CS 760: Machine Learning
Generative Models

University of Wisconsin-Madison

Outline

- Intro to Generative Models
  - Histograms, Parametrizing Distributions
- Flow-based Models
  - Transformations, training, sampling
- Generative Adversarial Networks (GANs)
  - Generators, discriminators, training, examples
- Diffusion Models

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Generative Models

- Goal: sample x ~ p(x)
  - x can be images, speech, songs, etc.
  - p() implicitly given by a training set x1… xn
  - want to sample (generate) “new” but realistic (coming from p or a similar distribution) x, not copying the training set
  - optionally condition on additional information y: x ~ p(x|y)
    - e.g. y=sketch on next slide

drawings by prof. Zhu's kids, many years ago

generative model output conditioned on the drawings and additional short text prompts, 2026/3

Applications: Generate Images

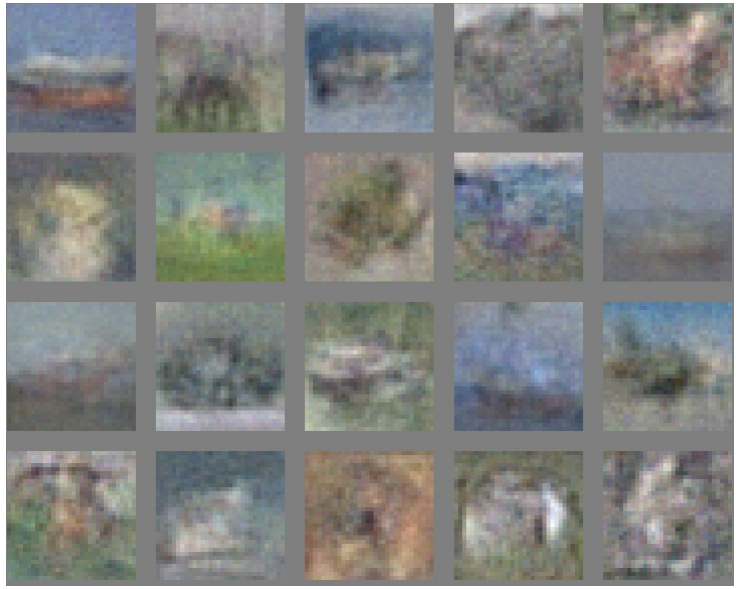
- Old idea---tremendous growth
- Historical evolution:

2006: Hinton et al

2013: Kingma & Welling

Applications: Generate Images

- More recently, GAN models: 2014
  - Goodfellow et al



Applications: Generate Images

- More recently, GAN models
  - StyleGAN, Karras, Laine, Aila, 2018

Applications: Generate Images

- Today, Diffusion Models: DALL·E 3, Stable Diffusion 3.5

Prompt: ~*~aesthetic~*~ #boho #fashion, full-body 30-something woman laying on microfloral grass, candid pose, overlay reads Stable Diffusion 3.5, cheerful cursive typography font.

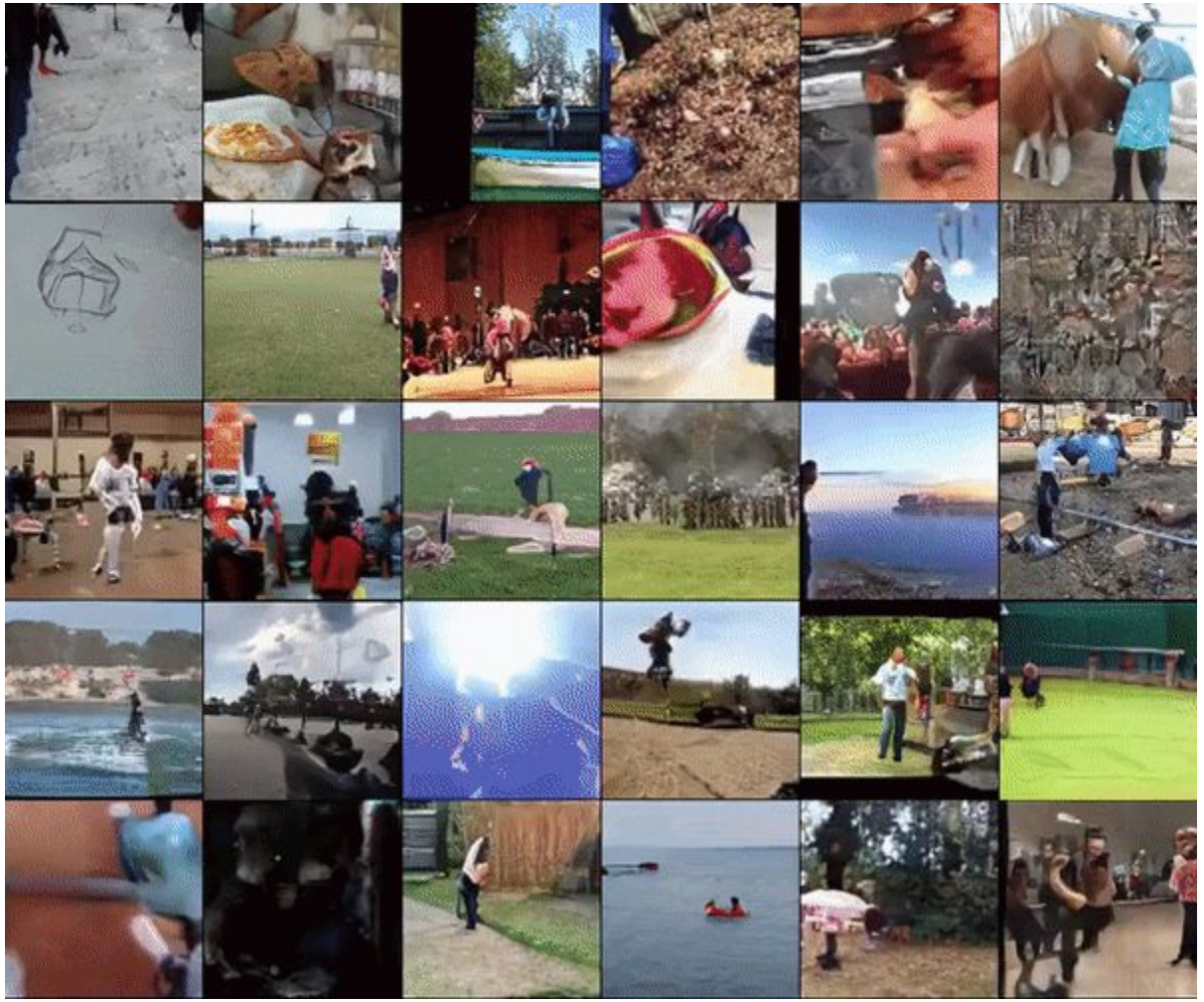
Applications: Generate Images/Video

- GANs can also generate video
  - Plus transfer:

CycleGAN: Zhu, Park, Isola & Efros, 2017

Applications: Generate Video

- GANs can also generate video (DVD-GAN, Clark et al)



Applications: Generate Video

- Diffusion model can generate long videos up to a minute long with high visual quality.

[OpenAI Sora]

Additional Applications

- **Compress** data
  - Can often do better than fixed methods like JPEG
  - Similar to nonlinear dimensionality reduction

- Obtain **good representations**
  - Then can fine-tune for particular tasks
  - Unlabeled data is cheap, labeled data is not.

Goal: Learn a Distribution

- Want to estimate p_{data} from samples

$$x^{(1)}, x^{(2)}, \ldots, x^{(n)} \sim p_{\text{data}}(x)$$

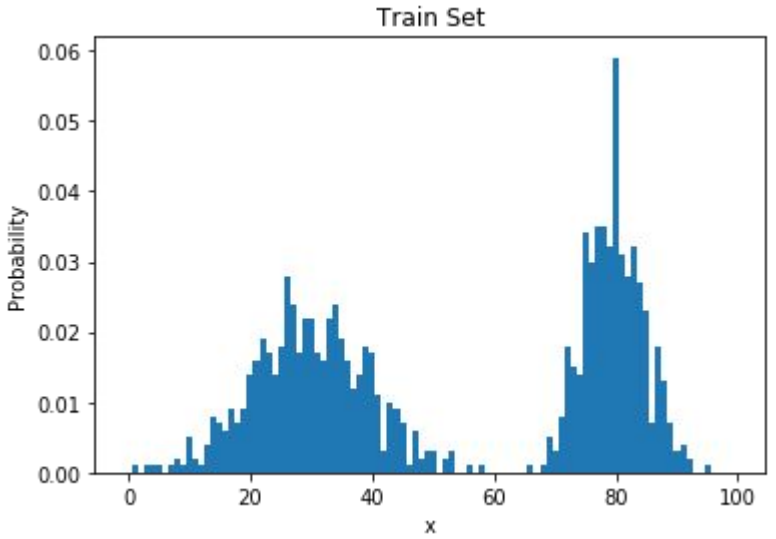
- Desired abilities:
  - Inference: compute p(x) for some x
  - Sampling: obtain a sample from p(x)

Goal: Learn a Distribution

- Want to estimate p_{data} from samples

$$x^{(1)}, x^{(2)}, \ldots, x^{(n)} \sim p_{\text{data}}(x)$$

- **One way**: build a histogram (piecewise constant probability density function):
- Bin data space into k intervals.
  - Estimate p_1, p_2, …, p_k
- Train this model:
  - Count times bin i appears in dataset



Histograms: Inference & Samples

- **Inference**: check our estimate of p_i
- **Sampling**: straightforward, select bin i with probability p_i, then select uniformly from bin i.

- But …
  - inefficient in high dimensions

Parametrizing Distributions

- Don't store each probability, store $p_\theta(x)$

- One approach: likelihood-based
  - We know how to train θ with **maximum likelihood**

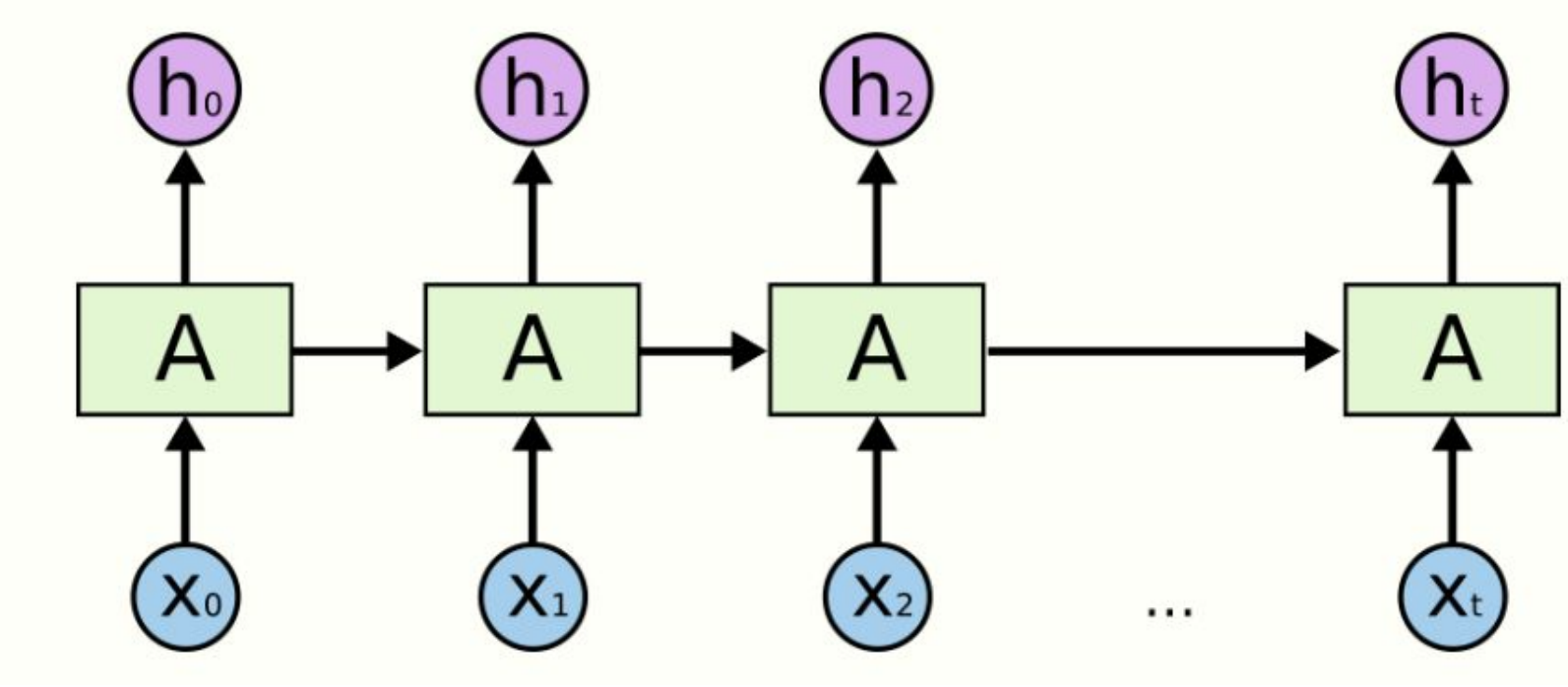
$$\arg\min_\theta -\frac{1}{n}\sum_{i=1}^{n} \log p_\theta(x^{(i)})$$

Parametrizing Distributions

- One approach: likelihood-based
  - We know how to train with **maximum likelihood**
  - Then, train with SGD
  - Just need to make some choices for $p_\theta(x)$
    - For example, recall Gaussian mixture models.
    - But many types of data have more complex underlying distributions.

Parametrizing Distributions: Autoregressive models

- e.g. recurrent neural networks, transformers.



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Flow Models

- One way to specify $p_\theta(x)$
- Use a latent variable z with a "simple" (e.g Gaussian) distribution.
- Then use a "complex" transformation, $x = f_\theta(z)$.
  - this generates a new item x
  - also induces $p_\theta(x)$ (next slide)
  - learn θ by maximum likelihood on training set

Flow Models: How to train?

- Relationship between densities of x and z

$$\mathbf{z} \sim \pi(\mathbf{z}), \mathbf{x} = f(\mathbf{z}), \mathbf{z} = f^{-1}(\mathbf{x})$$

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

[change of variables]

Determinant of Jacobian matrix

Lilian Weng. Flow-based Deep Generative Models

Flows: Transformations

- What kind of f transformations should we use? Desirable properties:
  - Invertible
  - determinant of Jacobian easy to compute

Example: RealNVP

y=f(x)

$$\mathbf{y}_{1:d} = \mathbf{x}_{1:d}$$

$$\mathbf{y}_{d+1:D} = \mathbf{x}_{d+1:D} \odot \exp\big(s(\mathbf{x}_{1:d})\big) + t(\mathbf{x}_{1:d})$$

keep first d-dimensions of x intact

affine on remaining dimensions

s, t arbitrary (nonlinear) functions, e.g. neural nets

Lilian Weng. Flow-based Deep Generative Models

Flow Models

- compose multiple “simple” transformations

$$x = f_{\theta_k}(f_{\theta_{k-1}}(\dots f_{\theta_1}(z)))$$

$$z = f^{-1}_{\theta_1}(f^{-1}_{\theta_2}(\dots f^{-1}_{\theta_k}(x)))$$

Flow Models

- Transform a simple distribution to a complex one via a chain of invertible transformations (the “flow”)

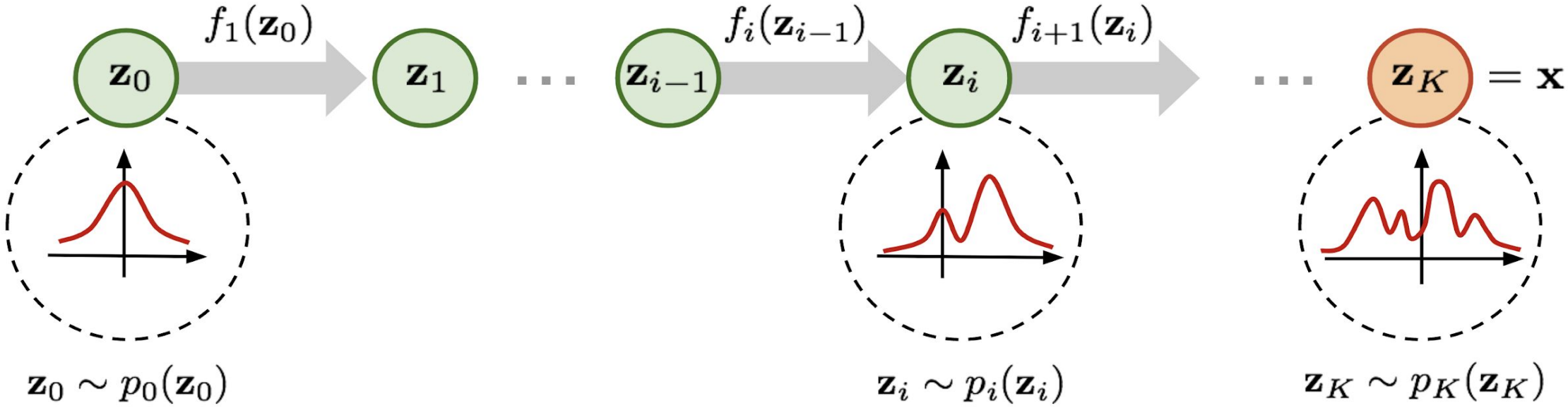
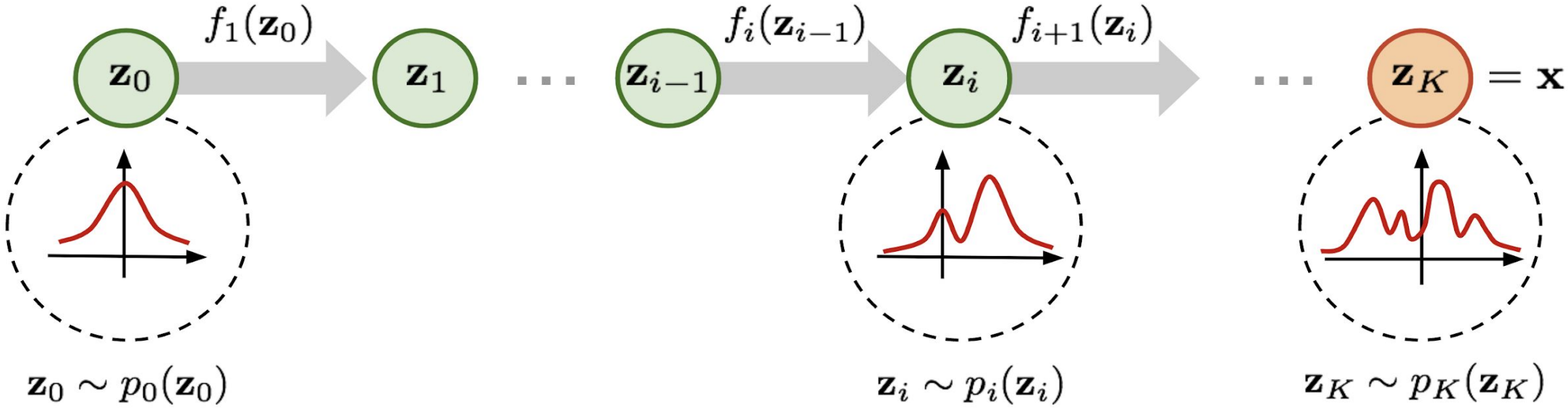


image from Lilian Weng

Flow Models: How to sample?

- Sample from z (the latent variable)---has a simple distribution that lets us do it: Gaussian, uniform, etc.
- Then run the sample z through the flow to get a sample x



Flow Models: Training

$$\max_\theta \sum_i \log\Big(p_x(x^{(i)};\theta)\Big) = \max_\theta \left(\sum_i \log\Big(p_z(f_\theta^{-1}(x^{(i)}))\Big) + \log\left|\frac{\partial f_\theta^{-1}(x^{(i)})}{\partial x}\right|\right)$$

Maximum Likelihood

Latent variable version

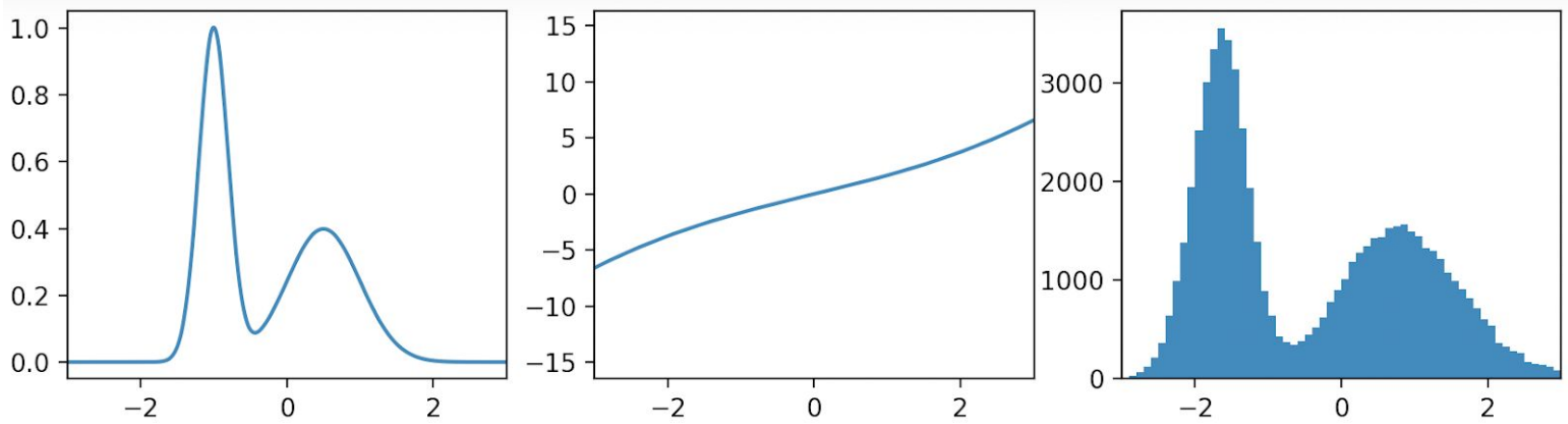
Determinant of Jacobian matrix

Flows: Example

- Inverse flow to a Gaussian (right)

Inverse Flow

- **Before** training:



- **After** training:

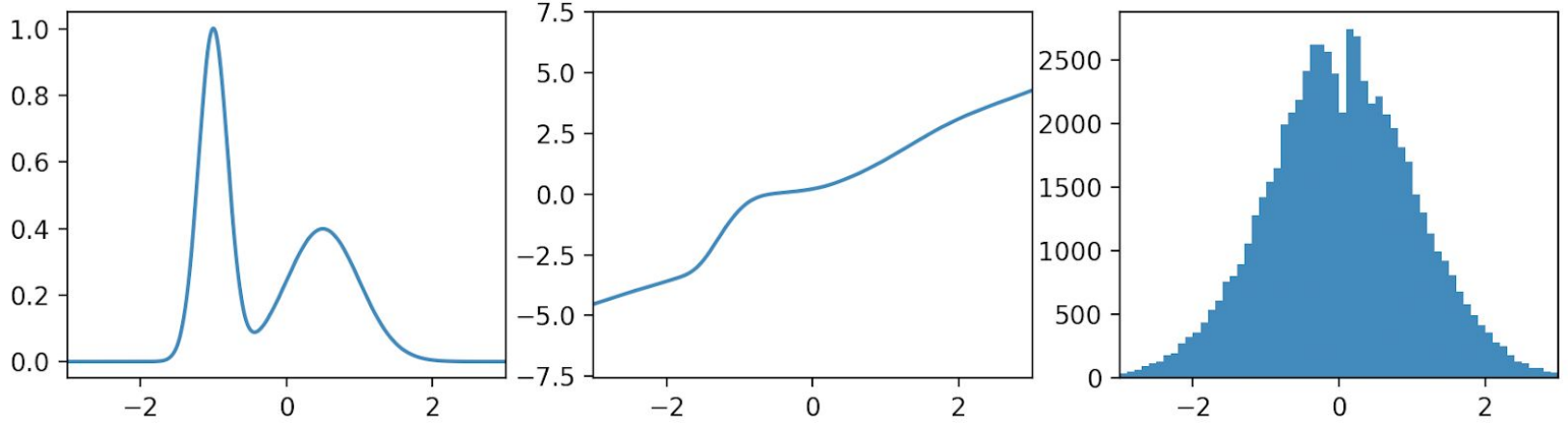


image from UC Berkeley: Deep Unsupervised Training

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GANs: Generative Adversarial Networks

- So far we've been modeling the density…
  - What if we just want to get high-quality samples?

- GANs do this.
  - Think of art forgery
  - Left: original
  - Right: forged version
  - Two-player game:
    - **Generator** wants to pass off the discriminator as an original
    - **Discriminator** wants to distinguish forgery from original

GANs: Basic Setup

- Let's set up networks that implement this idea:
  - **Discriminator** network D(x)=Pr(real img | x)
  - **Generator** network G(z) ∈ img space R^d

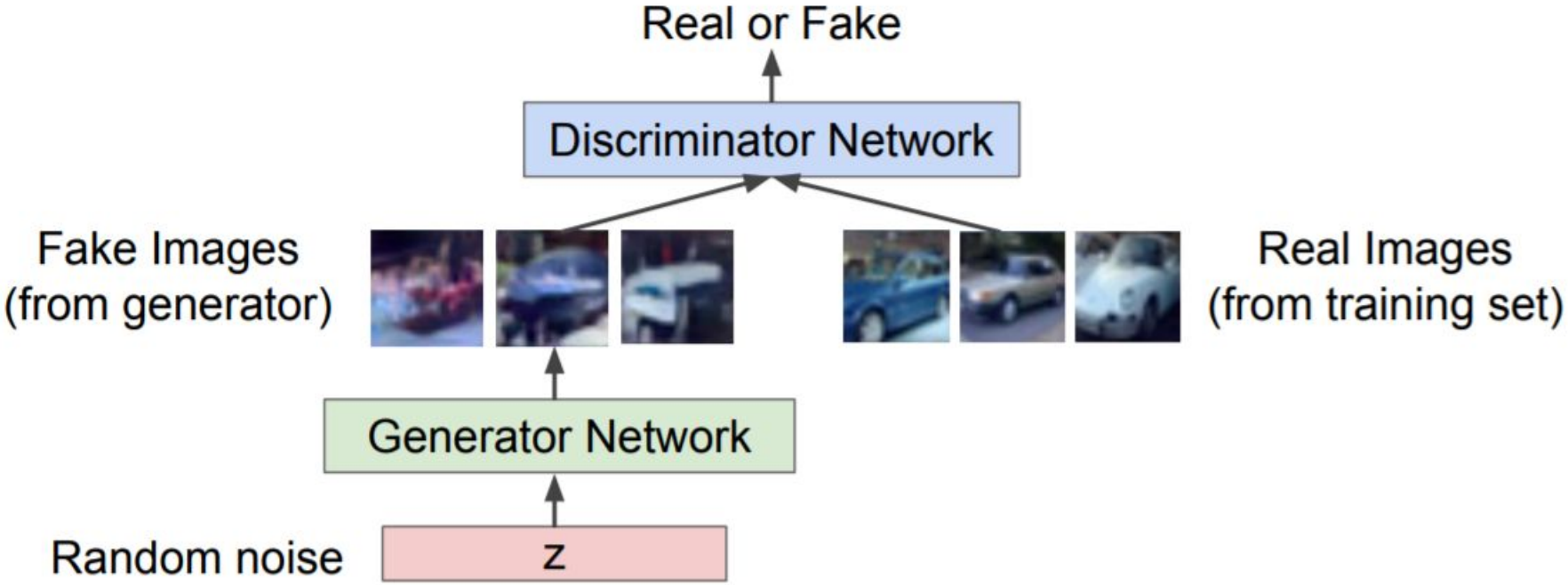


image from Stanford CS231n / Emily Denton

GAN Training: Discriminator

- How to train these networks? Two sets of parameters to learn: θ_d (discriminator) and θ_g (generator)

- Let's **fix** the generator. What should the discriminator do?
  - Distinguish fake and real data: binary classification.
  - Use the cross-entropy loss, we get

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

Real data, want to classify 1

Fake data, want to classify 0

GAN Training: Generator & Discriminator

- How to train these networks? Two sets of parameters to learn: θ_d (discriminator) and θ_g (generator)

- This makes the discriminator better, but also want to make the generator more capable of fooling it:
  - Two-player zero-sum game! Train jointly by solving minimax problem:

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

Real data, want to classify 1

Fake data, want to classify 0

GAN Training: Alternating Training

- So we have an optimization goal:

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

- Alternate training:
  - Gradient ascent: *fix generator*, make the discriminator better:

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

  - Gradient descent: *fix discriminator*, make the generator better

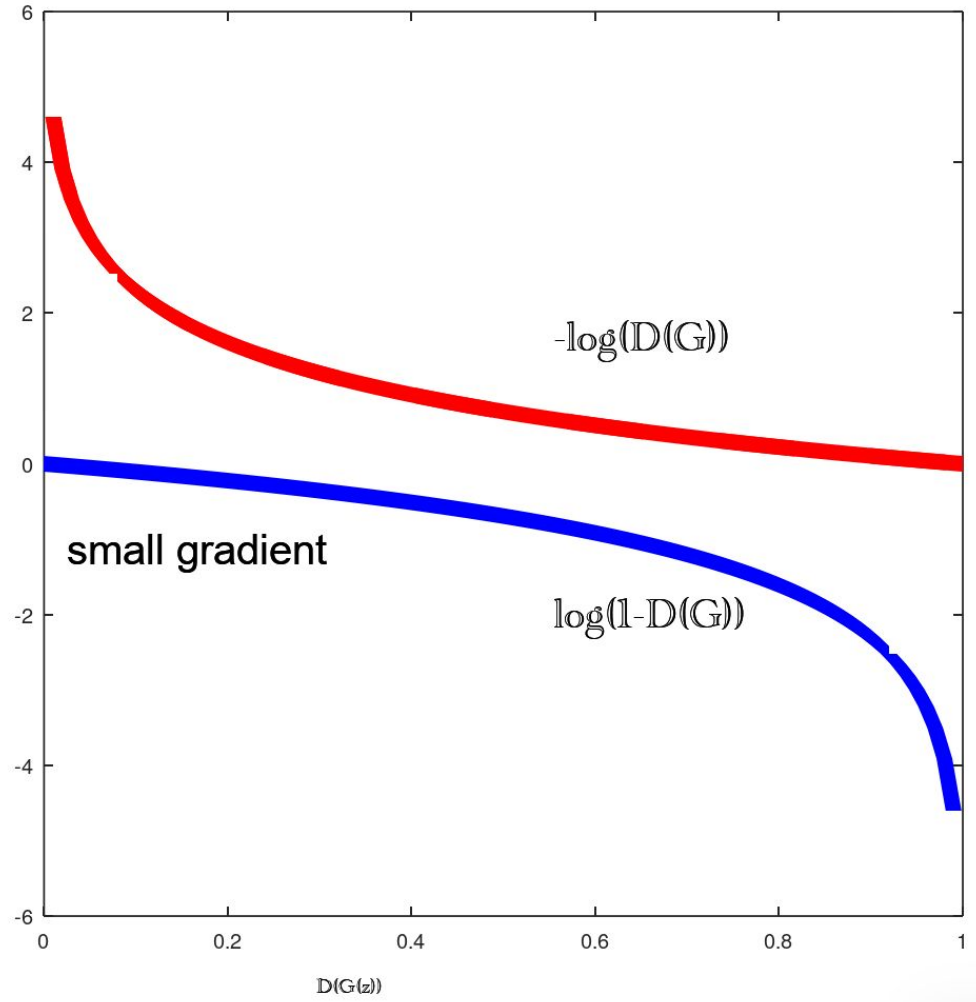
$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

GAN Training: Issues

- Small gradient for G initially when D(G)≈0
  - Replace the generator training with

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

  - Better gradient shape
    (but no longer a zero-sum game)
- Can still be challenging.
  Training often not stable



GAN Architectures

- Discriminator: image classification, use a CNN
- What should **generator** look like
  - Input: noise vector z.
  - Output: an image (i.e. a 3-channel x width x height volume)
  - Similar to a reversed CNN pattern…

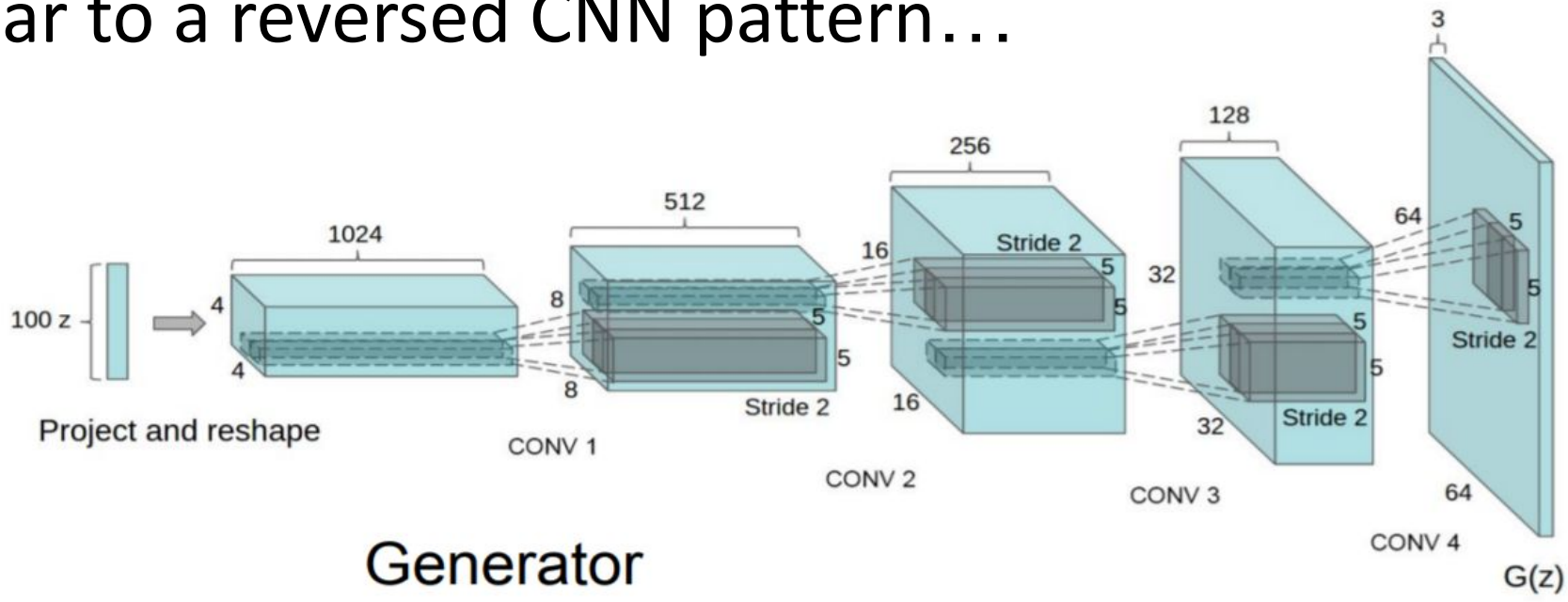


image from Radford et al ‘16

GANs: Example

- Output of a GAN after 5 epochs of training:

image from Radford et al ‘16

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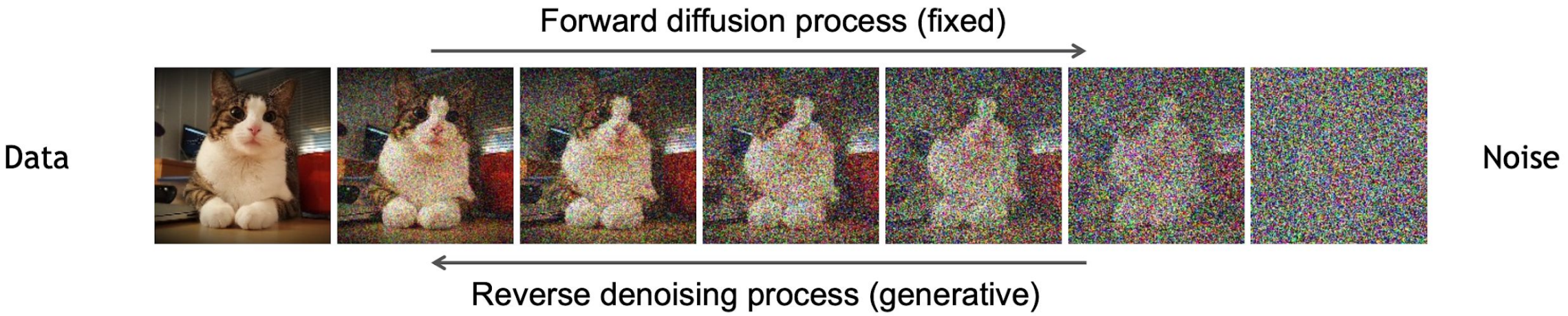
Diffusion Models (optional)

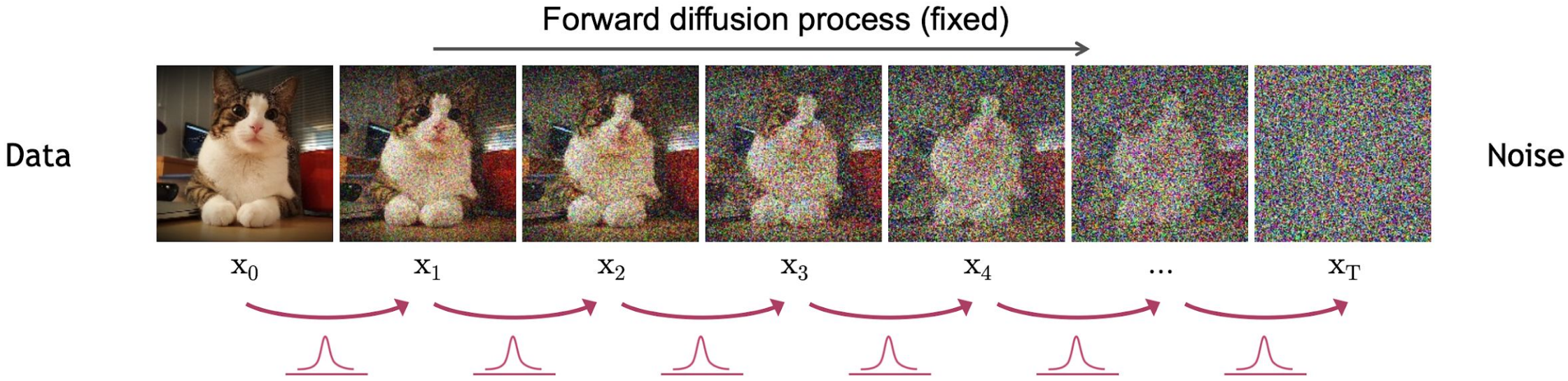
- **Learning to generate by denoising**
- Denoising diffusion models consist of two processes:
  - Forward diffusion process that gradually adds noise to input
  - Reverse denoising process that learns to generate data by denoising



Some slides were borrowed from
Denoising Diffusion-based Generative Modeling CVPR2022 tutorial
(https://cvpr2022-tutorial-diffusion-models.github.io/)

Diffusion Models (optional)

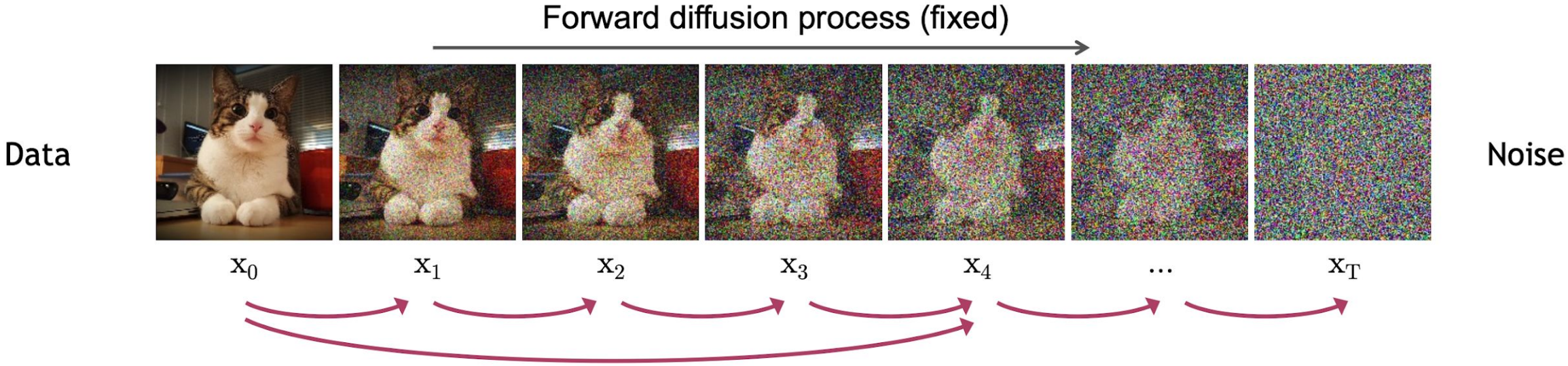
- The formal definition of the forward process in T steps:



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x_t}; \sqrt{1-\beta_t}\mathbf{x_{t-1}}, \beta_t\mathbf{I}) \quad \Rightarrow \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) \qquad \text{(joint)}$$

Diffusion Models (optional)

- Diffusion Kernel



Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}))$ (Diffusion Kernel)

For sampling: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\,\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

β_t values schedule (i.e., the noise schedule) is designed such that $\bar{\alpha}_T \to 0$ and $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

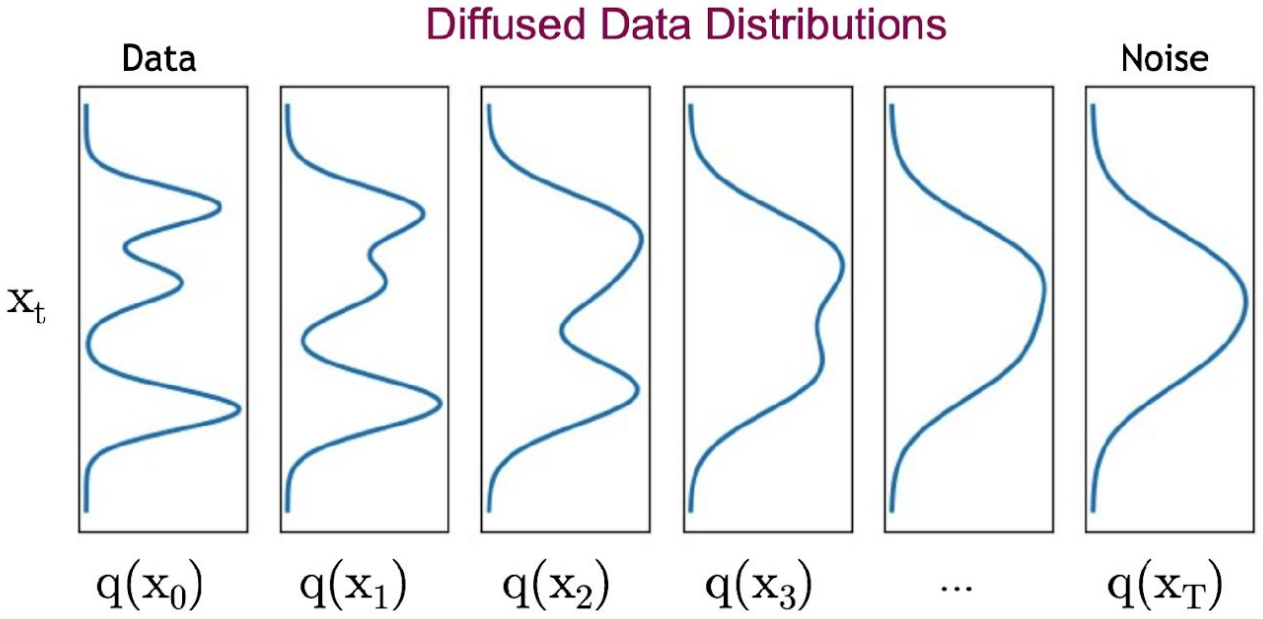
Diffusion Models (optional)

- What happens to a distribution in the forward diffusion?

So far, we discussed the diffusion kernel $q(\mathbf{x}_t|\mathbf{x}_0)$ but what about $q(\mathbf{x}_t)$?

$$\underbrace{q(\mathbf{x}_t)}_{\text{Diffused data dist.}} = \int \underbrace{q(\mathbf{x}_0, \mathbf{x}_t)}_{\text{Joint dist.}} d\mathbf{x}_0 = \int \underbrace{q(\mathbf{x}_0)}_{\text{Input data dist.}} \underbrace{q(\mathbf{x}_t|\mathbf{x}_0)}_{\text{Diffusion kernel}} d\mathbf{x}_0$$

The diffusion kernel is Gaussian convolution.



We can sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ by first sampling $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ and then sampling $\mathbf{x}_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$ (i.e., ancestral sampling).

Diffusion Models (optional)

- Generative Learning by Denoising

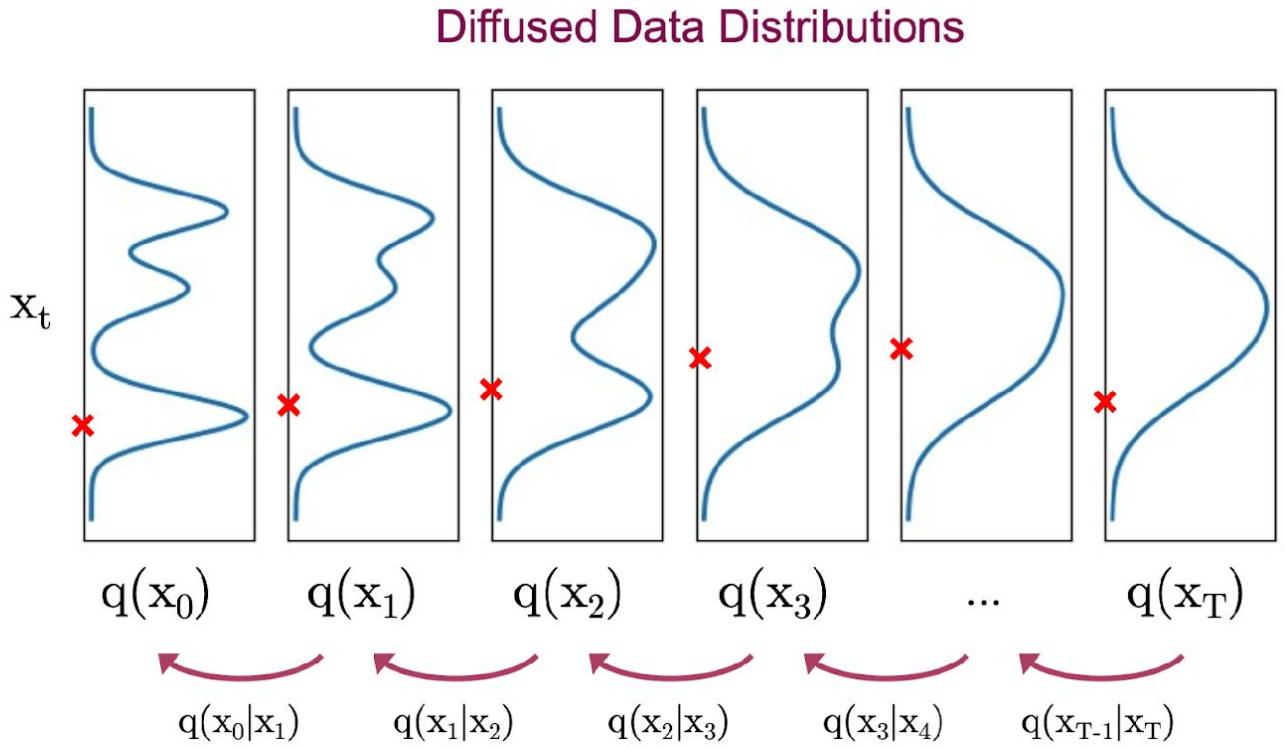
Recall, that the diffusion parameters are designed such that $q(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

Generation:

Sample $\mathbf{x}_T \sim \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$

Iteratively sample $\mathbf{x}_{t-1} \sim \underbrace{q(\mathbf{x}_{t-1}|\mathbf{x}_t)}$

True Denoising Dist.



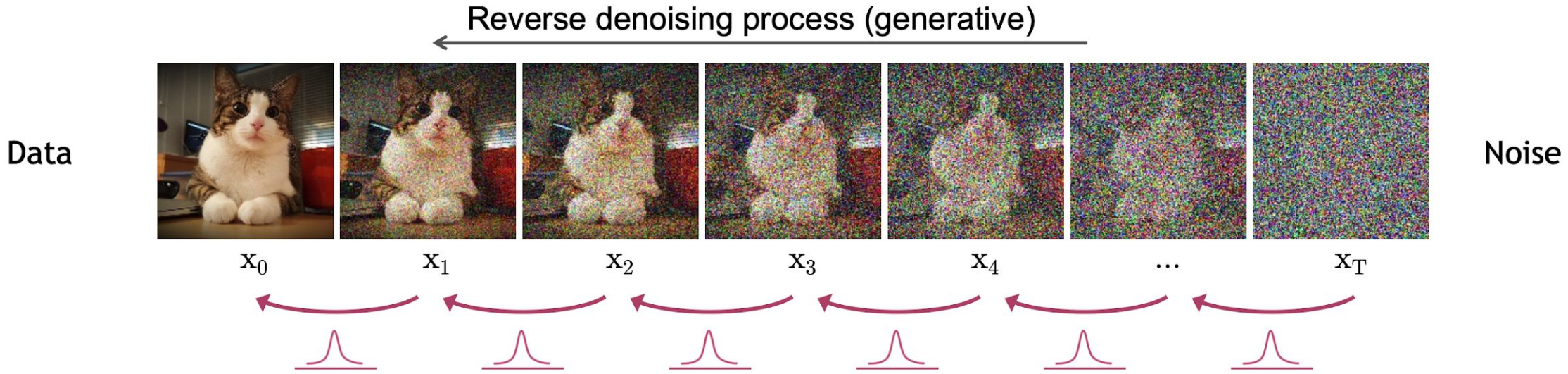
In general, $q(\mathbf{x}_{t-1}|\mathbf{x}_t) \propto q(\mathbf{x}_{t-1})q(\mathbf{x}_t|\mathbf{x}_{t-1})$ is intractable.

Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$? Yes, we can use a Normal distribution if β_t is small in each forward diffusion step.

Diffusion Models (optional)

- Reverse Denoising Process

Formal definition of forward and reverse processes in T steps:



$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}, \sigma_t^2\mathbf{I})$$

Trainable network
(U-net, Denoising Autoencoder)

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

Thanks Everyone!

Some of the slides in these lectures have been adapted/borrowed from materials developed by Misha Khodak, Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, Pedro Domingos, Jerry Zhu, Yingyu Liang, Volodymyr Kuleshov, Fei-Fei Li, Justin Johnson, Serena Yeung, Pieter Abbeel, Peter Chen, Jonathan Ho, Aravind Srinivas, Ruiqi Gao, Tengyang Xie