Google DeepMind

Diffusion Models

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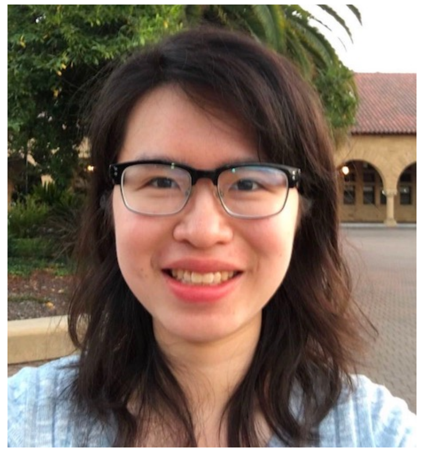
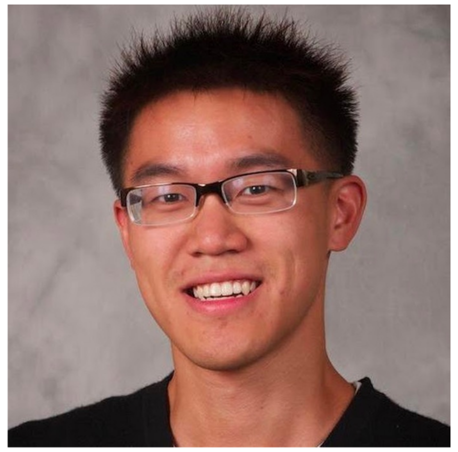
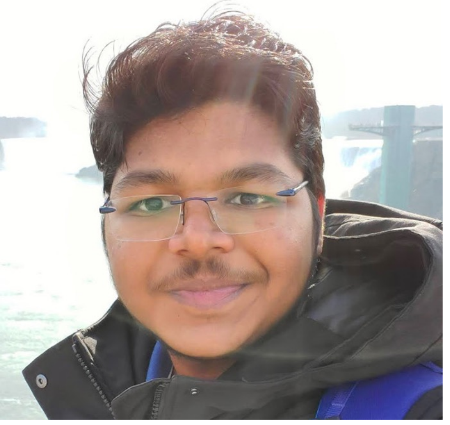
Acknowledgements







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

2022 / 2023 : The year of generative modeling?

Parti
Pathways Autoregressive Text-to-Image Model

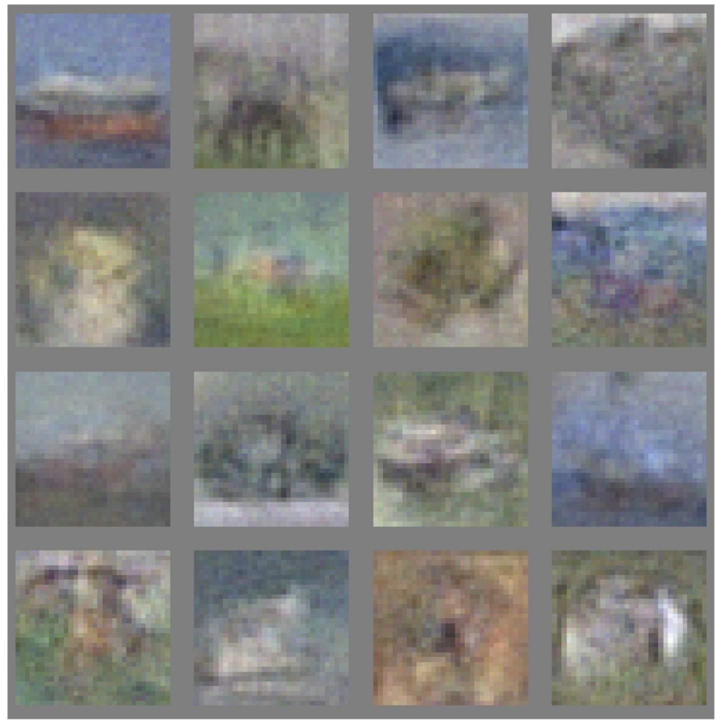
DALL·E 2

Stable Diffusion

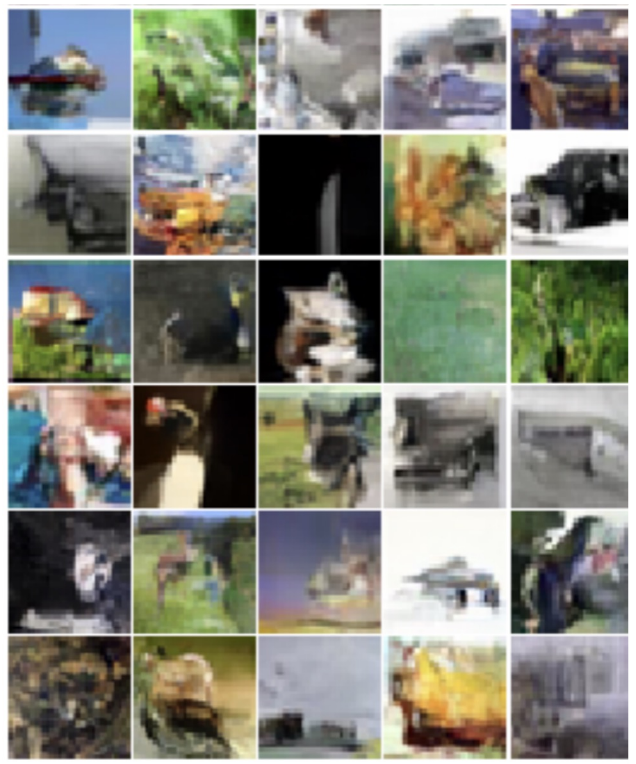
Where we came from

VAEs, 2013

GANs, 2014



PixelCNN, 2016



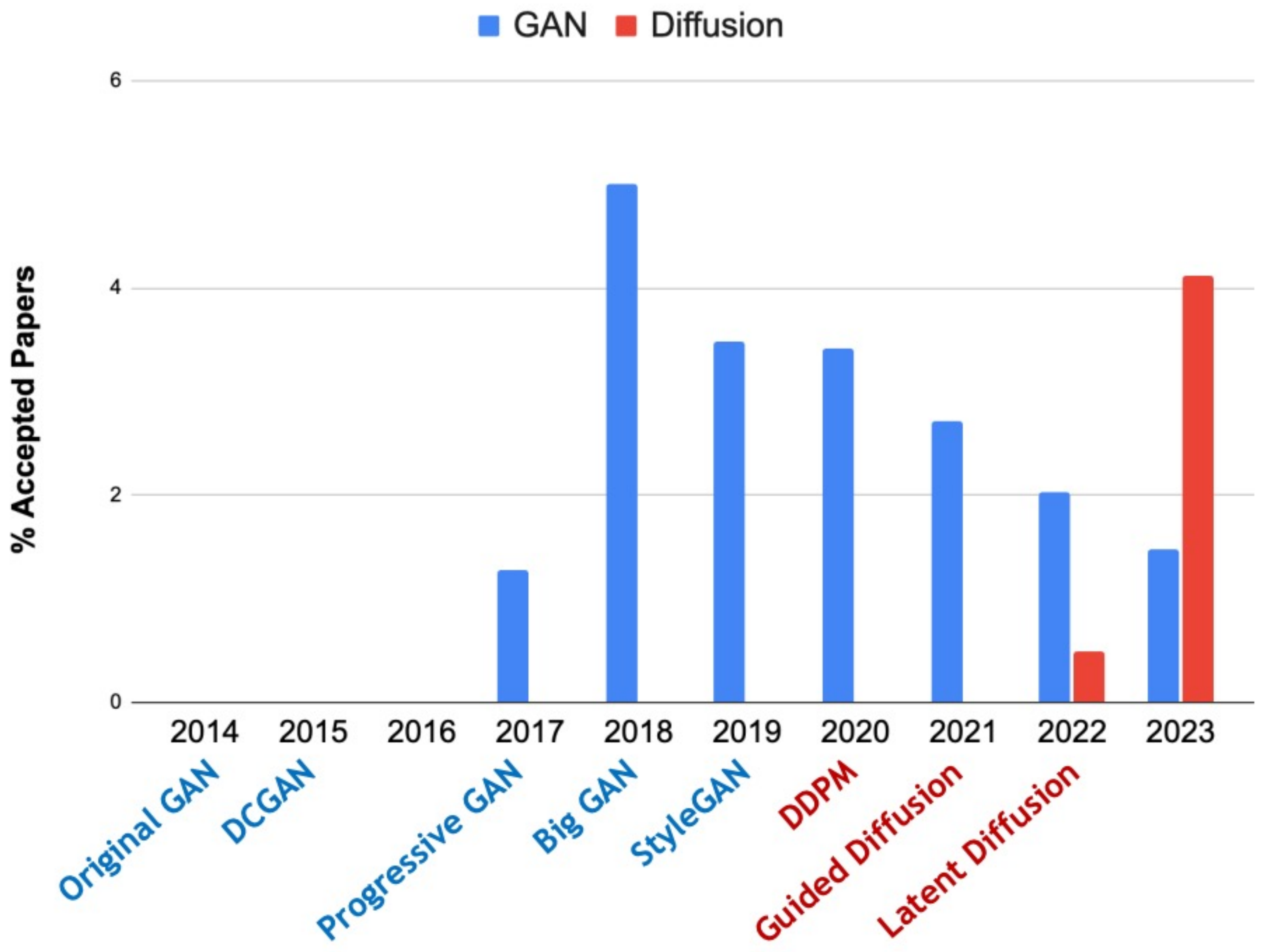
BigGAN, 2019

Imagen, 2022

The Landscape of Deep Generative Models

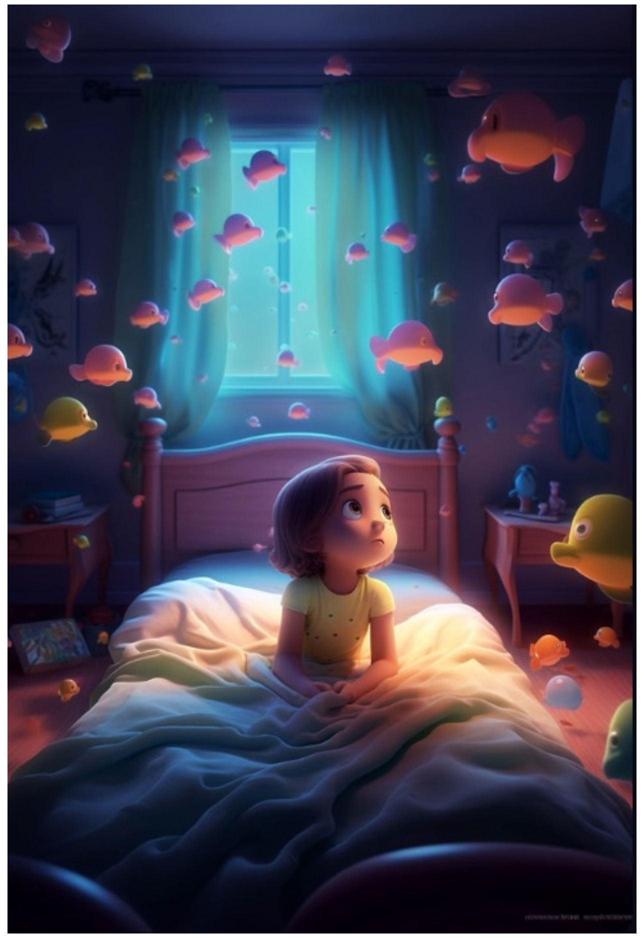
Diffusion models: a big bang to generative learning

Statistics of paper topics at CVPR



https://cvpr2023-tutorial-diffusion-models.github.io/

AI Art



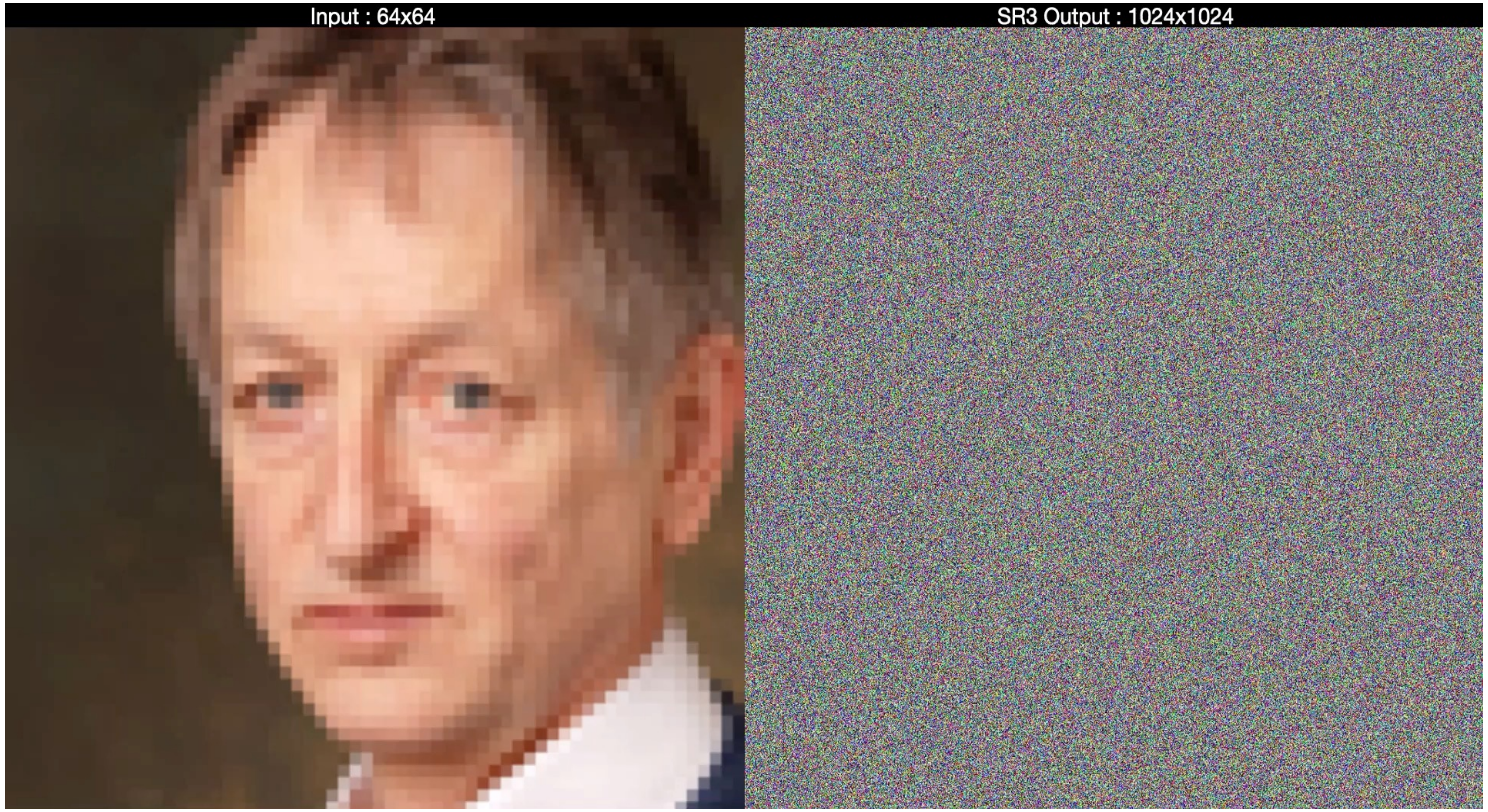
Midjourney v5

Video generation

AI Movie

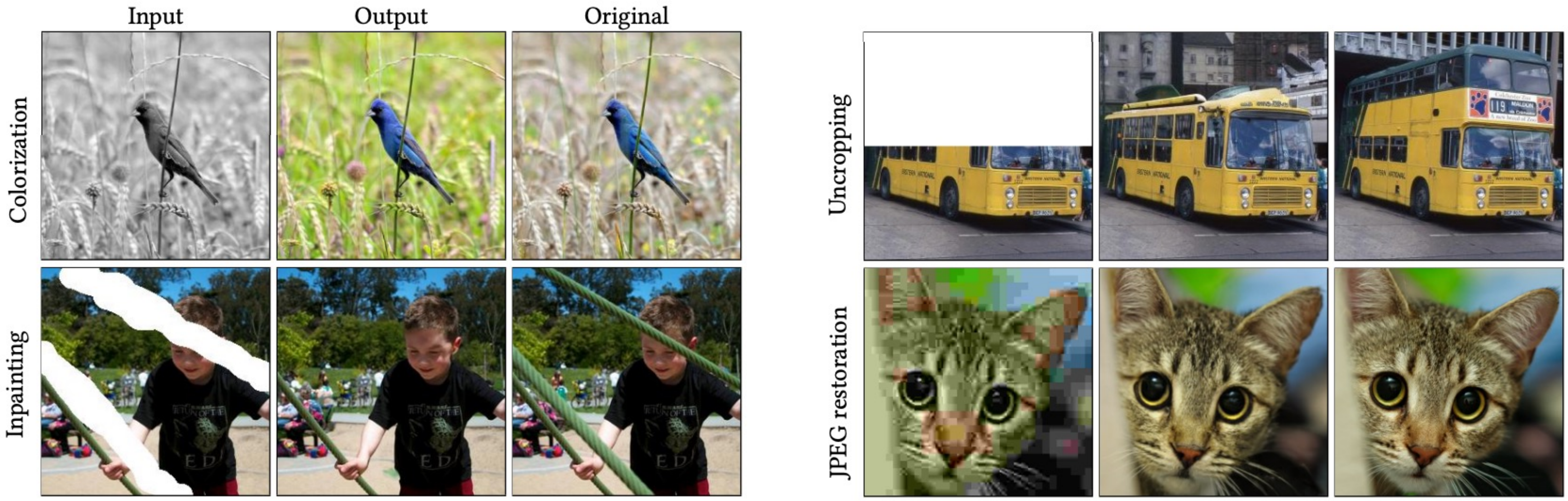
Midjourney Image + Runway Video + Triniti Audio + …

Applications: Super-resolution



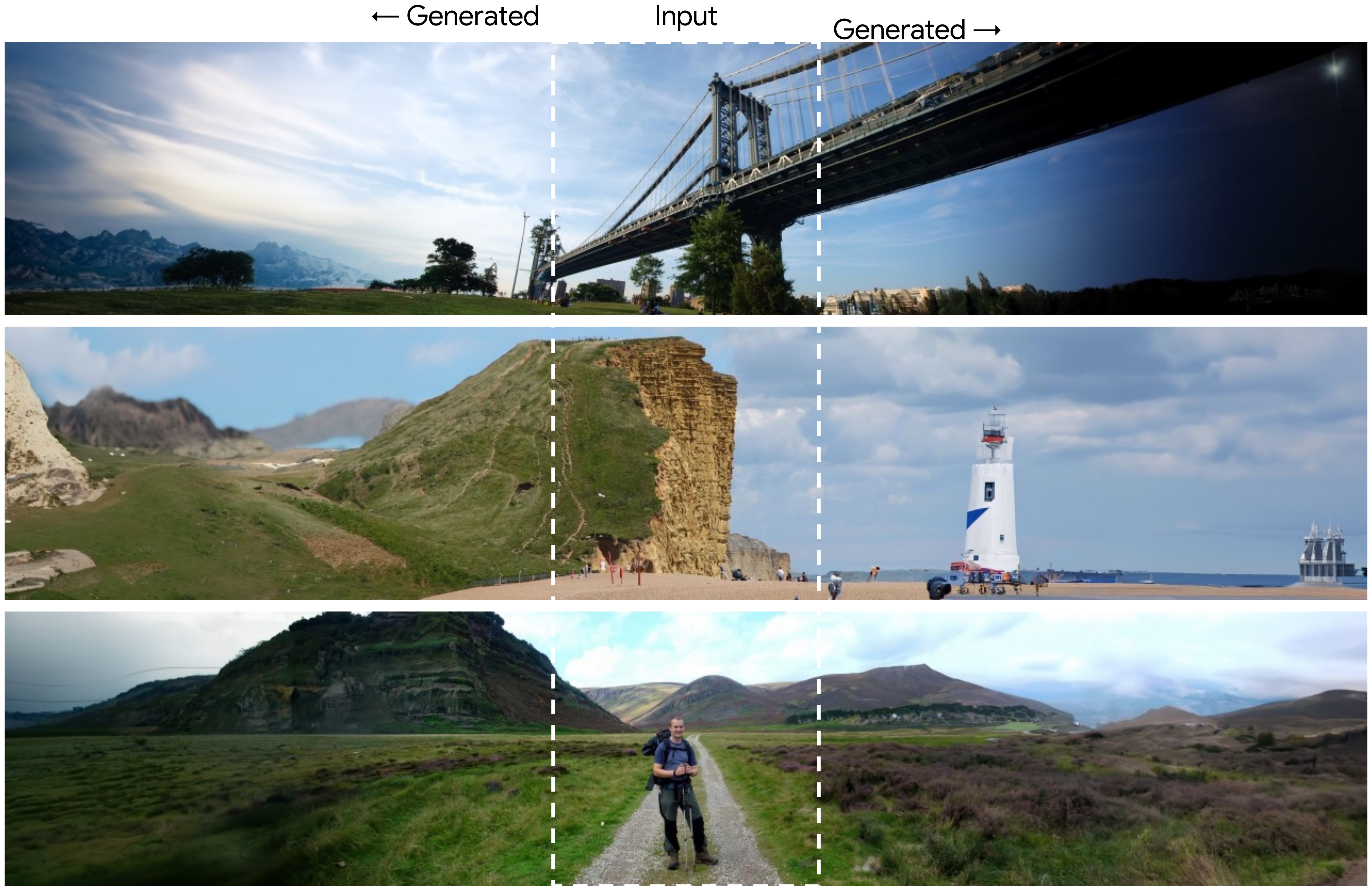
Palette: Image-to-Image Diffusion Models, 2022

Applications: Colorization, Inpainting, Restoration



Palette: Image-to-Image Diffusion Models, 2022

Applications: Outfilling



Palette: Image-to-Image Diffusion Models, 2022

Contents

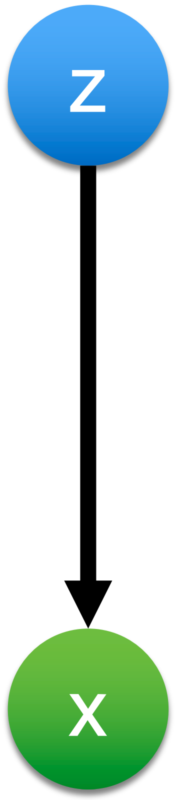
- Recap of variational autoencoders
- Diffusion models
    - Discrete-time framework
    - Continuous-time framework
- Case study: Imagen: high-fidelity text-to-image diffusion models

Not intended as a complete review of all recent work!

Variational Autoencoders

Latent variable model

latent variables



full image

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

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \mathbf{f}(\mathbf{z}))$$

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

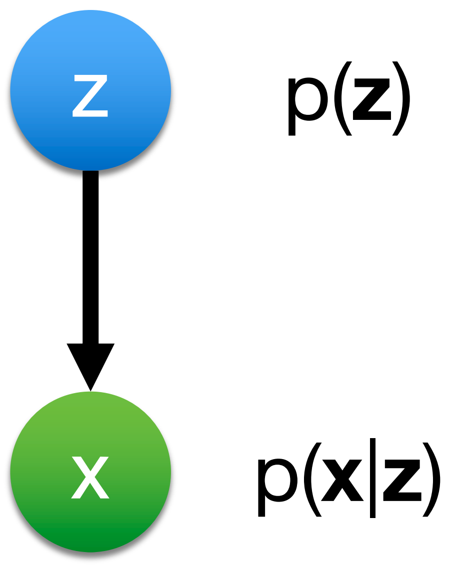
$$= \text{flexible distribution}$$

slide by Durk Kingma

Optimization

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \mathbf{f}(\mathbf{z}))$$

$$p(\mathbf{x}) = \int_{\mathbf{z}} p(\mathbf{x}|\mathbf{z})p(\mathbf{z})\, d\mathbf{z}$$
$$= \text{flexible distribution}$$



Generative model
p(x,z)

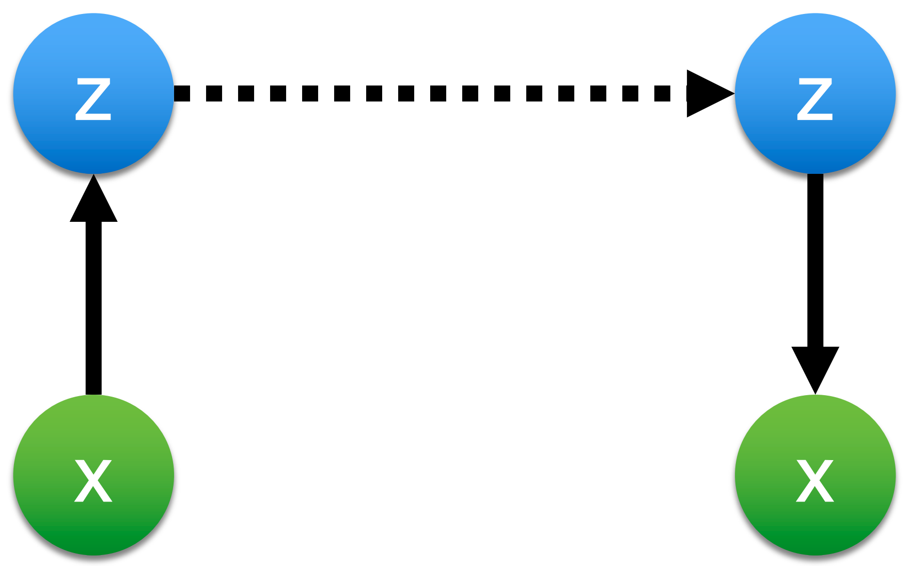
- Problem:
  - Marginal likelihood p(x) is intractable
  - So can't do maximum likelihood directly

Variational Autoencoders (VAEs)

- We introduce an **inference model** q(z|x)
- This allows us to efficiently optimize the log-likelihood, through the **evidence lower bound** (ELBO).

$$\log p(\mathbf{x}) \geq \mathrm{ELBO}(\mathbf{x}) = \mathbb{E}_{q(\mathbf{z}|\mathbf{x})}\left[\log \frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z}|\mathbf{x})}\right]$$

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



Inference model
q(z|x)

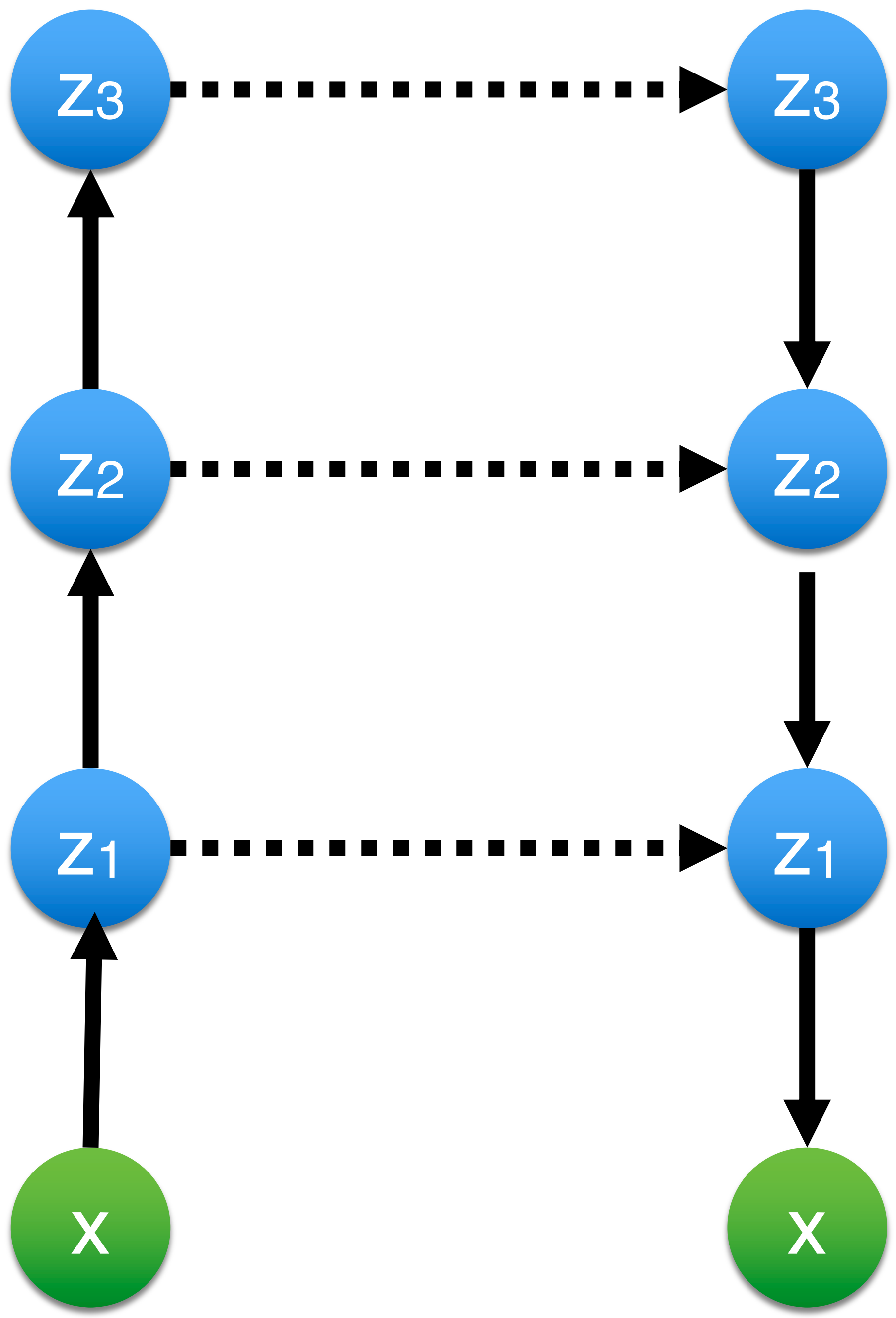
Generative model
p(x,z)

slide by Durk Kingma

[Kingma and Welling, 2013]

Hierarchical VAEs

- “Flat” VAEs suffer from simple priors
- Better likelihoods are achieved with hierarchies of latent variables



Inference model
q(z|x)

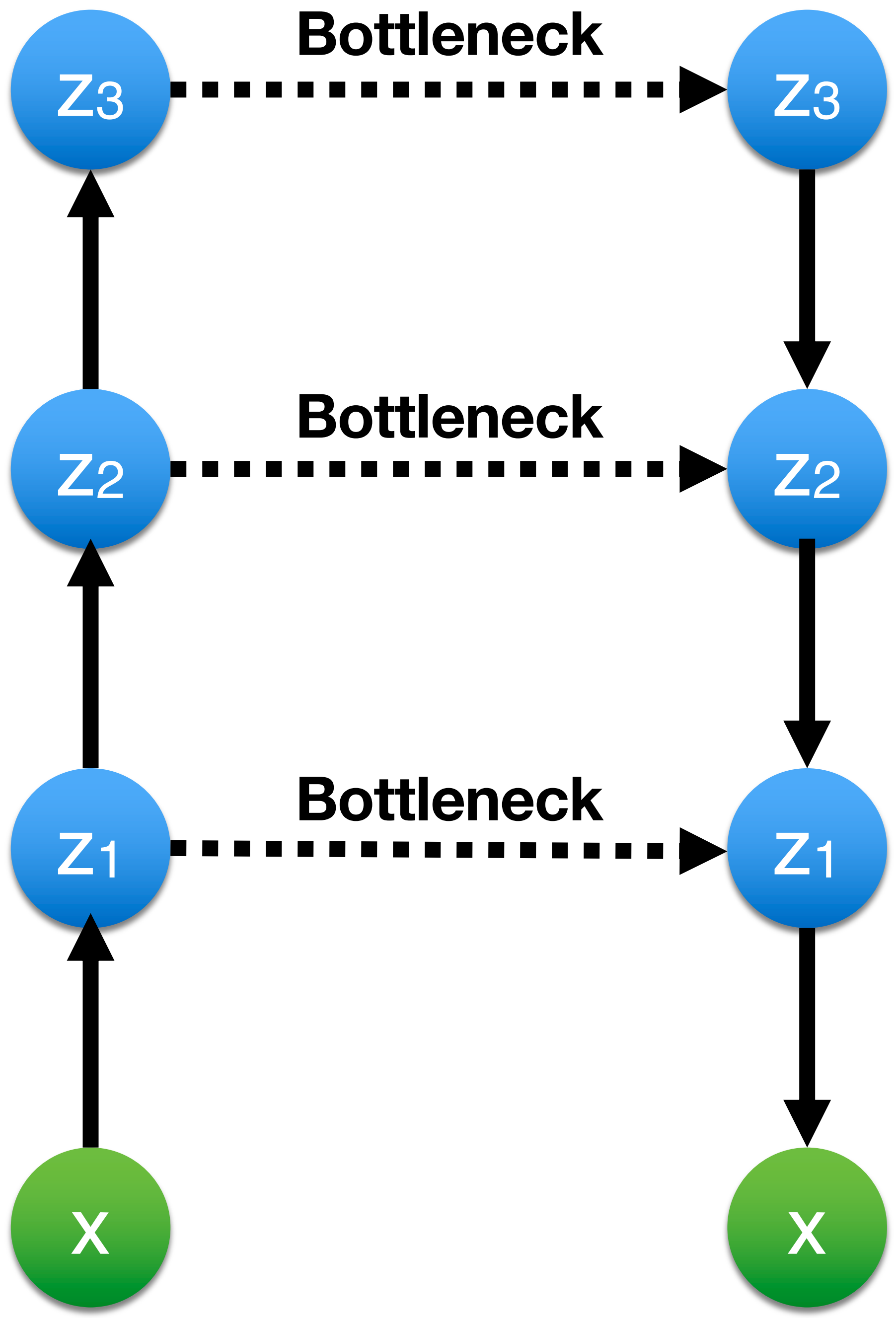
Generative model
p(x,z)

slide by Durk Kingma

[Kingma and Welling, 2017]

VAEs: challenges

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



Inference model
q(z|x)

Generative model
p(x,z)

slide by Durk Kingma

[Kingma and Welling, 2013]

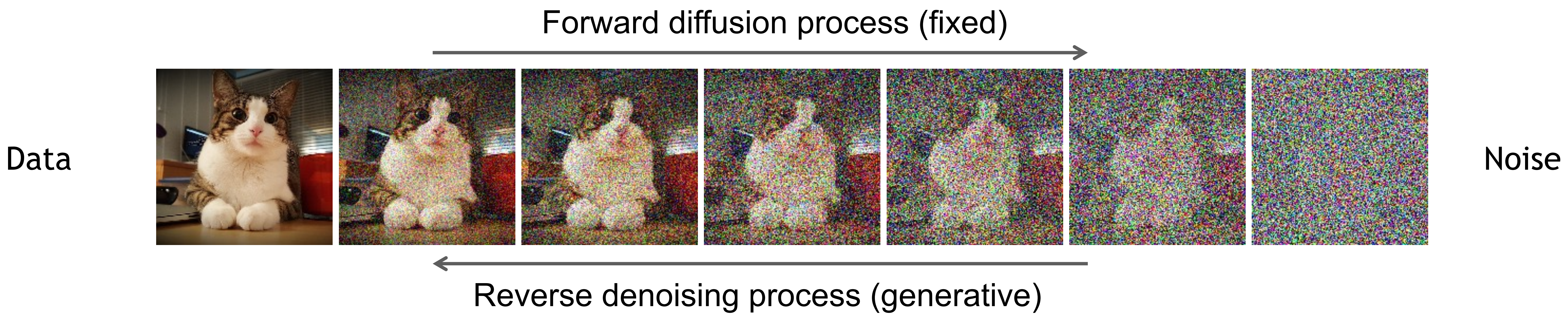
Diffusion Models

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]
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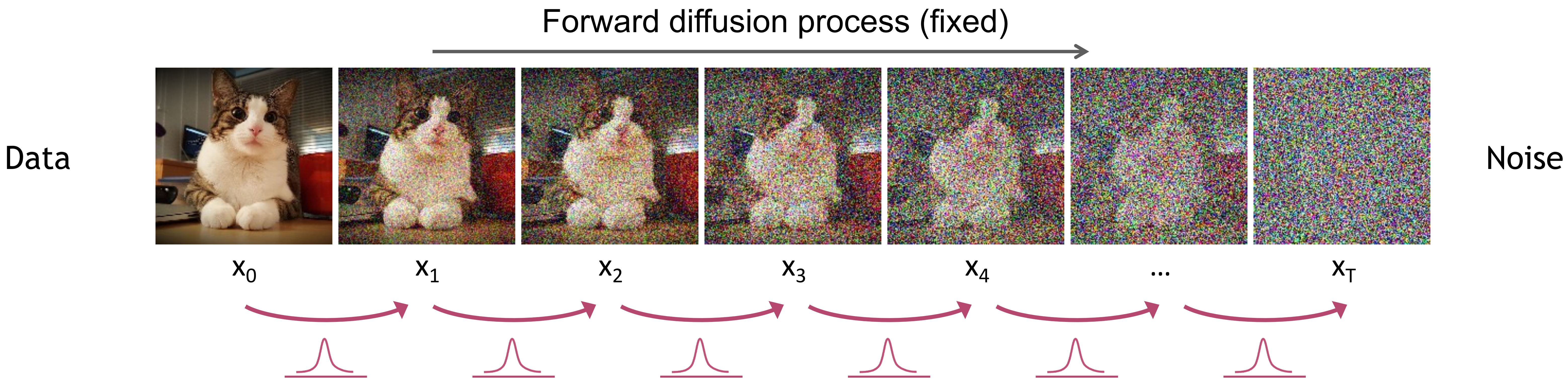
Forward Diffusion Process

The formal definition of the forward process in T steps:



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

Similar to the inference model in hierarchical VAEs.

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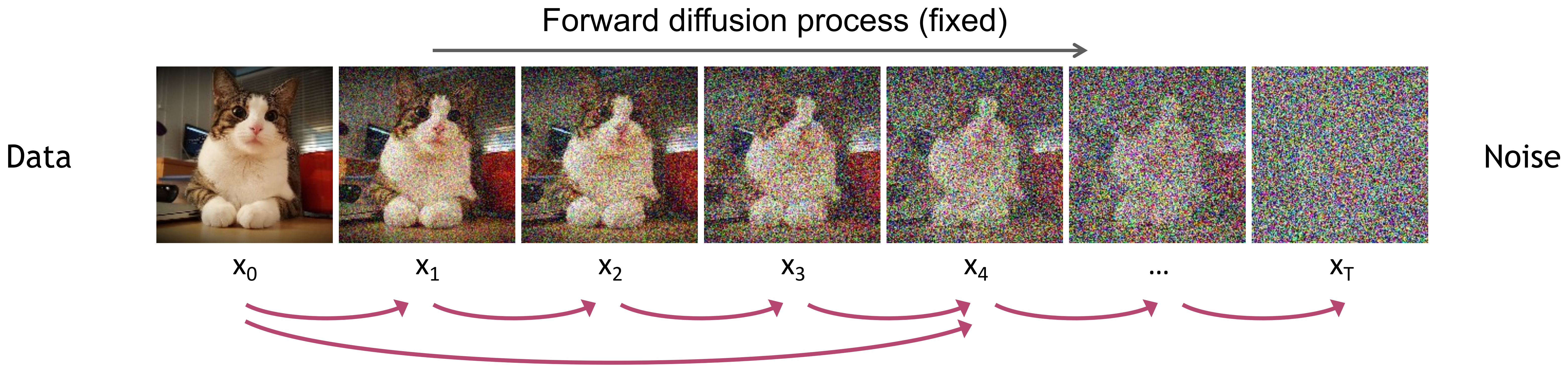
Diffusion Kernel



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 $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

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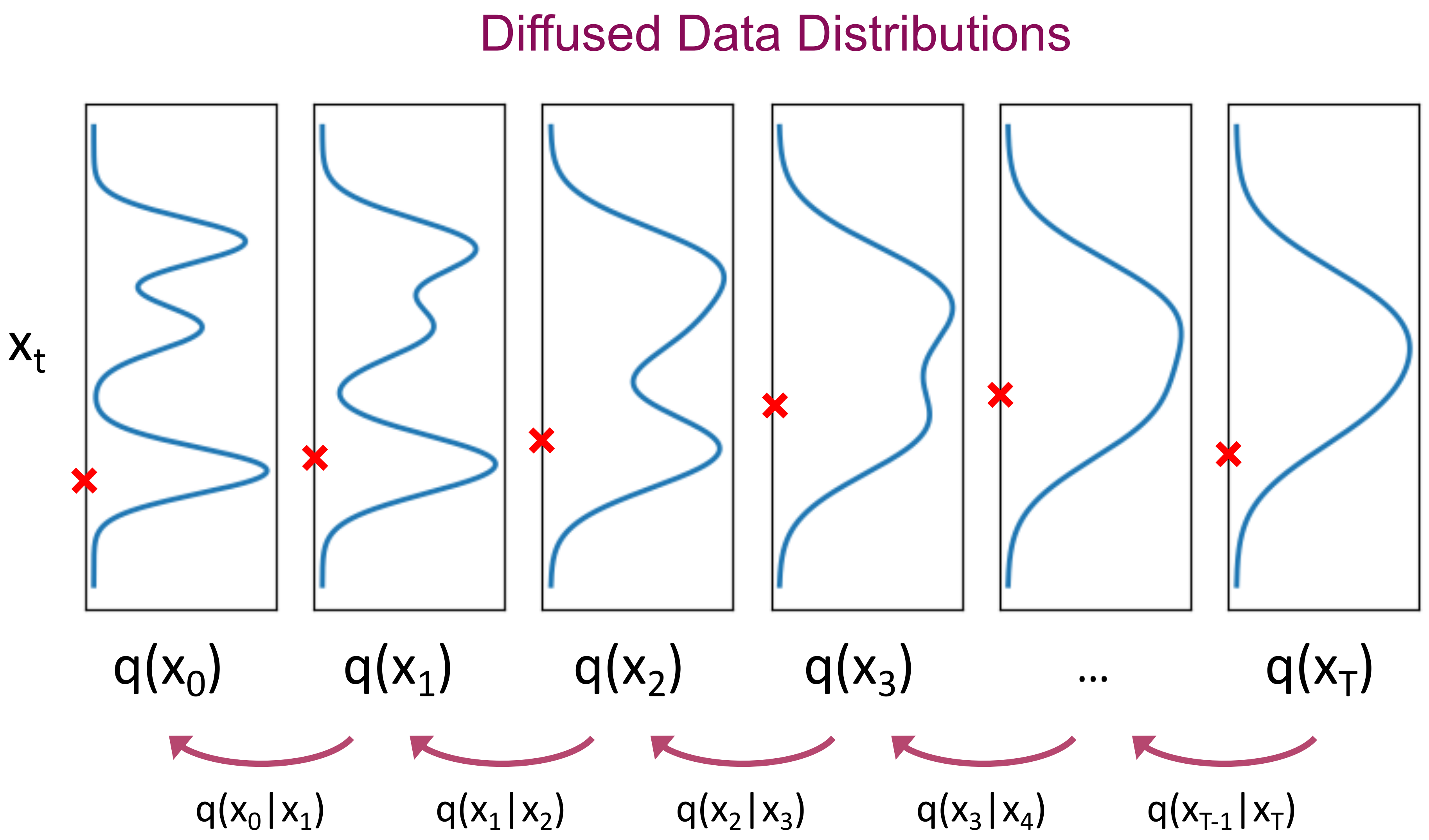
Generative Learning by Denoising

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 Normal distribution if β_t is small in each forward diffusion step.

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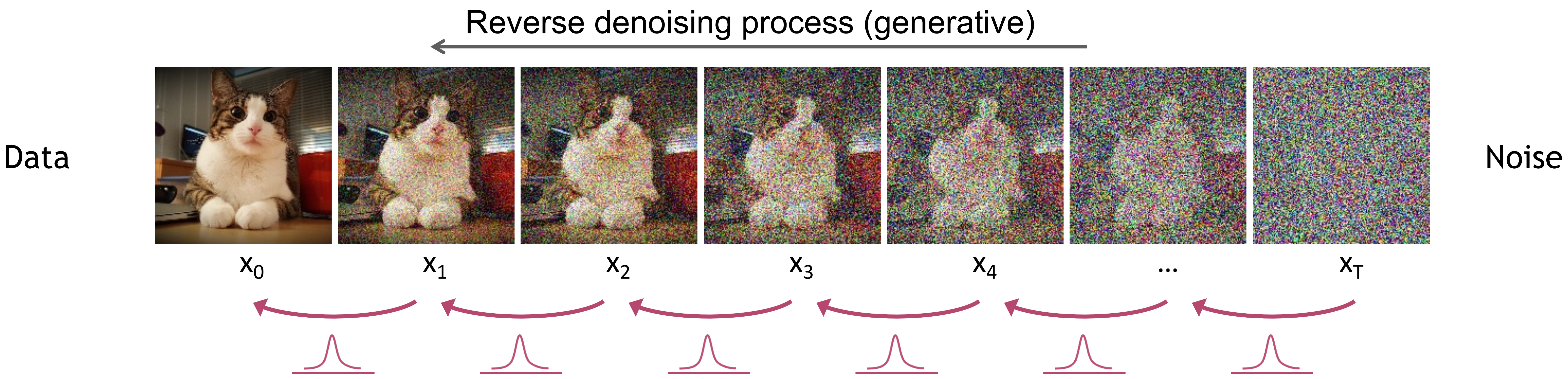
Reverse Denoising Process

Formal definition of forward and reverse processes in T steps:



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

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}_{\text{Trainable network (U-net, Denoising Autoencoder)}}, \sigma_t^2\mathbf{I})$$

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

Similar to the generative model in hierarchical VAEs.

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Learning Denoising Model

Variational upper bound

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

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

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

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

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

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

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

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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:

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

Recall that $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\ \mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\ \epsilon$. [Ho et al. NeurIPS 2020](https://arxiv.org/abs/2006.11239) 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

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

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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:

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

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Summary

Training and Sample Generation

Algorithm 1 Training

```
repeat
  x_0 ~ q(x_0)
  t ~ Uniform({1, ..., T})
  ε ~ N(0, I)
  Take gradient descent step on
      ∇_θ ||ε − ε_θ(√ᾱ_t x_0 + √(1 − ᾱ_t) ε, t)||^2
until converged
```

repeat

$\mathbf{x}_0 \sim q(\mathbf{x}_0)$

$t \sim \mathrm{Uniform}(\{1, \dots, T\})$

$\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

Take gradient descent step on

$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta\left(\boxed{\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}}, t\right) \right\|^2$$

until converged

Algorithm 2 Sampling

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

for $t = T, \dots, 1$ **do**

$\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

$$\mathbf{x}_{t-1} = \boxed{\frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right)} + \sigma_t \mathbf{z}$$

end for

return $\mathbf{x}_0$

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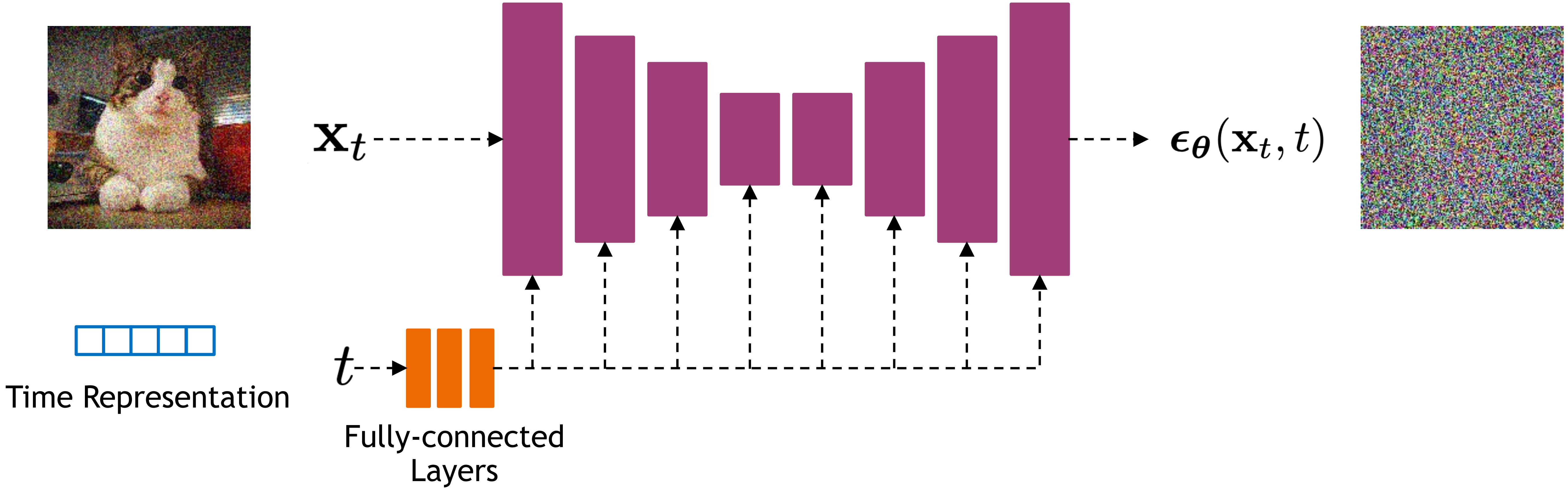
Implementation Considerations

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 Dharivwal and Nichol NeurIPS 2021)

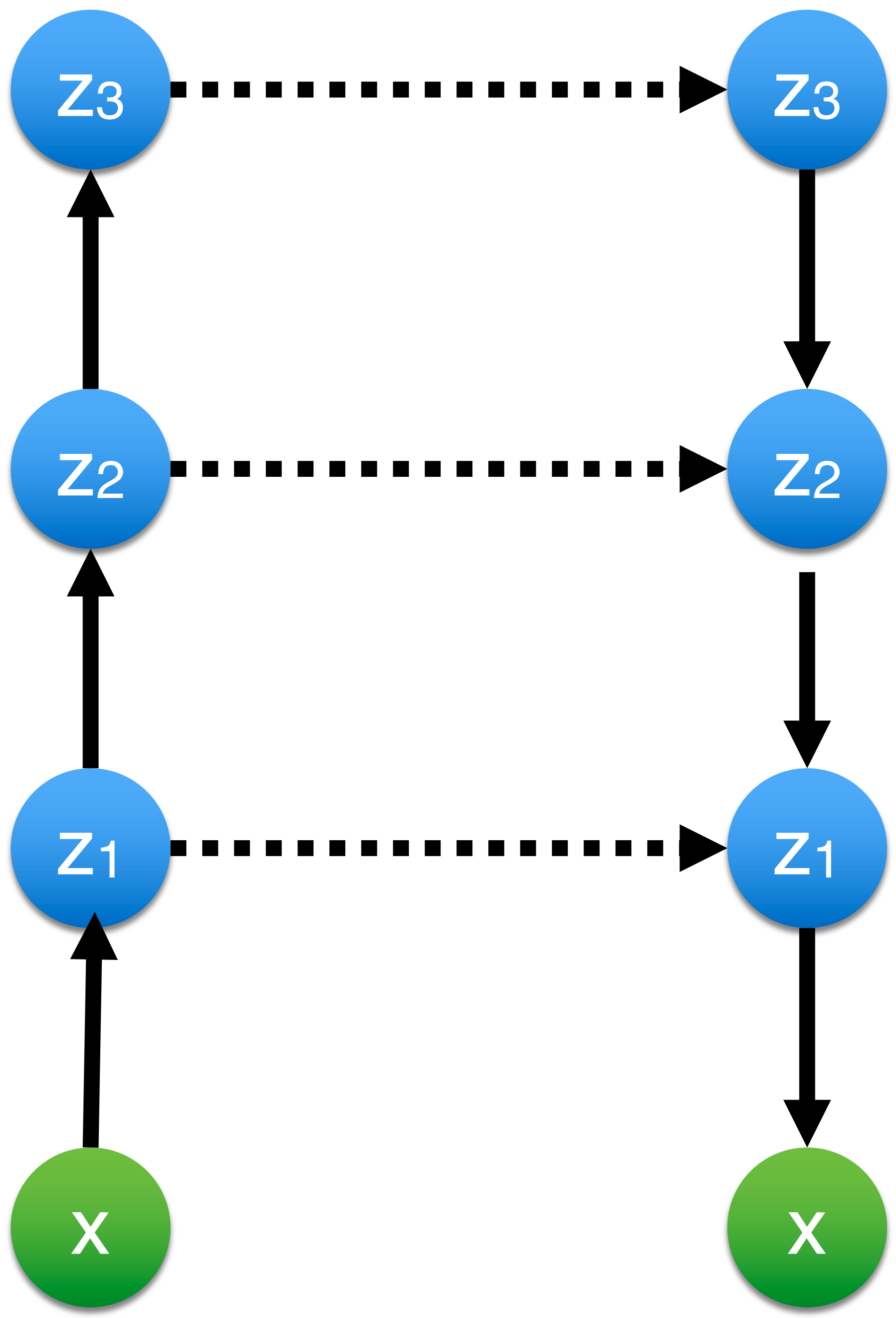
slide from https://cvpr2022-tutorial-diffusion-models.github.io/

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.



Inference model
q(z|x)

Generative model
p(x,z)

[Vahdat and Kautz, NVAE: A Deep Hierarchical Variational Autoencoder, NeurIPS 2020](#)
[Sønderby, et al.. Ladder variational autoencoders, NeurIPS 2016.](#)

Continuous-time diffusion models

Stochastic differential equation framework

Consider the limit of **many small steps**:

Forward diffusion process (fixed)

Data

Noise

$\mathbf{x}_0$ $\mathbf{x}_1$ ... ... $\mathbf{x}_T$

$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\,\mathbf{x}_{t-1}, \beta_t \mathbf{I})$$

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

Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", *ICLR*, 2021
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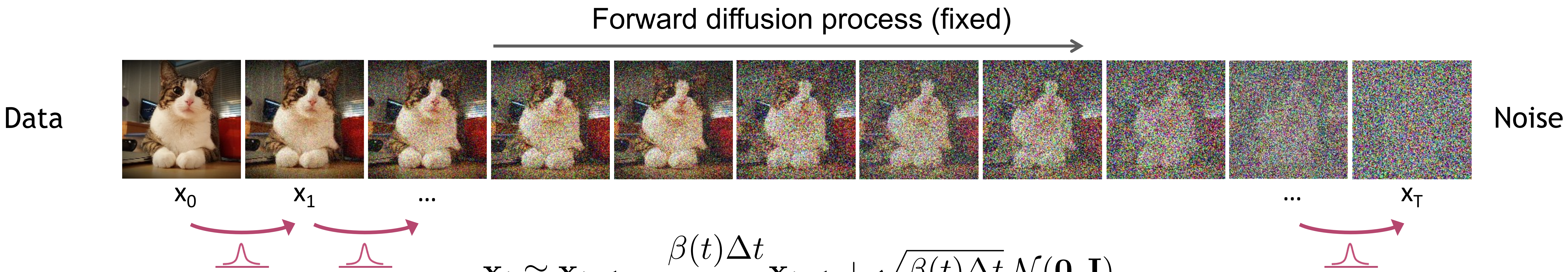
Forward Diffusion Process as Stochastic Differential Equation

Consider the limit of **many small steps:**



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

⬇

$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\boldsymbol{\omega}_t$$

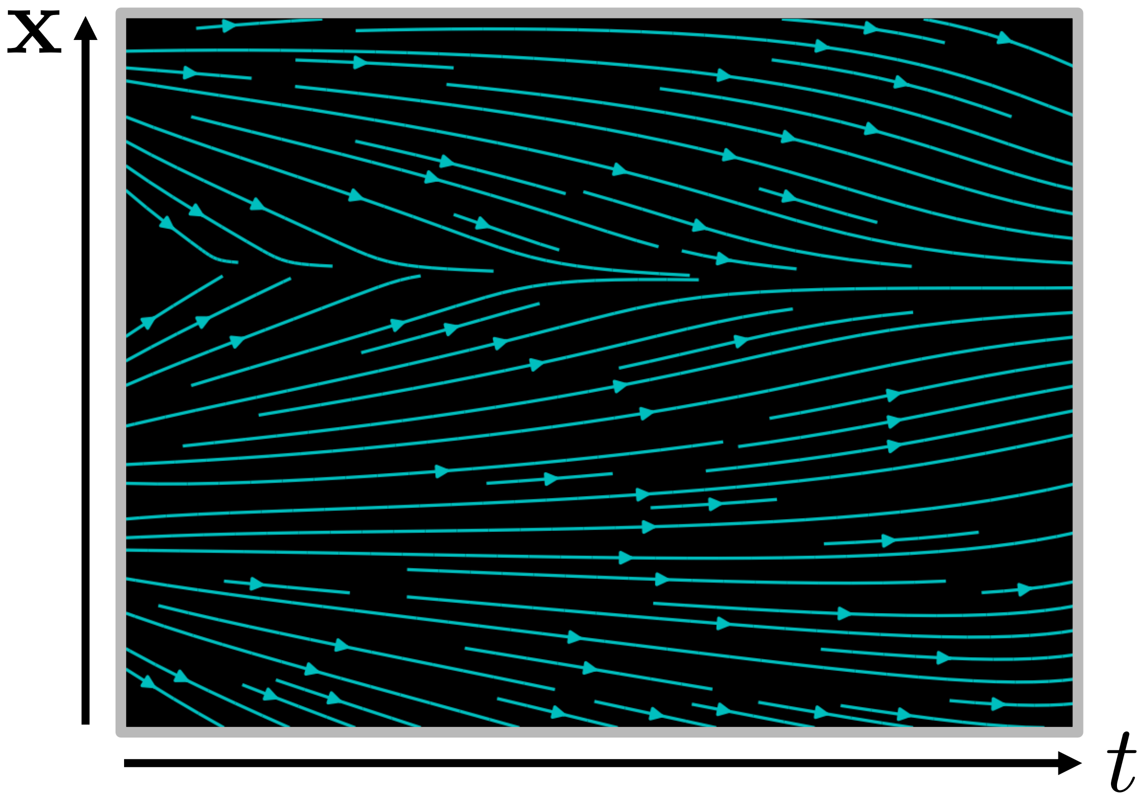
Stochastic Differential Equation (SDE)
describing the diffusion in infinitesimal limit

Song et al., "Score-Based Generative Modeling through Stochastic Differential Equations", *ICLR*, 2021
slide from https://cvpr2022-tutorial-diffusion-models.github.io/

Crash Course in Differential Equations

Ordinary Differential Equation (ODE):

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, t) \quad \text{or} \quad \mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t$$



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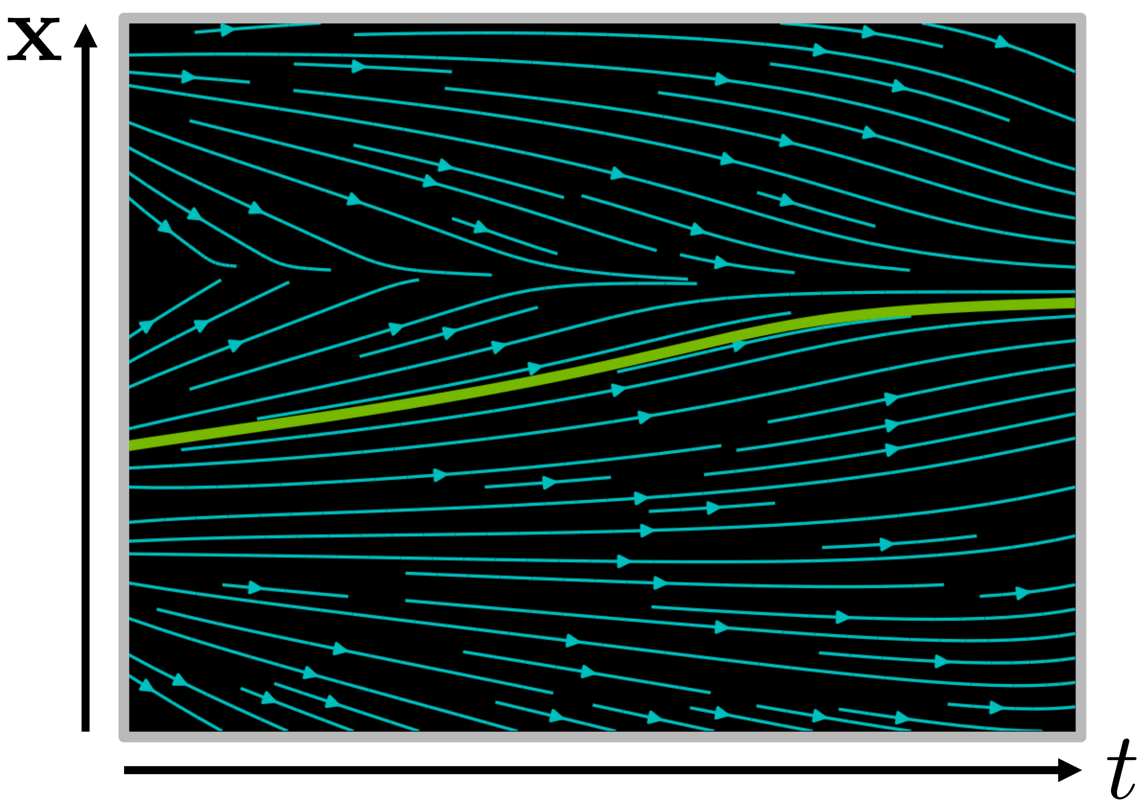


Analytical Solution:

$$\mathbf{x}(t) = \mathbf{x}(0) + \int_0^t \mathbf{f}(\mathbf{x}, \tau)\mathrm{d}\tau$$

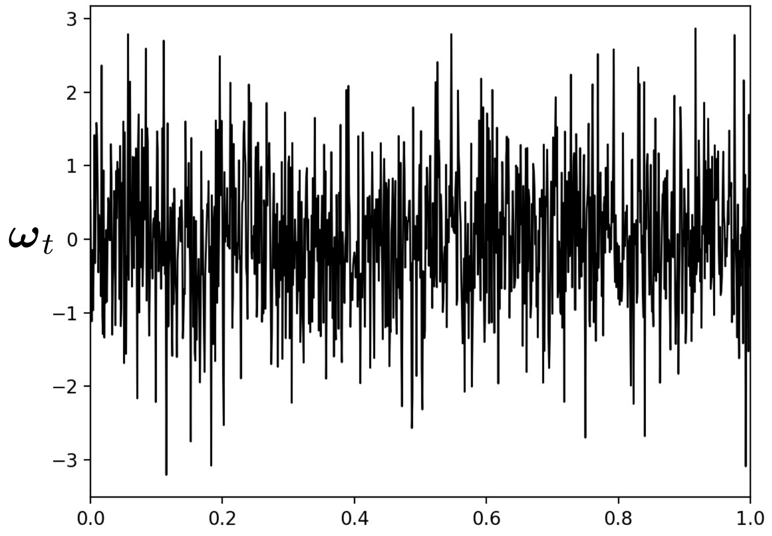
Iterative Numerical Solution:

$$\mathbf{x}(t + \Delta t) \approx \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t)\Delta t$$

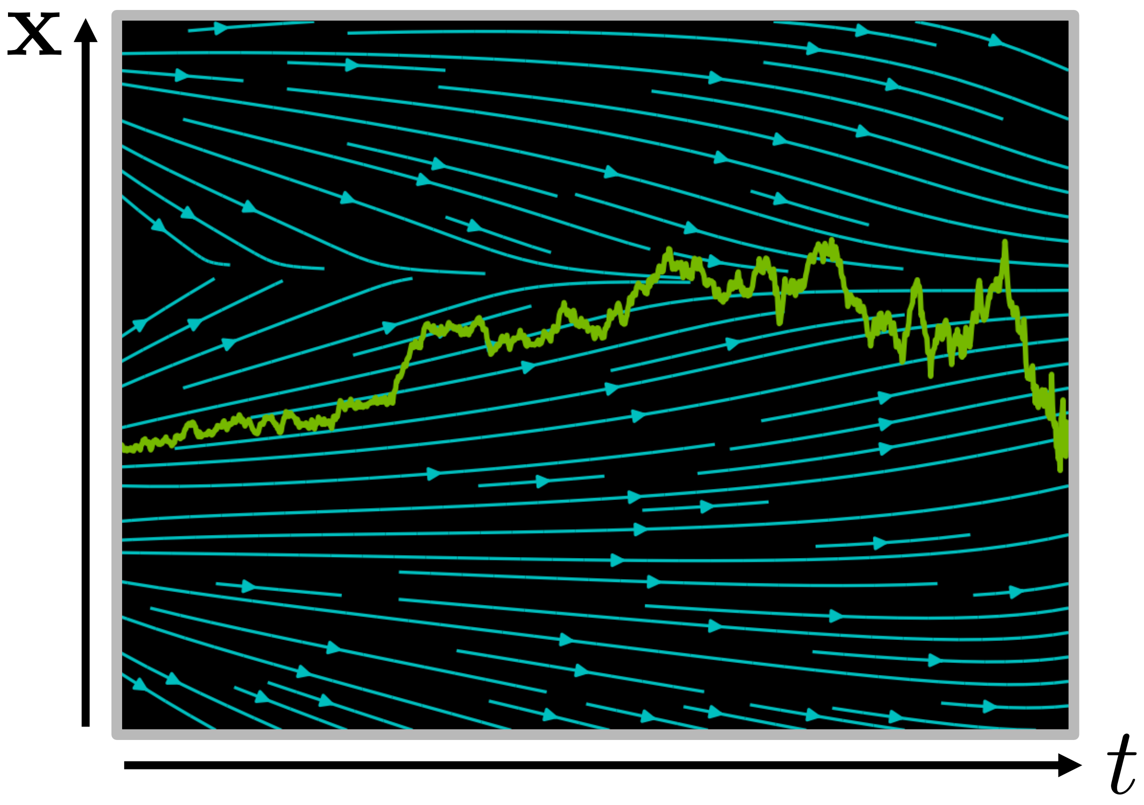
Stochastic Differential Equation (SDE):

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \underbrace{\mathbf{f}(\mathbf{x}, t)}_{\text{drift coefficient}} + \underbrace{\sigma(\mathbf{x}, t)}_{\text{diffusion coefficient}}\boldsymbol{\omega}_t$$

Wiener Process (Gaussian White Noise)



$$\left(\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + \sigma(\mathbf{x}, t)\mathrm{d}\boldsymbol{\omega}_t\right)$$

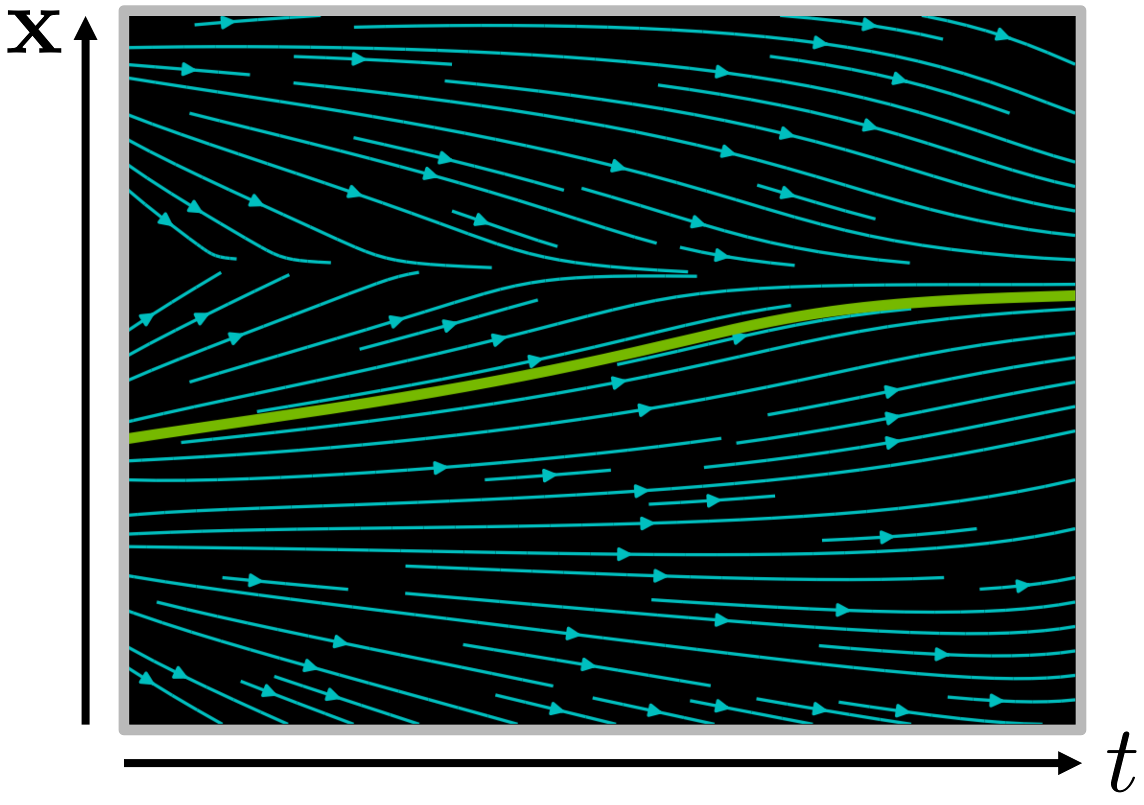


$$\mathbf{x}(t + \Delta t) \approx \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t)\Delta t + \sigma(\mathbf{x}(t), t)\sqrt{\Delta t}\,\mathcal{N}(\mathbf{0}, \mathbf{I})$$

Crash Course in Differential Equations

Ordinary Differential Equation (ODE):

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{f}(\mathbf{x}, t) \quad \text{or} \quad \mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t$$



Analytical Solution:

$$\mathbf{x}(t) = \mathbf{x}(0) + \int_0^t \mathbf{f}(\mathbf{x}, \tau)\mathrm{d}\tau$$

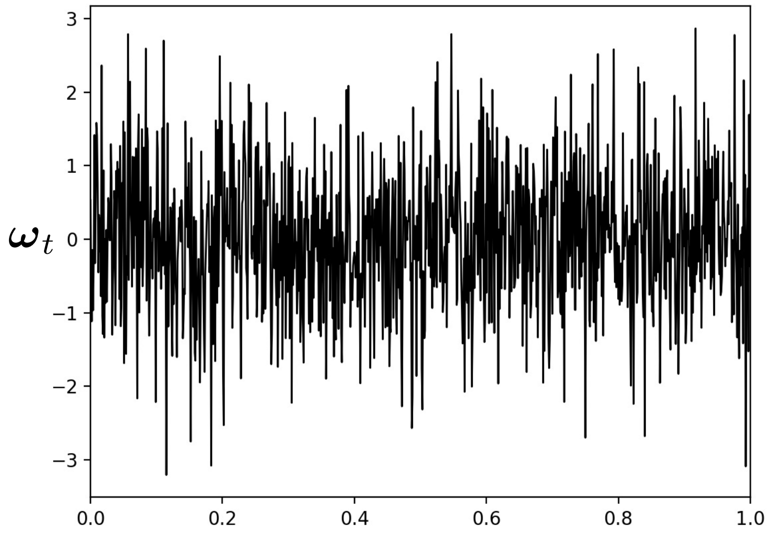
Iterative Numerical Solution:

$$\mathbf{x}(t + \Delta t) \approx \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t)\Delta t$$

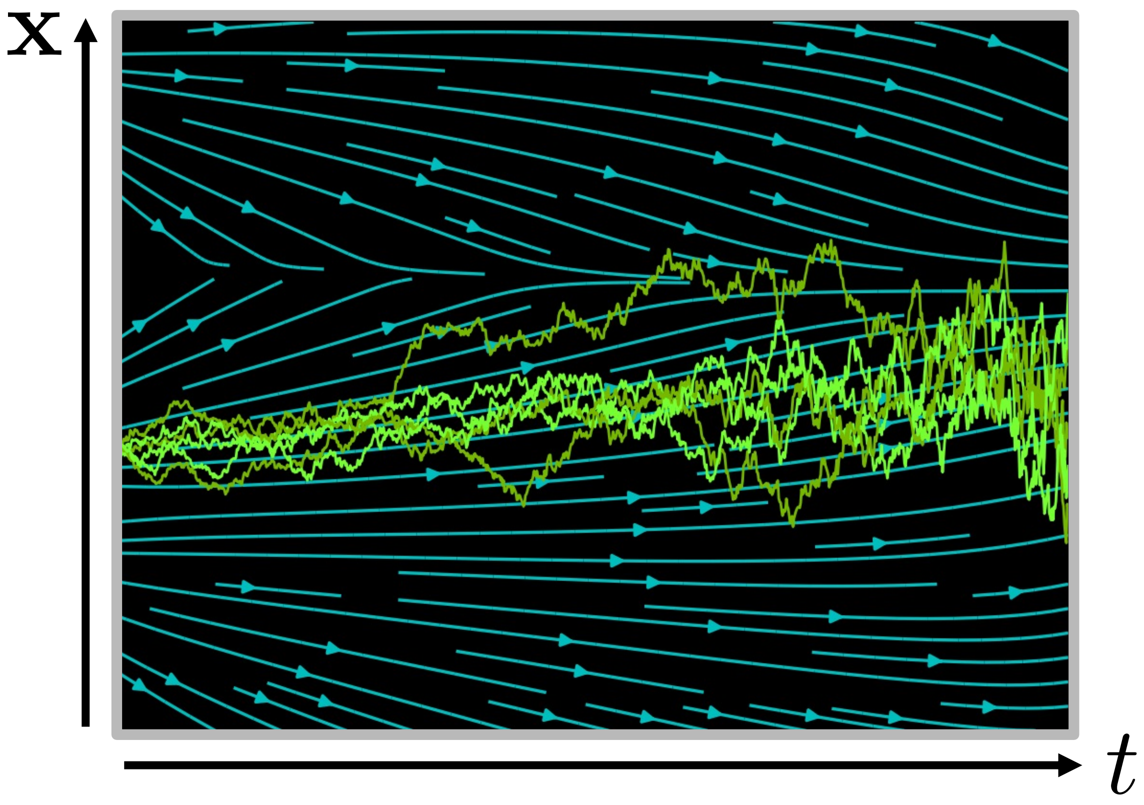
Stochastic Differential Equation (SDE):

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \underbrace{\mathbf{f}(\mathbf{x}, t)}_{\text{drift coefficient}} + \underbrace{\sigma(\mathbf{x}, t)}_{\text{diffusion coefficient}}\boldsymbol{\omega}_t$$

Wiener Process (Gaussian White Noise)

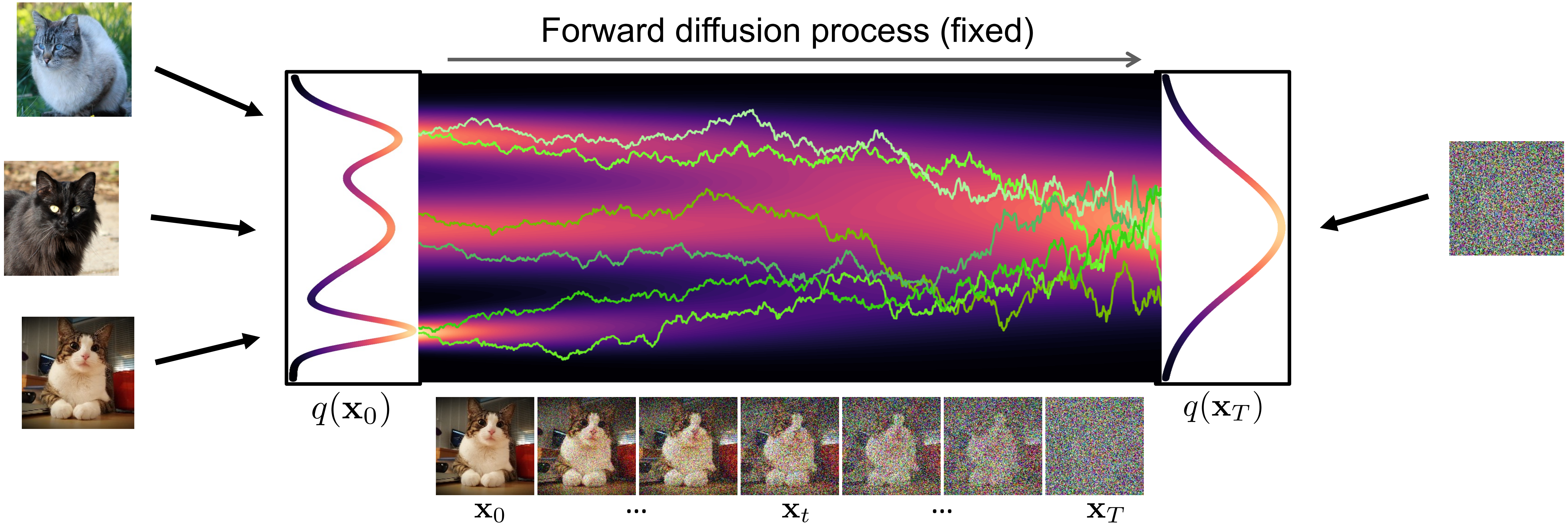


$$\left(\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + \sigma(\mathbf{x}, t)\mathrm{d}\boldsymbol{\omega}_t\right)$$



$$\mathbf{x}(t + \Delta t) \approx \mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t), t)\Delta t + \sigma(\mathbf{x}(t), t)\sqrt{\Delta t}\,\mathcal{N}(\mathbf{0}, \mathbf{I})$$

Forward Diffusion Process as Stochastic Differential Equation



Forward Diffusion SDE:

$$\mathrm{d}\mathbf{x}_t = \underbrace{-\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t}_{\substack{\text{drift term} \\ \text{(pulls towards mode)}}} + \underbrace{\sqrt{\beta(t)}\,\mathrm{d}\boldsymbol{\omega}_t}_{\substack{\text{diffusion term} \\ \text{(injects noise)}}}$$

Song et al., *ICLR*, 2021

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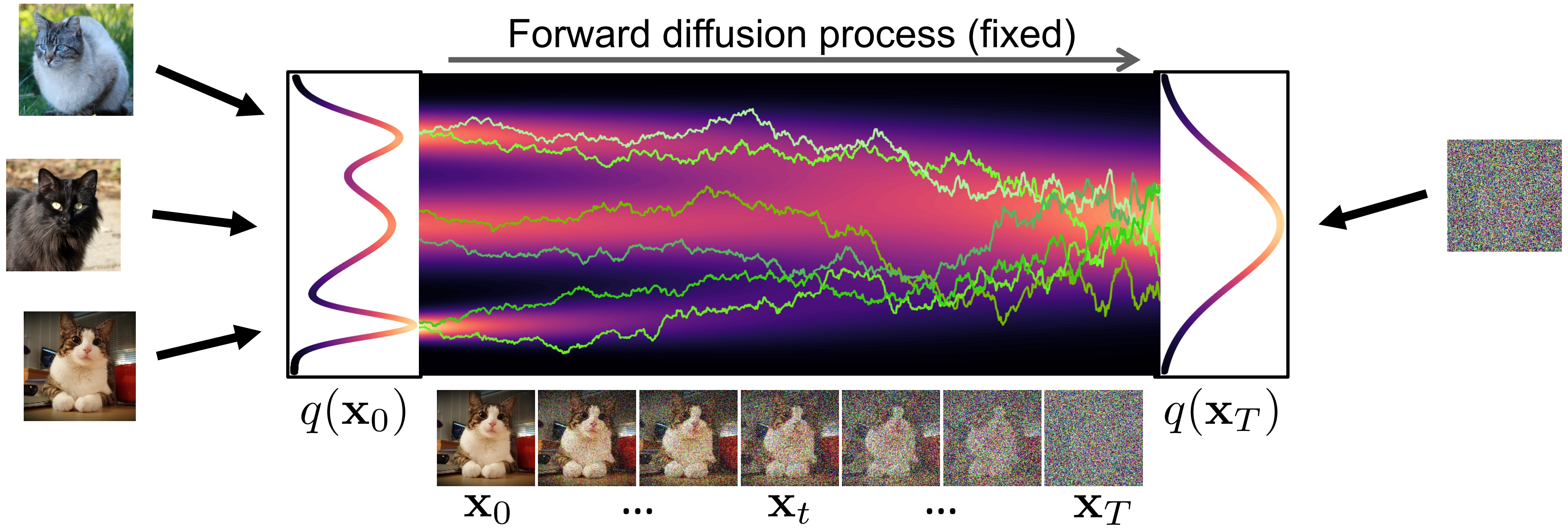
The Generative Reverse Stochastic Differential Equation



Forward Diffusion SDE:

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

Reverse Generative Diffusion SDE:

$$d\mathbf{x}_t = \overbrace{\left[-\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\underbrace{\color{red}{\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)}}_{\text{“Score Function”}}\right]}^{\text{drift term}} dt + \overbrace{\sqrt{\beta(t)}\, d\bar{\boldsymbol{\omega}}_t}^{\text{diffusion term}}$$

➡ **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: $\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\omega_t$

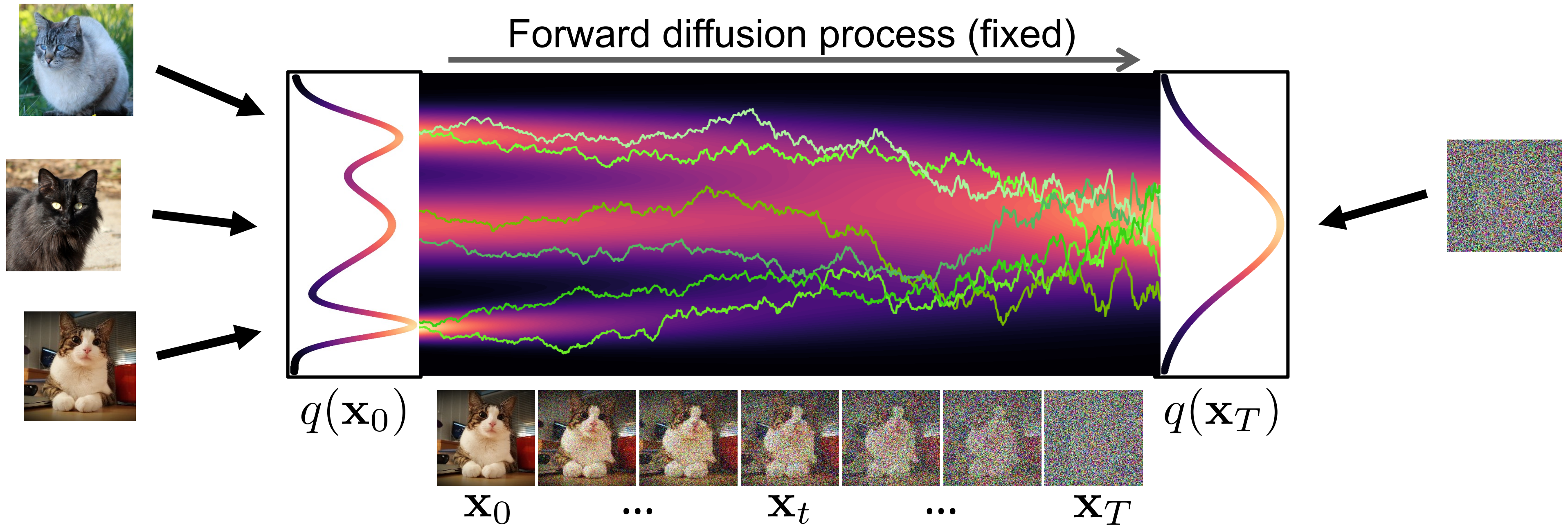
Reverse Generative Diffusion SDE:

$$\mathrm{d}\mathbf{x}_t = \overbrace{\left[-\frac{1}{2}\beta(t)\mathbf{x}_t - \beta(t)\underbrace{\nabla_{\mathbf{x}_t} \log q_t(\mathbf{x}_t)}_{\text{“Score Function”}}\right]\mathrm{d}t}^{\text{drift term}} + \overbrace{\sqrt{\beta(t)}\,\mathrm{d}\bar{\omega}_t}^{\text{diffusion term}}$$

➡ **Simulate reverse diffusion process: Data generation from random noise!**

Song et al., *ICLR*, 2021
Anderson, in *Stochastic Processes and their Applications*, 1982

Score Matching



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

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

➡ **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

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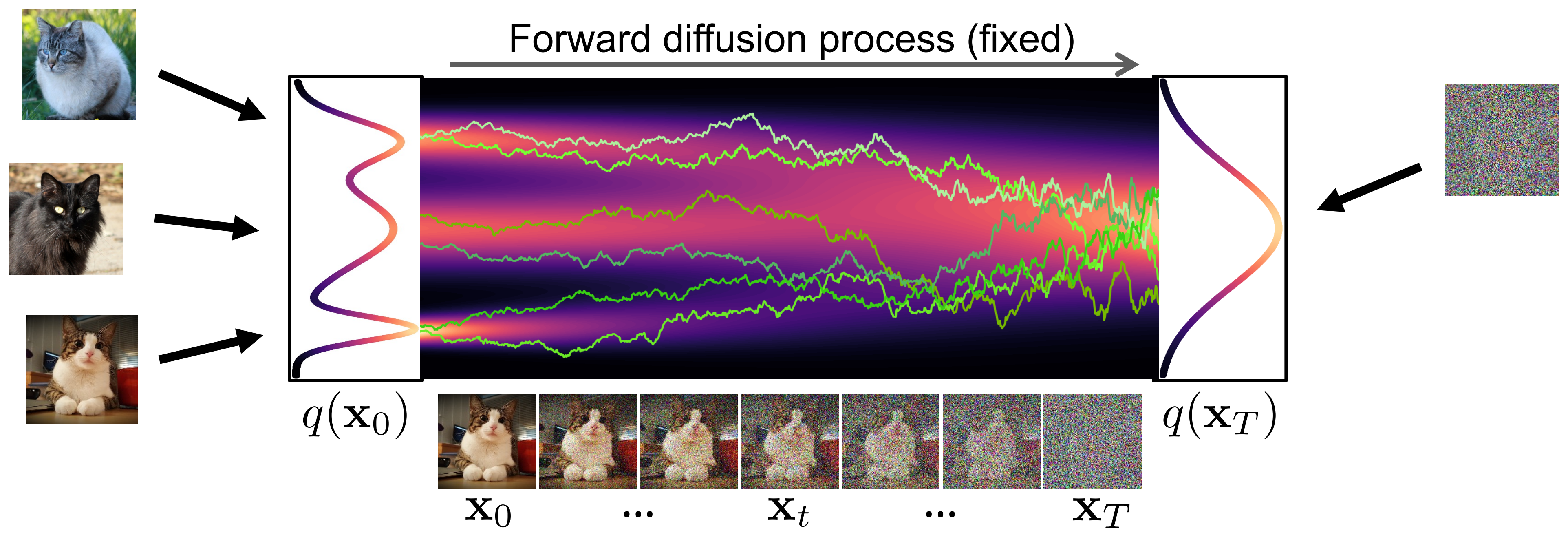
Denoising Score Matching



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

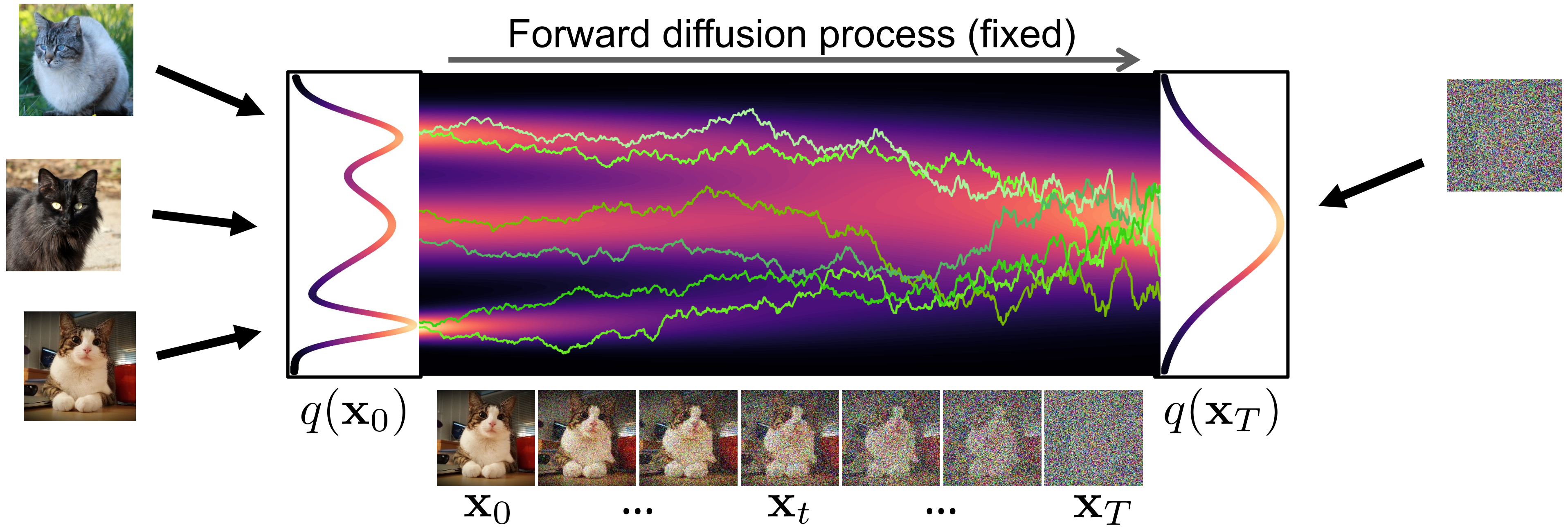
$$\min_{\boldsymbol{\theta}} \underbrace{\mathbb{E}_{t\sim\mathcal{U}(0,T)}}_{\text{diffusion time } t} \underbrace{\mathbb{E}_{\mathbf{x}_0\sim q_0(\mathbf{x}_0)}}_{\text{data sample } \mathbf{x}_0} \underbrace{\mathbb{E}_{\mathbf{x}_t\sim q_t(\mathbf{x}_t|\mathbf{x}_0)}}_{\text{diffused data sample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

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

Vincent, in *Neural Computation*, 2011
Song and Ermon, *NeurIPS*, 2019
Song et al. *ICLR*, 2021
slide from https://cvpr2022-tutorial-diffusion-models.github.io/

Denoising Score Matching

Epsilon-prediction parametrization



- **Denoising Score Matching:**

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

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

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

Vincent, in *Neural Computation*, 2011
Song and Ermon, *NeurIPS*, 2019
Song et al. *ICLR*, 2021
slide from https://cvpr2022-tutorial-diffusion-models.github.io/

What is the ELBO for continuous-time diffusion models?

Infinitely deep forward and backward models

Forward Diffusion SDE:

$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\mathbf{x}_t\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\boldsymbol{\omega}_t$$

Reverse Generative Diffusion SDE:

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

Forward joint distribution: $q(\mathbf{x}_{dt}, \ldots, \mathbf{x}_T | \mathbf{x}_0)$ (inference model)

Reverse joint distribution: $p(\mathbf{x}_0, \ldots, \mathbf{x}_T)$ (generative model)

Can be treated as an infinitely deep hierarchical VAE model

Kingma et al., "Variational diffusion models", NeurIPS 2021.

What is the ELBO for continuous-time diffusion models?

- [Kingma et al, 2021] showed that the negative ELBO in continuous time setting can be reduced to a simple variant:

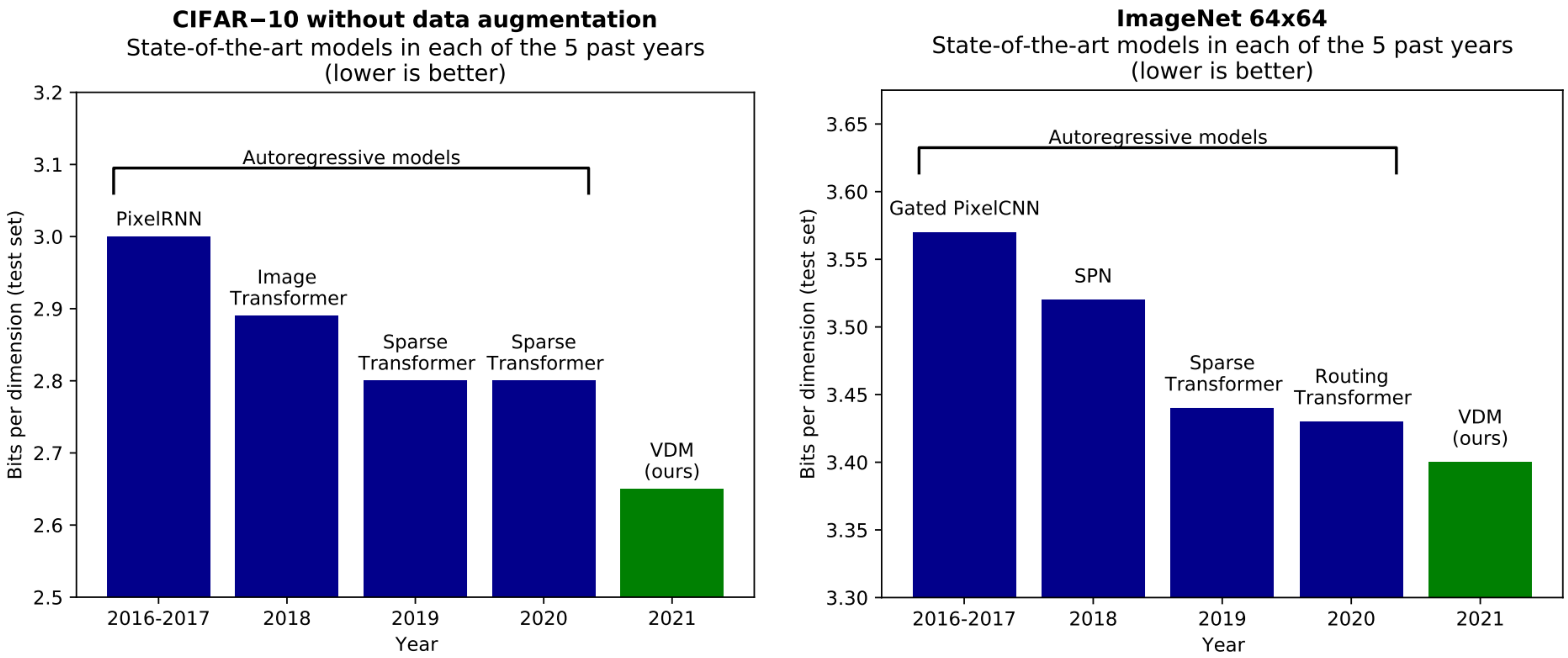
$$-\mathrm{ELBO}(\theta) = \frac{1}{2}\mathbb{E}_{t\sim\mathcal{U}(0,T)}\mathbb{E}_{\mathbf{x}_0\sim q_0(\mathbf{x}_0)}\mathbb{E}_{\boldsymbol{\epsilon}\sim\mathcal{N}(\mathbf{0},\mathbf{I})} -\frac{d\lambda}{dt}\cdot||\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_{\boldsymbol{\theta}}(\mathbf{x}_t,t)||_2^2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

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

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

Kingma et al., "Variational diffusion models", NeurIPS 2021.

Image density estimation benchmarks



Best likelihoods by far (at time of publication)

But…

- The best qualitative results are achieved with diffusion models that are trained with some reweighted objectives, seemingly not likelihood-based.
- **Is the log-likelihood objective (or the ELBO) flawed?**




Midjourney v5

Weighted diffusion objectives

Understanding diffusion objectives as the ELBO with data augmentation

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

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

- ELBO: $w(\lambda_t) = 1.$ ➡ Best for likelihood estimation.
- L_{simple} loss: $w(\lambda_t) = -1/(d\lambda/dt)$ ➡ Great for perceptual quality.

Kingma & Gao, "Understanding Diffusion Objectives\\as the ELBO with Data Augmentation", 2023.

Weighted diffusion objectives

Understanding diffusion objectives as the ELBO with data augmentation

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

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

- [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 noise perturbation):

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

$p_w(t)$: a distribution over t. $w(\lambda_t)$ equals its CDF.

$w(\lambda_t)$ controls the distribution of the data augmentation.

- Therefore, the ELBO objective is compatible with perceptual quality when combined with simple data augmentation.

Kingma & Gao, "Understanding Diffusion Objectives\\as the ELBO with Data Augmentation", 2023.

Intuition

What happens to an image with Gaussian noise perturbation?

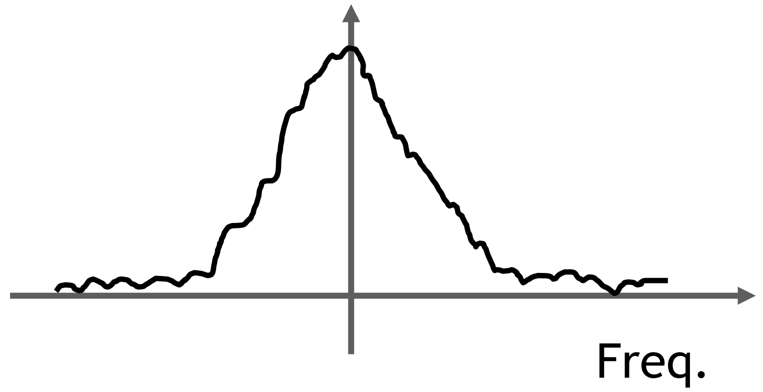
Recall that sampling from $q(\mathbf{x}_t|\mathbf{x}_0)$ is done using $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\ \mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\ \epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

$$\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\ \mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\ \epsilon$$

Fourier Transform

$$\mathcal{F}(\mathbf{x}_t) = \sqrt{\bar{\alpha}_t}\ \mathcal{F}(\mathbf{x}_0) + \sqrt{(1-\bar{\alpha}_t)}\ \mathcal{F}(\epsilon)$$

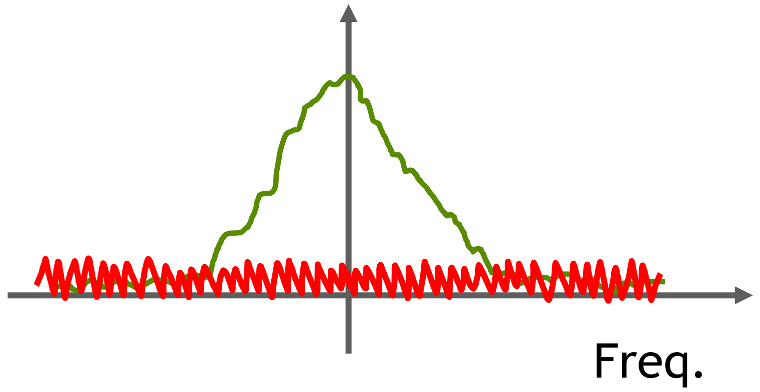
$|\mathcal{F}(\mathbf{x}_0)|$



Small t

$\bar{\alpha}_t \sim 1$

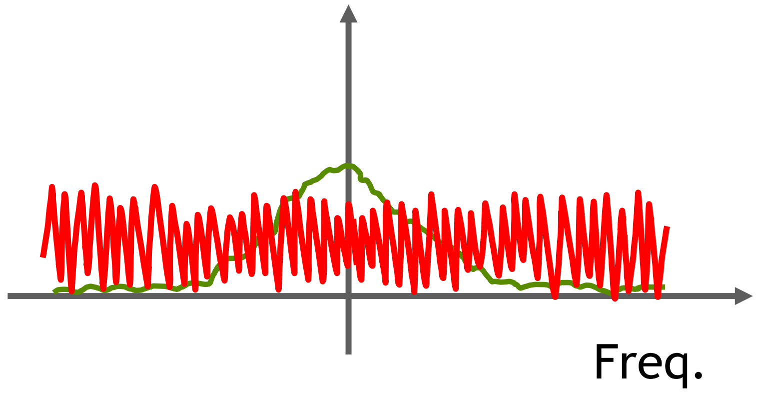
$|\mathcal{F}(\mathbf{x}_t)|$



Large t

$\bar{\alpha}_t \sim 0$

$|\mathcal{F}(\mathbf{x}_t)|$



As noise increases, the high frequency content is perturbed faster.

Content-Detail Tradeoff

Gaussian noise perturbation

Data  Noise

x z_0 z_{dt} z_{2dt} z_{3dt} … z_1

The model is required to capture high-frequency content (i.e., low-level details)

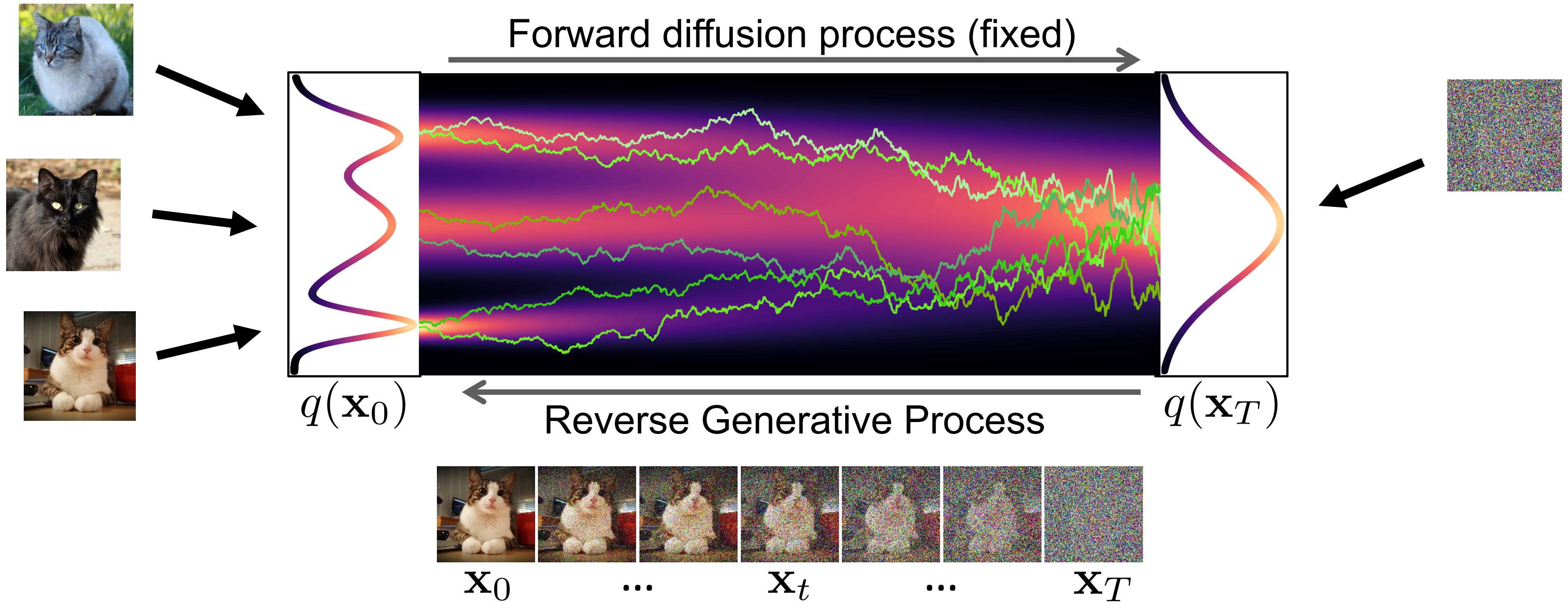
The model is specialized for capturing low-frequency content (i.e., high-level content)

With data augmentation, the model put more emphasis on modeling low-frequency content, which could be more important for human perception.

$w(\lambda_t)$ controls the balance between modeling content & details.

Probability Flow ODE

Alternative reverse process



- Consider reverse generative diffusion SDE:

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

- In distribution equivalent to "**Probability Flow ODE**":

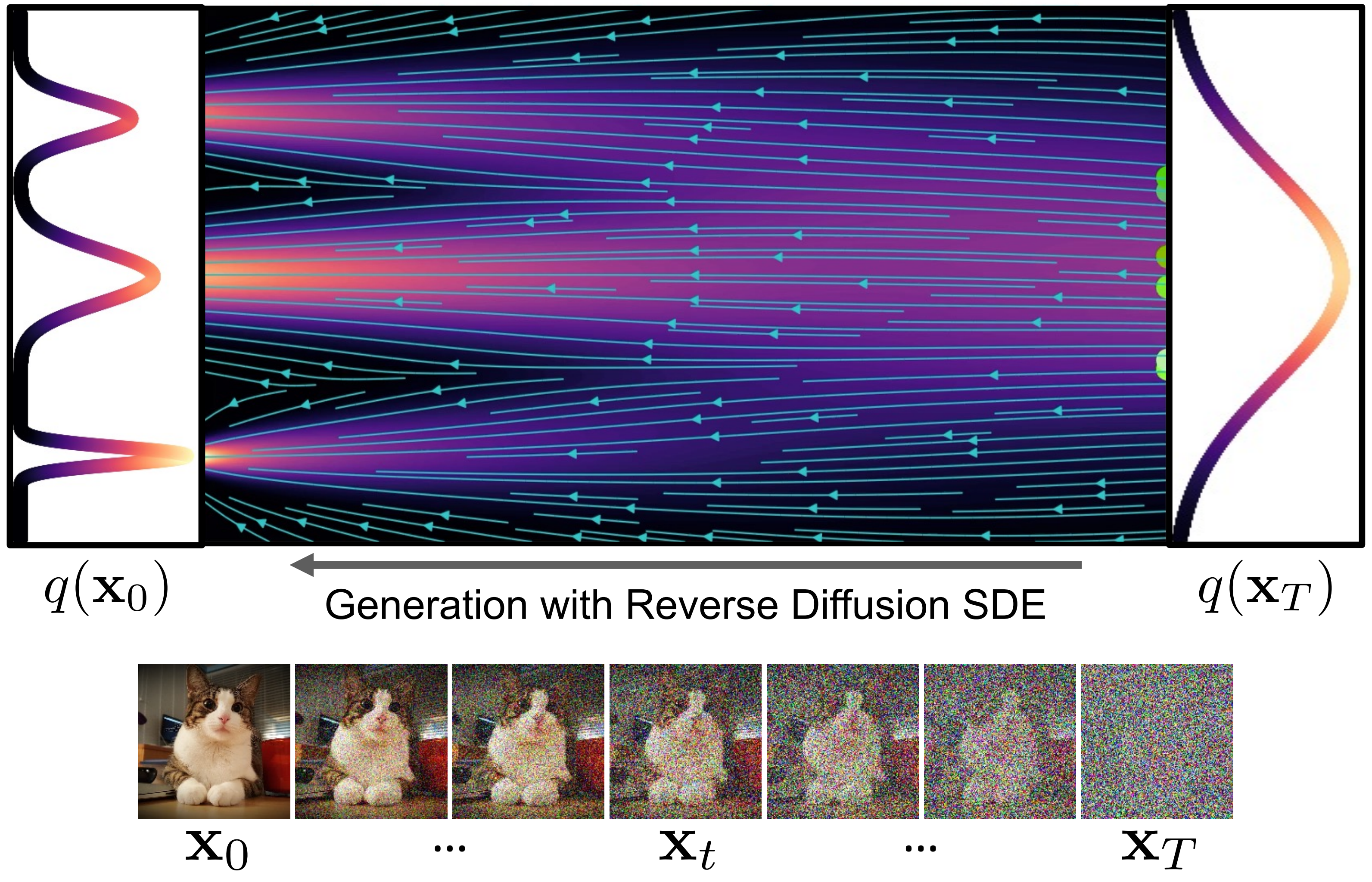
$$\mathrm{d}\mathbf{x}_t = -\frac{1}{2}\beta(t)\left[\mathbf{x}_t + \nabla_{\mathbf{x}_t}\log q_t(\mathbf{x}_t)\right]\mathrm{d}t$$

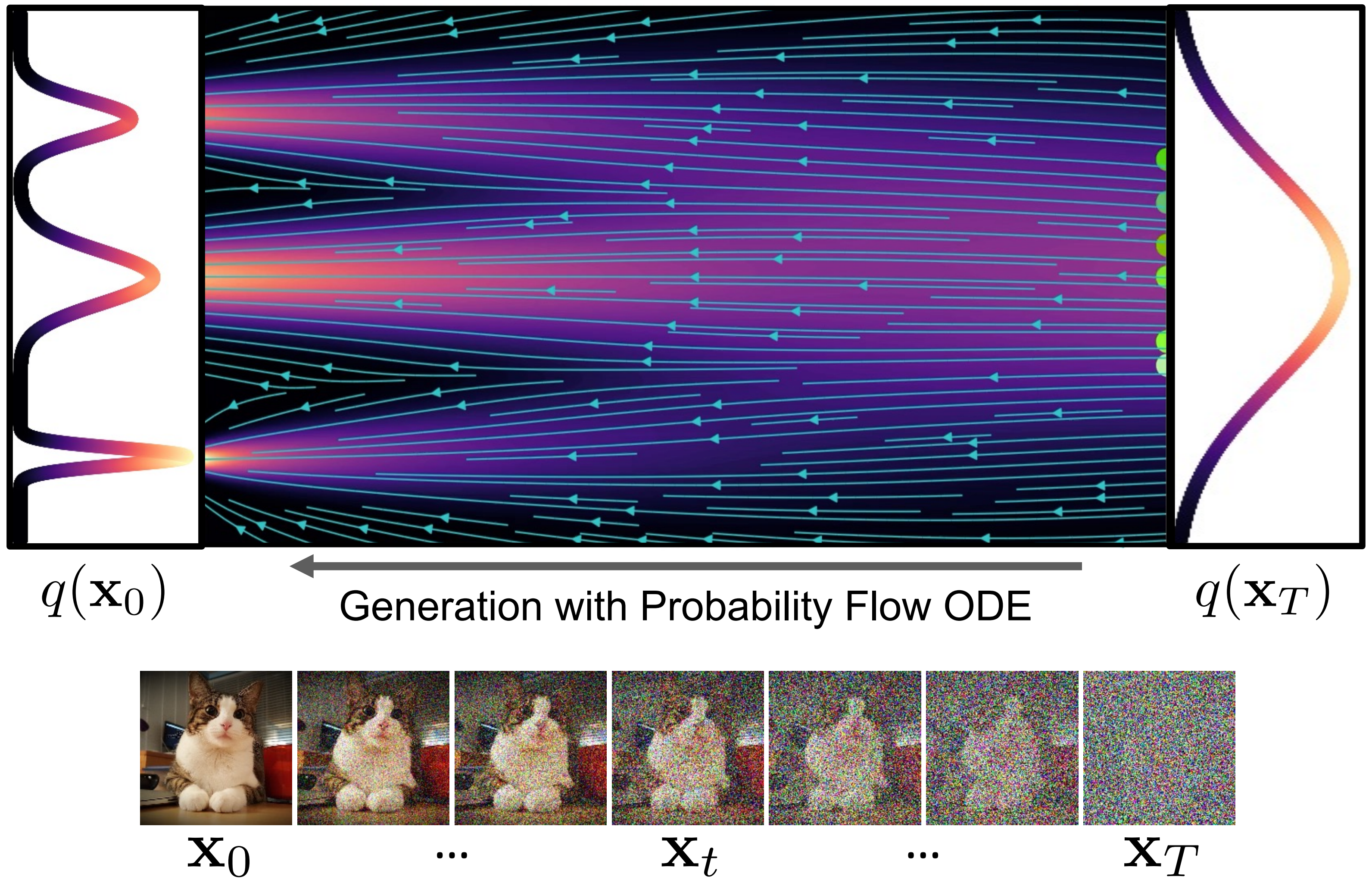
(solving this ODE results in the same $q_t(\mathbf{x}_t)$ when initializing $q_T(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$)

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

Song et al., *ICLR*, 2021

Synthesis with SDE vs. ODE





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

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

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

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

Song et al., *ICLR*, 2021

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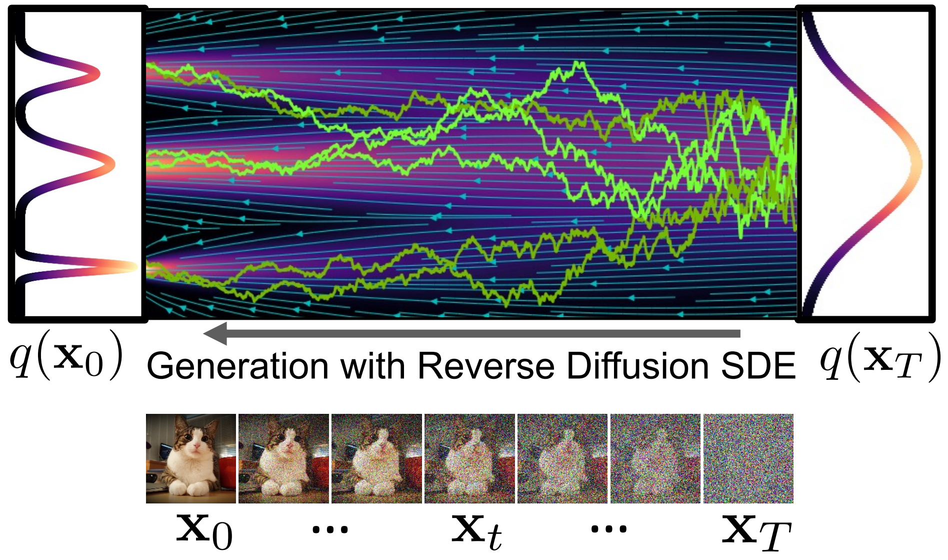
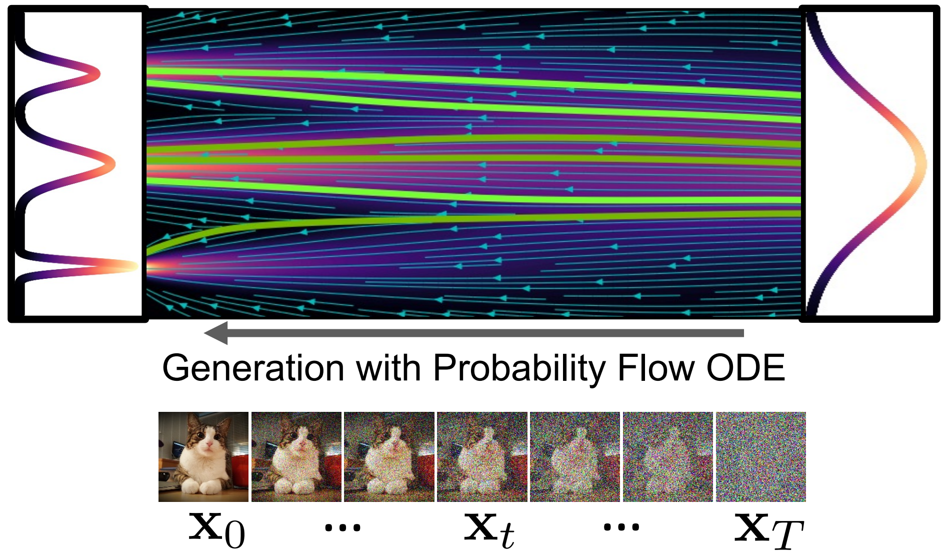
Sampling from “Continuous-Time” Diffusion Models

SDE vs. ODE Sampling: Pro’s and Con’s





Generative Diffusion SDE:

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

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

- *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:

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

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

Karras et al., “Elucidating the Design Space of Diffusion-Based Generative Models”, *arXiv*, 2022

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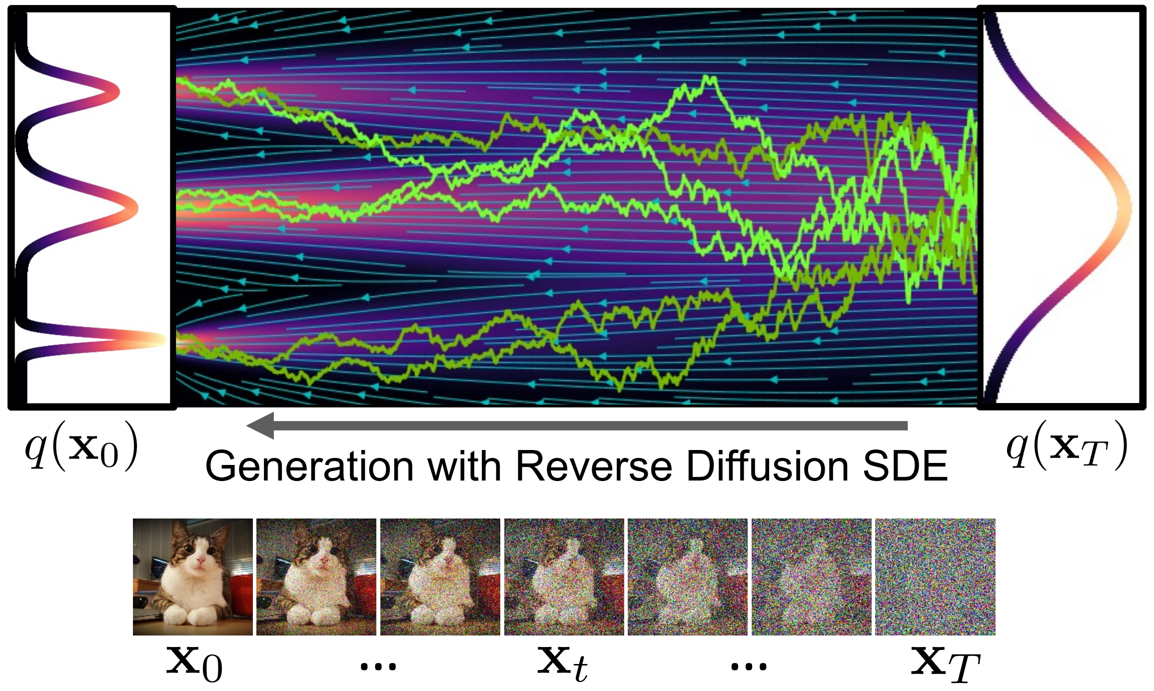
Sampling from "Continuous-Time" Diffusion Models

How to solve the generative SDE or ODE in practice?



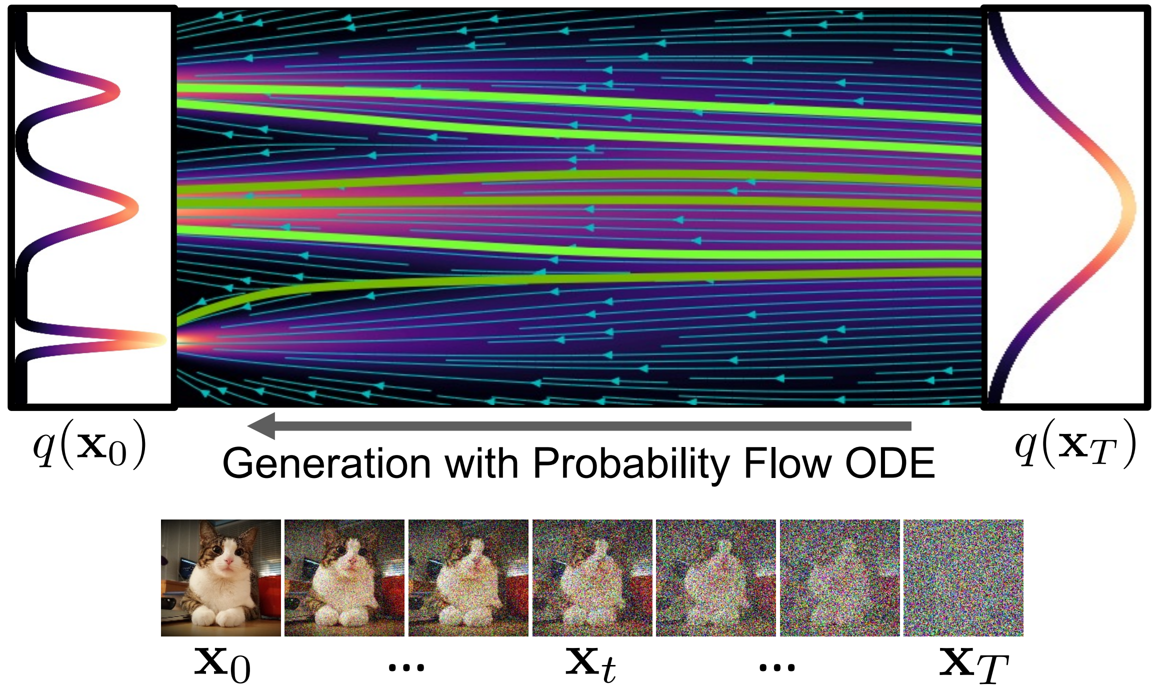
Generative Diffusion SDE:

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

- *Euler-Maruyama*:

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

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



Probability Flow ODE:

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

- *Euler's Method*:

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

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

Song et al., *ICLR*, 2021

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How to make sampling faster?

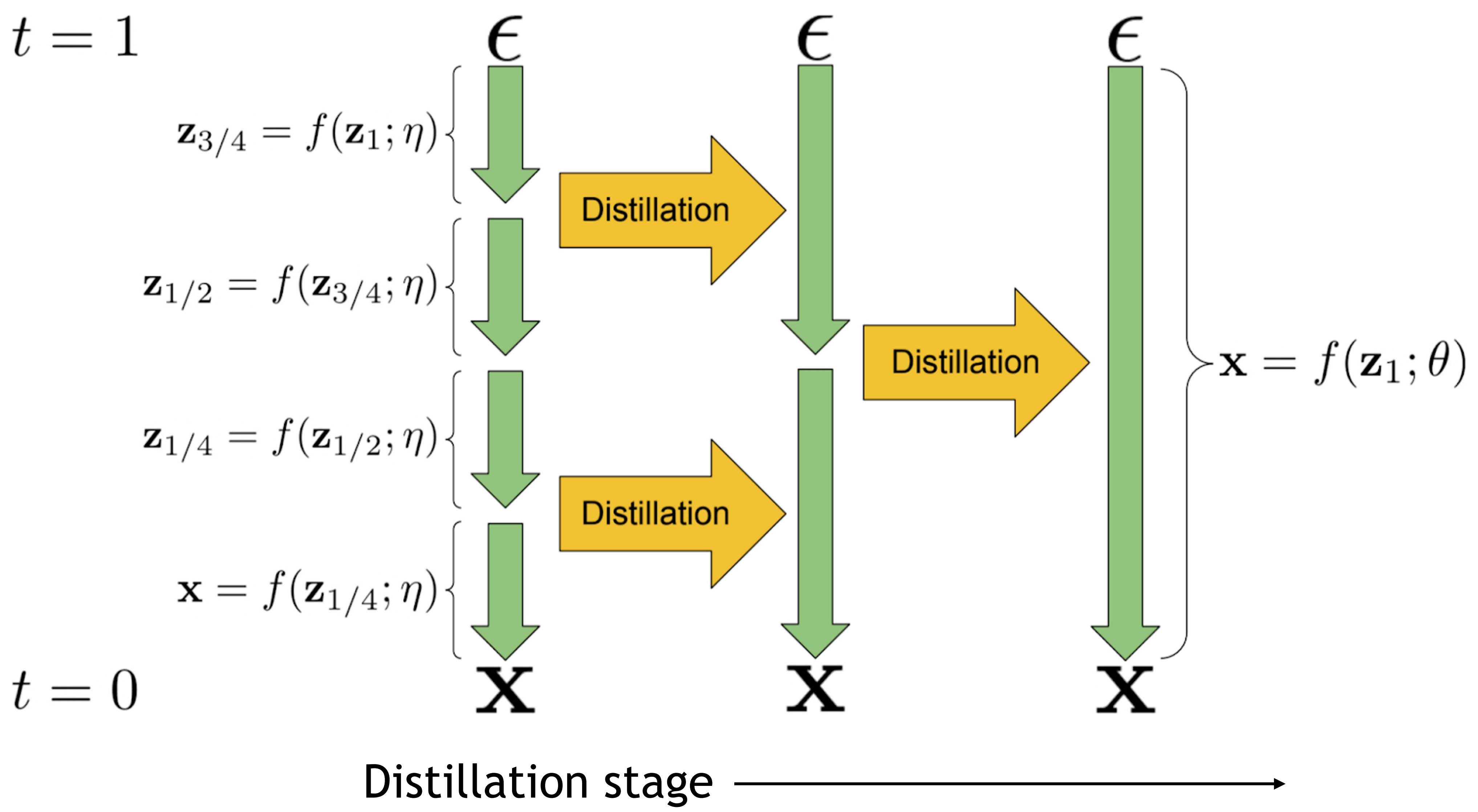
- One bottleneck of diffusion models is its slowness in sampling: need 10-1000+ steps to generate high quality samples
- Generative models need to be fast for practical use.

- One solution: distill diffusion models into models using just 1-8 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.



Salimans & Ho, “Progressive distillation for fast sampling of diffusion models”, ICLR 2022.

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**
    $\mathbf{x} \sim \mathcal{D}$
    $t = i/N, \quad i \sim Cat[1, 2, \ldots, N]$
    $\epsilon \sim N(0, I)$
    $\mathbf{z}_t = \alpha_t \mathbf{x} + \sigma_t \epsilon$
    `# 2 steps of DDIM with teacher`
    $t' = t - 0.5/N, \quad t'' = t - 1/N$
    $\mathbf{z}_{t'} = \alpha_{t'} \hat{\mathbf{x}}_\eta(\mathbf{z}_t) + \frac{\sigma_{t'}}{\sigma_t}(\mathbf{z}_t - \alpha_t \hat{\mathbf{x}}_\eta(\mathbf{z}_t))$
    $\mathbf{z}_{t''} = \alpha_{t''} \hat{\mathbf{x}}_\eta(\mathbf{z}_{t'}) + \frac{\sigma_{t''}}{\sigma_{t'}}(\mathbf{z}_{t'} - \alpha_{t'} \hat{\mathbf{x}}_\eta(\mathbf{z}_{t'}))$
    $\tilde{\mathbf{x}} = \frac{\mathbf{z}_{t''} - (\sigma_{t''}/\sigma_t)\mathbf{z}_t}{\alpha_{t''} - (\sigma_{t''}/\sigma_t)\alpha_t}$ ▷ 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

Salimans & Ho, "Progressive distillation for fast sampling of diffusion models", ICLR 2022.

On Distillation of Guided Diffusion Models

Meng et al., CVPR 2023 award nominated

Now also works with

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

Text-guided generation (1 step)

Text-guided generation (4 steps)

Text-guided generation (2 steps)

Class-conditional generation (1 step)

Image inpainting (2 steps)

Image to image translation (3 steps)

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.

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

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.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

Imagen

By Google (imagen.research.google)

A dragon fruit wearing karate belt in the snow.

Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.

“toilet paper with real cactus spikes”
by Irina Blok

[Saharia et al., “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding”, arXiv 2022.](#)

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

Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

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Explicit Conditional Training

Conditional sampling can be considered as training $p(\mathbf{x}|\mathbf{y})$ where $\mathbf{y}$ is the input conditioning (e.g., text) and $\mathbf{x}$ is generated output (e.g., image)

Train the score model for $\mathbf{x}$ conditioned on $\mathbf{y}$ using:

$$\mathbb{E}_{(\mathbf{x},\mathbf{y})\sim p_{\text{data}}(\mathbf{x},\mathbf{y})}\mathbb{E}_{\epsilon\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\mathbb{E}_{t\sim\mathcal{U}[0,T]}\ ||\epsilon_\theta(\mathbf{x}_t, t; \mathbf{y}) - \epsilon||_2^2$$

The conditional score is simply a U-Net with $\mathbf{x_t}$ and $\mathbf{y}$ together in the input.

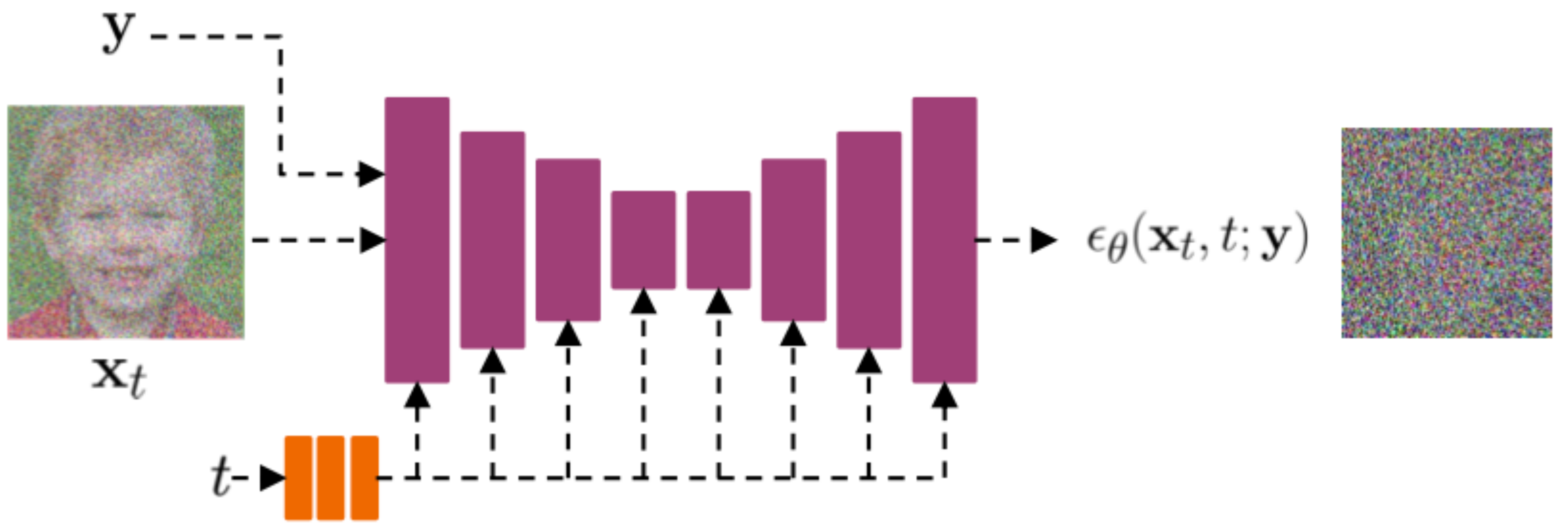
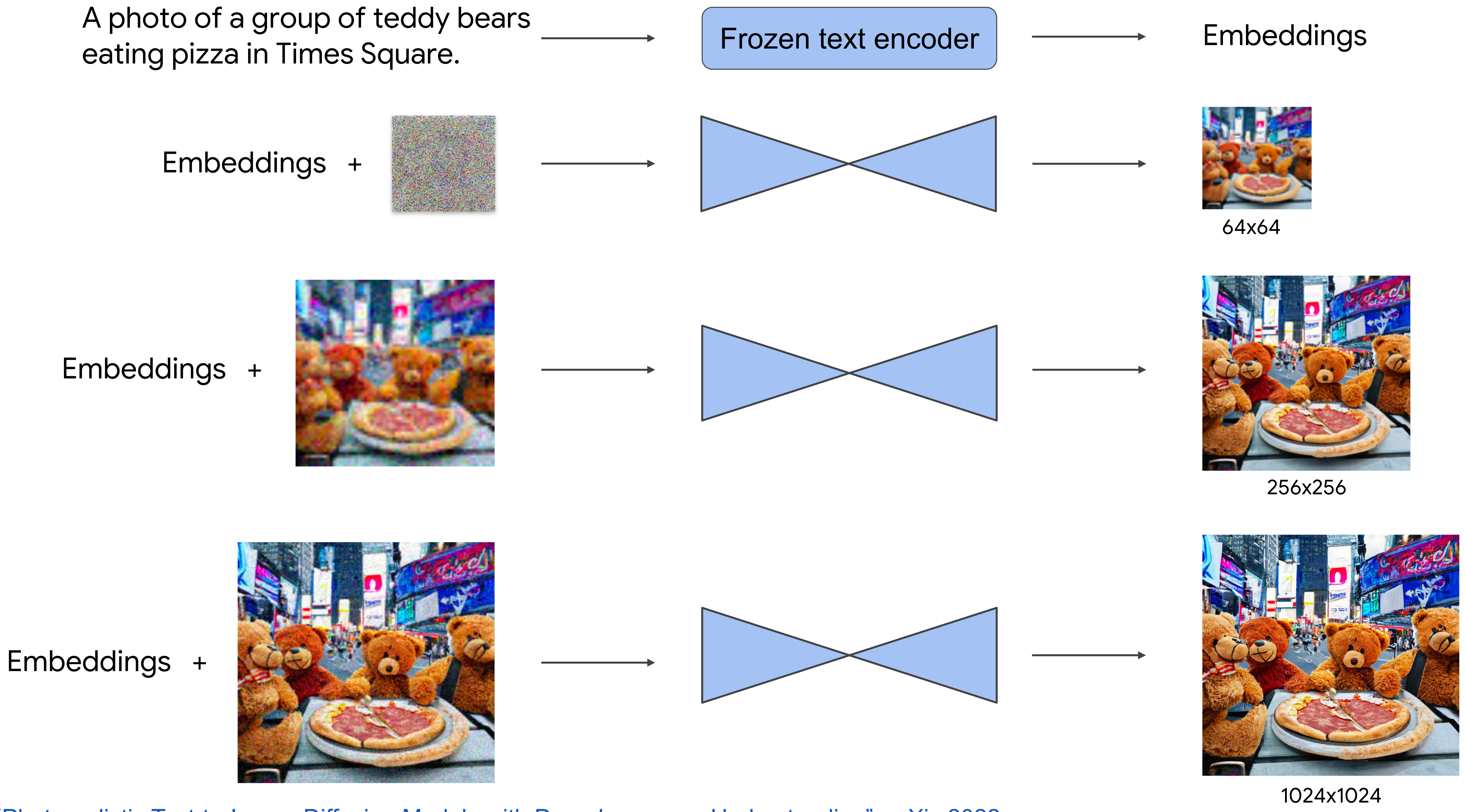


Imagen: Cascaded generation pipeline



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

Classifier Guidance

Sampler technique

- Assume pairs of data (x, 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 c.
- Cons: need to train an additional classifier. Increase model complexity.

Dhariwal and Nichol, "Diffusion models beat GANs on image synthesis", NeurIPS 2021.

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

$$\nabla_{\mathbf{x}_t} \log \tilde{p}_\theta(\mathbf{x}_t|\mathbf{c}) = (1+\omega)\underbrace{\nabla_{\mathbf{x}_t} \log p_\theta(\mathbf{x}_t|\mathbf{c})}_{\text{From the conditional diffusion model}} - \omega\underbrace{\nabla_{\mathbf{x}_t} \log p_\theta(\mathbf{x}_t)}_{\text{From the unconditional diffusion model}}.$$

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

Ho & Salimans, "Classifier-Free Diffusion Guidance", 2021.

Classifier-free guidance

Trade-off for sample quality and sample diversity

Non-guidance

$\omega = 1$

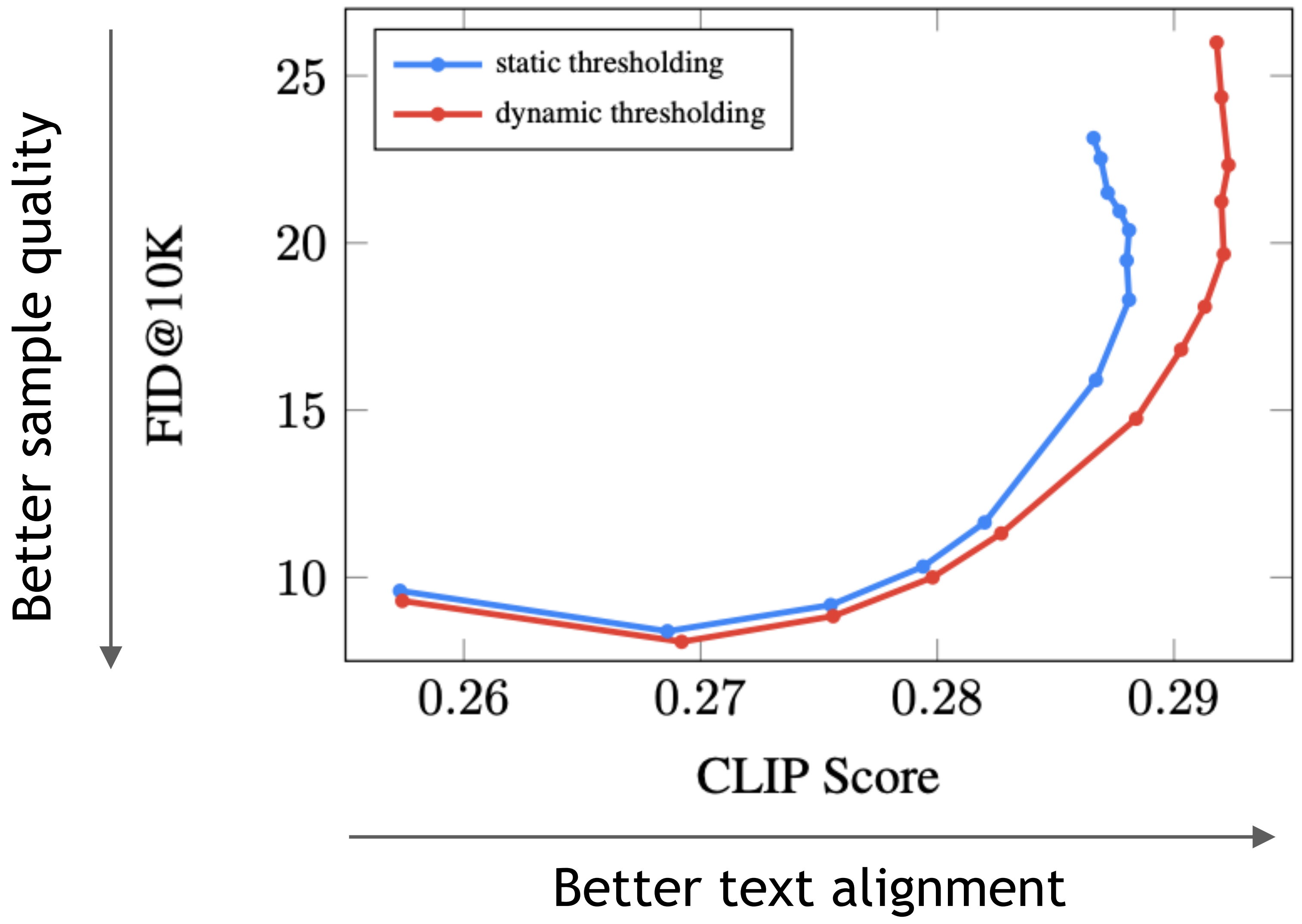
$\omega = 3$

Large guidance weight (ω) usually leads to better individual sample quality but less sample diversity.

[Ho & Salimans, "Classifier-Free Diffusion Guidance", 2021.](#)

Classifier-free guidance in Imagen

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



Saharia et al., "Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding", arXiv 2022.

“watercolor greeting card of thank you so much!”