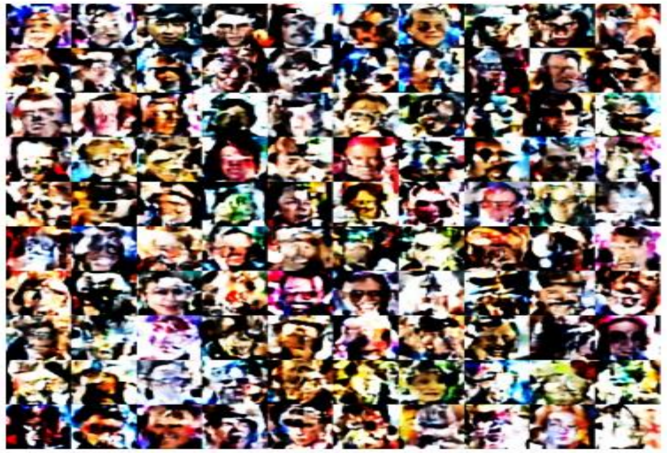
  (E100, G100->12288)

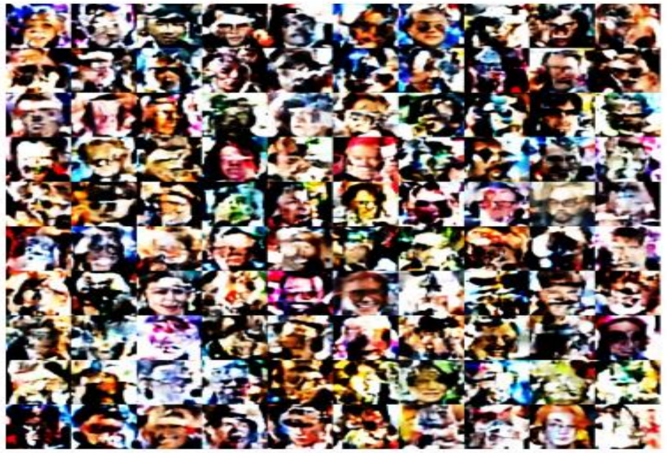
CelebA: Energy Based Models

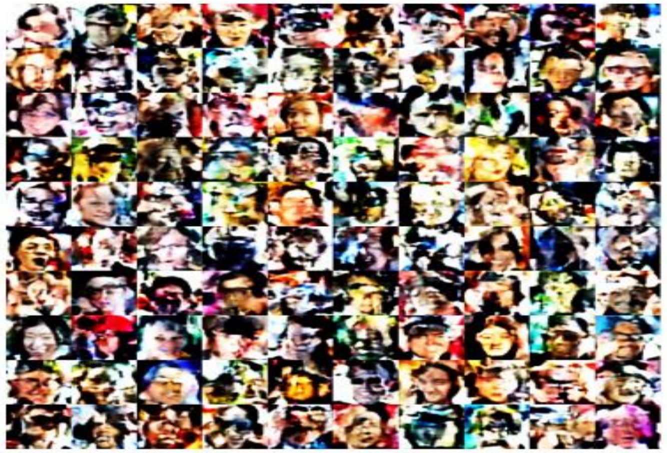

(a) True model sample


(b) KL sampler


(c) TemperFlow


(d) Metropolis–Hastings


(e) Hamiltonian Monte Carlo

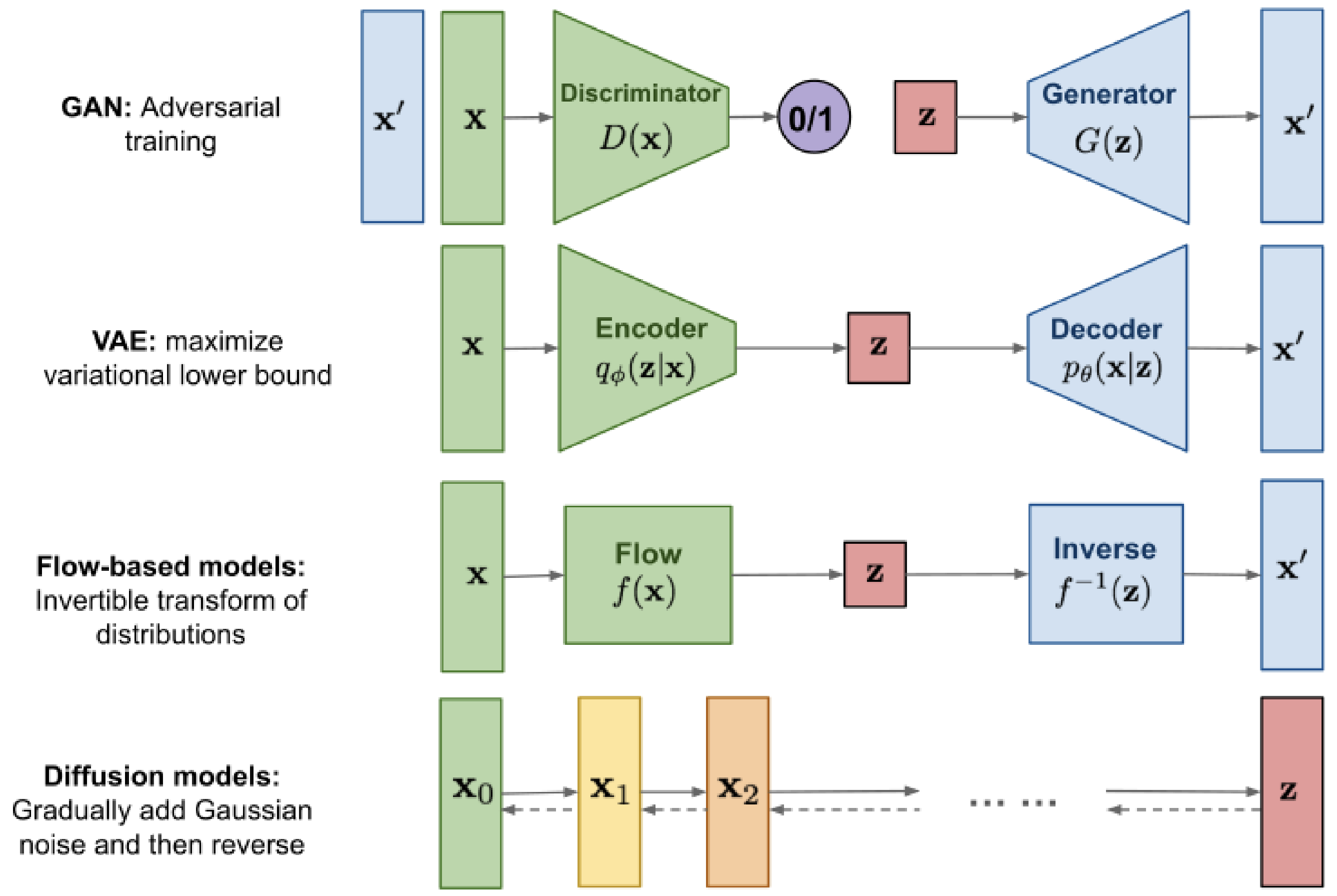

(f) Parallel tempering

Summary

- Sampling is a fundamental yet challenging task in statistics and machine learning
- Modern deep learning techniques can help solve classical sampling problems
- Many interesting and open problems to be explored

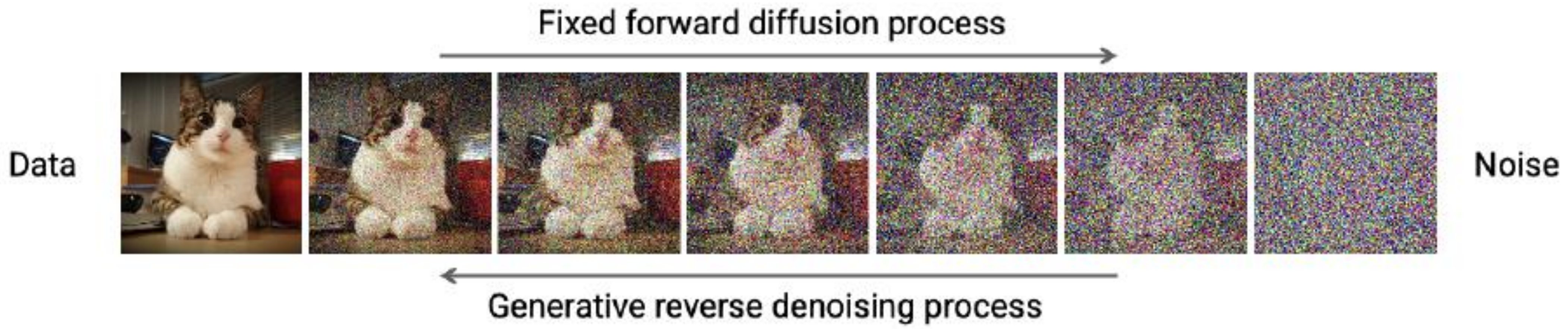
Content

GAN, VAE, Flow, and DM



GAN: Adversarial training
$\mathbf{x}'$
$\mathbf{x}$
Discriminator $D(\mathbf{x})$
0/1
$\mathbf{z}$
Generator $G(\mathbf{z})$
$\mathbf{x}'$
VAE: maximize variational lower bound
$\mathbf{x}$
Encoder $q_\phi(\mathbf{z}|\mathbf{x})$
$\mathbf{z}$
Decoder $p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$
Flow-based models: Invertible transform of distributions
$\mathbf{x}$
Flow $f(\mathbf{x})$
$\mathbf{z}$
Inverse $f^{-1}(\mathbf{z})$
$\mathbf{x}'$
Diffusion models: Gradually add Gaussian noise and then reverse
$\mathbf{x}_0$
$\mathbf{x}_1$
$\mathbf{x}_2$
... ...
$\mathbf{z}$

Denoising Diffusion Models

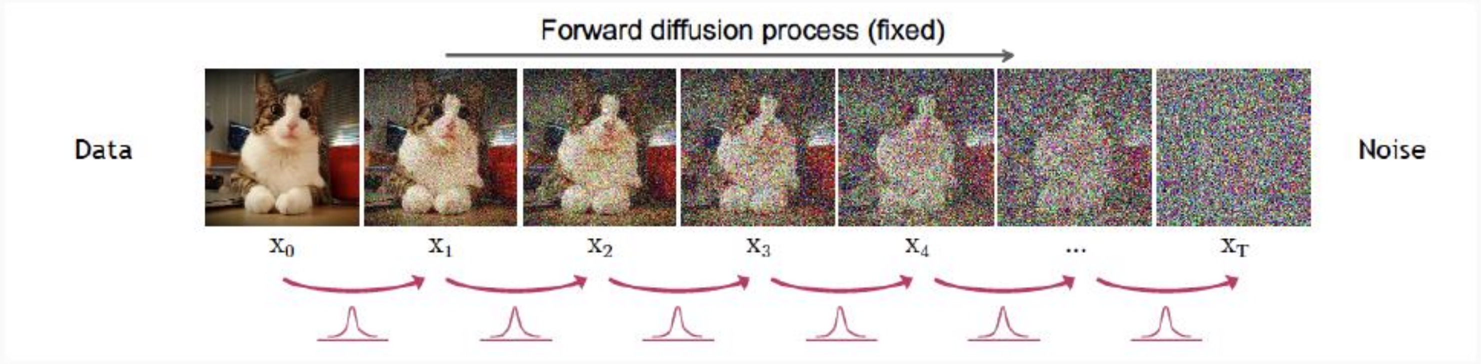

Fixed forward diffusion process
Data
Noise
Generative reverse denoising process

Forward Diffusion Process

- The latent dimension is exactly equal to the data dimension
- The structure of the latent encoder at each timestep is not learned; it is pre-defined as a linear Gaussian model. In other words, it is a Gaussian distribution centered around the output of the previous timestep
- The Gaussian parameters of the latent encoders vary over time in such a way that the distribution of the latent at final timestep T is a standard Gaussian

Forward Diffusion Process

The formal definition of the forward process in T steps:

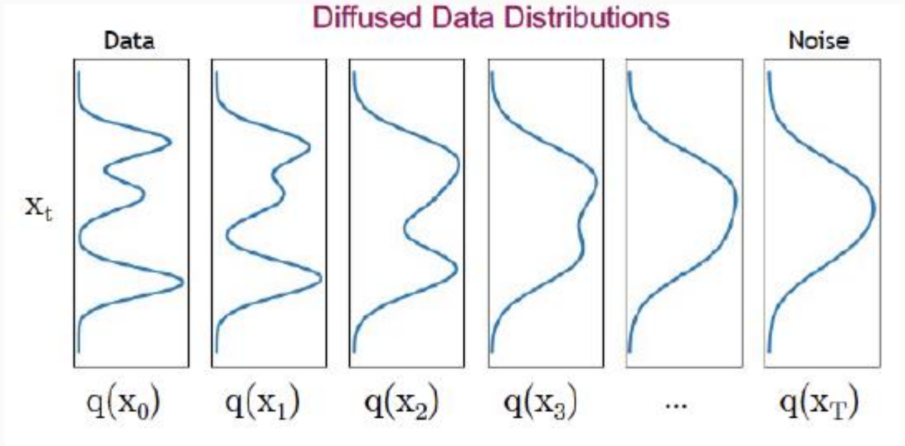


$$x_t \big| x_{t-1} \sim N(\sqrt{1-\beta_t}\; x_{t-1}, \beta_t I)$$

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$

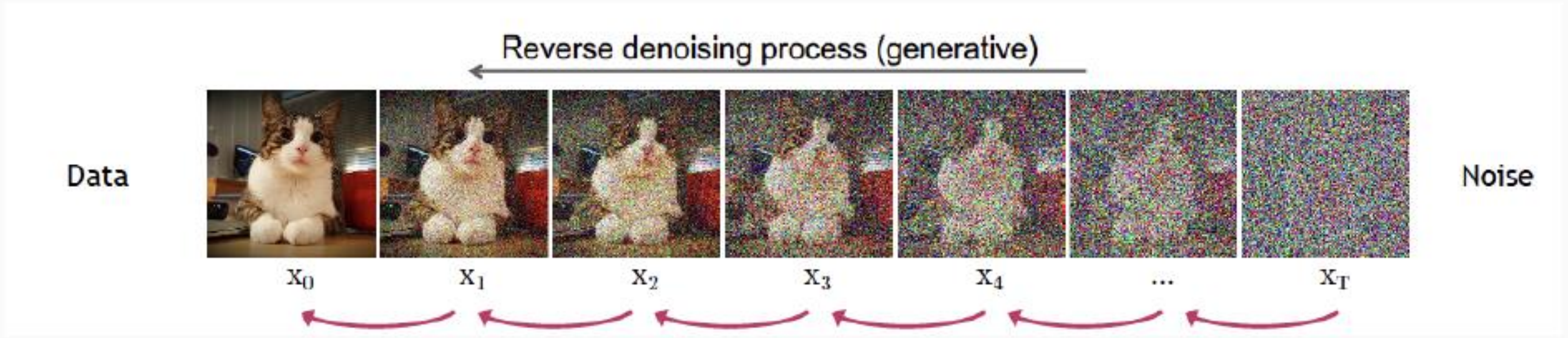
Diffusion Kernel

- Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$
- $x_t | x_0 \sim N(\sqrt{\bar{\alpha}_t}\, x_0, (1-\bar{\alpha}_t)I)$
- For sampling: $x_t = \sqrt{\bar{\alpha}_t}\, x_0 + \sqrt{1-\bar{\alpha}_t}\, \epsilon$, where $\epsilon \sim N(0, I)$
- β_t is designed such that $\bar{\alpha}_T \to 0$ and $x_T | x_0 \dot{\sim} N(0, I)$
- Marginally, $q(x_t) = \int q(x_0) q(x_t | x_0) dx_0$



Reverse Denoising Process

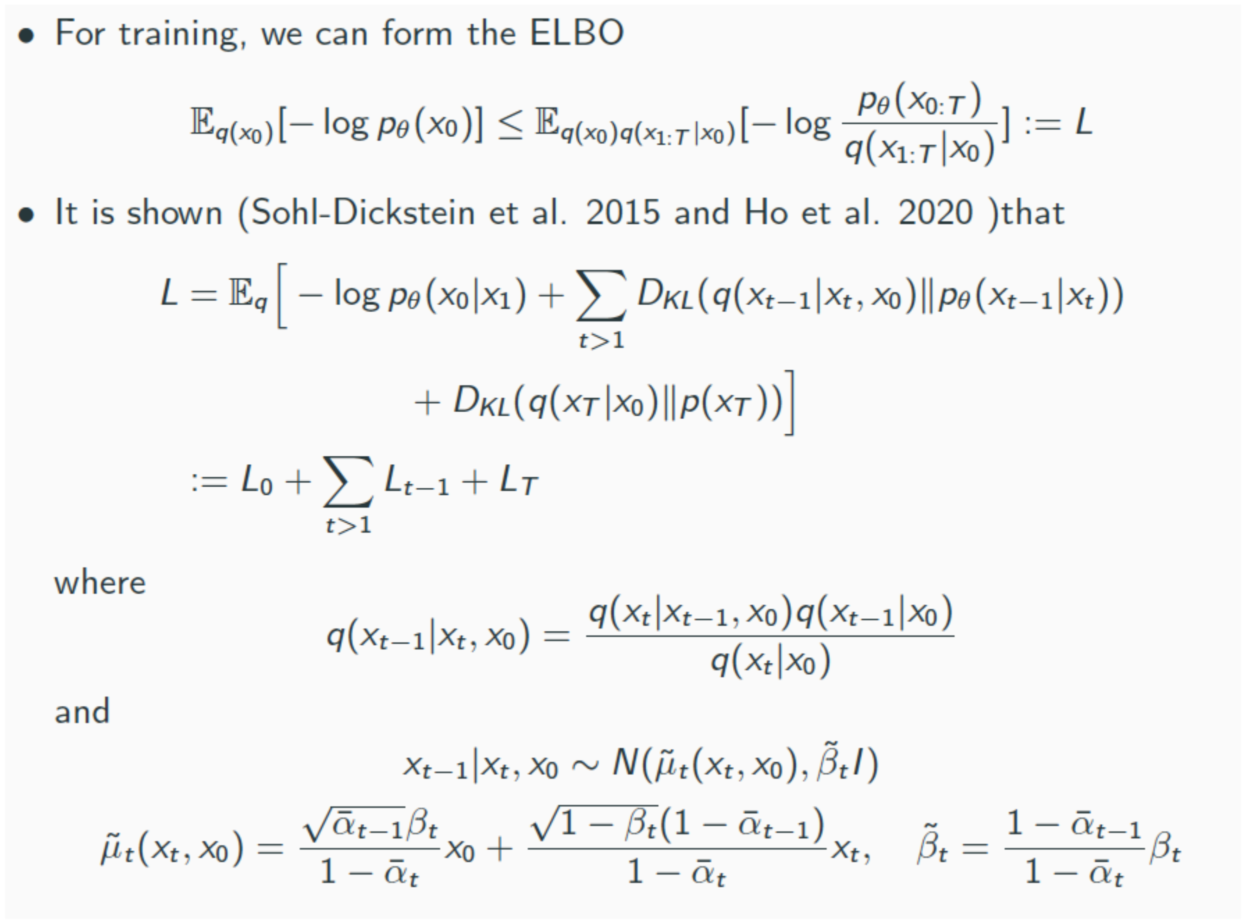
Formal definition of reverse processes in T steps:



$$x_T \sim N(0, I), \quad x_{t-1}|x_t \sim N(\mu_\theta(x_t, t), \sigma_t^2 I)$$

$$p_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

Learning Denoising Model



- For training, we can form the ELBO

$$\mathbb{E}_{q(x_0)}[-\log p_\theta(x_0)] \le \mathbb{E}_{q(x_0)q(x_{1:T}|x_0)}[-\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)}] := L$$

- It is shown (Sohl-Dickstein et al. 2015 and Ho et al. 2020)that

$$\begin{aligned} L &= \mathbb{E}_q\Big[-\log p_\theta(x_0|x_1) + \sum_{t>1} D_{KL}(q(x_{t-1}|x_t, x_0)\|p_\theta(x_{t-1}|x_t)) \\ &\qquad + D_{KL}(q(x_T|x_0)\|p(x_T))\Big] \\ &:= L_0 + \sum_{t>1} L_{t-1} + L_T \end{aligned}$$

where

$$q(x_{t-1}|x_t, x_0) = \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_t|x_0)}$$

and

$$x_{t-1}|x_t, x_0 \sim N(\tilde{\mu}_t(x_t, x_0), \tilde{\beta}_t I)$$

$$\tilde{\mu}_t(x_t, x_0) = \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}x_0 + \frac{\sqrt{1-\beta_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}x_t, \quad \tilde{\beta}_t = \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

Learning Denoising Model

- $\mathbb{E}_{q_{x_1|x_0}}[-\log p_\theta(x_0|x_1)]$ can be interpreted as a reconstruction term; like its analogue in the ELBO of a vanilla VAE, this term can be approximated and optimized using a Monte Carlo estimate.
- $D_{KL}(q(x_T|x_0)||p(x_T))$ represents how close the distribution of the final noisified input is to the standard Gaussian prior. It has no trainable parameters, and is also equal to zero under our assumptions.
- $\mathbb{E}_{q(x_t|x_0)}[D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))]$ is a denoising matching term. We learn desired denoising transition step $p_\theta(x_{t-1}|x_t)$ as an approximation to tractable, ground-truth denoising transition step $q(x_{t-1}|x_t, x_0)$.

Reparameterizing the Denoising Model

- Due to the normal distributions, the KL divergence has a simple form:

$$L_{t-1} = D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) = \mathbb{E}_q\left[\frac{1}{2\sigma_t^2}\|\tilde{\mu}_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2\right] + C$$

- Ho et al. (2020) observe that:

$$\tilde{\mu}_t(x_t, x_0) = \frac{1}{\sqrt{1-\beta_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon)$$

- Ho et al. (2020) propose to represent the mean of the denoising model using a noise-prediction network:

$$\mu_\theta(x_t, t) = \frac{1}{\sqrt{1-\beta_t}}(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t))$$

Reparameterizing the Denoising Model

- With this reparametrization

$$L_{t-1} = \mathbb{E}_{x_0 \sim q(x_0), \epsilon \sim N(0,I)} \left[\frac{\beta_t^2}{2\sigma_t^2(1-\beta_t)(1-\bar{\alpha}_t)} ||\epsilon - \epsilon_\theta(x_t, t)||^2 \right] + C$$

where $x_t = \sqrt{\bar{\alpha}_t}\ x_0 + \sqrt{1 - \bar{\alpha}_t \epsilon}$

- Ho et al. (2020) observe that simply setting the time dependent coefficient being 1 improves sample quality. So, they propose to use:

$$L_{\text{simple}} = \mathbb{E}_{x_0 \sim q(x_0), \epsilon \sim N(0,I), t \sim Unif[1,T]} \left|\left| \epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\ x_0 + \sqrt{1 - \bar{\alpha}_t}\ \epsilon, t) \right|\right|^2$$

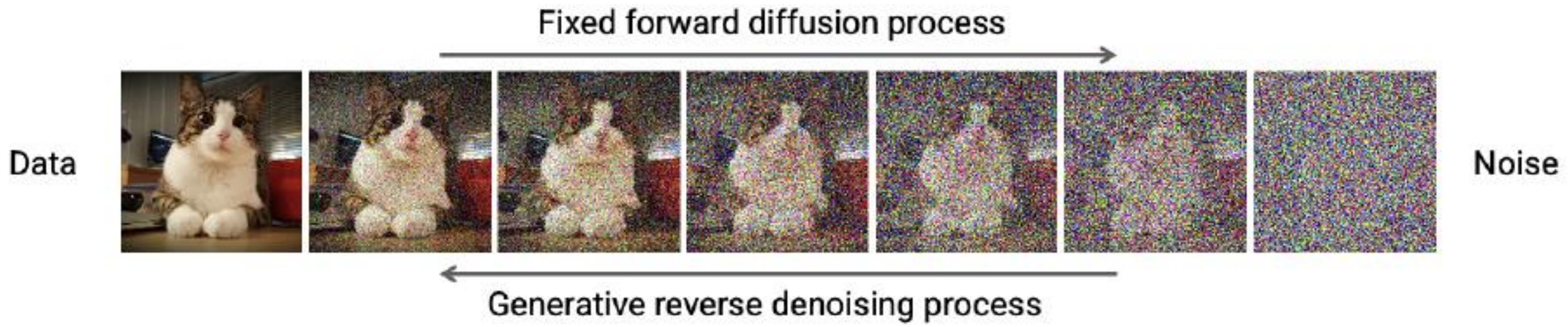
Algorithm

Algorithm 1 Training

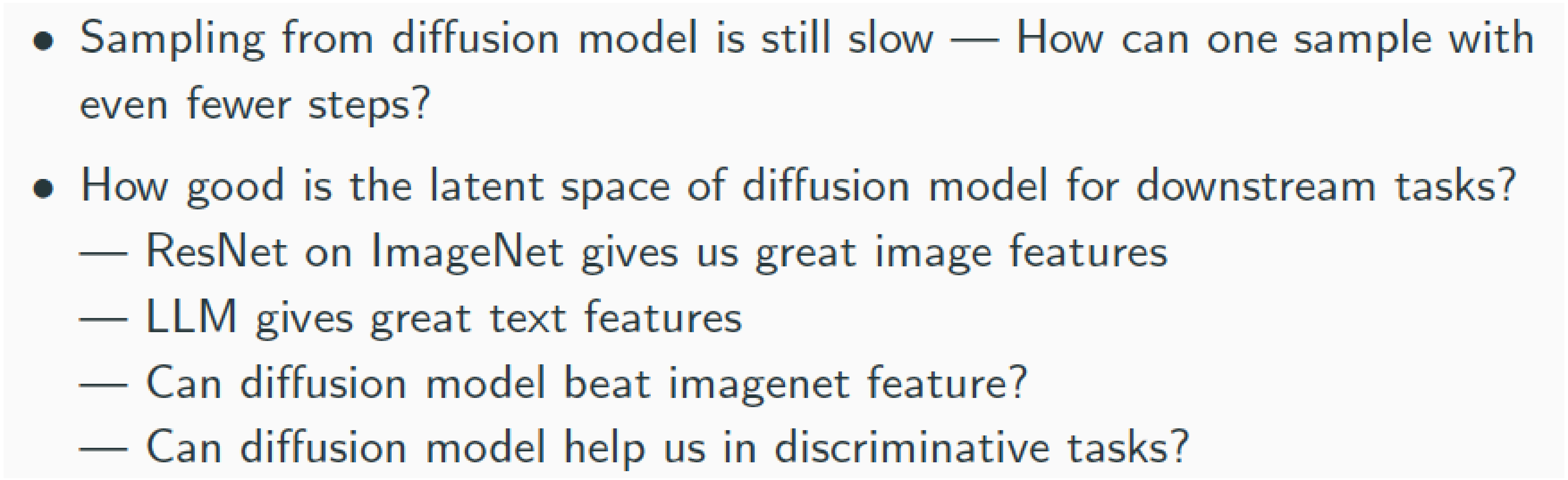
```
1: repeat
2:   $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3:   $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
4:   $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5:   Take gradient descent step on
         $\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\boxed{\sqrt{\bar\alpha_t}\mathbf{x}_0 + \sqrt{1-\bar\alpha_t}\boldsymbol{\epsilon}}, t) \right\|^2$
6: until converged
```

Algorithm 2 Sampling

```
1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: for $t = T, \ldots, 1$ do
3:   $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4:   $\mathbf{x}_{t-1} = \boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar\alpha_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)} + \sigma_t \mathbf{z}$
5: end for
6: return $\mathbf{x}_0$
```


Fixed forward diffusion process
Data
Noise
Generative reverse denoising process

Open Problems



- Sampling from diffusion model is still slow — How can one sample with even fewer steps?
- How good is the latent space of diffusion model for downstream tasks?
  — ResNet on ImageNet gives us great image features
  — LLM gives great text features
  — Can diffusion model beat imagenet feature?
  — Can diffusion model help us in discriminative tasks?

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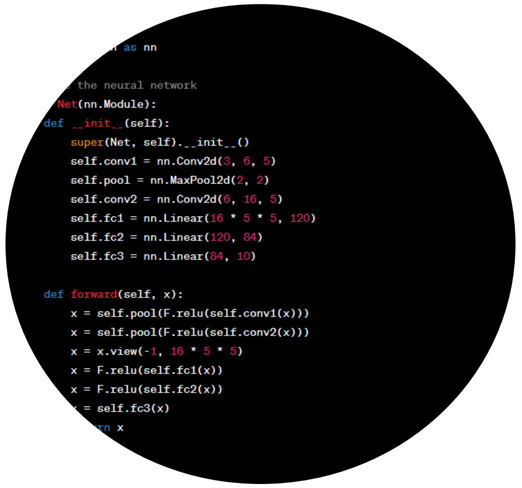
How to succeed in this course?



```
        n as nn

  e the neural network
 Net(nn.Module):
def __init__(self):
    super(Net, self).__init__()
    self.conv1 = nn.Conv2d(3, 6, 5)
    self.pool = nn.MaxPool2d(2, 2)
    self.conv2 = nn.Conv2d(6, 16, 5)
    self.fc1 = nn.Linear(16 * 5 * 5, 120)
    self.fc2 = nn.Linear(120, 84)
    self.fc3 = nn.Linear(84, 10)

def forward(self, x):
    x = self.pool(F.relu(self.conv1(x)))
    x = self.pool(F.relu(self.conv2(x)))
    x = x.view(-1, 16 * 5 * 5)
    x = F.relu(self.fc1(x))
    x = F.relu(self.fc2(x))
     = self.fc3(x)
      rn x
```

Practice

Explore

Visualize

Discuss

Ask