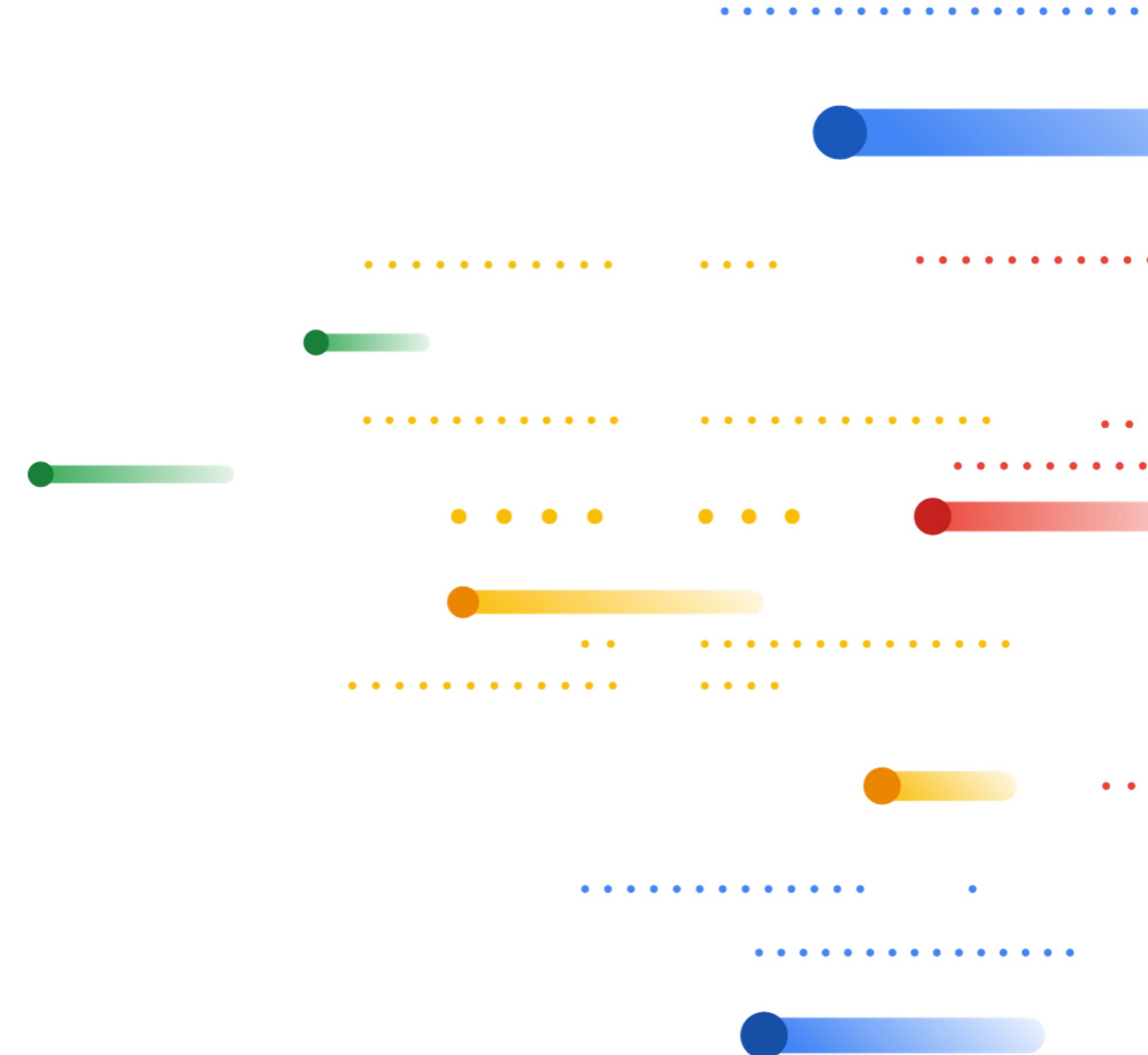


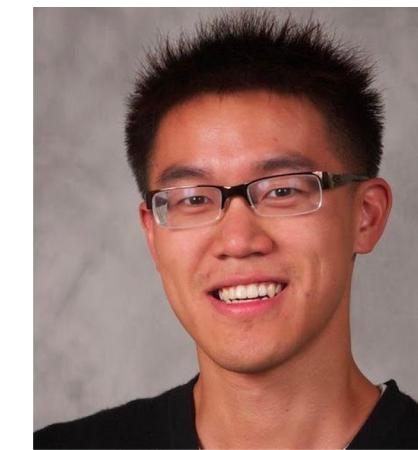
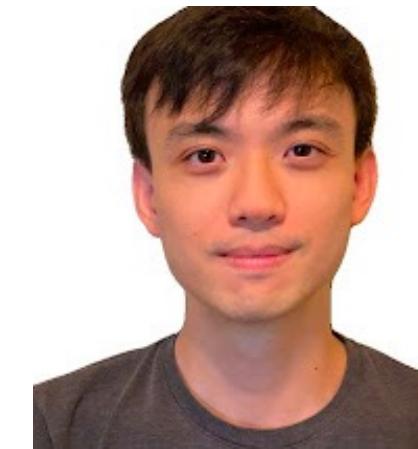


Variational Autoencoders and Diffusion Models

Ruiqi Gao @Stanford cs231n
May 25, 2023



Acknowledgements



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

Contents

- Deep generative models and applications in computer vision
- Variational Autoencoders
- Diffusion models
 - Discrete-time diffusion models
 - Continuous-time diffusion models: differential equation framework
- Case study: Imagen: high-fidelity text-to-image diffusion models

Not intended as a complete review of all recent work!

Deep Generative Models

Deep Generative Models

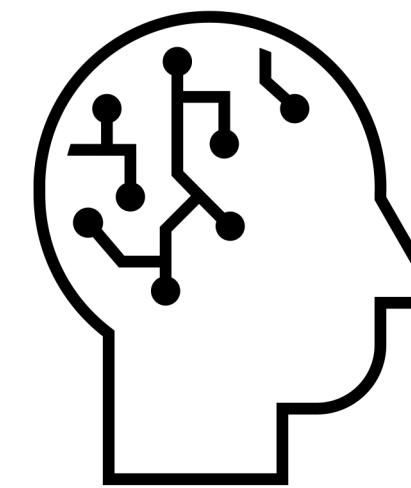
Learning to generate data



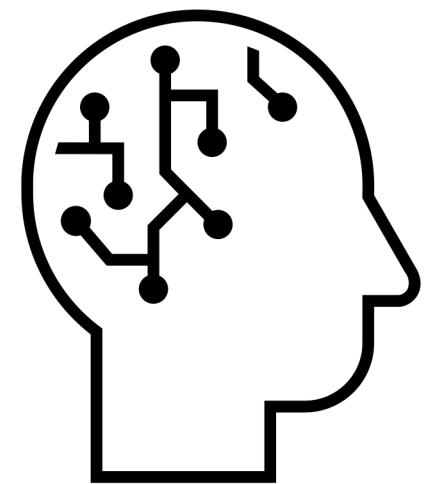
Samples from a Data Distribution

Train

A thick green arrow pointing to the right, indicating the direction of the training process.



Neural Network



Sample

A thick green arrow pointing to the right, indicating the direction of sampling from the trained model.



Application (1): Content Generation

StyleGAN3 example images



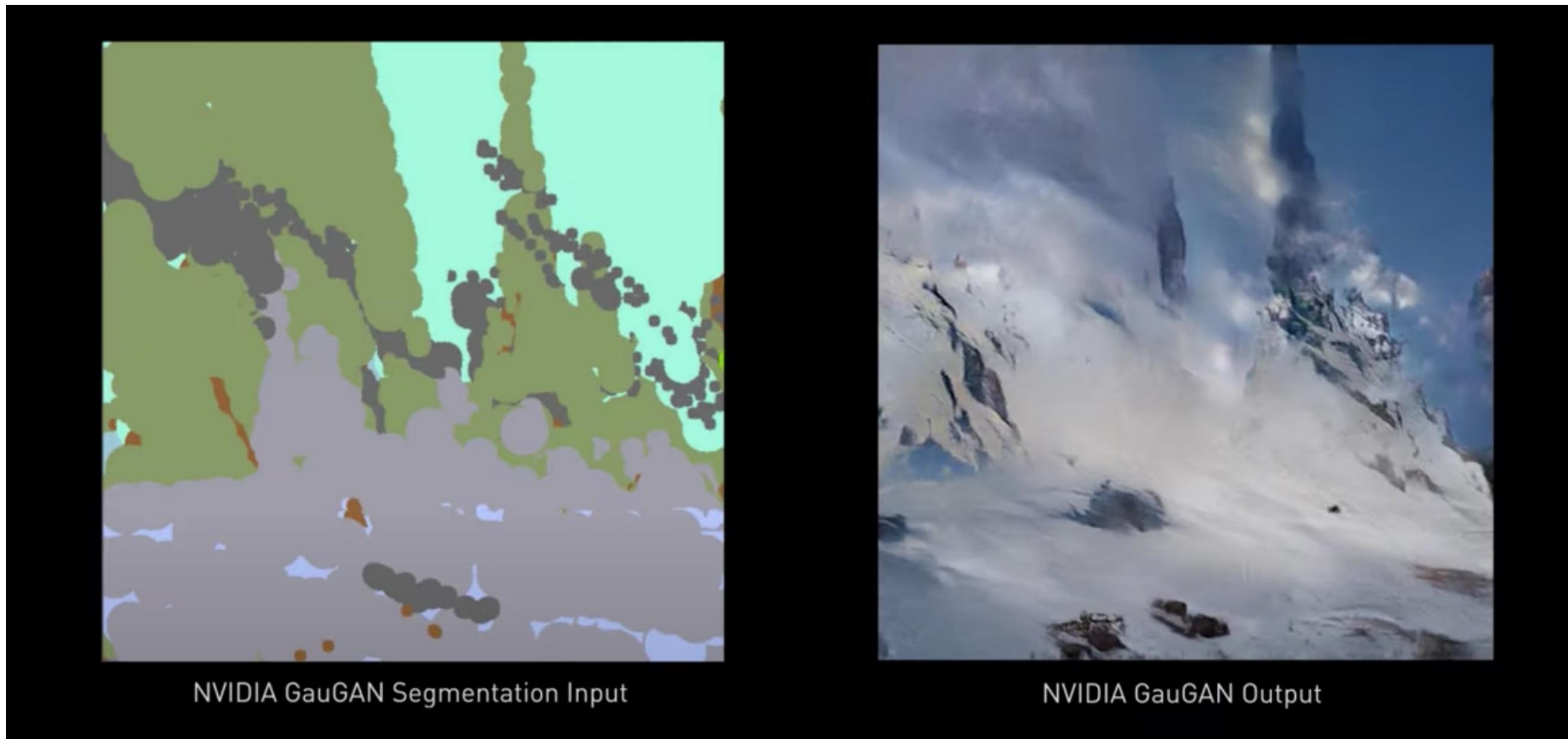
Application (2): Representation Learning

Learning from limited labels



Application (3): Artistic Tools

NVIDIA GauGAN



2022 / 2023 : The year of generative modeling?



Parti
Pathways Autoregressive Text-to-Image Model

DALL·E 2

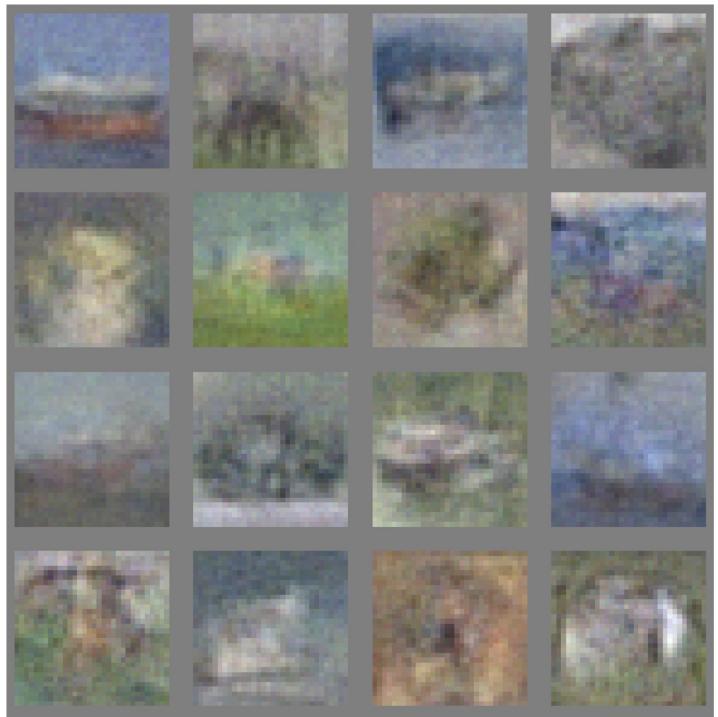
Stable Diffusion

Where we came from

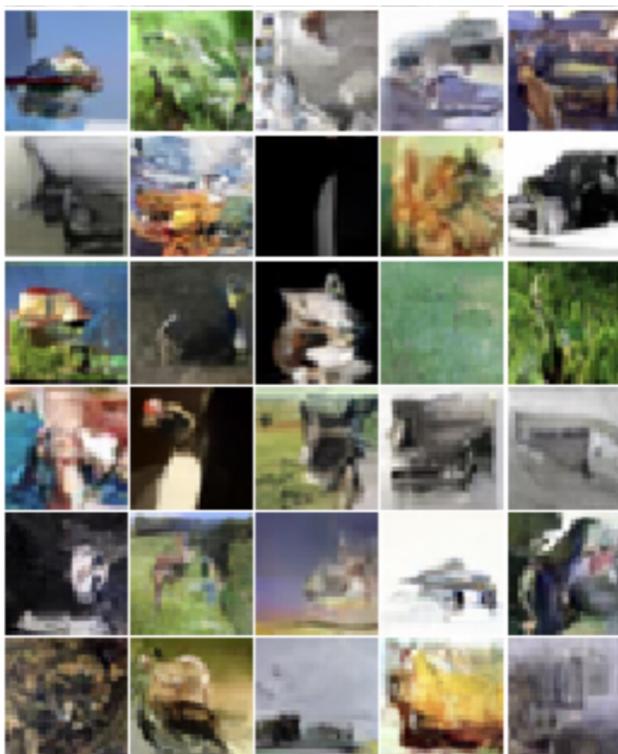
VAEs, 2013



GANs, 2014



PixelCNN, 2016



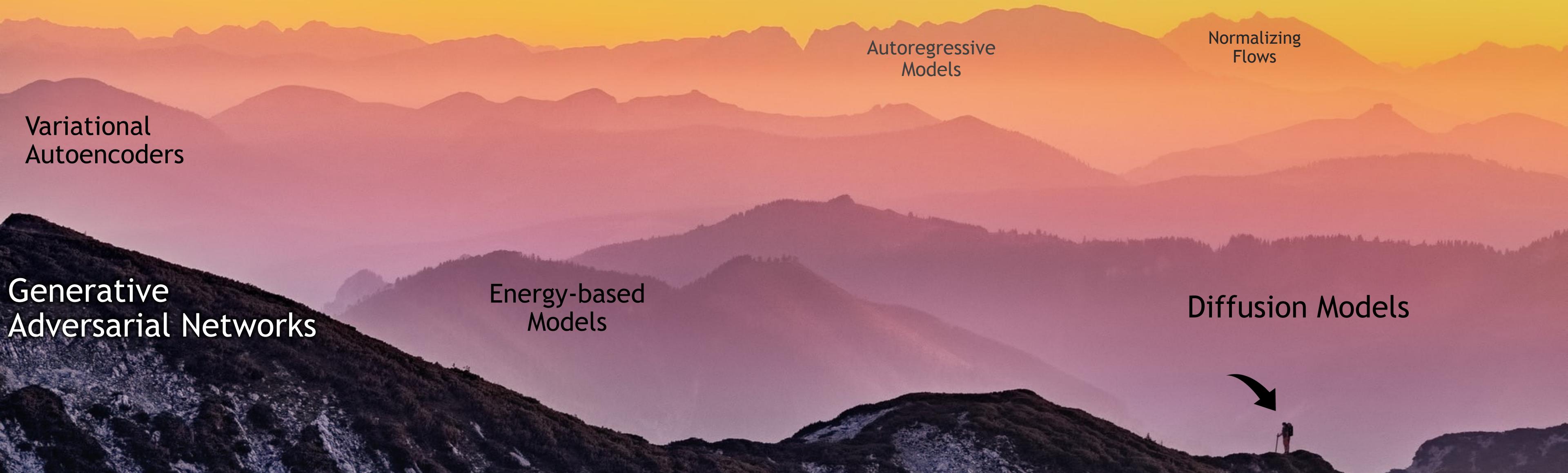
BigGAN, 2019



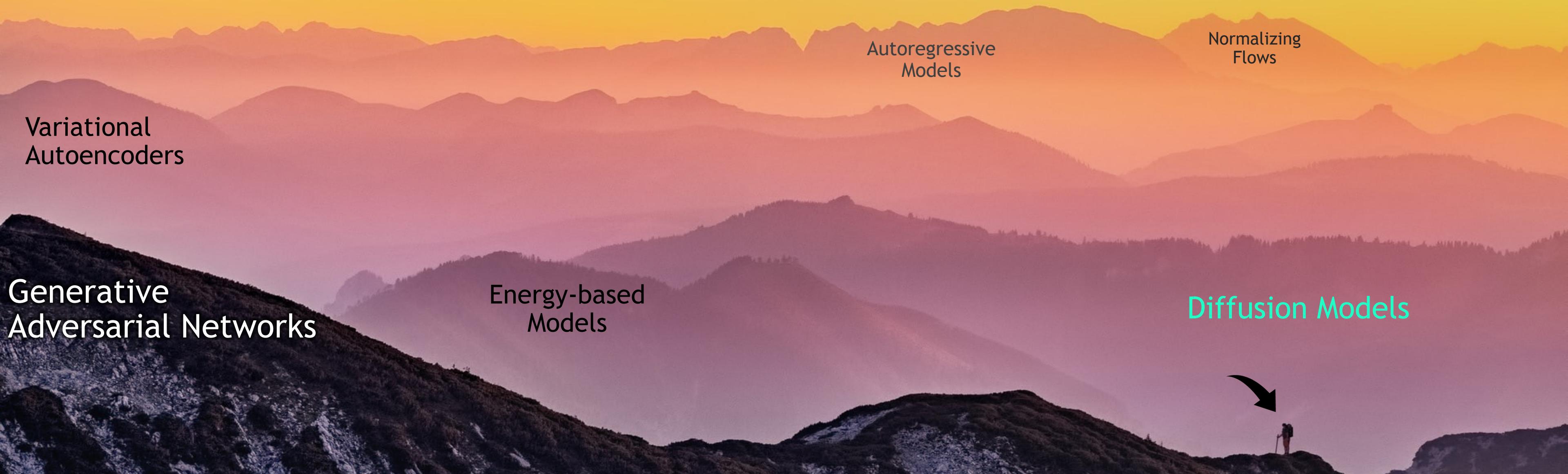
Imagen, 2022



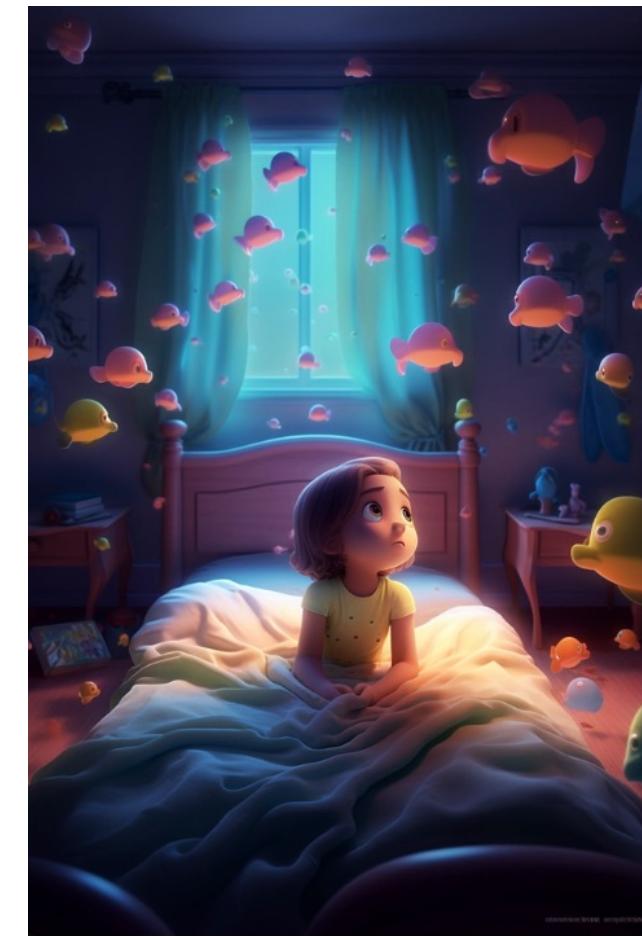
The Landscape of Deep Generative Models



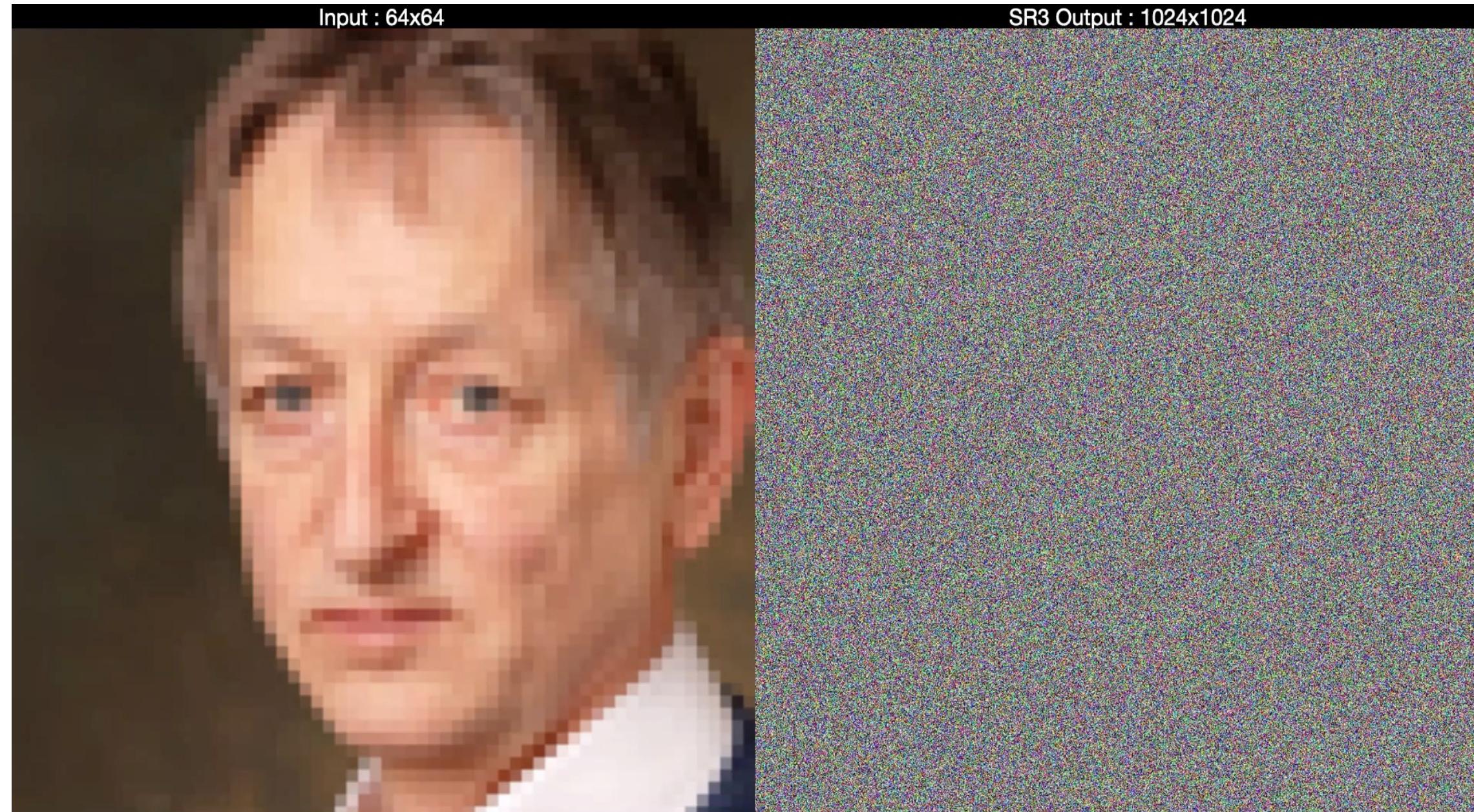
The Landscape of Deep Generative Models



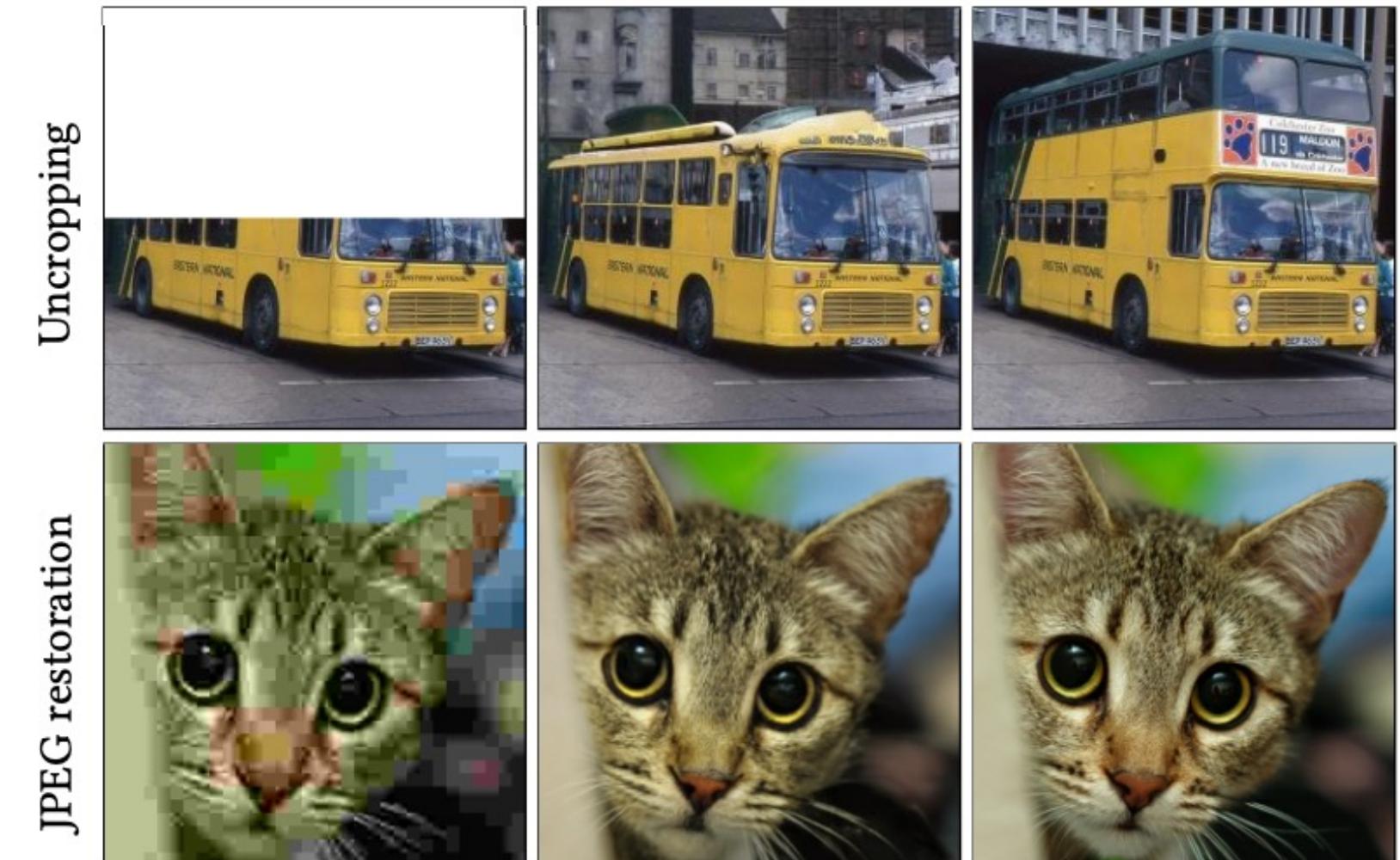
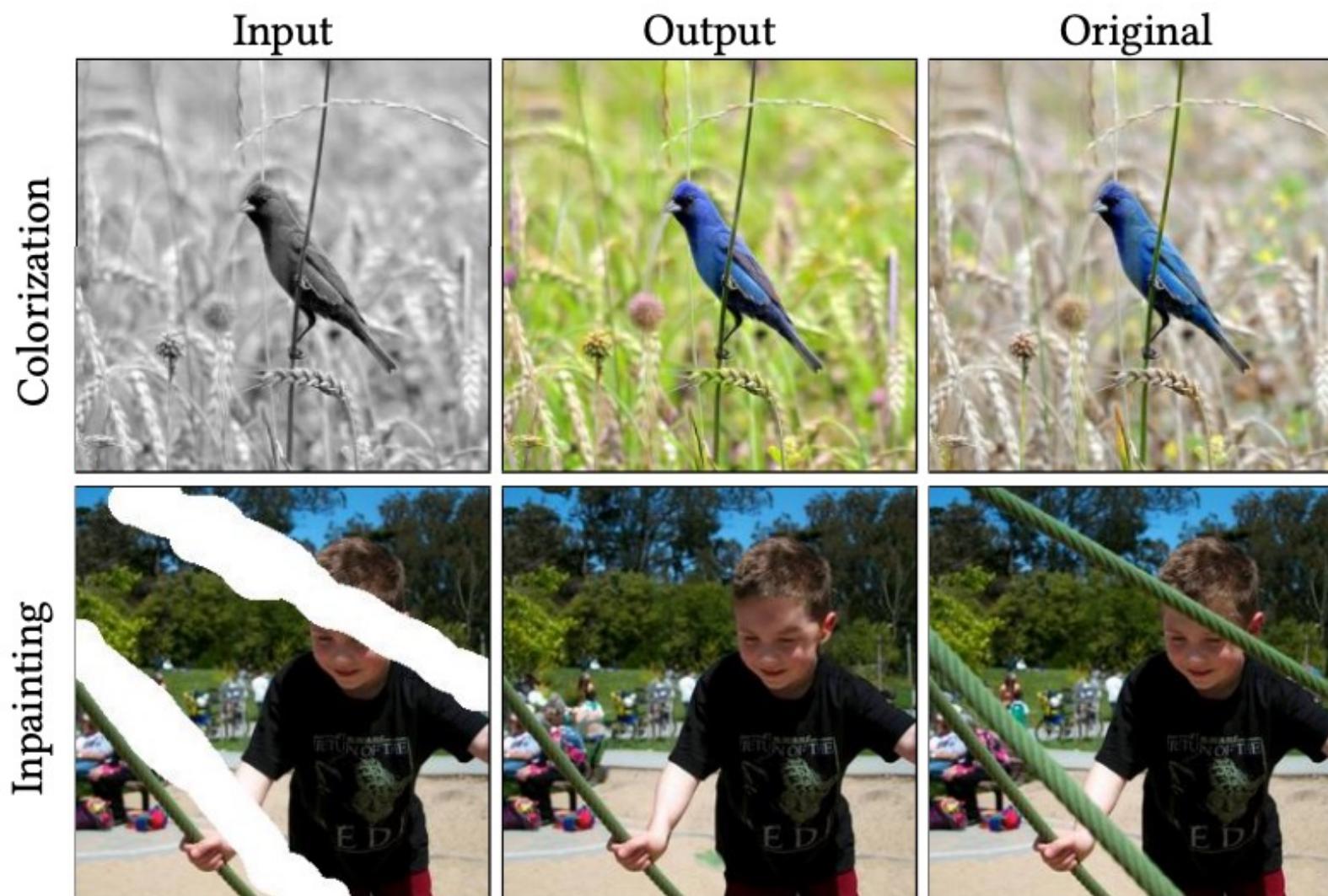
AI Art



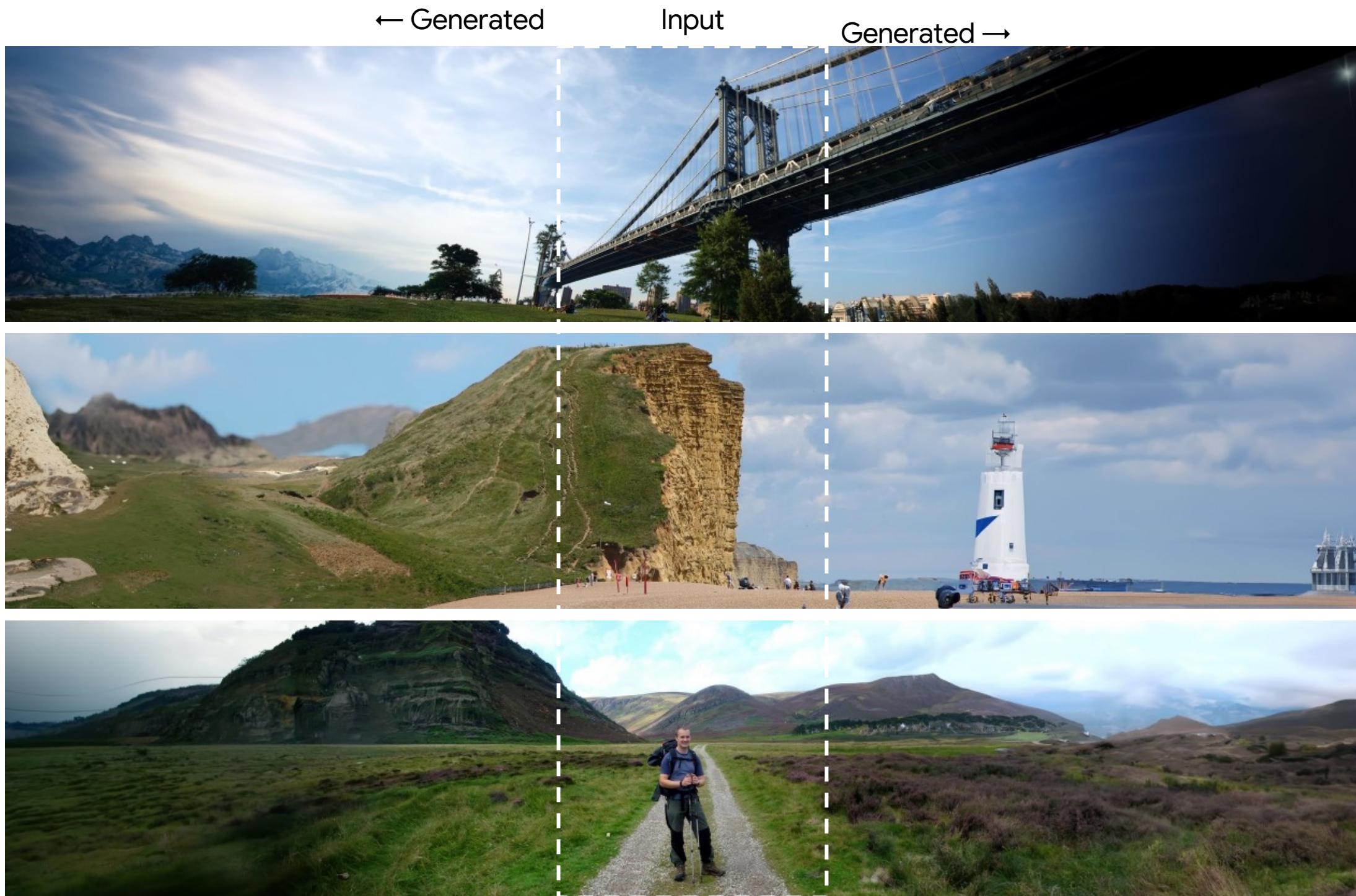
Applications: Super-resolution



Applications: Colorization, Inpainting, Restoration

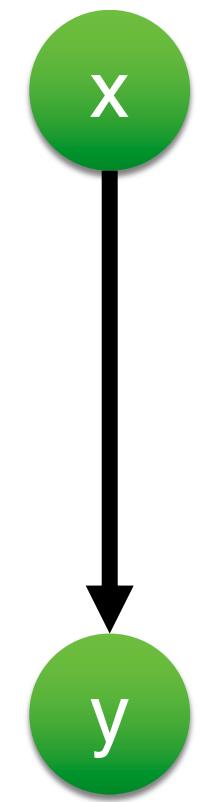


Applications: Outfilling



Variational Autoencoders

Classifying chocolate

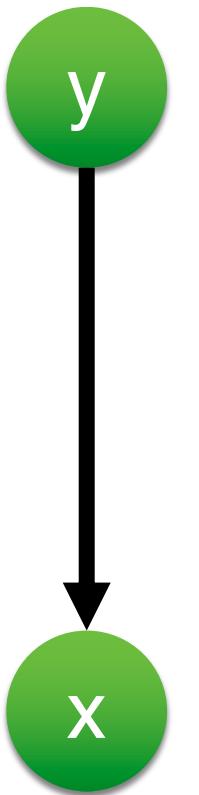


$$p(y|x) = \text{Categorical}(y; f(x))$$

“chocolate”

Generating chocolate

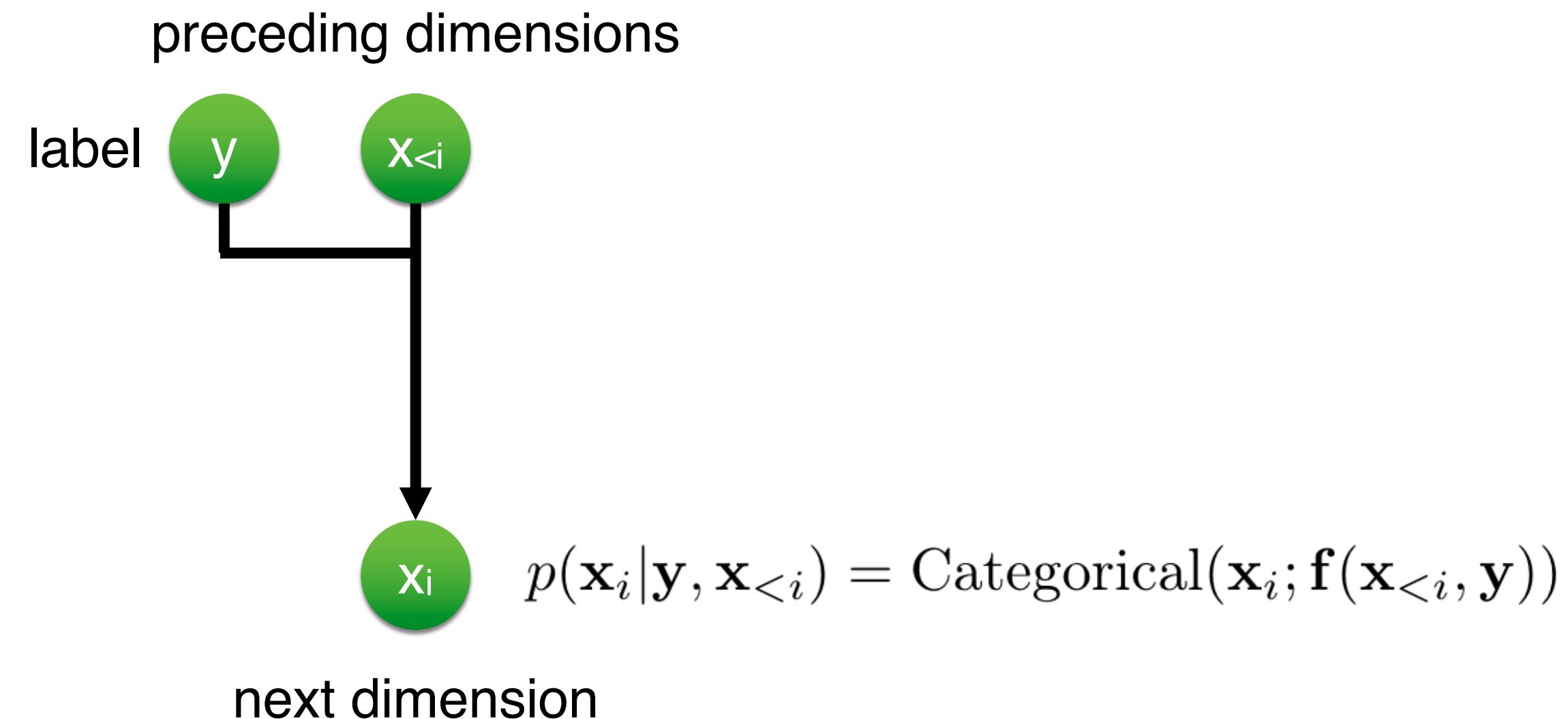
“chocolate”



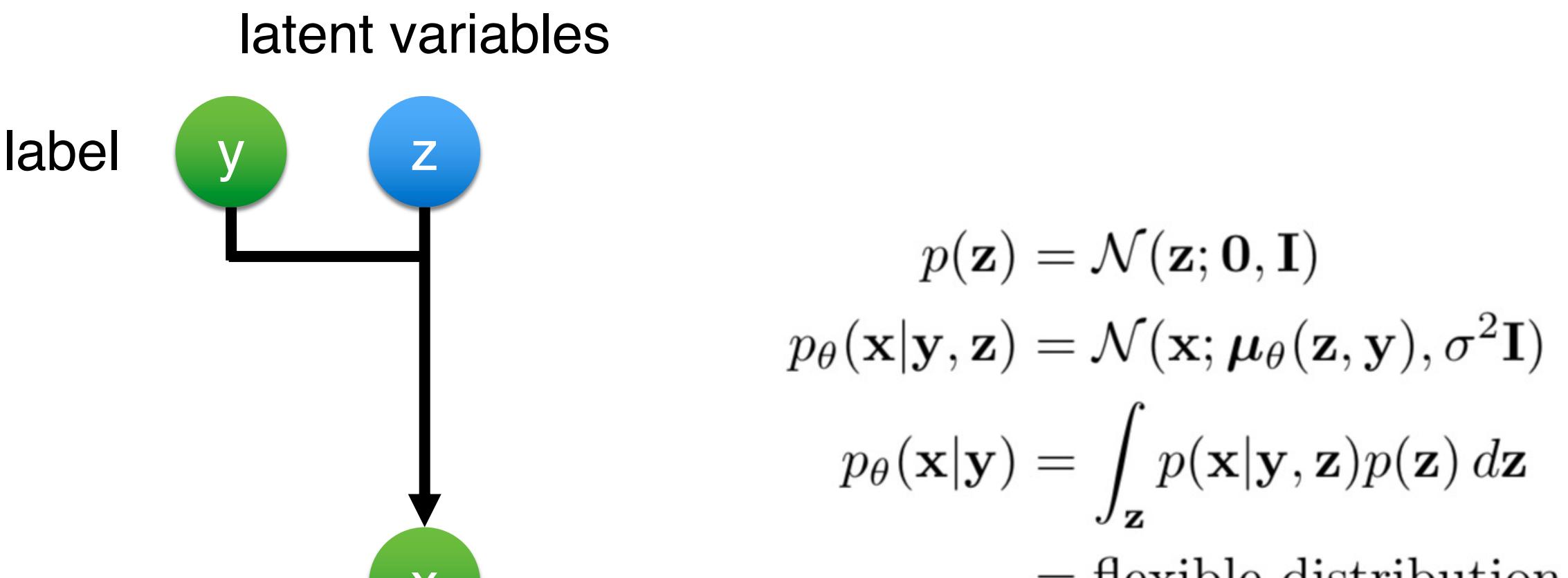
$$p(\mathbf{x}|\mathbf{y}) = ?$$



Autoregressive approach

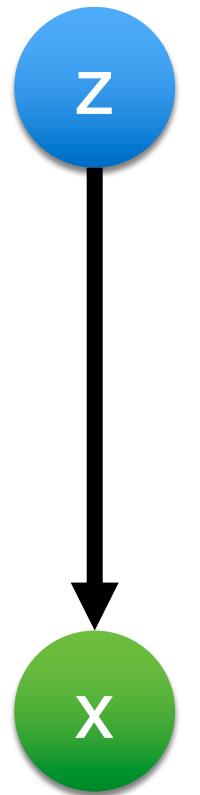


Latent variable approach



Latent variable approach - without y

latent variables



full image



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

$$p_{\theta}(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{\theta}(\mathbf{z}), \sigma^2 \mathbf{I})$$

$$p_{\theta}(\mathbf{x}) = \int_{\mathbf{z}} p_{\theta}(\mathbf{x}|\mathbf{z})p(\mathbf{z}) d\mathbf{z}$$

= flexible distribution

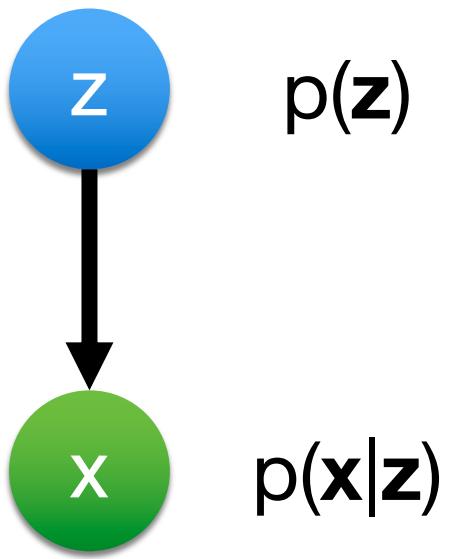
Optimization

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

$$p_\theta(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_\theta(\mathbf{z}), \sigma^2 \mathbf{I})$$

$$p_\theta(\mathbf{x}) = \int_{\mathbf{z}} p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z}) d\mathbf{z}$$

= flexible distribution



- Problem:
 - Marginal likelihood $p(\mathbf{x})$ is intractable
 - So can't do maximum likelihood directly

Generative model
 $p(\mathbf{x}, \mathbf{z})$

Variational Autoencoders (VAEs)

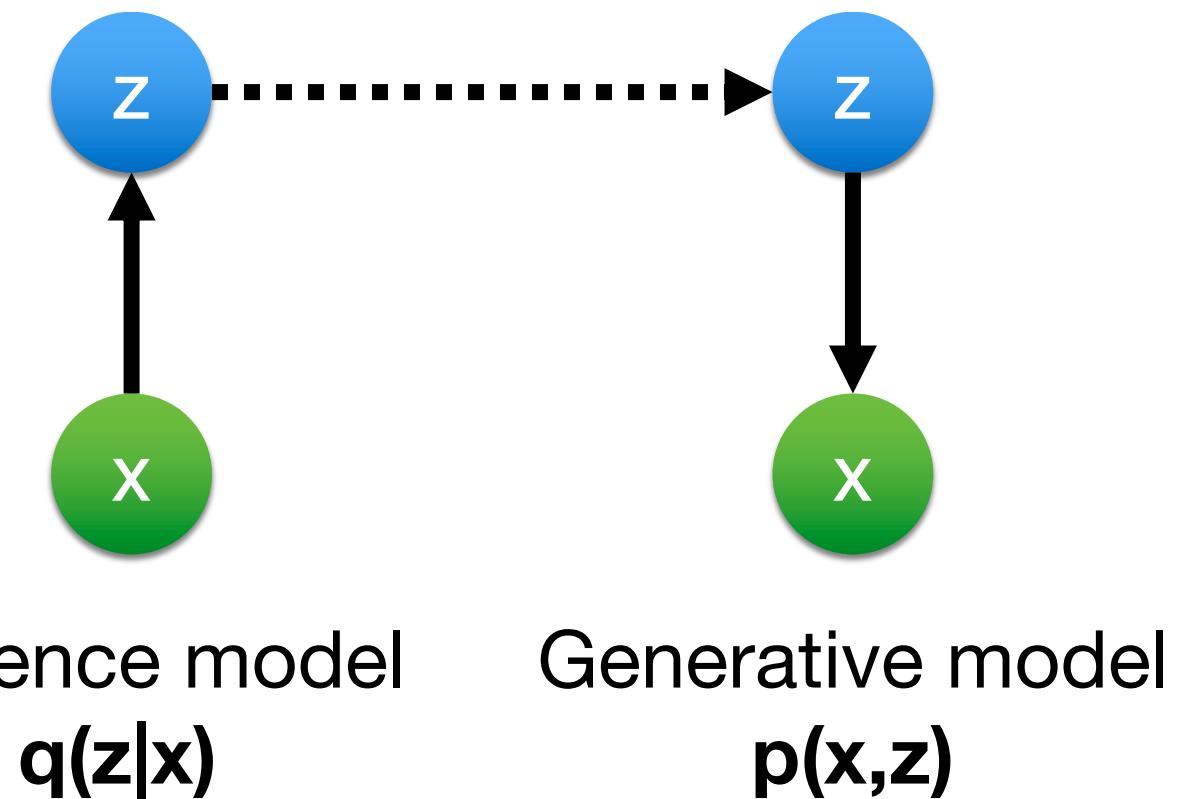
- We introduce an **inference model** $q(z|x)$

$$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \Sigma_\phi(x))$$

- This allows us to efficiently optimize the log-likelihood, through the **evidence lower bound** (ELBO).

$$\log p_{\theta,\phi}(x) \geq \text{ELBO}(x) = \mathbb{E}_{q_\phi(z|x)} \left[\log \frac{p_\theta(x, z)}{q_\phi(z|x)} \right]$$

- We optimize $q(z|x)$ and $p(x,z)$ jointly w.r.t. ELBO
- Bound is tight with the right $q(z|x)$



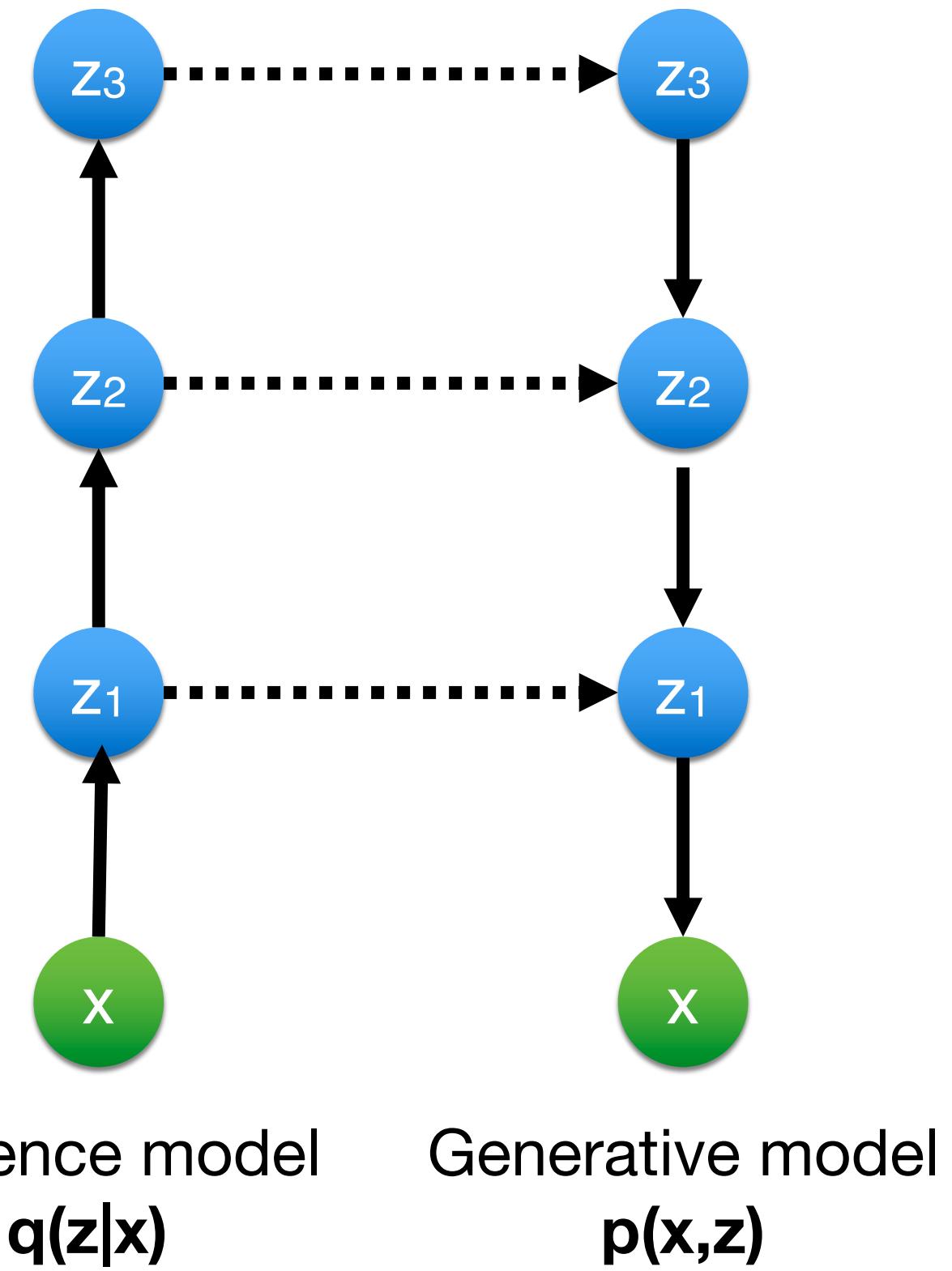
Hierarchical VAEs

- “Flat” VAEs suffer from simple priors
- Making both inference model and generative model hierarchical

$$q_\phi(\mathbf{z}_{1,2,3}|\mathbf{x}) = q_\phi(\mathbf{z}_1|\mathbf{x})q_\phi(\mathbf{z}_2|\mathbf{z}_1)q_\phi(\mathbf{z}_3|\mathbf{z}_2)$$

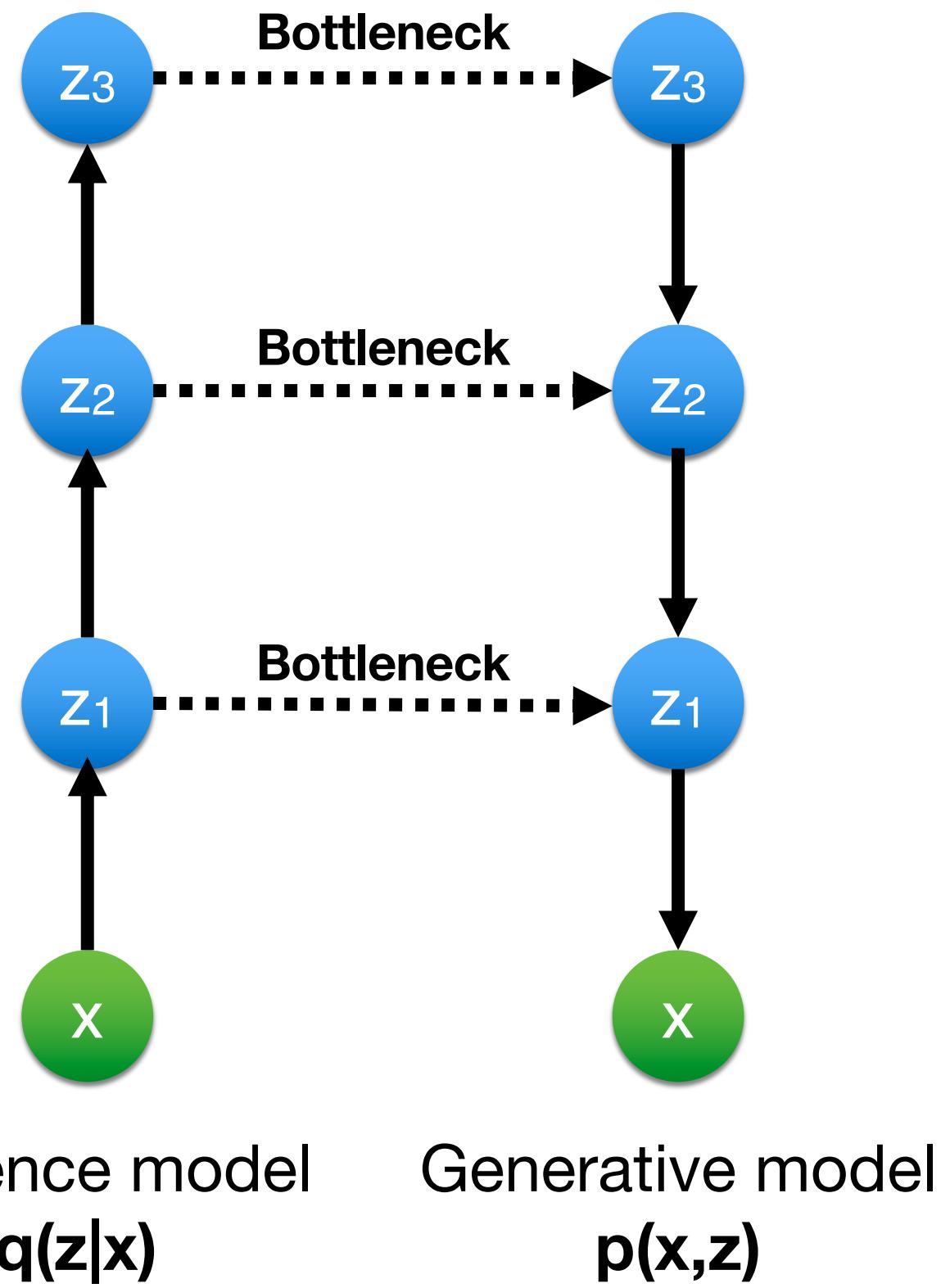
$$p_\theta(\mathbf{z}_{1,2,3}) = p_\theta(\mathbf{z}_3)p_\theta(\mathbf{z}_2|\mathbf{z}_3)p_\theta(\mathbf{z}_1|\mathbf{z}_2)p_\theta(\mathbf{x}|\mathbf{z}_1)$$

- Better likelihoods are achieved with hierarchies of latent variables



VAEs: challenges

- Optimization can be difficult for large models
- The ELBO enforces an **information bottleneck** (through its loss function) at the latent variables 'z', making VAE optimization prone to **bad local minima**.
- **Posterior collapse** is a dreaded bad local minimum where the latents do not transmit any information.



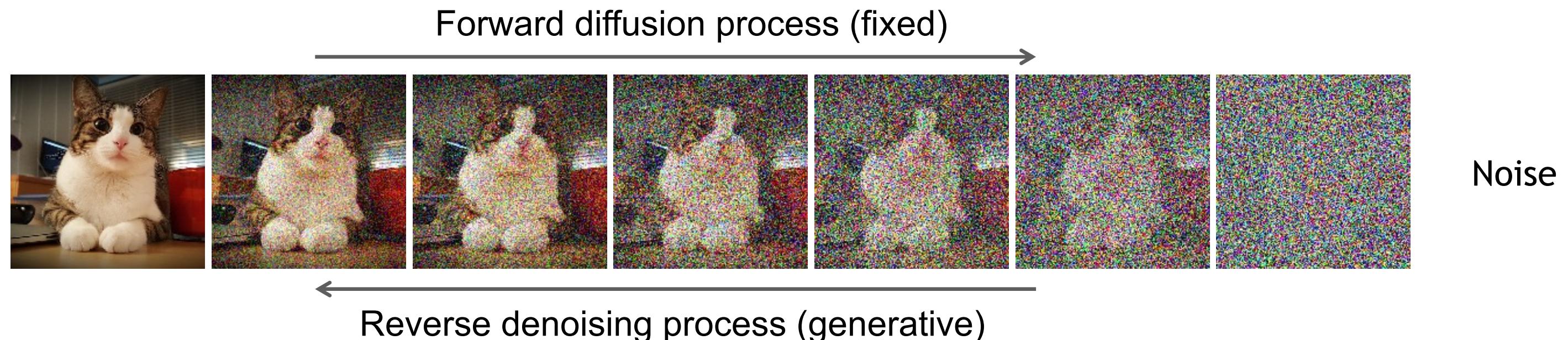
Diffusion Models

Denoising Diffusion Models

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



[Sohl-Dickstein et al., Deep Unsupervised Learning using Nonequilibrium Thermodynamics, ICML 2015](#)

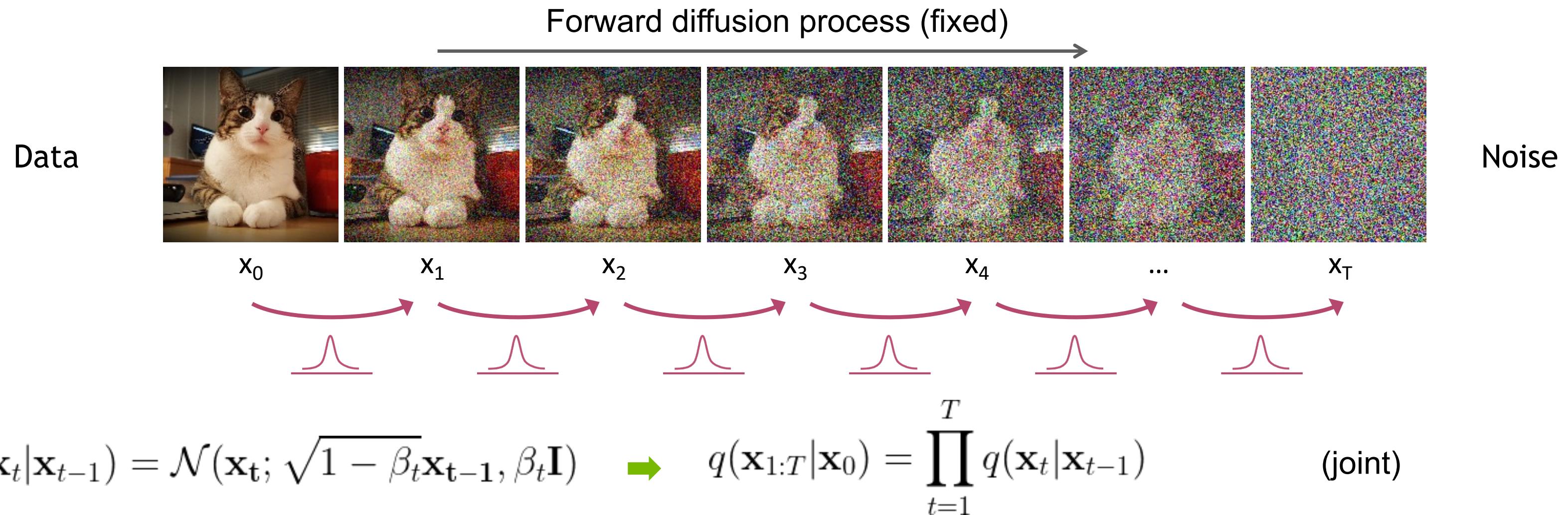
[Ho et al., Denoising Diffusion Probabilistic Models, NeurIPS 2020](#)

[Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021](#)

slide from <https://cvpr2022-tutorial-diffusion-models.github.io/>

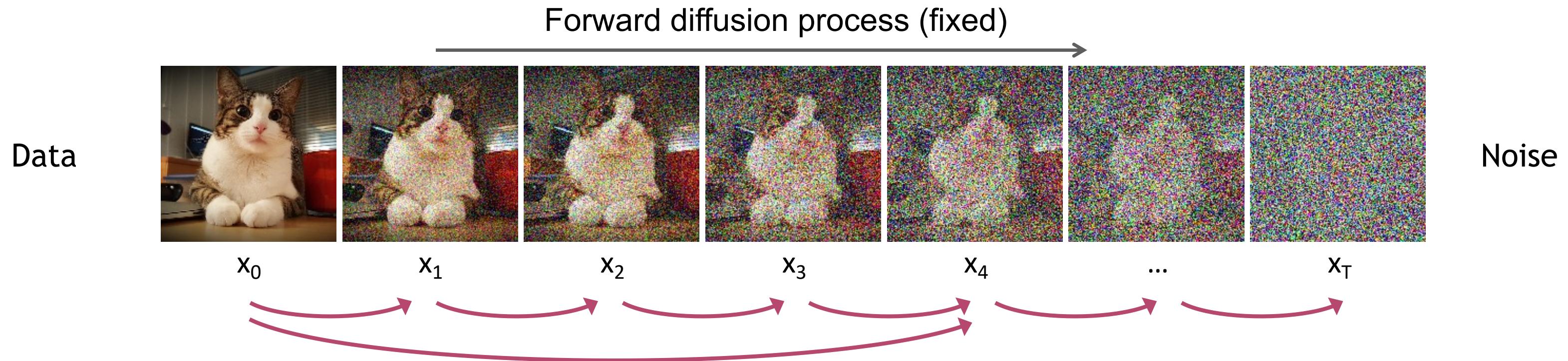
Forward Diffusion Process

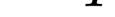
The formal definition of the forward process in T steps:



Similar to the inference model in hierarchical VAEs.

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

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

Generative Learning by Denoising

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

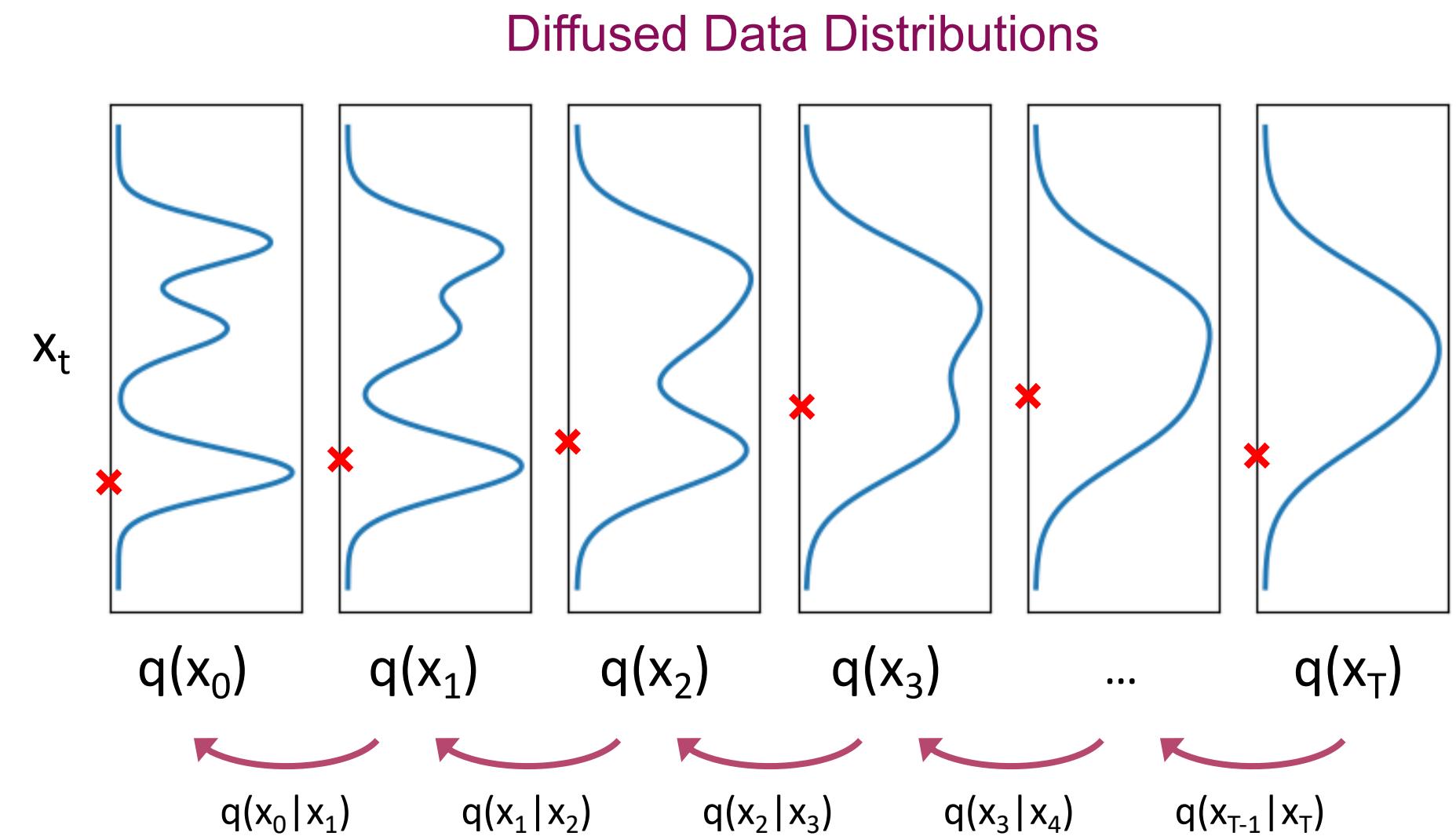
Generation:

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

Iteratively sample $\mathbf{x}_{t-1} \sim \underbrace{q(\mathbf{x}_{t-1} | \mathbf{x}_t)}_{\text{True Denoising Dist.}}$

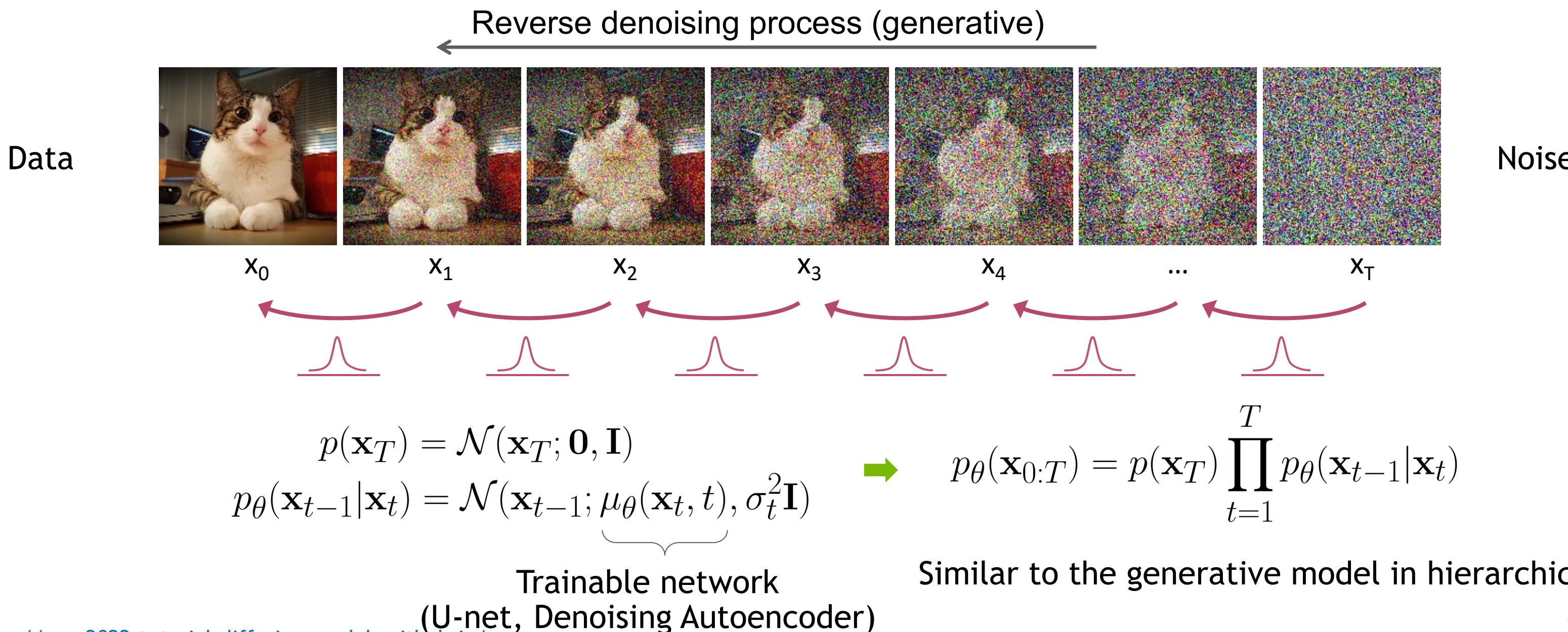
In general, $q(\mathbf{x}_{t-1} | \mathbf{x}_t) \propto q(\mathbf{x}_{t-1})q(\mathbf{x}_t | \mathbf{x}_{t-1})$ is intractable.

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



Reverse Denoising Process

Formal definition of forward and reverse processes in T steps:



Learning Denoising Model

Variational upper bound

For training, we can form variational upper bound (negative ELBO) that is commonly used for training variational autoencoders:

$$\mathbb{E}_{q(\mathbf{x}_0)} [-\log p_\theta(\mathbf{x}_0)] \leq \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)} \right] =: L$$

Sohl-Dickstein et al. ICML 2015 and Ho et al. NeurIPS 2020 show that:

$$L = \mathbb{E}_q \left[\underbrace{D_{\text{KL}}(q(\mathbf{x}_T|\mathbf{x}_0)||p(\mathbf{x}_T))}_{L_T} + \sum_{t>1} \underbrace{D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)||p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t))}_{L_{t-1}} \underbrace{-\log p_\theta(\mathbf{x}_0|\mathbf{x}_1)}_{L_0} \right]$$

where $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ is the tractable posterior distribution:

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

$$\text{where } \tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t}\mathbf{x}_0 + \frac{\sqrt{1-\beta_t}(1-\bar{\alpha}_{t-1})}{1-\bar{\alpha}_t}\mathbf{x}_t \text{ and } \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

Parameterizing the Denoising Model

Since both $q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0)$ and $p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$ are Normal distributions, the KL divergence has a simple form:

$$L_{t-1} = D_{\text{KL}}(q(\mathbf{x}_{t-1}|\mathbf{x}_t, \mathbf{x}_0) || p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)) = \mathbb{E}_q \left[\frac{1}{2\sigma_t^2} \|\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) - \mu_\theta(\mathbf{x}_t, t)\|^2 \right] + C$$

Recall that $\mathbf{x}_t = \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$. [Ho et al. NeurIPS 2020](#) observe that:

$$\tilde{\mu}_t(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{1 - \beta_t}} \left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1 - \bar{\alpha}_t}} \epsilon \right)$$

They propose to represent the mean of the denoising model using a *noise-prediction* network:

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

With this parameterization

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\frac{\beta_t^2}{2\sigma_t^2(1 - \beta_t)(1 - \bar{\alpha}_t)} \|\epsilon - \underbrace{\epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)}_{\mathbf{x}_t}\|^2 \right] + C$$

Training Objective Weighting

Trading likelihood for perceptual quality

$$L_{t-1} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[\underbrace{\frac{\beta_t^2}{2\sigma_t^2(1 - \beta_t)(1 - \bar{\alpha}_t)}}_{\lambda_t} \|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2 \right]$$

The time dependent λ_t ensures that the training objective is weighted properly for the maximum data likelihood training.

However, this weight is often very large for small t's.

Ho et al. NeurIPS 2020 observe that simply setting $\lambda_t = 1$ improves sample quality. So, they propose to use:

$$L_{\text{simple}} = \mathbb{E}_{\mathbf{x}_0 \sim q(\mathbf{x}_0), \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I}), t \sim \mathcal{U}(1, T)} \left[\underbrace{\|\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2}_{\mathbf{x}_t} \right]$$

Summary

Training and Sample Generation

Algorithm 1 Training

```
1: repeat
2:    $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ 
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
```

Algorithm 2 Sampling

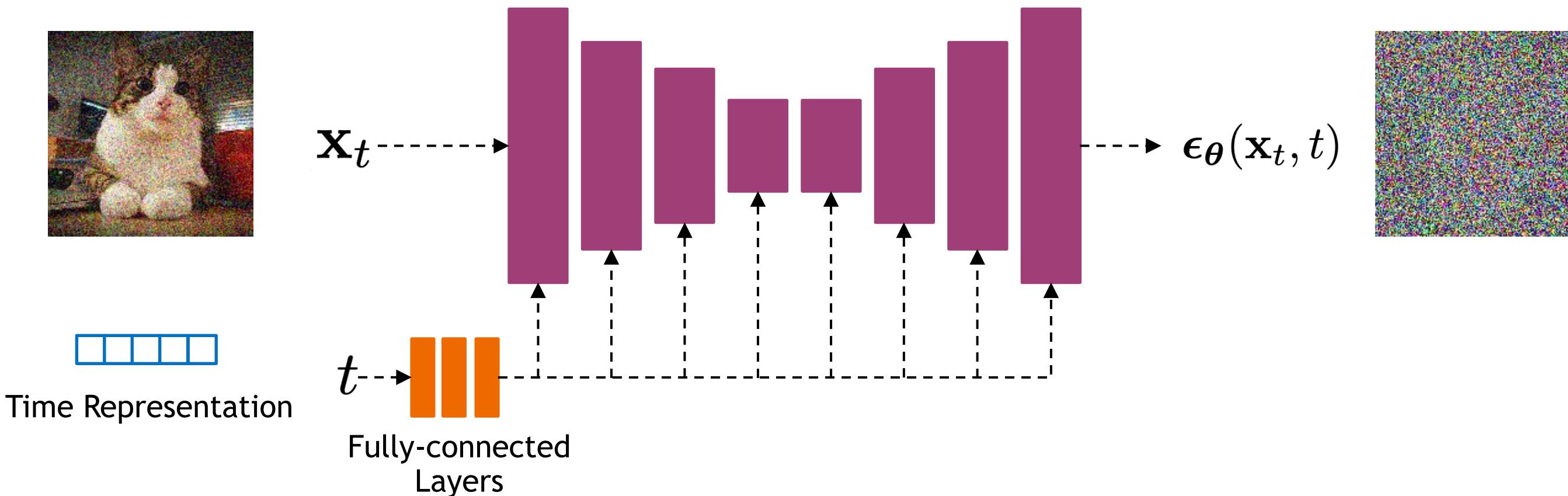
```
1:  $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
2: for  $t = T, \dots, 1$  do
3:    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ 
4:   
$$\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left( \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}} \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t,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

5: end for
6: return  $\mathbf{x}_0$ 
```

Implementation Considerations

Network Architectures

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_\theta(\mathbf{x}_t, t)$



Time representation: sinusoidal positional embeddings or random Fourier features.

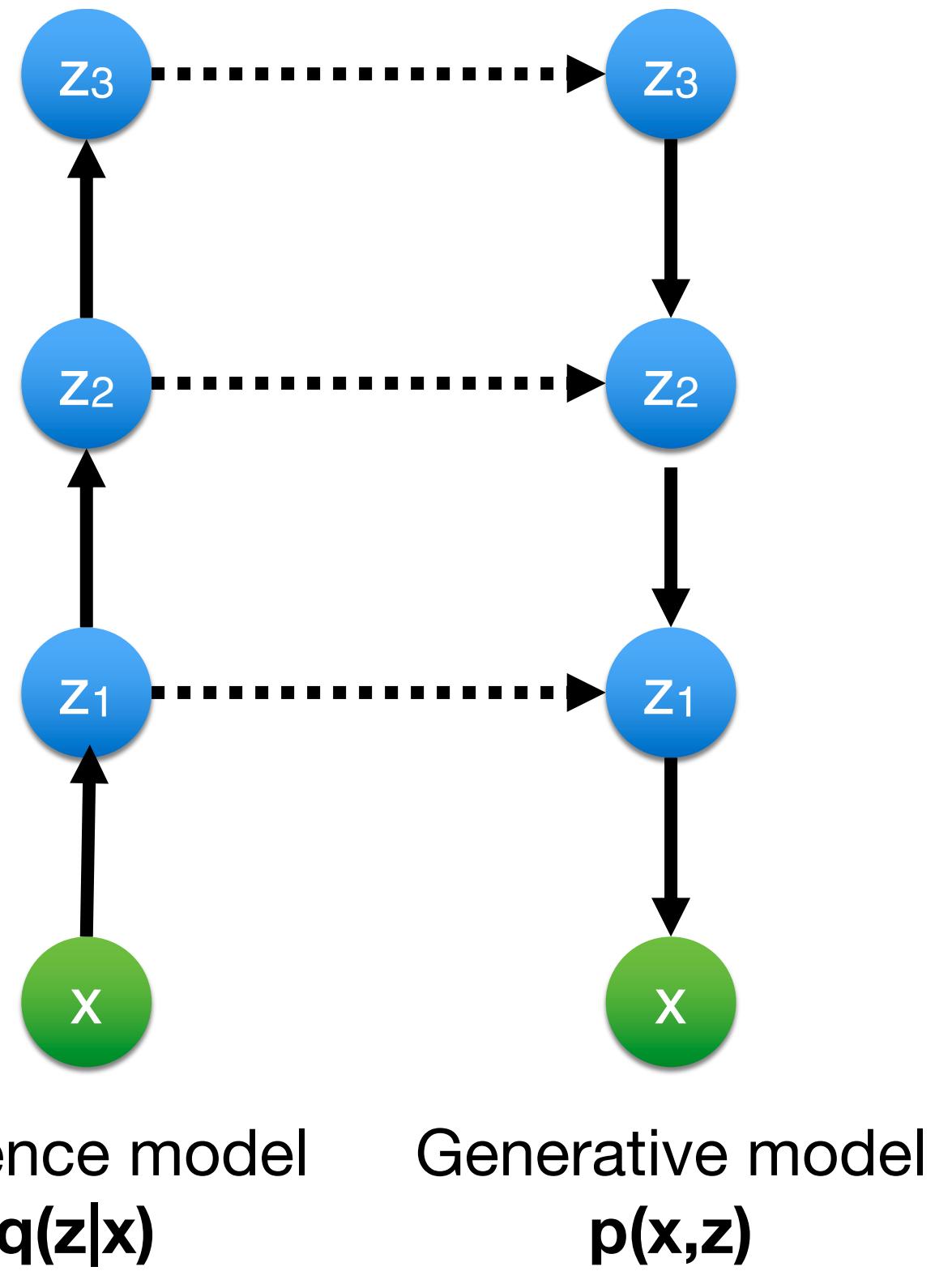
Time features are fed to the residual blocks using either simple spatial addition or using adaptive group normalization layers. (see [Dhariwal and Nichol NeurIPS 2021](#))

Connection to VAEs

Diffusion models can be considered as a special form of hierarchical VAEs.

However, in diffusion models:

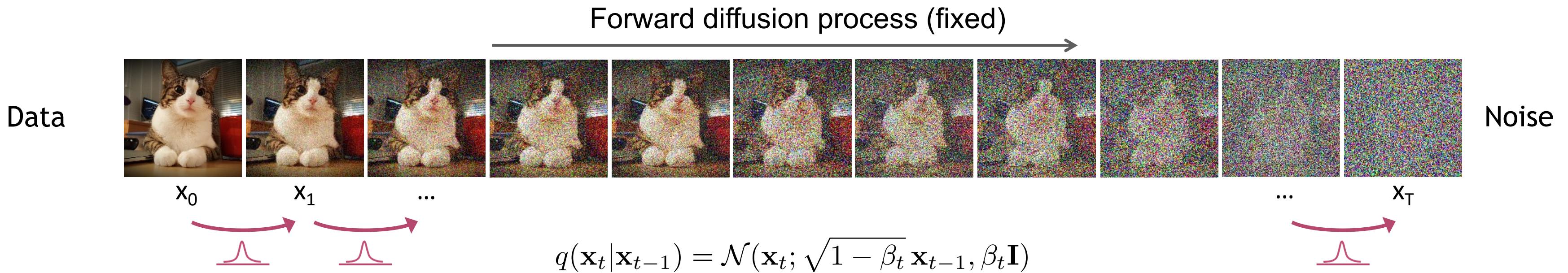
- The inference model is fixed: easier to optimize
- The latent variables have the same dimension as the data.
- The ELBO is decomposed to each time step: fast to train
 - Can be made extremely deep (even infinitely deep)
- The model is trained with some reweighting of the ELBO.



Continuous-time diffusion models

Stochastic differential equation framework

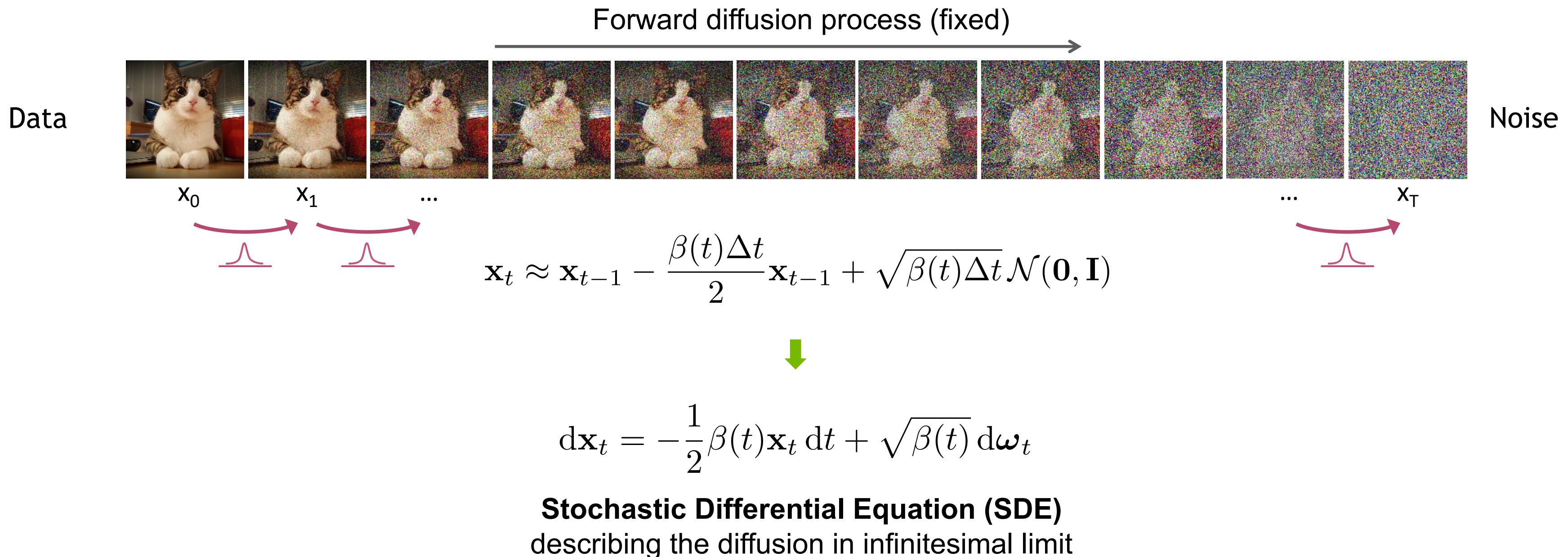
Consider the limit of many small steps:



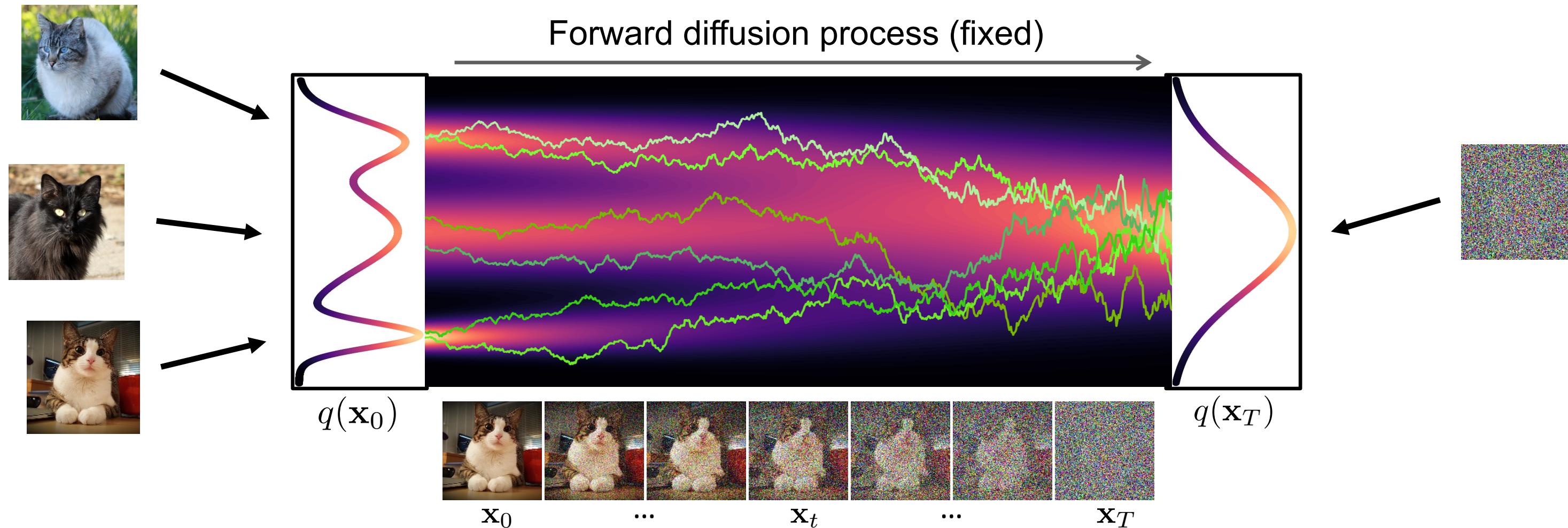
$$\begin{aligned}
 \mathbf{x}_t &= \sqrt{1 - \beta_t} \mathbf{x}_{t-1} + \sqrt{\beta_t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \\
 &= \sqrt{1 - \beta(t)\Delta t} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (\beta_t := \beta(t)\Delta t) \\
 \rightarrow \quad \mathbf{x}_t &\approx \mathbf{x}_{t-1} - \frac{\beta(t)\Delta t}{2} \mathbf{x}_{t-1} + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I}) \quad (\text{Taylor expansion})
 \end{aligned}$$

Forward Diffusion Process as Stochastic Differential Equation

Consider the limit of many small steps:



Forward Diffusion Process as Stochastic Differential Equation

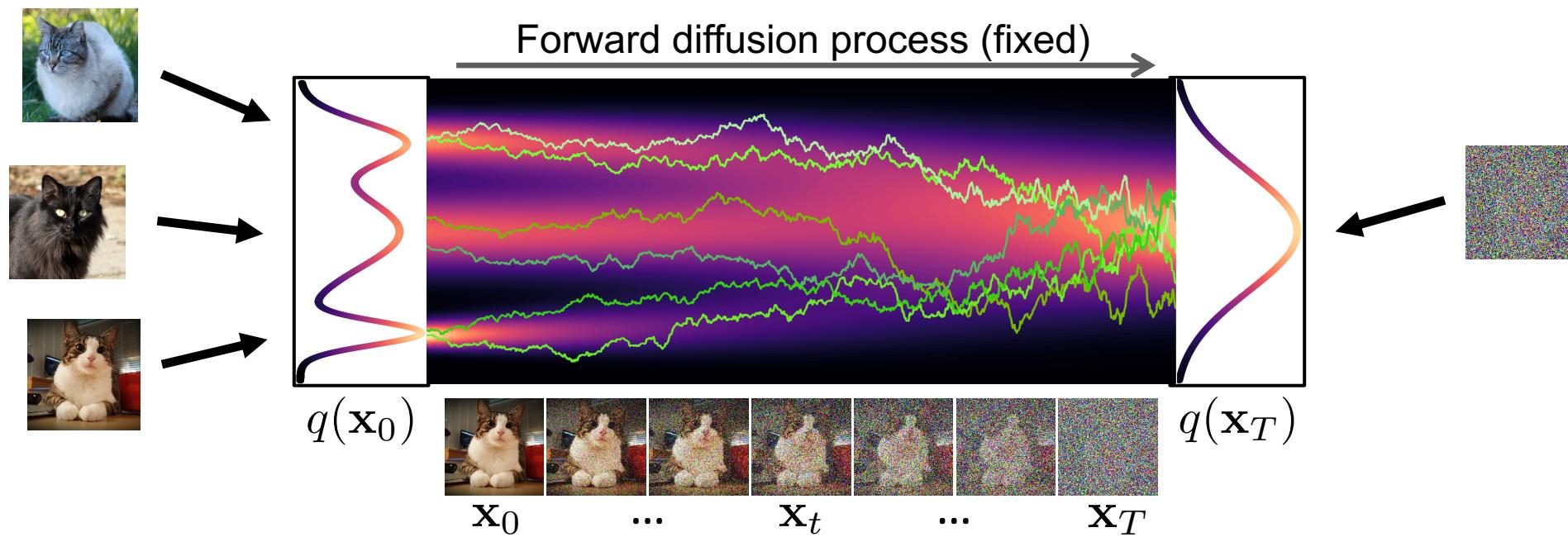


Forward Diffusion SDE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)} d\omega_t$$

drift term
(pulls towards mode) diffusion term
(injects noise)

The Generative Reverse Stochastic Differential Equation



Forward Diffusion SDE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t dt + \sqrt{\beta(t)} d\omega_t$$

Reverse Generative Diffusion SDE:

→ Simulate reverse diffusion process: Data generation from random noise!

Song et al., ICLR, 2021

Anderson, in Stochastic Processes and their Applications, 1982

slide from <https://cvpr2022-tutorial-diffusion-models.github.io/>

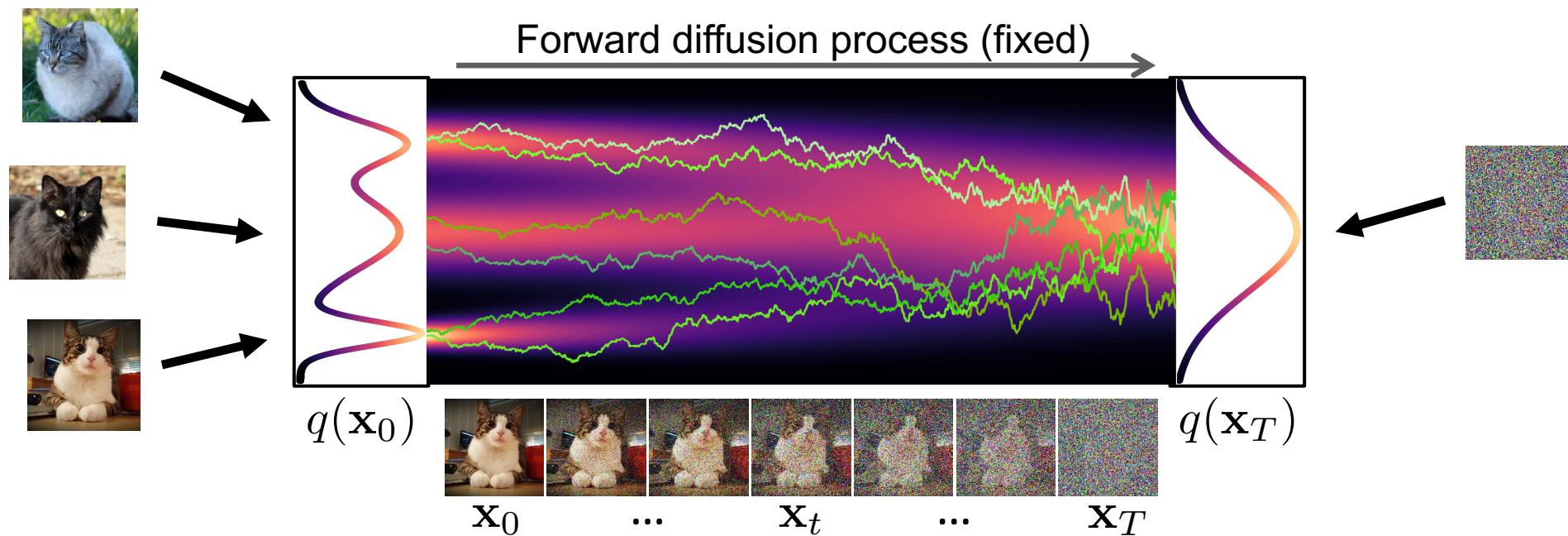
The Generative Reverse Stochastic Differential Equation

But how to get the score function $\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)$?

Forward Diffusion SDE:

Reverse Generative Diffusion SDE:

Score Matching



- Naïve idea, learn model for the score function by direct regression?

$$\min_{\theta} \underbrace{\mathbb{E}_{t \sim \mathcal{U}(0, T)}}_{\text{diffusion time } t} \underbrace{\mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t)}}_{\text{diffused data } \mathbf{x}_t} \underbrace{\tilde{w}(t)}_{\text{weighting function}} \cdot \underbrace{\|\mathbf{s}_{\theta}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)\|_2^2}_{\text{score of diffused data (marginal)}}$$

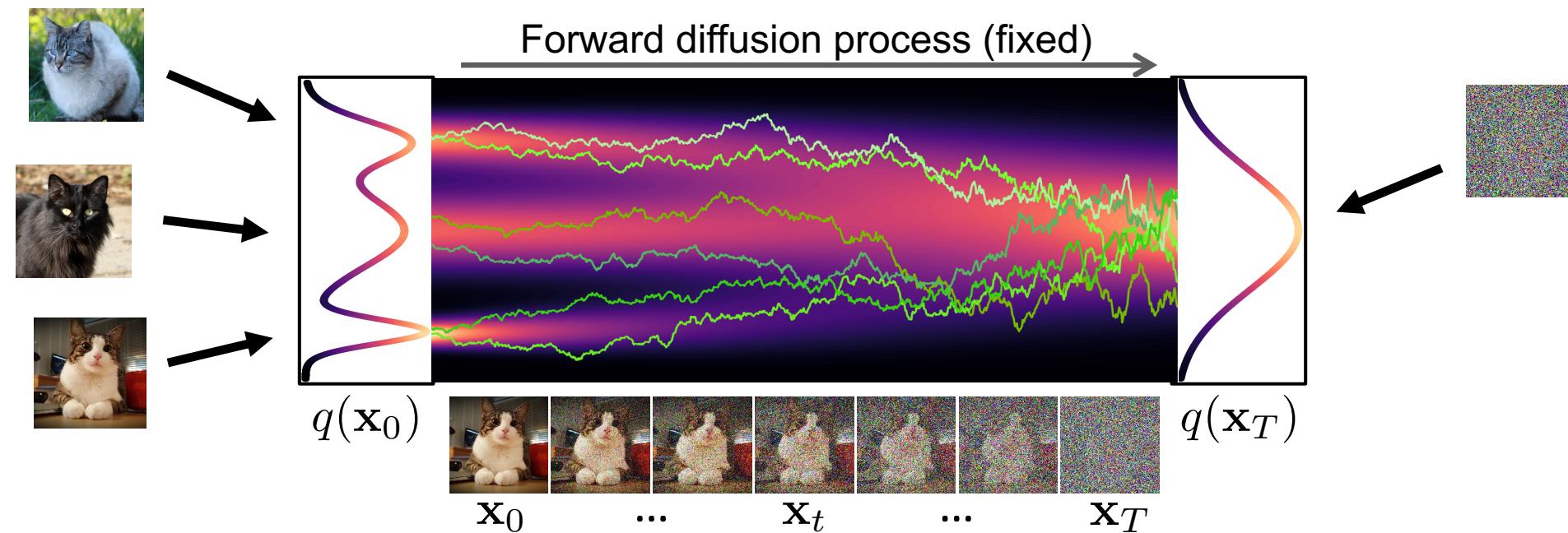
→ But $\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)$ (**score of the *marginal diffused density* $q_t(\mathbf{x}_t)$**) is not tractable!

[Vincent, "A Connection Between Score Matching and Denoising Autoencoders", Neural Computation, 2011](#)

[Song and Ermon, "Generative Modeling by Estimating Gradients of the Data Distribution", NeurIPS, 2019](#)

slide from <https://cvpr2022-tutorial-diffusion-models.github.io/>

Denoising Score Matching



- Instead, diffuse individual data points \mathbf{x}_0 . Diffused $q_t(\mathbf{x}_t|\mathbf{x}_0)$ **is** tractable!
- **Denoising Score Matching:**

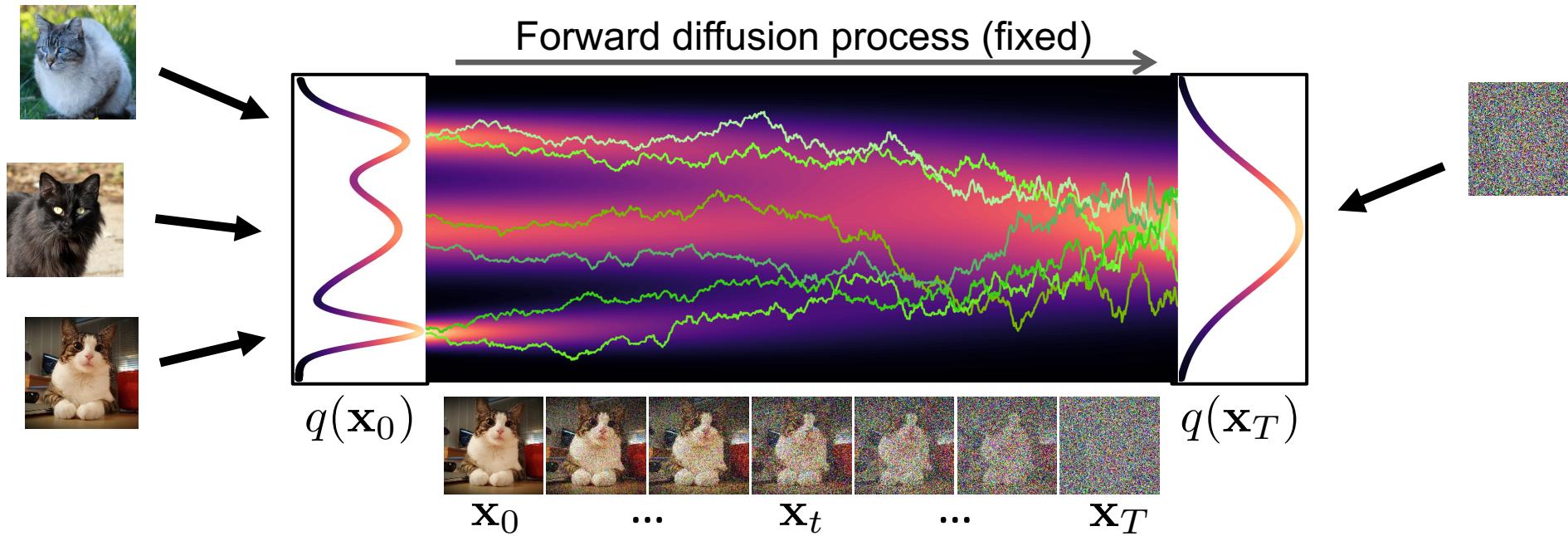
$$\min_{\theta} \underbrace{\mathbb{E}_{t \sim \mathcal{U}(0,T)}}_{\text{diffusion time } t} \underbrace{\mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)}}_{\text{data sample } \mathbf{x}_0} \underbrace{\mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t|\mathbf{x}_0)}}_{\text{diffused data sample } \mathbf{x}_t} \underbrace{\tilde{w}(t) \cdot ||\mathbf{s}_{\theta}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t|\mathbf{x}_0)||_2^2}_{\begin{array}{l} \text{weighting function} \\ \text{neural network} \\ \text{score of diffused data sample} \end{array}}$$

[Vincent, in Neural Computation, 2011](#)
[Song and Ermon, NeurIPS, 2019](#)
[Song et al. ICLR, 2021](#)
 slide from <https://cvpr2022-tutorial-diffusion-models.github.io/>

→ **After expectations,** $\mathbf{s}_{\theta}(\mathbf{x}_t, t) \approx \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)$!

Denoising Score Matching

Epsilon-prediction parametrization



- **Denoising Score Matching:**

$$\min_{\theta} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t | \mathbf{x}_0)} \tilde{w}(t) \cdot \|\mathbf{s}_{\theta}(\mathbf{x}_t, t) - \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t | \mathbf{x}_0)\|_2^2$$

- Re-parametrized sampling: $\mathbf{x}_t = \alpha_t \mathbf{x}_0 + \sigma_t \boldsymbol{\epsilon}$ $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

- Score function: $\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t | \mathbf{x}_0) = -\nabla_{\mathbf{x}_t} \frac{(\mathbf{x}_t - \alpha_t \mathbf{x}_0)^2}{2\sigma_t^2} = -\frac{\mathbf{x}_t - \alpha_t \mathbf{x}_0}{\sigma_t^2} = -\frac{\alpha_t \mathbf{x}_0 + \sigma_t \boldsymbol{\epsilon} - \alpha_t \mathbf{x}_0}{\sigma_t^2} = -\frac{\boldsymbol{\epsilon}}{\sigma_t}$

- Neural network model: $\mathbf{s}_{\theta}(\mathbf{x}_t, t) := -\frac{\boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)}{\sigma_t}$

Vincent, in *Neural Computation*, 2011
 Song and Ermon, *NeurIPS*, 2019
 Song et al. *ICLR*, 2021

→ $\min_{\theta} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \hat{w}(t) \cdot \|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\theta}(\mathbf{x}_t, t)\|_2^2$ $\hat{w}(t) = \frac{\tilde{w}(t)}{\sigma_t}$

What is the ELBO for continuous-time diffusion models?

- Denoising Score Matching:

$$\min_{\theta} \mathbb{E}_{t \sim \mathcal{U}(0, T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \hat{w}(t) \cdot \|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, t)\|_2^2$$

- [Kingma et al, 2021] showed that the variational upper bound (negative ELBO) can be reduced to a simple variant:

$$-\text{ELBO}(\theta) = \frac{1}{2} \mathbb{E}_{t \sim \mathcal{U}(0, T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} - \frac{d\lambda}{dt} \cdot \|\epsilon - \epsilon_{\theta}(\mathbf{x}_t, t)\|_2^2 + \text{const}$$

where $\mathbf{x}_t = \alpha_t \mathbf{x}_0 + \sigma_t \epsilon$

$$\lambda = \log \frac{\alpha_t^2}{\sigma_t^2} \quad (\text{signal-to-noise ratio of timestep } t)$$

- In practice, different loss weightings trade off between model with good perceptual quality vs. high log-likelihood:

- Perceptual quality, e.g., $\hat{w}(t) = 1$
- High likelihood: -ELBO



How to explain such discrepancy?
Can we still trust ELBO / maximum likelihood?

Weighted diffusion objectives

Understanding diffusion objectives as the ELBO with data augmentation

- Summarize different types of diffusion objectives as the following **weighted diffusion objective**:

$$\mathcal{L}_w(\theta) = \frac{1}{2} \mathbb{E}_{t \sim \mathcal{U}(0,T)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \left[w(t) \cdot -\frac{d\lambda}{dt} \cdot \|\epsilon - \epsilon_\theta(\mathbf{x}_t, t)\|_2^2 \right]$$

- [Kingma & Gao, 2023] showed that if $w(t)$ is a monotonically increasing function, then the weighted diffusion objective is equivalent to the **negative ELBO with data augmentation** (Gaussian addition noise):

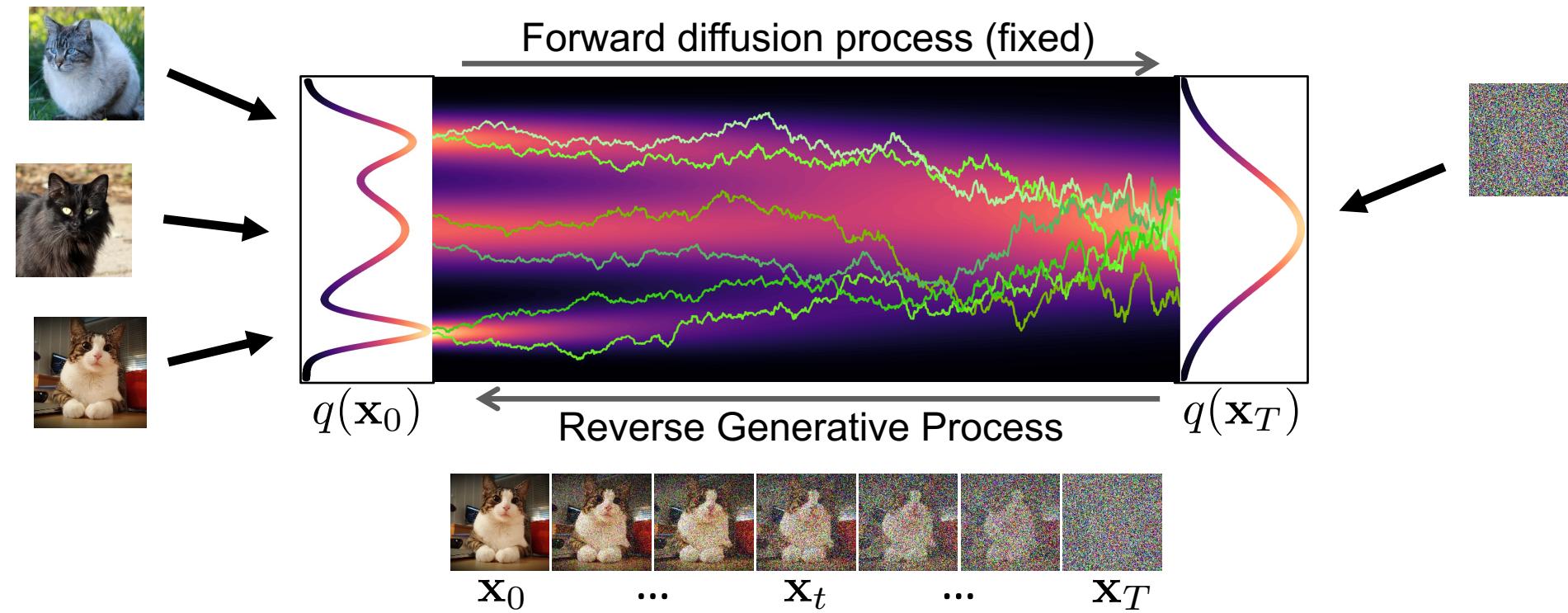
$$\mathcal{L}_w(\theta) \geq \underbrace{\mathbb{E}_{t \sim p_w(t)} \mathbb{E}_{\mathbf{x}_0 \sim q_0(\mathbf{x}_0)} \mathbb{E}_{\mathbf{x}_t \sim q_t(\mathbf{x}_t | \mathbf{x}_0)} [-\log p(\mathbf{x}_t)]}_{\text{Neg. log lik. of noise-perturbed data}} + \text{const}$$

where $p_w(t) \propto \frac{dw(t)}{dt}$

- Therefore, the ELBO objective is compatible with perceptual quality when combined with simple data augmentation (additive noise)

Probability Flow ODE

Alternative reverse process



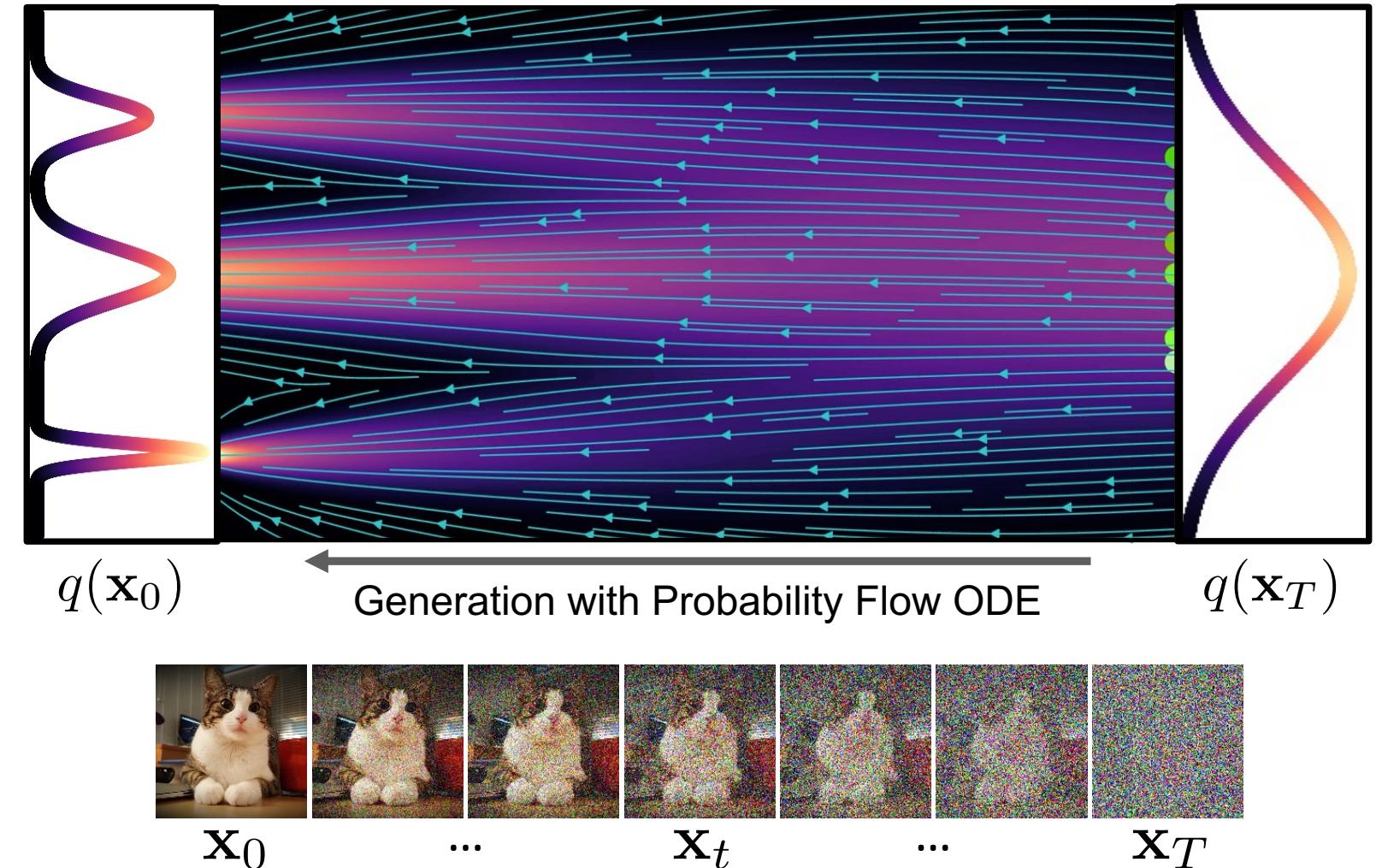
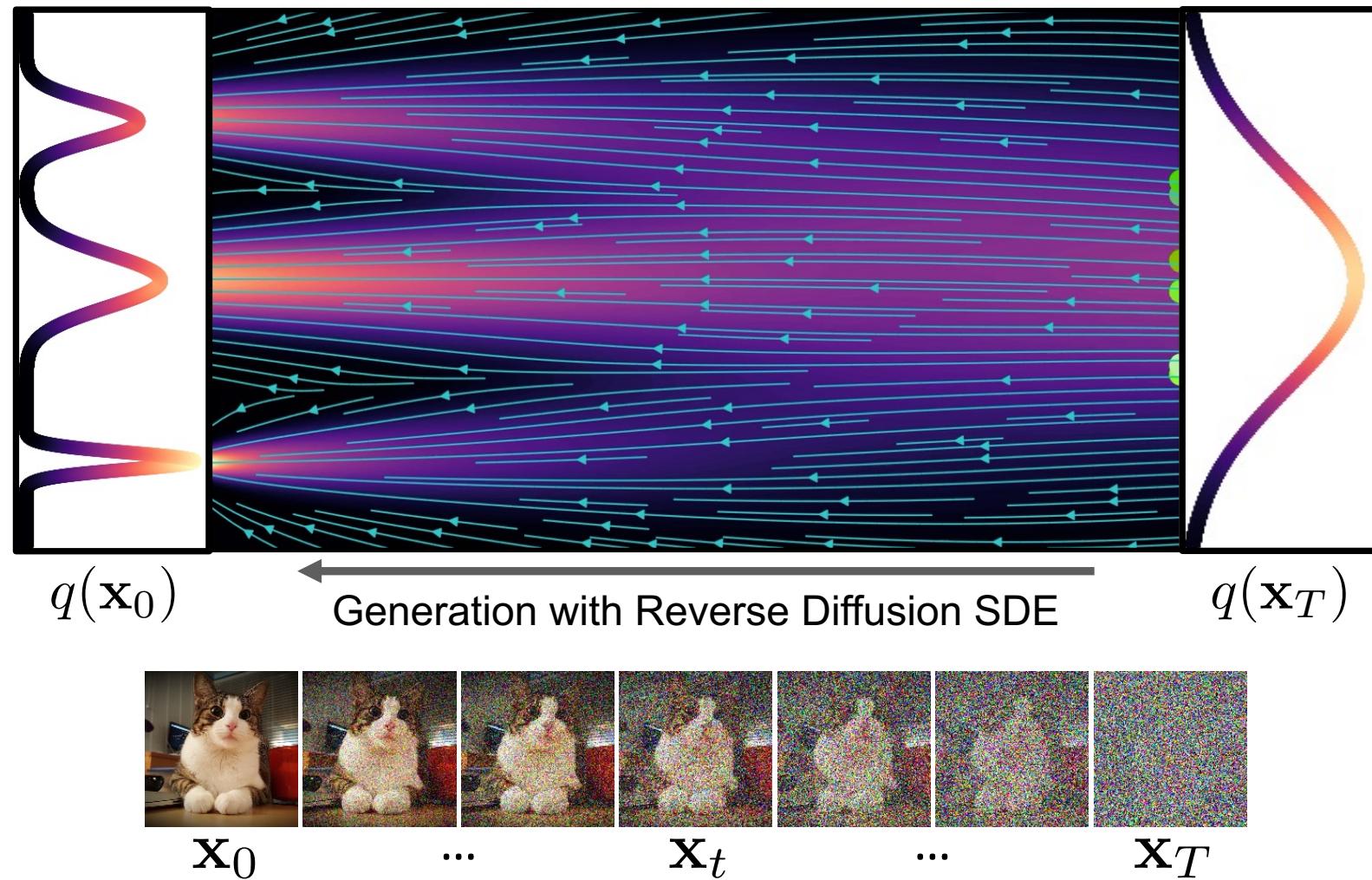
- Consider reverse generative diffusion SDE:
- In distribution equivalent to "Probability Flow ODE":
(solving this ODE results in the same $q_t(\mathbf{x}_t)$ when initializing $q_T(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$)

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + 2\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)] dt + \sqrt{\beta(t)} d\bar{\omega}_t$$

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + \nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)] dt$$

Deterministic mapping from \mathbf{x}_T to \mathbf{x}_0

Synthesis with SDE vs. ODE



- **Generative Reverse Diffusion SDE (stochastic):**

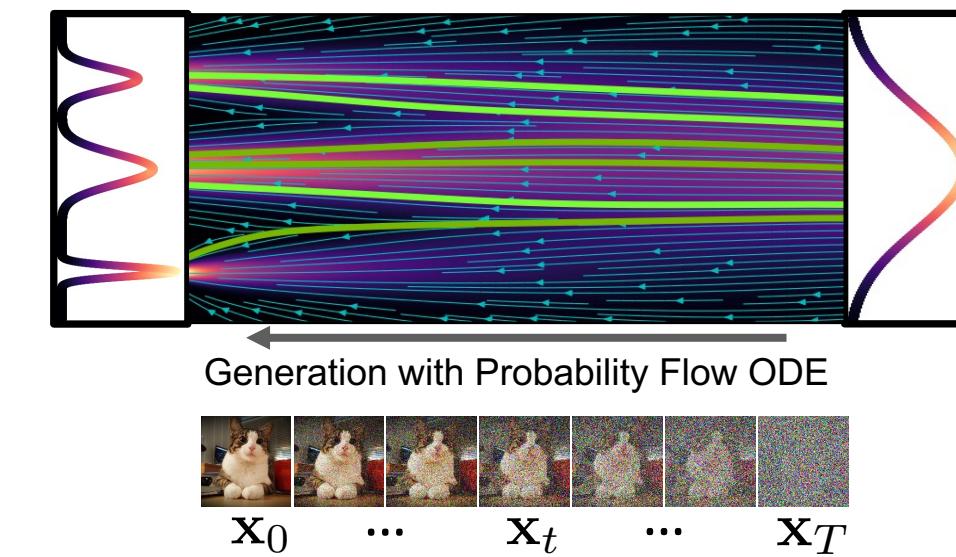
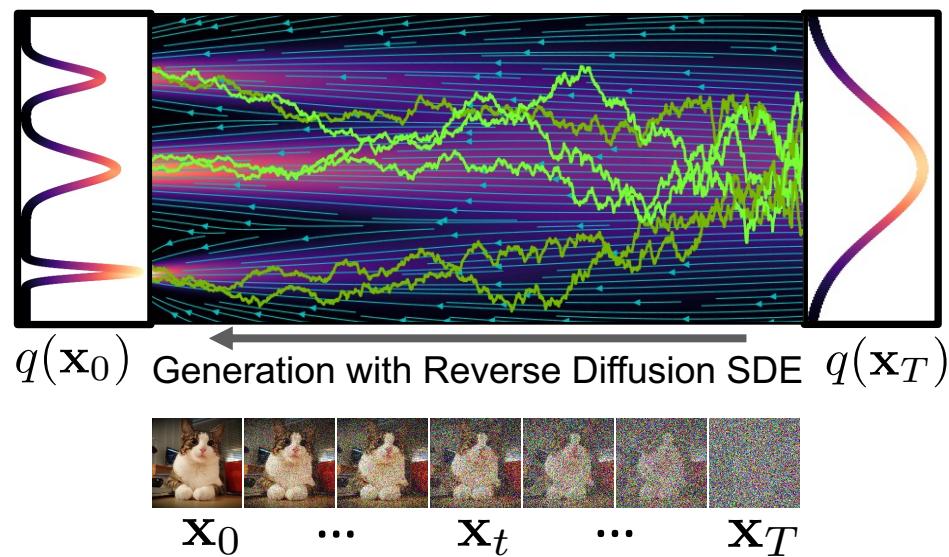
$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + 2\mathbf{s}_{\theta}(\mathbf{x}_t, t)] dt + \sqrt{\beta(t)} d\bar{\omega}_t$$

- **Generative Probability Flow ODE (deterministic):**

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + \mathbf{s}_{\theta}(\mathbf{x}_t, t)] dt$$

Sampling from “Continuous-Time” Diffusion Models

SDE vs. ODE Sampling: Pro’s and Con’s



Generative Diffusion SDE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)[\mathbf{x}_t + 2\mathbf{s}_{\theta}(\mathbf{x}_t, t)]dt + \sqrt{\beta(t)}d\bar{\omega}_t$$

$$d\mathbf{x}_t = \underbrace{-\frac{1}{2}\beta(t)[\mathbf{x}_t + \mathbf{s}_{\theta}(\mathbf{x}_t, t)]dt}_{\text{Probability Flow ODE}} - \underbrace{\frac{1}{2}\beta(t)\mathbf{s}_{\theta}(\mathbf{x}_t, t)dt}_{\text{Langevin dynamics}} + \sqrt{\beta(t)}d\bar{\omega}_t$$

- **Pro:** Continuous noise injection can help to compensate errors during diffusion process (Langevin sampling actively pushes towards correct distribution).
- **Con:** Often slower, because the stochastic terms themselves require fine discretization during solve.

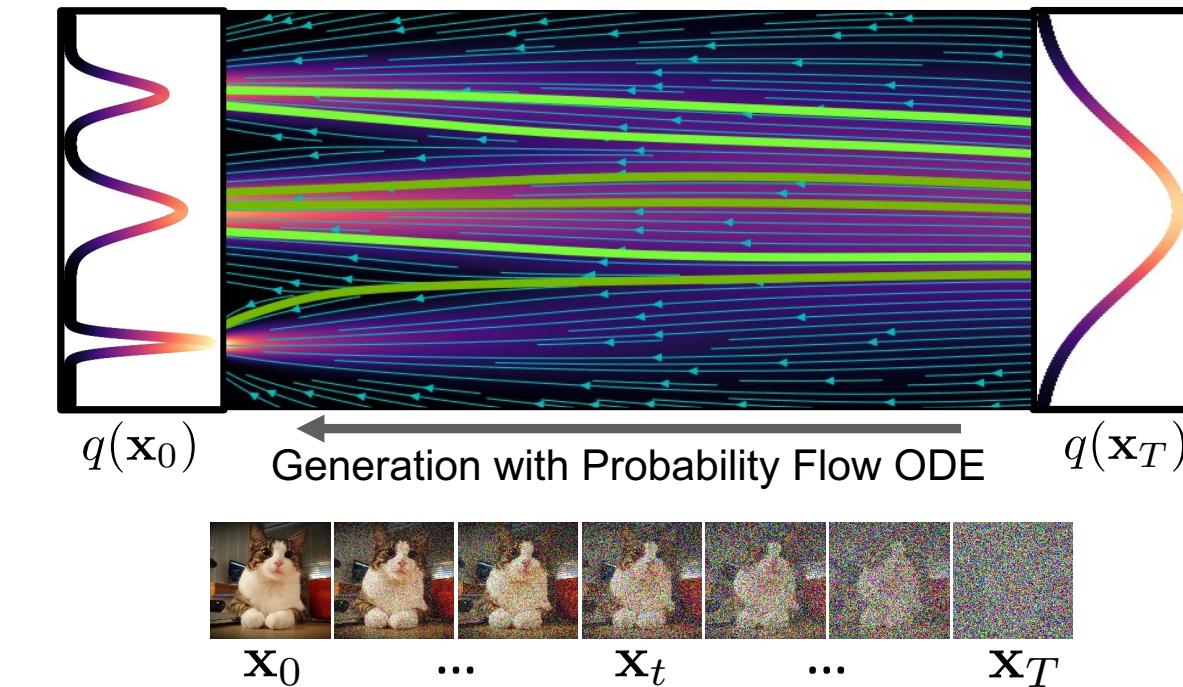
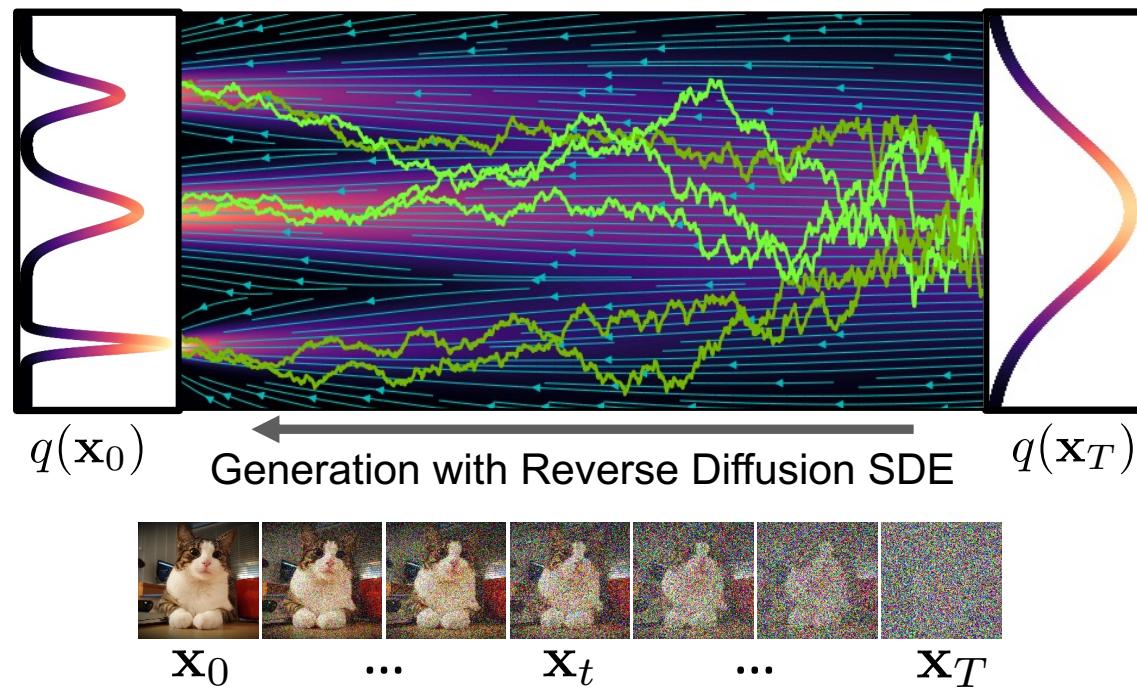
Probability Flow ODE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t)[\mathbf{x}_t + \mathbf{s}_{\theta}(\mathbf{x}_t, t)]dt$$

- **Pro:** Can leverage fast ODE solvers. Best when targeting very fast sampling.
- **Con:** No “stochastic” error correction, often slightly lower performance than stochastic sampling.

Sampling from “Continuous-Time” Diffusion Models

How to solve the generative SDE or ODE in practice?



Generative Diffusion SDE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + 2\mathbf{s}_{\theta}(\mathbf{x}_t, t)] dt + \sqrt{\beta(t)} d\bar{\omega}_t$$

→ *Euler-Maruyama:*

$$\mathbf{x}_{t-1} = \mathbf{x}_t + \frac{1}{2}\beta(t) [\mathbf{x}_t + 2\mathbf{s}_{\theta}(\mathbf{x}_t, t)] \Delta t + \sqrt{\beta(t)\Delta t} \mathcal{N}(\mathbf{0}, \mathbf{I})$$

→ *Ancestral Sampler* (discrete-time) is also a generative SDE sampler!

Probability Flow ODE:

$$d\mathbf{x}_t = -\frac{1}{2}\beta(t) [\mathbf{x}_t + \mathbf{s}_{\theta}(\mathbf{x}_t, t)] dt$$

→ *Euler's Method:*

$$\mathbf{x}_{t-1} = \mathbf{x}_t + \frac{1}{2}\beta(t) [\mathbf{x}_t + \mathbf{s}_{\theta}(\mathbf{x}_t, t)] \Delta t$$

→ In practice: DDIM sampler, another solver of the ODE.

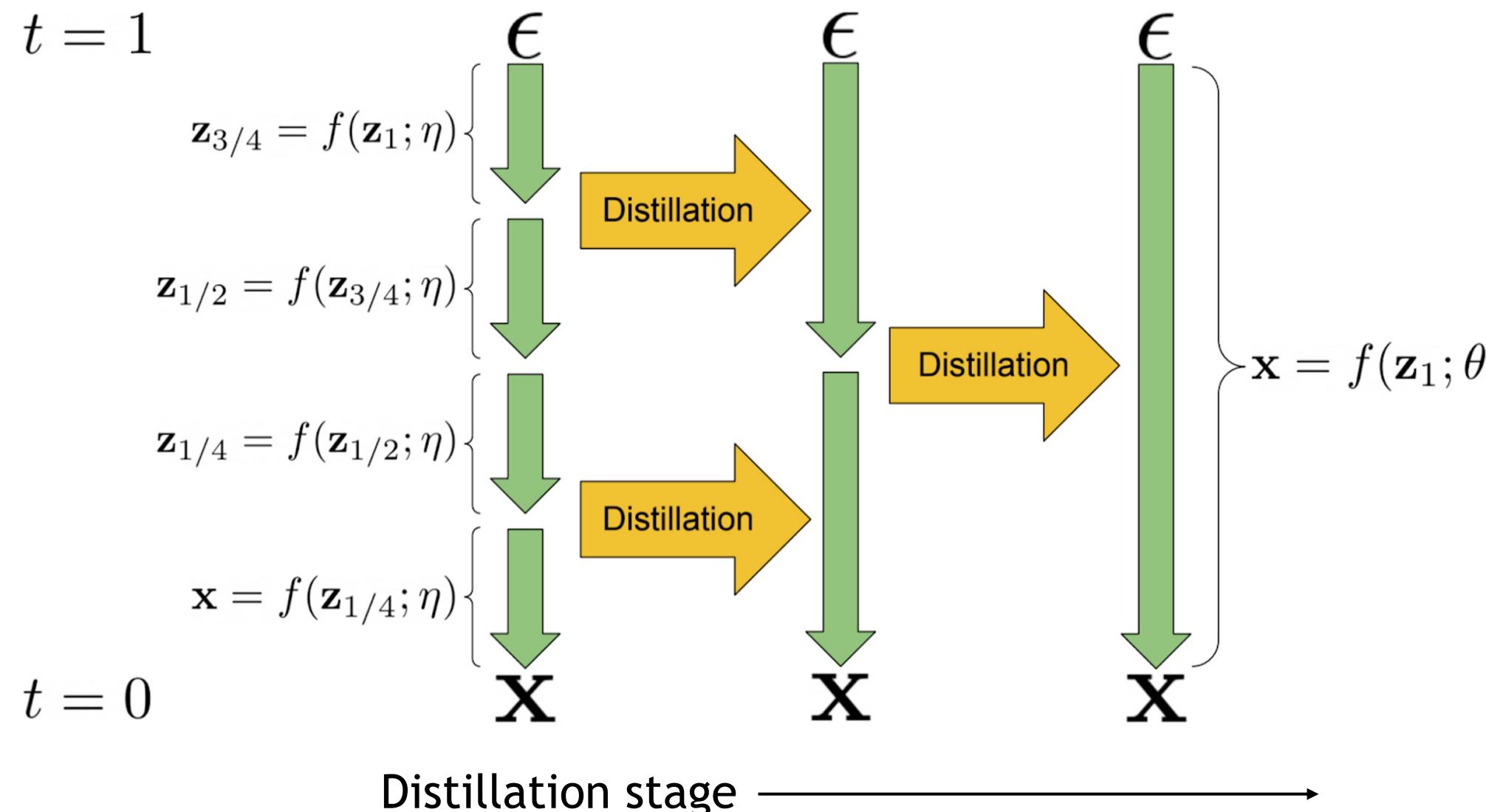
How to make sampling faster?

- One bottleneck of diffusion models is its slowness in sampling: need 10-1000+ steps to generate high quality samples
- Generative models need to be fast for practical use.
- One solution: distill diffusion models into models using just 4-8 sampling steps!
 - *Progressive distillation for fast sampling of diffusion models, Salimans & Ho, ICLR 2022*
 - *On Distillation of Guided Diffusion Models, Meng et al., CVPR 2023*

Progressive distillation

How to make sampling faster?

- Distill a deterministic ODE sampler (i.e. DDIM sampler) to the same model architecture.
- At each stage, a “student” model is learned to distill two adjacent sampling steps of the “teacher” model to one sampling step.
- At next stage, the “student” model from previous stage will serve as the new “teacher” model.



Algorithm 1 Standard diffusion training

Require: Model $\hat{\mathbf{x}}_\theta(\mathbf{z}_t)$ to be trained
Require: Data set \mathcal{D}
Require: Loss weight function $w()$

while not converged **do**

- $\mathbf{x} \sim \mathcal{D}$ ▷ Sample data
- $t \sim U[0, 1]$ ▷ Sample time
- $\epsilon \sim N(0, I)$ ▷ Sample noise
- $\mathbf{z}_t = \alpha_t \mathbf{x} + \sigma_t \epsilon$ ▷ Add noise to data

$\tilde{\mathbf{x}} = \mathbf{x}$ ▷ Clean data is target for $\hat{\mathbf{x}}$

$\lambda_t = \log[\alpha_t^2 / \sigma_t^2]$ ▷ log-SNR

$L_\theta = w(\lambda_t) \|\tilde{\mathbf{x}} - \hat{\mathbf{x}}_\theta(\mathbf{z}_t)\|_2^2$ ▷ Loss

$\theta \leftarrow \theta - \gamma \nabla_\theta L_\theta$ ▷ Optimization

end while

Algorithm 2 Progressive distillation

Require: Trained teacher model $\hat{\mathbf{x}}_\eta(\mathbf{z}_t)$
Require: Data set \mathcal{D}
Require: Loss weight function $w()$
Require: Student sampling steps N

for K iterations **do**

- $\theta \leftarrow \eta$ ▷ Init student from teacher

while not converged **do**

- $\mathbf{x} \sim \mathcal{D}$
- $t = i/N, i \sim Cat[1, 2, \dots, N]$
- $\epsilon \sim N(0, I)$
- $\mathbf{z}_t = \alpha_t \mathbf{x} + \sigma_t \epsilon$
- # 2 steps of DDIM with teacher
- $t' = t - 0.5/N, t'' = t - 1/N$
- $\mathbf{z}_{t'} = \alpha_{t'} \hat{\mathbf{x}}_\eta(\mathbf{z}_t) + \frac{\sigma_{t'}}{\sigma_t} (\mathbf{z}_t - \alpha_t \hat{\mathbf{x}}_\eta(\mathbf{z}_t))$
- $\mathbf{z}_{t''} = \alpha_{t''} \hat{\mathbf{x}}_\eta(\mathbf{z}_{t'}) + \frac{\sigma_{t''}}{\sigma_{t'}} (\mathbf{z}_{t'} - \alpha_{t'} \hat{\mathbf{x}}_\eta(\mathbf{z}_{t'}))$
- $\tilde{\mathbf{x}} = \frac{\mathbf{z}_{t''} - (\sigma_{t''}/\sigma_t) \mathbf{z}_t}{\alpha_{t''} - (\sigma_{t''}/\sigma_t) \alpha_t}$ ▷ Teacher $\hat{\mathbf{x}}$ target
- $\lambda_t = \log[\alpha_t^2 / \sigma_t^2]$
- $L_\theta = w(\lambda_t) \|\tilde{\mathbf{x}} - \hat{\mathbf{x}}_\theta(\mathbf{z}_t)\|_2^2$
- $\theta \leftarrow \theta - \gamma \nabla_\theta L_\theta$

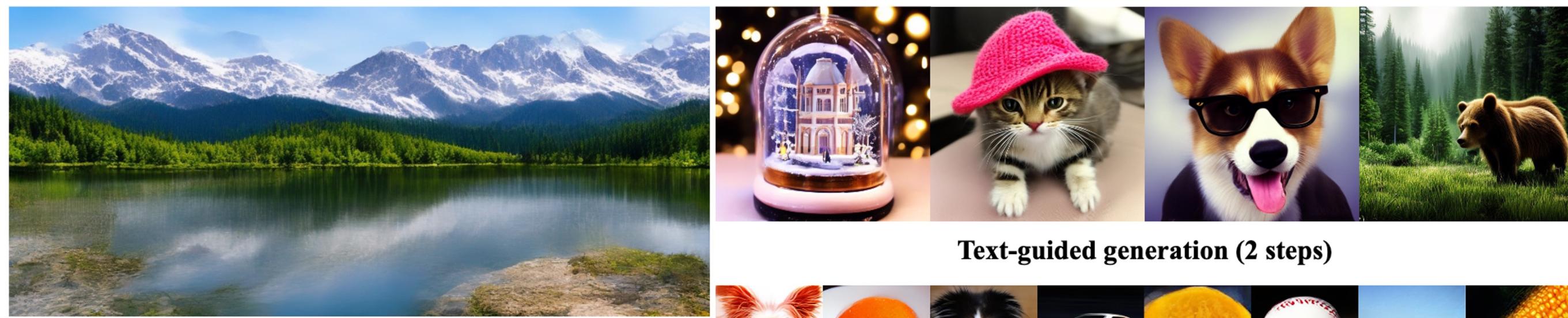
end while

- $\eta \leftarrow \theta$ ▷ Student becomes next teacher
- $N \leftarrow N/2$ ▷ Halve number of sampling steps

end for

On Distillation of Guided Diffusion Models

Meng et al., CVPR 2023 award nominated



Text-guided generation (1 step)



Class-conditional generation (1 step)



Input

Mask

Result 1

Result 2

Image inpainting (2 steps)



Text-guided generation (4 steps)



Image to image translation (3 steps)

Now also works with

- CF-Guidance
- Stochastic sampling
- Text-to-image/video
- Image-to-image
- Inpainting
- Latent Diffusion

Case study: Imagen

Imagen: text-to-image diffusion models

By Google (imagen.research.google)

Input: text; Output: 1kx1k images

- An unprecedented degree of photorealism
 - SOTA automatic scores & human ratings
- A deep level of language understanding
- Extremely simple
 - no latent space, no quantization



A brain riding a rocketship heading towards the moon.

Imagen

By Google (imagen.research.google)



A photo of a Shiba Inu dog with a backpack riding a bike. It is wearing sunglasses and a beach hat.

Imagen

By Google (imagen.research.google)



A dragon fruit wearing karate belt in the snow.

“toilet paper with real
cactus spikes”
by Irina Blok



What goes to Imagen?

Data

- Image-text pairs
- LAION-400M
- Internal (~500M images)

Model

- Diffusion models
- Cascading super-res
- Frozen text encoders

Sampler

- Classifier-free guidance
- Maximizing text-alignment

Scaling up

What goes to Imagen?

Data

- Image-text pairs
- LAION-400M
- Internal (~500M images)

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- Diffusion models
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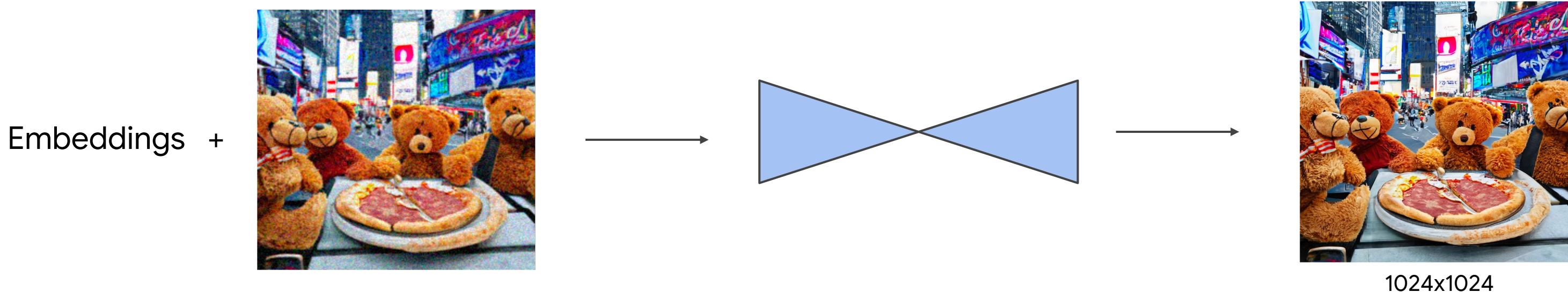
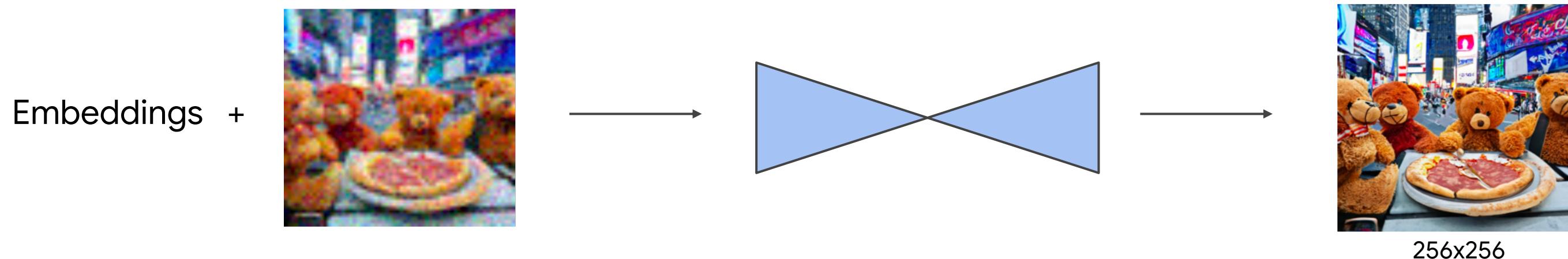
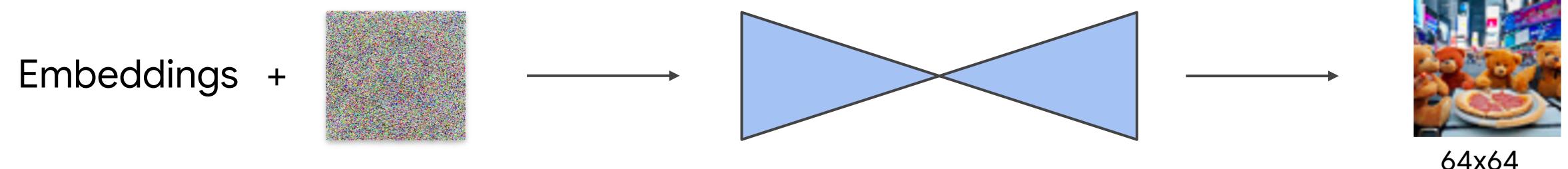
Sampler

- Classifier-free guidance
- Maximizing text-alignment

Scaling up

Imagen: Cascaded generation pipeline

A photo of a group of teddy bears eating pizza in Times Square. → Frozen text encoder → Embeddings



Classifier Guidance

Sampler technique

- Assume pairs of data (\mathbf{x}, \mathbf{c}) . A classifier guidance diffusion model consists of
 - A trained conditional diffusion model
 - A trained classifier model on noisy data \mathbf{x}_t
- During sampling, at each denoising step, modify the score function to

$$\nabla_{\mathbf{x}_t} \log \tilde{p}_{\theta,\phi}(\mathbf{x}_t|\mathbf{c}) = \nabla_{\mathbf{x}_t} \log p_\theta(\mathbf{x}_t|\mathbf{c}) + \omega \nabla_{\mathbf{x}_t} \log p_\phi(\mathbf{c}|\mathbf{x}_t).$$

From the conditional
diffusion model

From the classifier
model

- Upweight samples that the classifier assigns high probability with, better alignment with \mathbf{c} .
- Cons: need to train an additional classifier. Increase model complexity.

Classifier-free Guidance

Sampler technique

- Assume there're two diffusion models, one conditional model and one unconditional model.
- By Bayes' rule we can define an implicit classifier

$$p_\theta(\mathbf{c}|\mathbf{x}_t) \propto p_\theta(\mathbf{x}_t|\mathbf{c})/p_\theta(\mathbf{x}_t).$$

- The modified score function during sampling then becomes

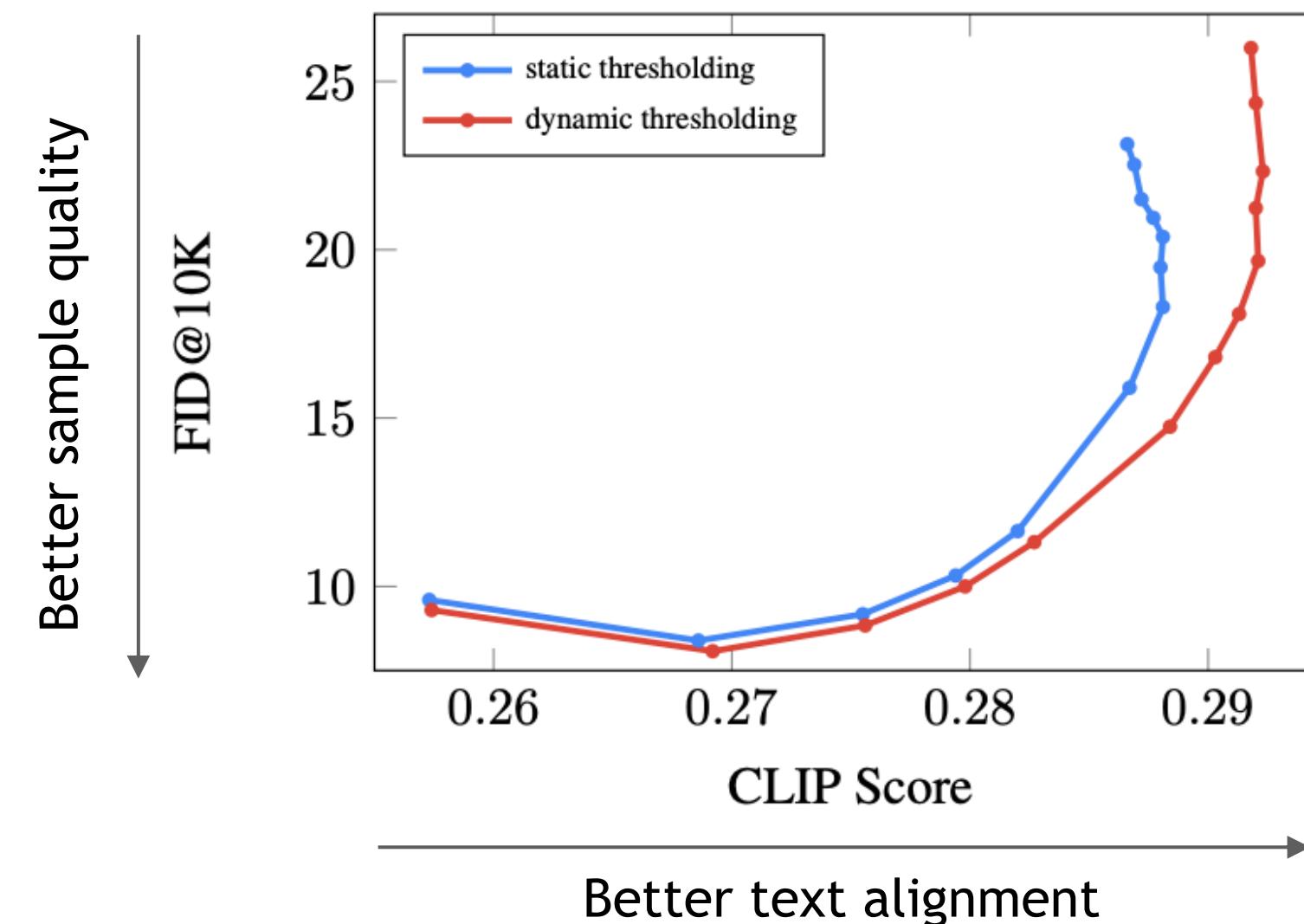
$$\nabla_{\mathbf{x}_t} \log \tilde{p}_\theta(\mathbf{x}_t|\mathbf{c}) = (1 + \omega) \nabla_{\mathbf{x}_t} \log p_\theta(\mathbf{x}_t|\mathbf{c}) - \omega \nabla_{\mathbf{x}_t} \log p_\theta(\mathbf{x}_t).$$

From the conditional diffusion model From the unconditional diffusion model

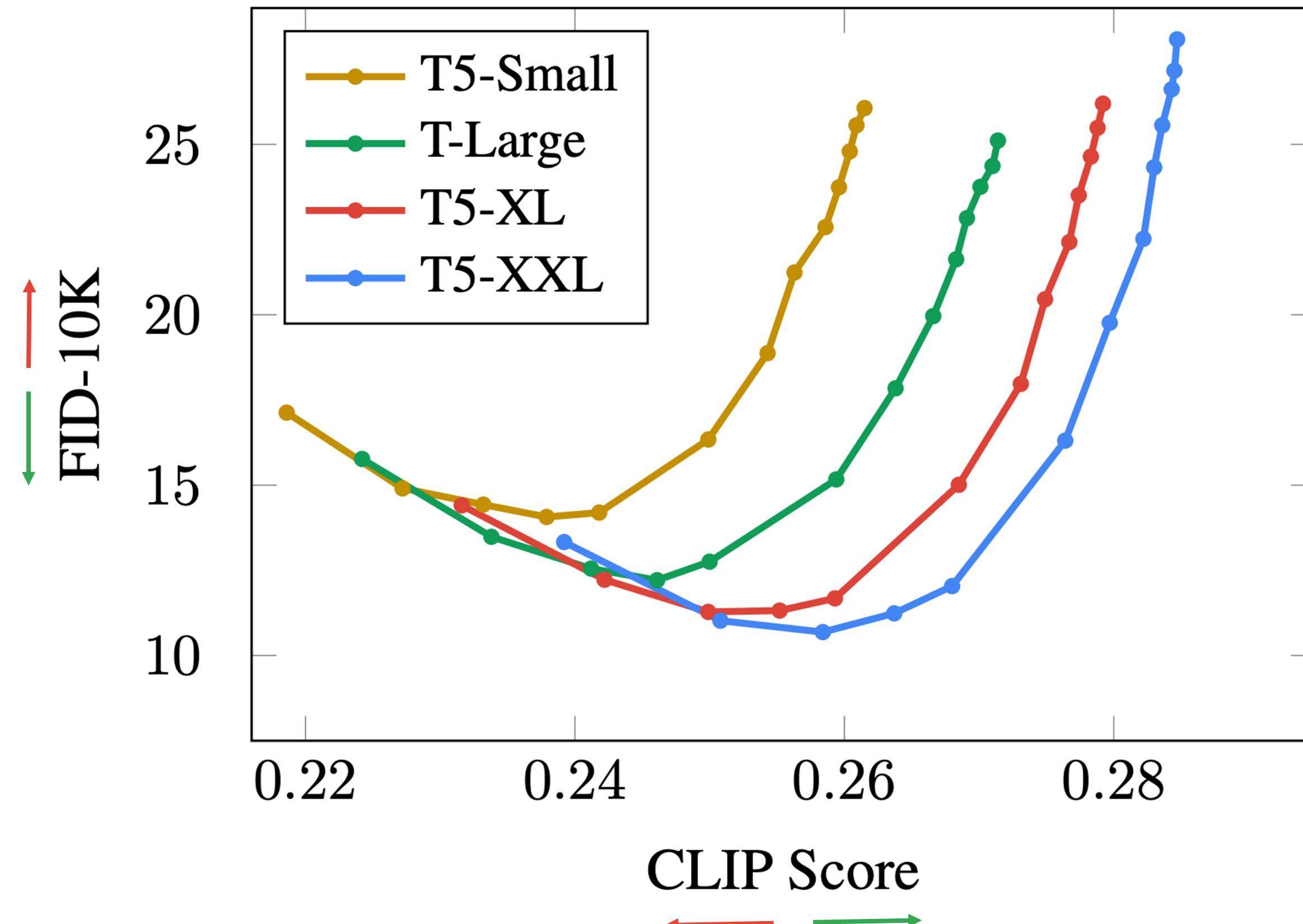
- The two models can share weights, with the unconditional model taking a null class label \mathbf{c} .

Classifier-free guidance in Imagen

- Large classifier-free guidance weights → better text alignment, worse image fidelity



Larger Text Encoders → Better Alignment, Better Fidelity



Can we generalize this to video?

Imagen Video (imagen.research.google/video)

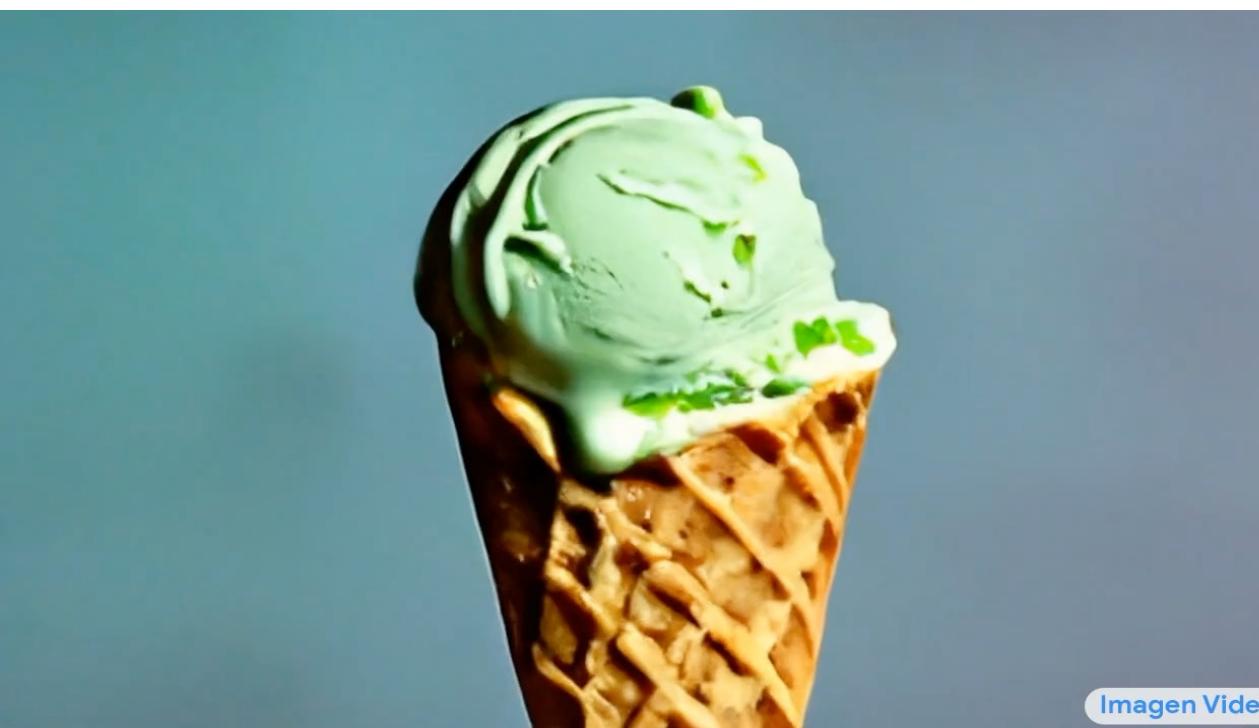
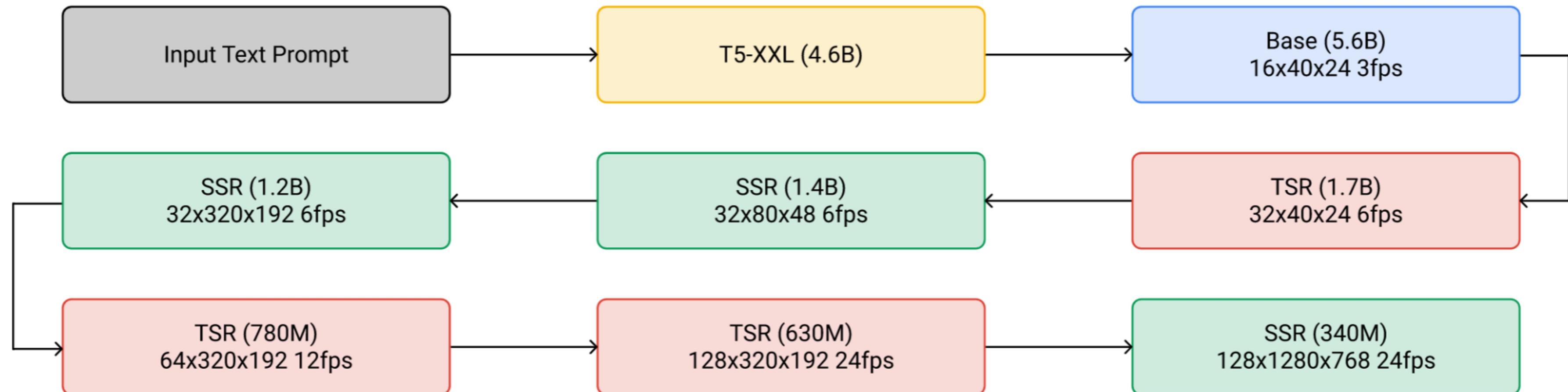


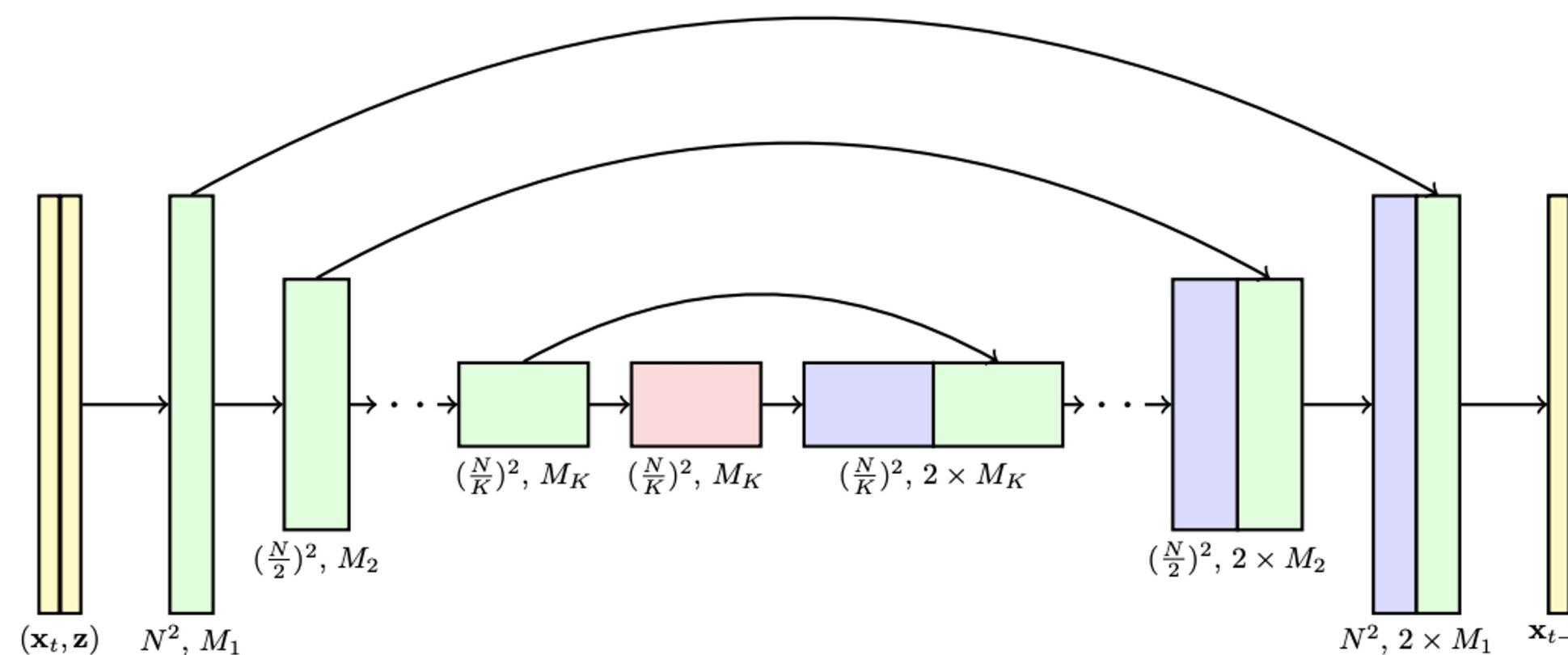
Imagen Video generalizes Imagen to the video domain using a cascade of super-resolution diffusion models in space and time



Video diffusion models

Ho & Salimans, et al. <https://video-diffusion.github.io/>

- Image → Video: Just add another dimension to the data tensor
- Image architecture: 2D UNet
- Video architecture: 3D UNet, space-time separable
 - repeat the 2D UNet over frames
 - additional layers to mix over time using attention or convolution





Wooden figurine surfing on a surfboard in space.

Imagen Video



Imagen Video



Flying through an intense battle between pirate ships in a stormy ocean.

Imagen Video

*“watercolor greeting card of
thank you so much!”*

