

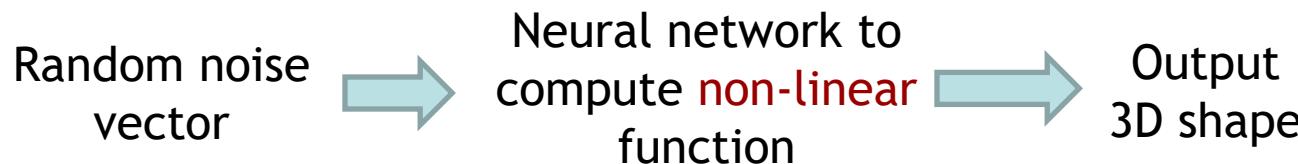
CMSC740

Advanced Computer Graphics

Matthias Zwicker
Fall 2025

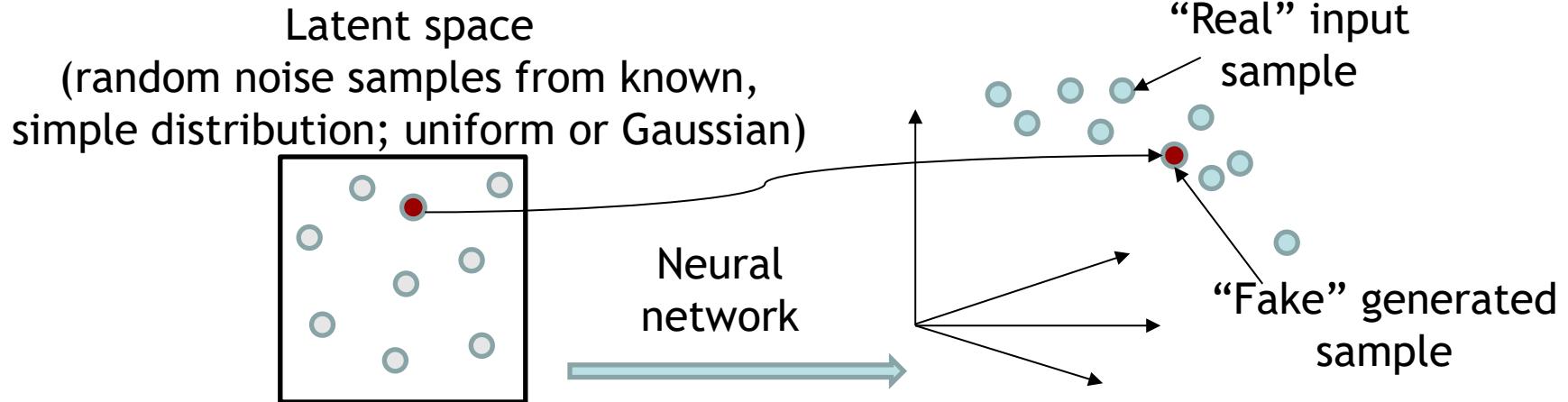
Unsupervised, generative models

- Given: database of objects
- Goal: mechanism that produces random new objects that “look just like objects from the database”
- “Random (Gaussian, uniform) noise -> neural network -> object”, where object can be almost anything (image, video, 3D shape, text, etc.)



- Applications in graphics: automatically generate images, videos, shapes, textures, animations, ...

Abstract point of view



Objects in database interpreted as
points in high dimensional space
(images, shapes, etc.), i.e., samples
of non-uniform probability density

- Generative model: mechanism (neural network) that maps random samples from latent space to points in high dimensional space, such that **distribution (density) of generated points matches distribution of given data**
- Applications: generate arbitrary amounts of new data samples that “look like” samples from given data distribution (images, video, 3D shapes, text, etc.)

Examples

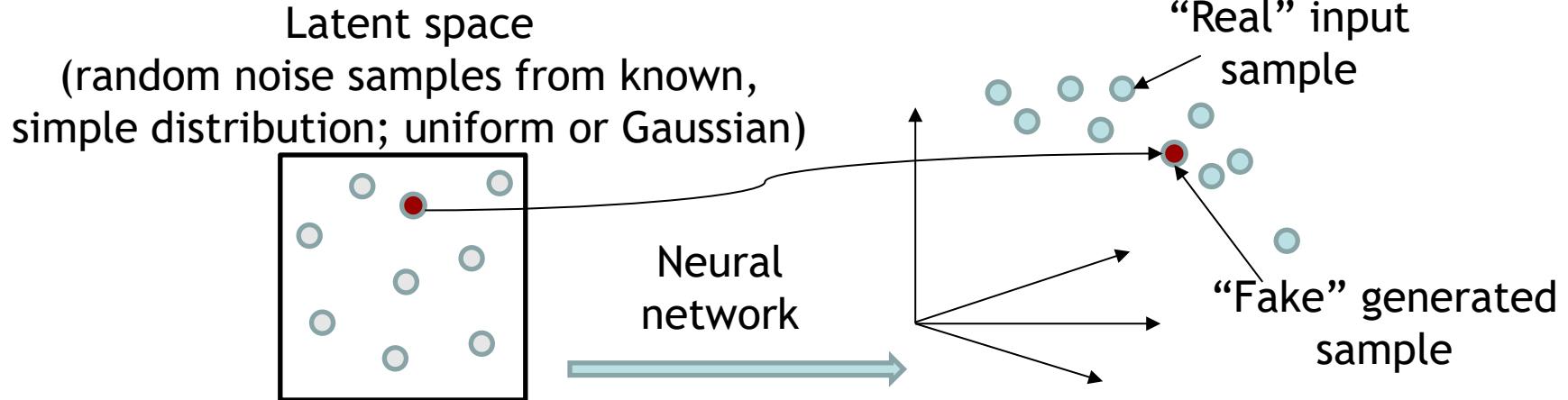


StyleGan (2018) samples, input distribution given by millions of facial images
<https://en.wikipedia.org/wiki/StyleGAN>

Stable diffusion (2022), input distribution given by hundreds of millions of internet images
https://en.wikipedia.org/wiki/Stable_Diffusion

In practice, often **conditional** generative modeling: provide additional input (condition, such as text label) to model, which then samples from conditional density; same techniques generally apply to unconditional and conditional generative modeling

Abstract point of view



Objects in database interpreted as
points in high dimensional space
(images, shapes, etc.), i.e., samples
of non-uniform probability density

- Challenge: how to formulate the training objective (loss function)?
- Notes
 - Difference between generated and true data density quantified using **divergence** (similar to metric, but to quantify similarities/distances of probability distributions)
 - Large amount of training data (millions of images, etc.) typically necessary to obtain high-quality generative models ([empirical neural scaling laws](#))

Training objectives

Alternatives

- Estimate **probability density of true and generated data as continuous functions**, then minimize difference (**divergence**) between two densities
 - Various divergence measures as generalizations of squared Euclidean distance
 - “Learning Generative Models using Denoising Density Estimators”, <https://github.com/siavashBigdeli/DDE>
- Design learning objective that **minimizes the divergence between generated and input density without explicitly estimating the densities at all**
 - Generative adversarial networks, https://en.wikipedia.org/wiki/Generative_adversarial_network
- Estimate **generated density** at any location in high dimensional data space, then maximize **log-likelihood of input data samples** produced by generator
 - Maximum likelihood estimation, https://en.wikipedia.org/wiki/Maximum_likelihood_estimation
 - Flow-based generative models, https://en.wikipedia.org/wiki/Flow-based_generative_model
 - Variational autoencoders (ELBO approximation), https://en.wikipedia.org/wiki/Variational_autoencoder
- Estimate **gradient of density (score)** of input data, then use an **iterative procedure to sample** from it
 - Langevin sampling, https://en.wikipedia.org/wiki/Metropolis-adjusted_Langevin_algorithm, <https://github.com/ermongroup/ncsn>
- Design process that iteratively maps input density to simple (Gaussian density), then learn to **invert** it using (approximate) maximum likelihood objective
 - Diffusion models, <https://lilianweng.github.io/posts/2021-07-11-diffusion-models/> (has nice overview of other models also)
 - Highly related to Langevin sampling

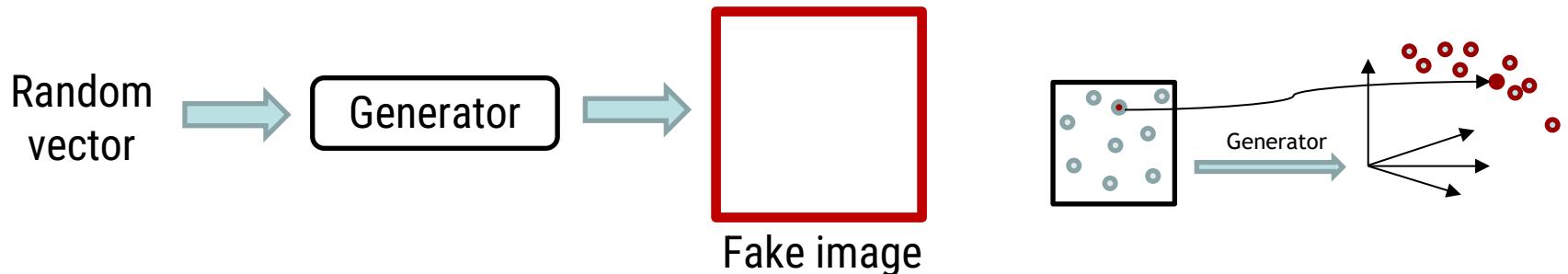
Generative Adversarial Nets

Basic mechanism introduced by Goodfellow
et al., 2014

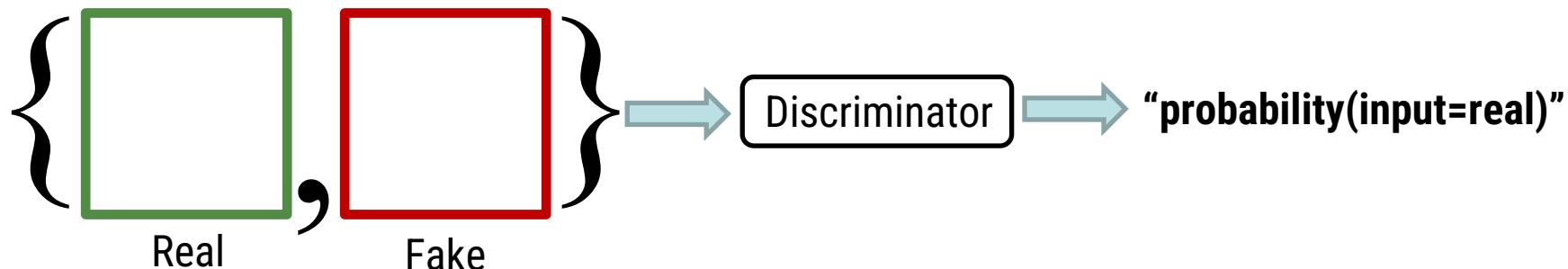
<https://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf>

Generative adversarial networks

- Generator network to synthesize objects



- Discriminator network to predict whether object is real



- Train generator and discriminator simultaneously

- Generator training objective: maximize "probability(fake input=real)" of discriminator
- Discriminator training objective: minimize "probability(fake input=real)", maximize "probability(real input = real)"

Mathematical formulation

<https://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf>

- Generator G , generated object $G(z)$, random input z from known density p_z (uniform, Gaussian)
- Discriminator D , probability that object x is real $D(x)$
- Given data density p_{data} , training objective:

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

Two-player minimax game,
optimize parameters of neural networks implementing D, G

Training

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

- Expected values in GAN objectives are integrals, evaluate using Monte Carlo sampling
 - Integrals (expected values) turn into sums over samples
- Sampling p_{data} simply by randomly selecting input sample
- Sampling $p_{\mathbf{z}}$ simple, since $p_{\mathbf{z}}$ uniform or Gaussian
- Switch between gradient descent steps to optimize generator (min in training objective), discriminator training (max)

Theoretical analysis

<https://papers.nips.cc/paper/5423-generative-adversarial-nets.pdf>

- GAN training minimizes Jensen-Shannon divergence between generated and given data distribution https://en.wikipedia.org/wiki/Jensen%E2%80%93Shannon_divergence
- Training converges such that generated = given distribution under some assumptions
 - Unlimited capacity of networks
 - Unlimited amount of training data
- Annotated proof
<https://srome.github.io/An-Annotated-Proof-of-Generative-Adversarial-Networks-with-Implementation-Notes/>

KL divergence

- Kullback-Leibler (KL) divergence (discrete case) given by relative entropy

$$D_{\text{KL}}(P \parallel Q) = \sum_{x \in \mathcal{X}} P(x) \log\left(\frac{P(x)}{Q(x)}\right)$$

- Set of discrete events X , two different probability distributions P, Q for the events x
- Interpretation
 - Assume we have optimal code for X under distribution $\textcolor{red}{Q}$ (optimal code uses fewer bits for events with higher probability)
 - KL divergence is number of extra (“wasted”) bits used when encoding events distributed according to $\textcolor{red}{P}$, in average
 - Not symmetric
- Continuous version: replace sum with integral

JS divergence

- Jensen-Shannon (JS) divergence is symmetrized version of KL divergence

$$\text{JSD}(P \parallel Q) = \frac{1}{2} D_{KL}(P \parallel M) + \frac{1}{2} D_{KL}(Q \parallel M)$$

$$M = \frac{1}{2}(P + Q)$$

- Square root of JS is a **metric**
 - Distance between identical points is zero, otherwise always positive, symmetric, triangle inequality
- GAN objective can be modified to minimize other metrics, such as Wasserstein distance
(Kantorovich-Rubinstein metric, earth mover's distance) https://en.wikipedia.org/wiki/Wasserstein_GAN

Proof steps

- For a given generator width PDF p_G , optimal discriminator is

$$D(x) = \frac{p_{data}}{p_{data} + p_G}$$

- Plugging D_G into $V(D, G)$ get $C(G)$ defined as

$$C(G) = -\log 4 + 2 \cdot JSD(p_{data} | p_G)$$

which is 0 only when $p_G = p_{data}$

- When p_G converges to p_{data} , optimal discriminator becomes

$$D_G^* = \frac{p_{data}}{p_{data} + p_G} = \frac{1}{2}$$

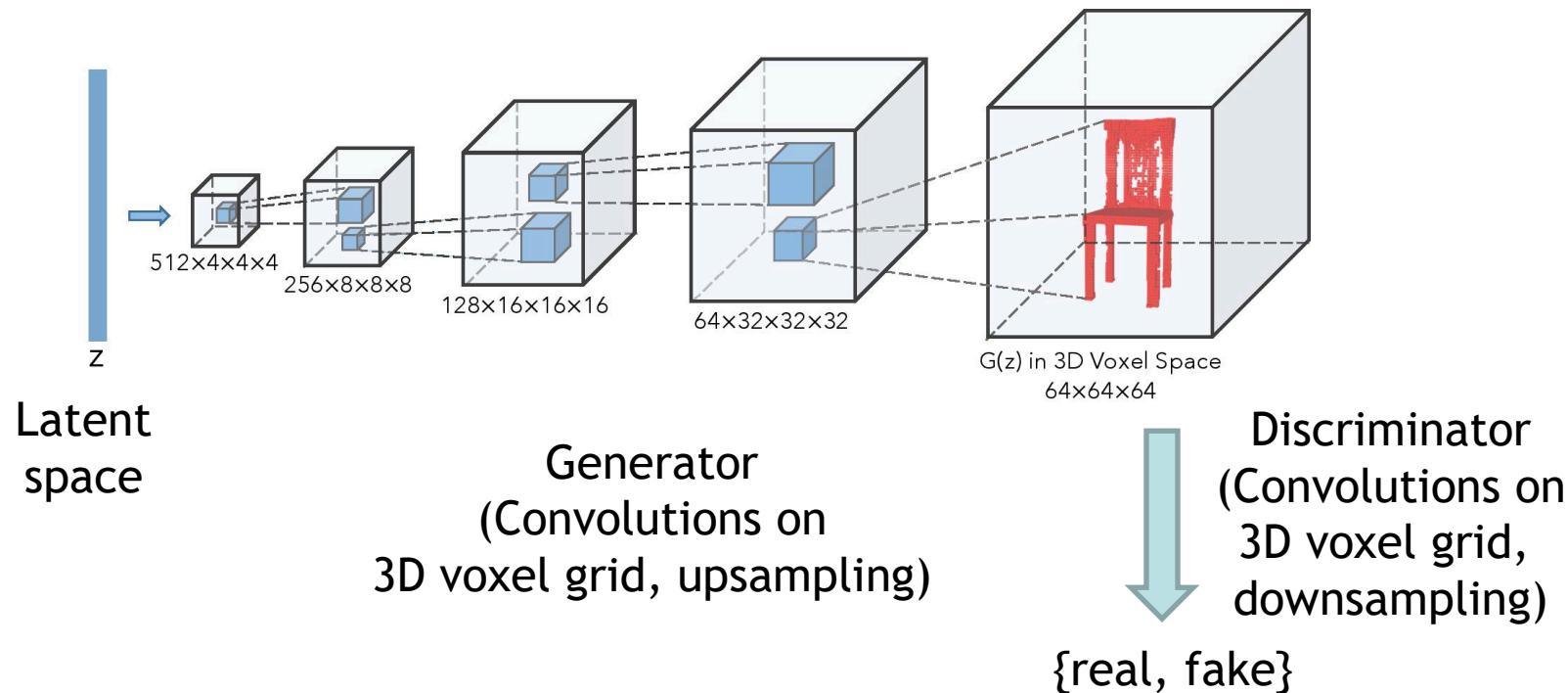
- Hence, at optimum of $V(D, G)$, $p_G = p_{data}$, $D_G^* = 1/2$
- Separate proof for convergence of training procedure

GAN applications

- Original GAN paper [Goodfellow et al. 2014] showed image generation
- Applications to many other types of data
 - Video
 - Shapes/3D models
 - Audio
 - Text
 - Medical data
 - Etc.

ShapeGAN

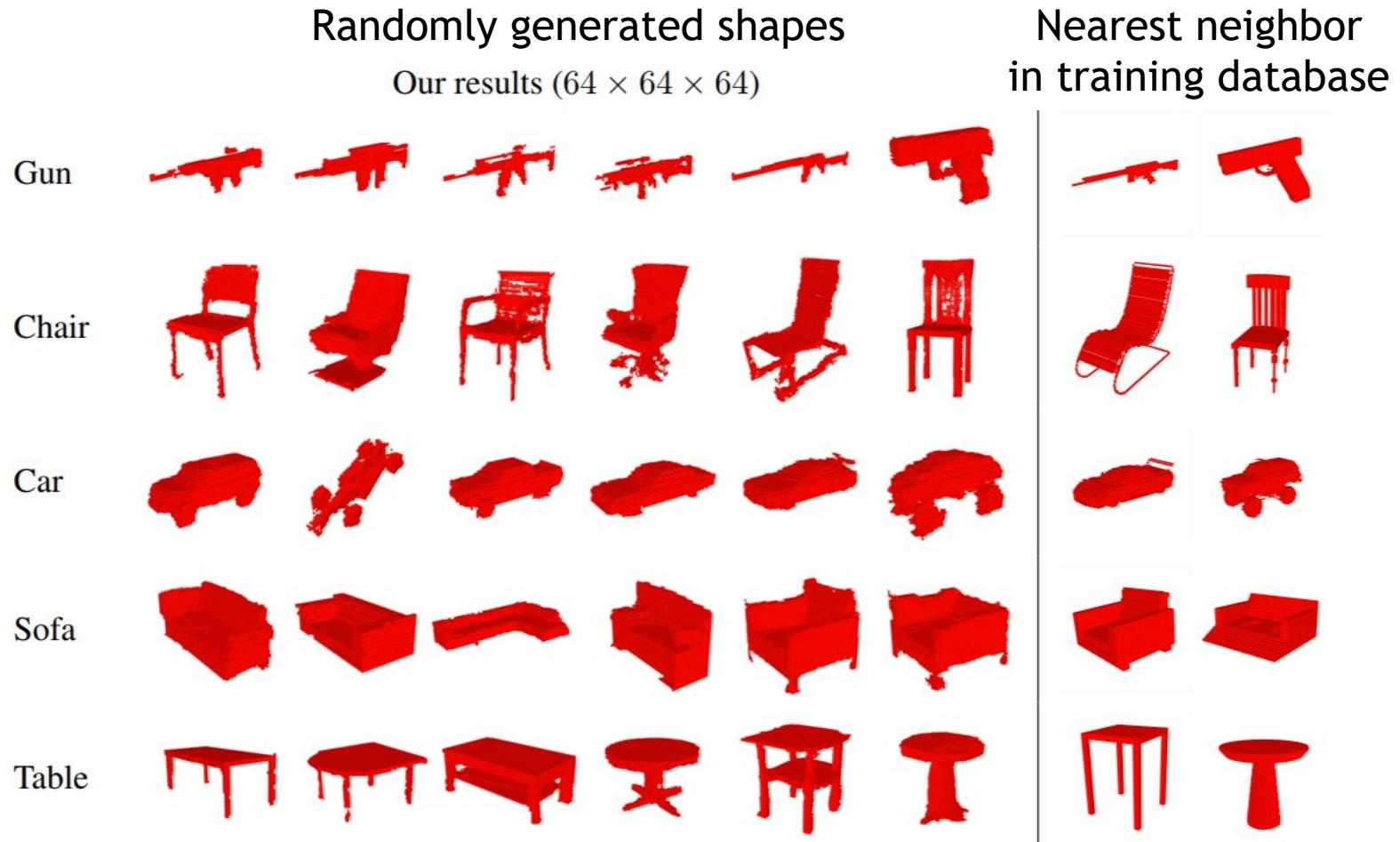
- “Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling”, Wu et al., NIPS 2016, <http://3dgan.csail.mit.edu/>



Results

<http://3dgan.csail.mit.edu/>

- Trained on ShapeNet



<http://3dgan.csail.mit.edu/>

GAN pros/cons

- Pros
 - Theoretical guarantees to obtain generator for input data distribution
 - Conceptually simple formulation and training
 - Fast sample generation (no iteration required)
- Cons
 - Training convergence unstable in practice
 - Requires manual hyper-parameter tuning
 - Tends to produce “mode collapse” (favors sample quality over diversity of samples)
- Note: theory of GANs isn’t specific to using neural networks as generators, discriminators
- Much recent research on various improvements (different discriminator/generator architectures, ways to feed random input into generator, other divergence metrics)
 - For example, StyleGAN3, NeurIPS 2021 <https://github.com/NVlabs/stylegan3>
- Illustrative animations of GAN training: <https://poloclub.github.io/ganlab/>

Diffusion Models

Basic mechanism introduced by Sohl-Dickstein et al., 2015

<https://arxiv.org/pdf/1503.03585.pdf>

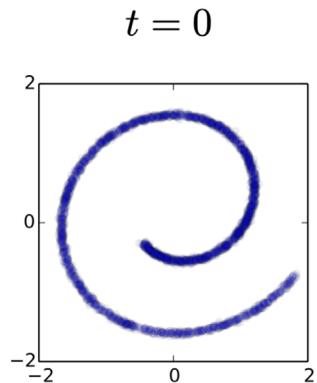
Diffusion models

- Basic idea: define forward diffusion process that iteratively maps input density to simple density (Gaussian) by adding noise, then learn to **invert** it

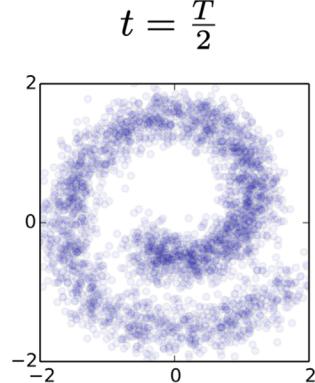
Forward diffusion, iteratively adding Gaussian noise to data points



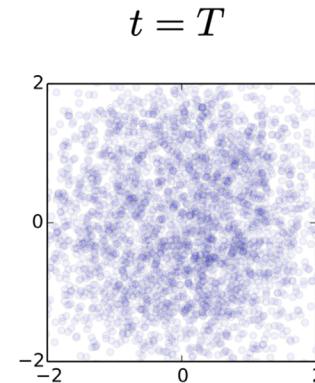
Input data
distribution
 q



$t = 0$



$t = \frac{T}{2}$



$t = T$

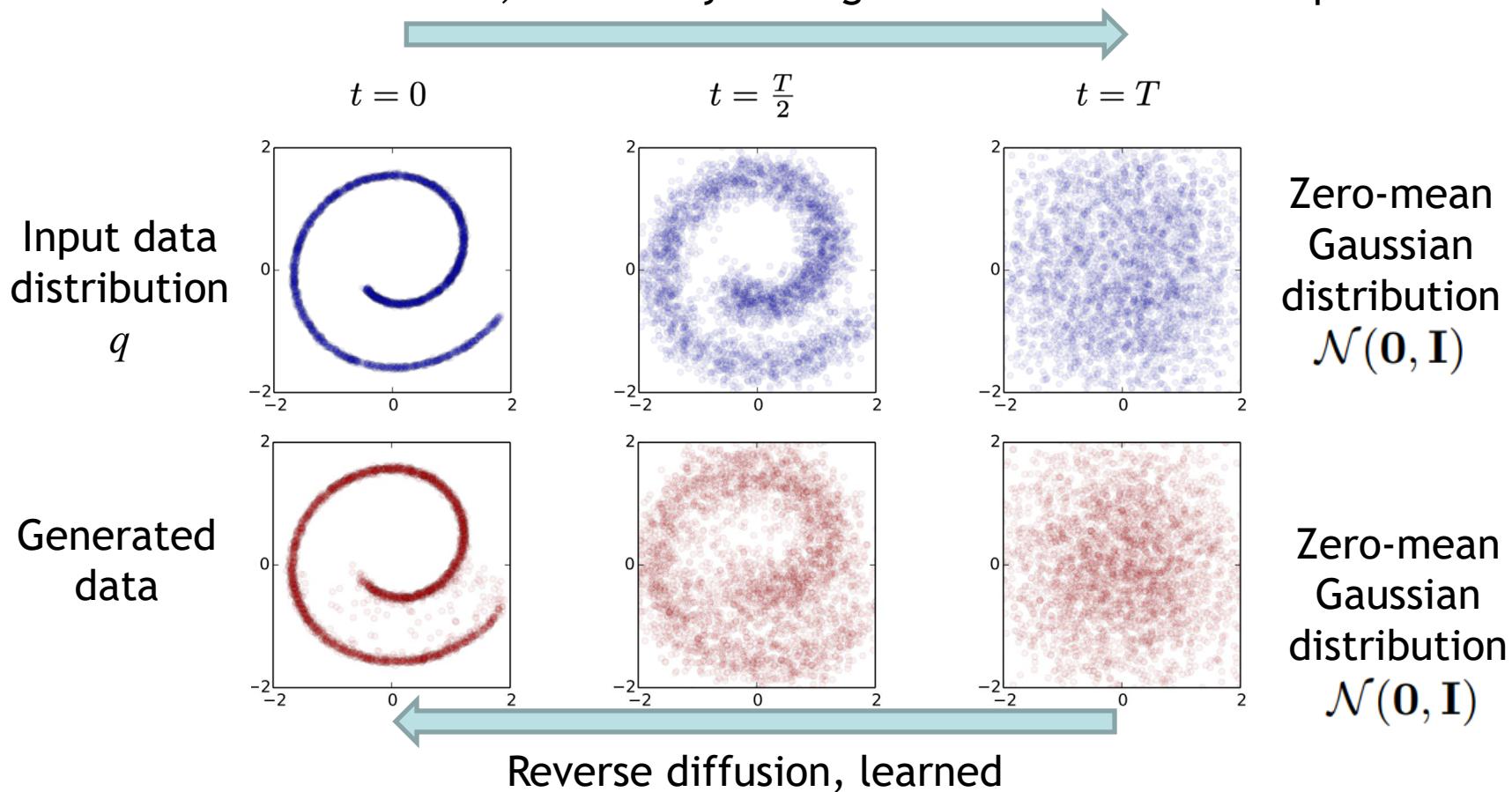
Zero-mean
Gaussian
distribution
 $\mathcal{N}(\mathbf{0}, \mathbf{I})$

Input data
density $q(x_0)$

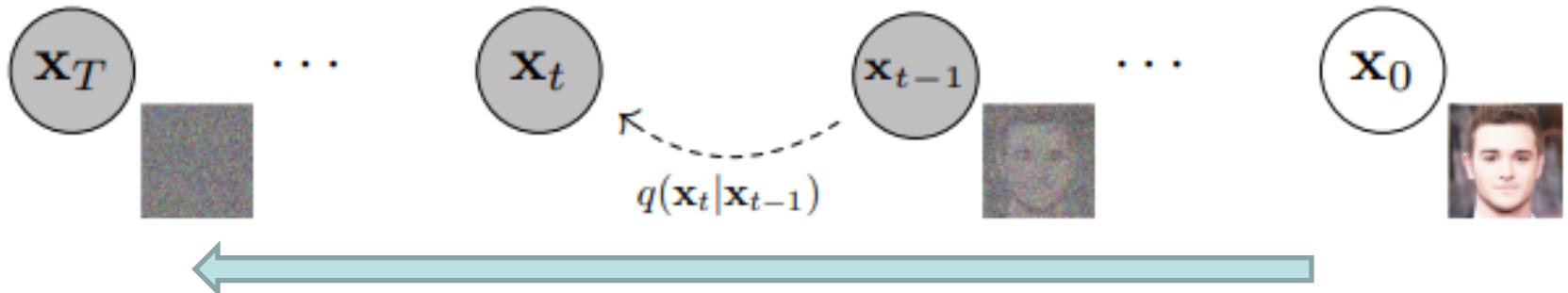
Diffusion models

- Basic idea: define forward diffusion process that iteratively maps input density to simple density (Gaussian) by adding noise, then learn to **invert** it

Forward diffusion, iteratively adding Gaussian noise to data points



Forward diffusion

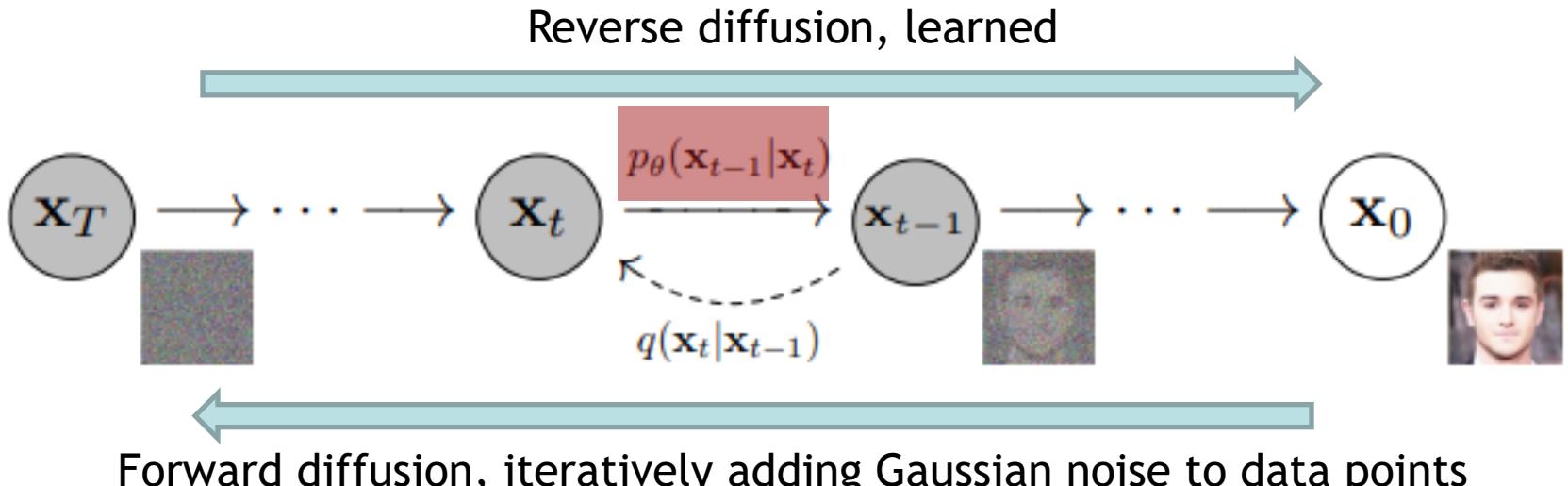


- Forward diffusion defined as adding Gaussian noise N with given variance β_t in each time step t
$$q(\mathbf{x}_t | \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \text{mean}, \text{covariance})$$

Shrink mean towards 0 Diagonal covariance, independent noise at each pixel

$$q(\mathbf{x}_{1:T} | \mathbf{x}_0) = \prod_{t=1}^T q(\mathbf{x}_t | \mathbf{x}_{t-1})$$

Reverse diffusion



- Need to know conditional probability $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ of reverse diffusion step; by sampling $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ we can make backward steps
- Key observation: if noise β_t small enough, reverse diffusion $p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t)$ has same form has forward step, here Gaussian ([Feller, 1949](#))

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

- But **mean $\boldsymbol{\mu}_\theta$ is unknown** at this point (will be able to compute variance $\boldsymbol{\Sigma}_\theta$ explicitly)
- **Goal of training:** generator network with parameters θ will be trained to predict mean $\boldsymbol{\mu}_\theta$ in each step t

Reverse diffusion

- Joint density of entire reverse trajectory using generator with parameters θ

$$p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) \quad p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

For $T \rightarrow \infty$, isotropic Gaussian distribution

- Marginal density $p_\theta(\mathbf{x}_0)$ of generated output data \mathbf{x}_0 using generator with parameters θ

$$p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} = \int p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) d\mathbf{x}_{1:T}$$

Integrate
over all
steps along
reverse
diffusion

- Given generator with fixed parameters θ , $p_\theta(\mathbf{x}_0)$ is well defined, but integral is intractable to compute in practice
- (extremely high dimensional)

Generated output density

- Intuition: (marginal) output density $p_\theta(\mathbf{x}_0)$ for each output \mathbf{x}_0 is integral over all backward trajectories starting from Gaussian distributed \mathbf{x}_T and ending up at \mathbf{x}_0

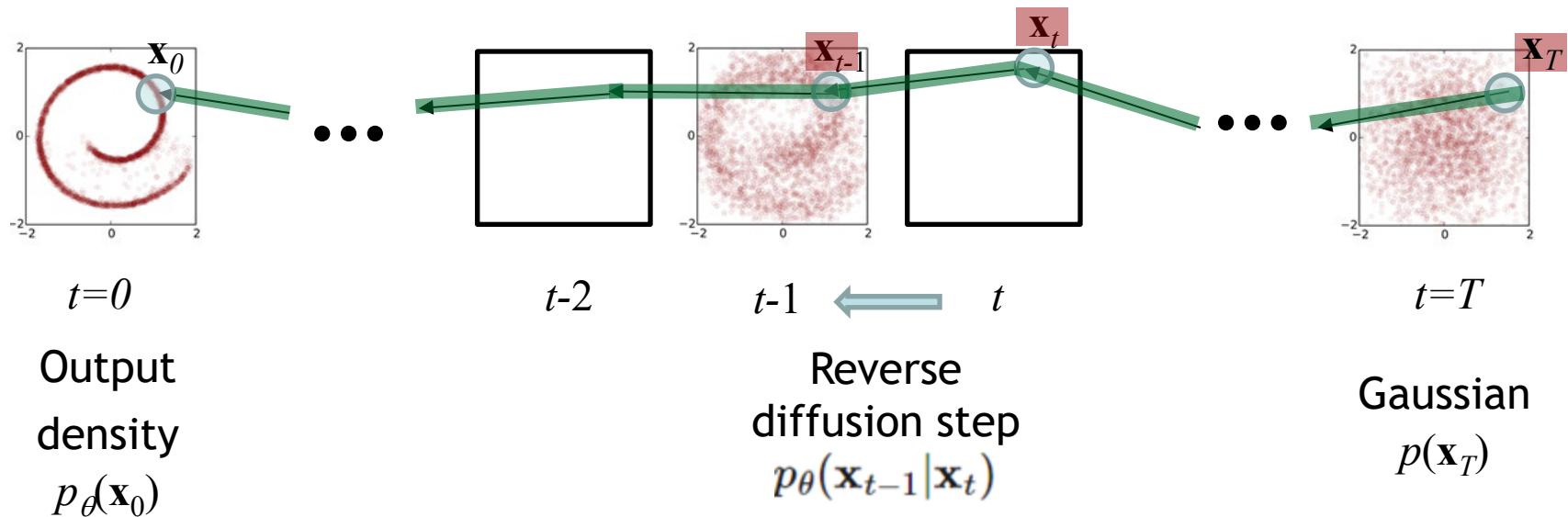
$$p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} = \int_{\text{Trajectory from time } T \text{ back to 0}} p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) d\mathbf{x}_{1:T}$$

Generated output density

- Intuition: (marginal) output density $p_\theta(\mathbf{x}_0)$ for each output \mathbf{x}_0 is integral over all backward trajectories starting from Gaussian distributed \mathbf{x}_T and ending up at \mathbf{x}_0

$$p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} = \int p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) d\mathbf{x}_{1:T}$$

Trajectory from
time T back to 0

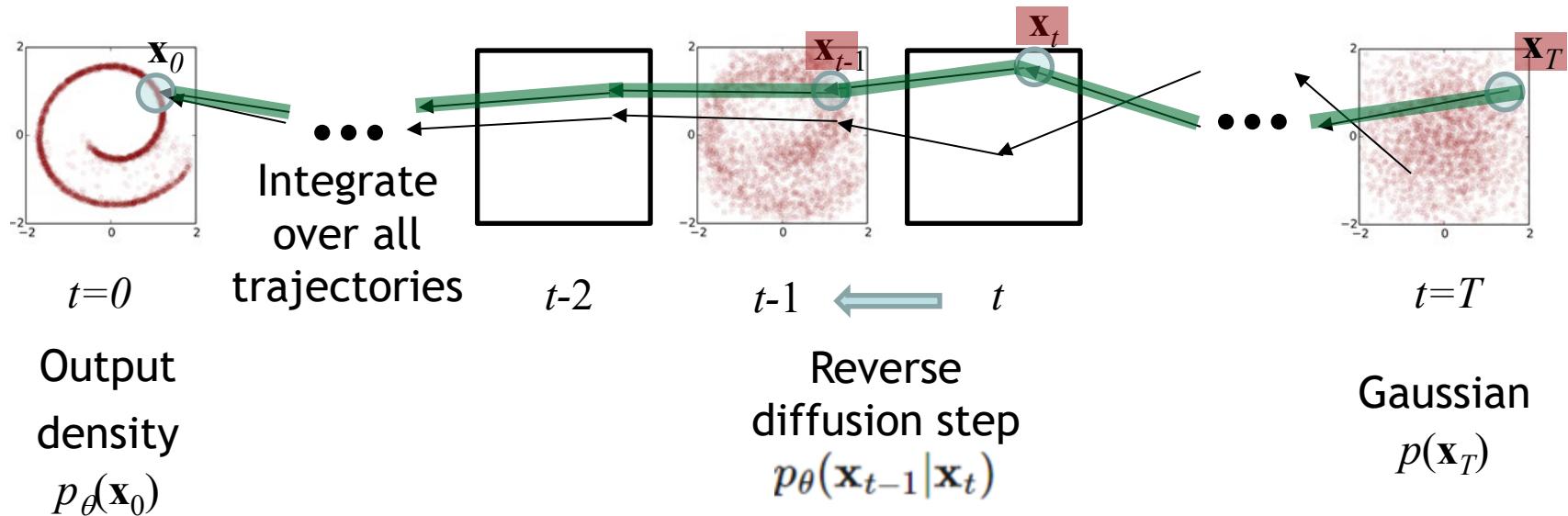


Generated output density

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$$p_\theta(\mathbf{x}_0) = \int p_\theta(\mathbf{x}_{0:T}) d\mathbf{x}_{1:T} = \int p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) d\mathbf{x}_{1:T}$$

Trajectory from
time T back to 0



Training objective

- Minimize negative log-likelihood (i.e., maximize likelihood) of generated output data $-\mathbb{E}_{q(\mathbf{x}_0)} \log p_{\theta}(\mathbf{x}_0)$
 - “The density of generated data, evaluated where the input data is [to estimate expected value], should be as high as possible” (density of input data denoted q)
 - “Randomly select set of training data points \mathbf{x}_0 [for Monte Carlo estimation of $\mathbb{E}_{q(\mathbf{x}_0)}$], evaluate their density under the current generator $p_{\theta}(\mathbf{x}_0)$, and minimize sum of negative logs” (equivalent to maximizing sum of densities)

Training objective

- Goal: Train generator θ to predict Gaussian distributions (means μ_θ) in each step t

$$p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_\theta(\mathbf{x}_t, t), \boldsymbol{\Sigma}_\theta(\mathbf{x}_t, t))$$

to minimize negative log-likelihood

$$\begin{aligned} & -\mathbb{E}_{q(\mathbf{x}_0)} \log p_\theta(\mathbf{x}_0) \\ &= -\mathbb{E}_{q(\mathbf{x}_0)} \log \left(\int p(\mathbf{x}_T) \prod_{t=1}^T p_\theta(\mathbf{x}_{t-1} | \mathbf{x}_t) d\mathbf{x}_{1:T} \right) \end{aligned}$$

In theory, could optimize this directly over generator parameters θ , but integral not tractable in practice

Practical training objective

- For practical training, need to approximate training objective based on negative log-likelihood
- Here, approach based on “Denoising Diffusion Probabilistic Models”, 2020

<https://arxiv.org/pdf/2006.11239.pdf>

Practical training objective

- After some math and approximations, find that minimizing negative log-likelihood can be achieved by minimizing KL divergence

Desired inverse diffusion step

$$D_{\text{KL}}(q(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{x}_0) \| p_\theta(\mathbf{x}_t | \mathbf{x}_{t+1}))$$

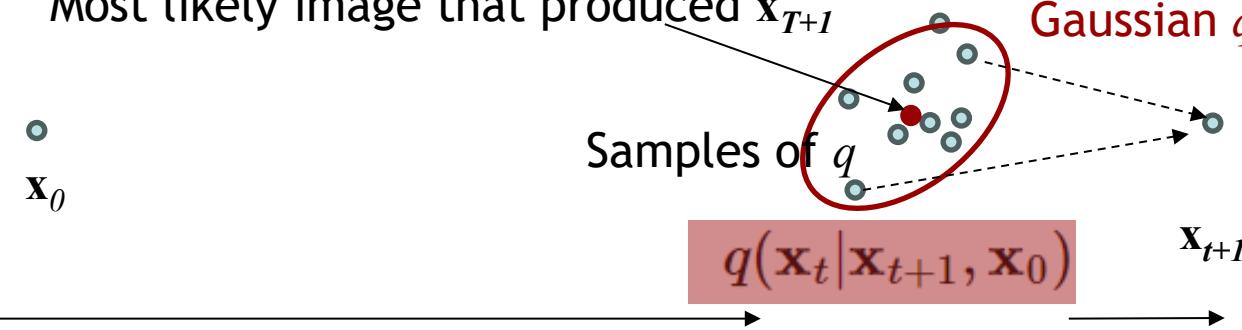
where $q(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{x}_0)$ is Gaussian with known parameters $\tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\boldsymbol{\beta}}_t \mathbf{I}$

$$q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_{t-1}; \tilde{\boldsymbol{\mu}}(\mathbf{x}_t, \mathbf{x}_0), \tilde{\boldsymbol{\beta}}_t \mathbf{I})$$

- “If we knew original image \mathbf{x}_0 , then we could know which image \mathbf{x}_{t-1} most likely produced \mathbf{x}_t in forward diffusion step”; would allow us to make inverse step
- However, during reverse diffusion, \mathbf{x}_0 unknown, cannot use $q(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{x}_0)$ directly in reverse diffusion

Visualization

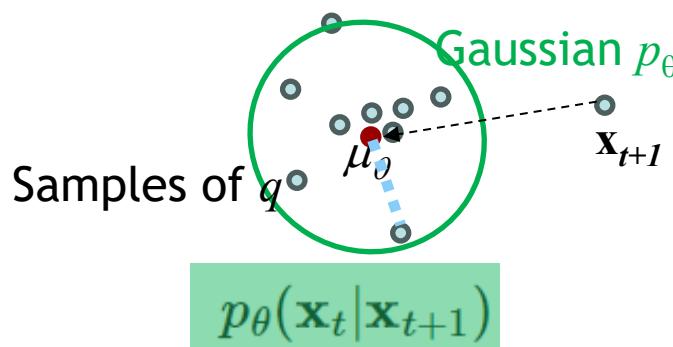
Most likely image that produced \mathbf{x}_{T+1}



Forward diffusion, known distributions

$$\text{Minimize } D_{\text{KL}}(q(\mathbf{x}_t | \mathbf{x}_{t+1}, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_t | \mathbf{x}_{t+1}))$$

Key observation: KL is minimized when mean μ_{θ} of p_{θ} minimizes L2 distance to mean of q ; achieved by minimizing L2 distance between samples of q and mean μ_{θ} of p_{θ}



Reverse diffusion, distribution p_{θ} of reverse step to be learned

Minimizing KL divergence

- Minimizing KL divergence means minimizing prediction error for mean, over all input data \mathbf{x}_0 and noise vectors ε

Loss to be minimized

$$L_t = \mathbb{E}_{\mathbf{x}_0, \varepsilon} \left[\frac{1}{2\|\Sigma_{\theta}(\mathbf{x}_t, t)\|_2^2} \left\| \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_{\theta}(\mathbf{x}_t, t) \right\|^2 \right]$$

Known Predicted by generator

$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0)$ — $\mu_{\theta}(\mathbf{x}_t, t)$

- “For all input images \mathbf{x}_0 and noise ε , train generator μ_{θ} to denoise image \mathbf{x}_t , which predicts mean $\tilde{\mu}(\mathbf{x}_t, \mathbf{x}_0)$ “

Minimizing KL divergence

- Paper shows: predicting denoised image (i.e., sample of q) is equivalent to predicting noise ϵ_t that was added

Known noise ϵ_t
applied in
forward diffusion

$L_t = \mathbb{E}_{\mathbf{x}_0, \epsilon} \left[\frac{(1 - \alpha_t)^2}{2\alpha_t(1 - \bar{\alpha}_t)\|\Sigma_{\theta}\|_2^2} \|\epsilon_t - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon_t, t)\|^2 \right]$

Known noise ϵ_t applied
to input data \mathbf{x}_0

Minimize loss wrt.
parameters θ

Noise predicted by
generator network, parameters θ

Noisy input
image at time t

$\alpha_t = 1 - \beta_t$ $\bar{\alpha}_t = \prod_{i=1}^t \alpha_i$ $\epsilon_{t-1}, \epsilon_{t-2}, \dots \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

Variances used in forward diffusion Gaussian noise

Summary

- Approximation of training objective (minimizing negative log-likelihood of generated data density) can be achieved by training noise prediction network ε_θ
- Training
 - Construct noisy data by adding known noise vectors to clean data points, noise magnitudes (variance) given by time t
 - Given noisy inputs, time t , train network ε_θ (noisy image, t) to predict noise

Training & sampling algorithms

Algorithm 1 Training

```
1: repeat
2:    $\mathbf{x}_0 \sim q(\mathbf{x}_0)$       // randomly select input image
3:    $t \sim \text{Uniform}(\{1, \dots, T\})$ 
4:    $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
5:   Take gradient descent step on
     
$$\nabla_{\theta} \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}, t)\|^2$$

6: until converged
```



Simplified training objective,
works better in practice

$$\alpha_t = 1 - \beta_t \quad \bar{\alpha}_t = \prod_{i=1}^t \alpha_i$$

Variances used in forward diffusion

Training & sampling algorithms

Algorithm 1 Training

```

1: repeat
2:    $\mathbf{x}_0 \sim q(\mathbf{x}_0)$  // randomly select input image
3:    $t \sim \text{Uniform}(\{1, \dots, T\})$ 
4:    $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
5:   Take gradient descent step on
      
$$\nabla_{\theta} \|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2$$

6: until converged

```

Simplified training objective,
works better in practice

$$\alpha_t = 1 - \beta_t \quad \bar{\alpha}_t = \prod_{i=1}^t \alpha_i$$

Variances used in forward diffusion

Algorithm 2 Sampling

```

1:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$  // start with Gaussian noise image
2: for  $t = T, \dots, 1$  do
3:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$  if  $t > 1$ , else  $\mathbf{z} = \mathbf{0}$ 
4:    $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon_{\theta}(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$ 
5: end for
6: return  $\mathbf{x}_0$ 

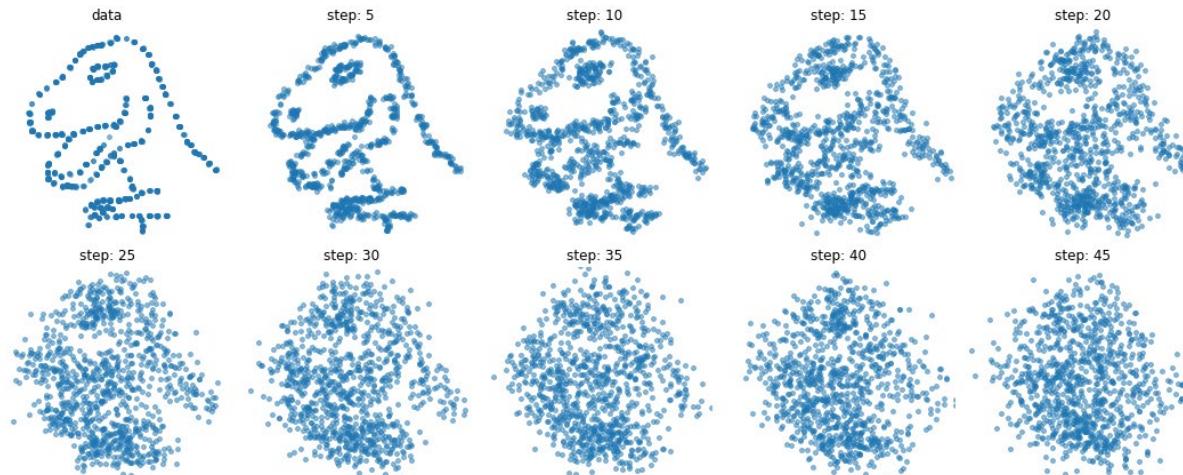
```

subtract add new
 predicted noise noise

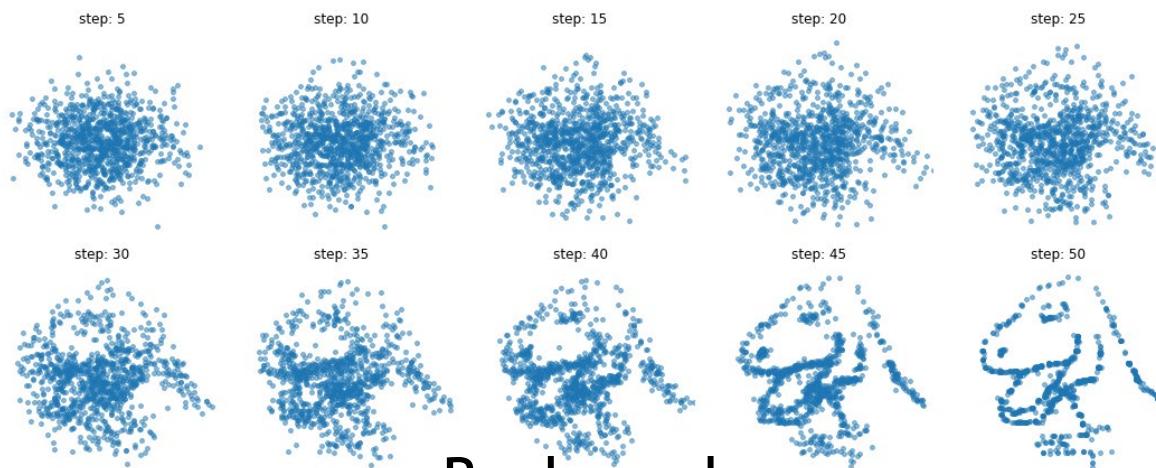
Sample Gaussian $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$, different
choices for σ_t in practice, such as $\sigma_t^2 = \beta_t$

Educational 2D model

<https://github.com/tanelp/tiny-diffusion>



Forward



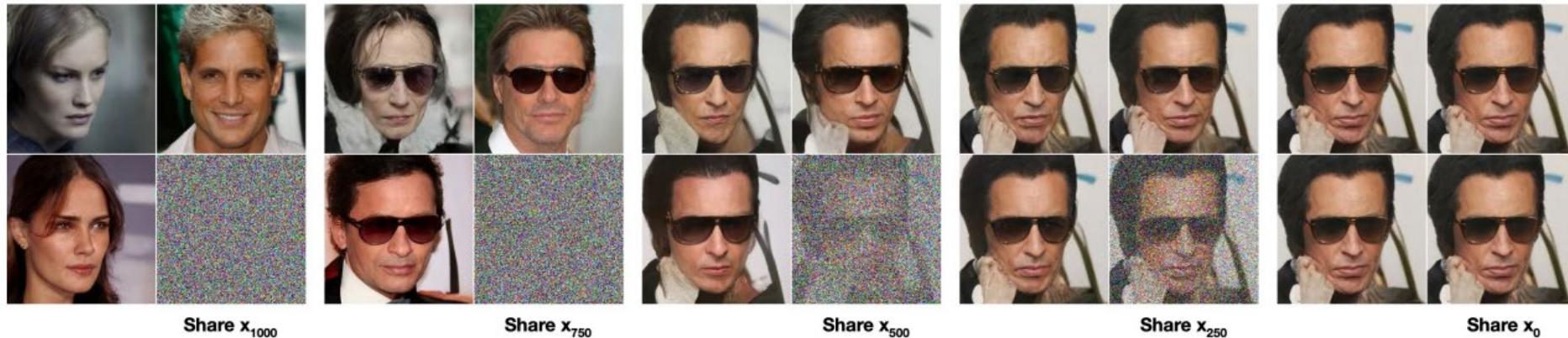
Backward

Results

Gaussian
noise

Reverse diffusion steps by sampling $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$

Input data
distribution



Different end points of reverse trajectories starting at different t