

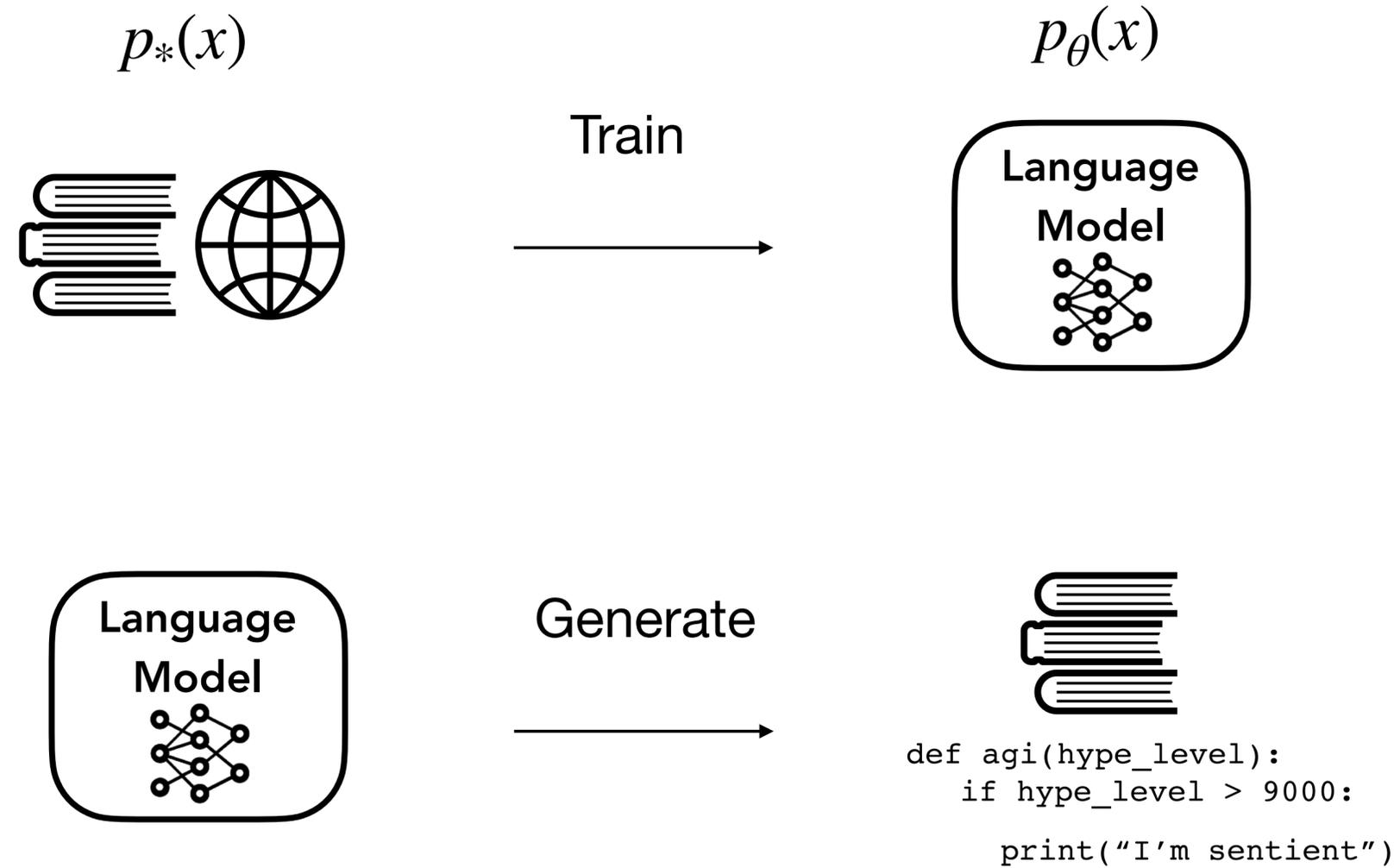
Denoising diffusion models

Sean Welleck

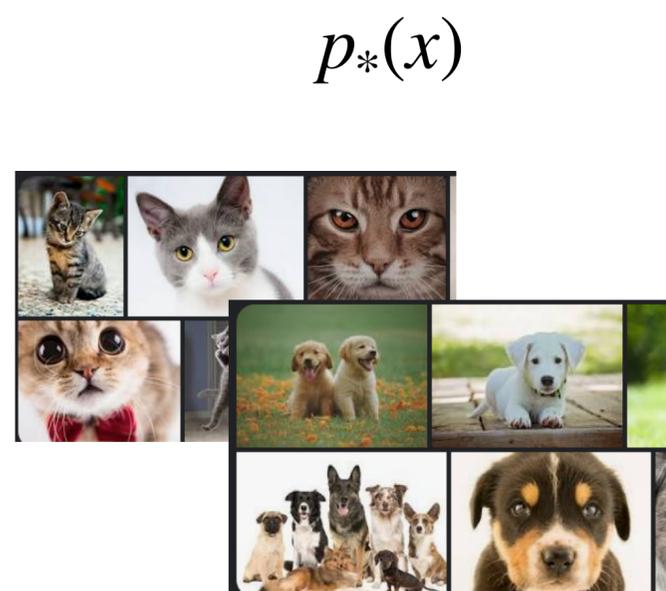
July 27 2022

Some content inspired or adapted from:
[\[MIT Lecture: Diffusion Probabilistic Models, Jascha Sohl-Dickstein\]](#)
[\[CVPR 2022 Tutorial\]](#)
[\[IRCAM diffusion notebooks\]](#)
[\[Lillian Weng's Blog\]](#)
[\[Yang Song's Blog\]](#)
Papers referenced in slides

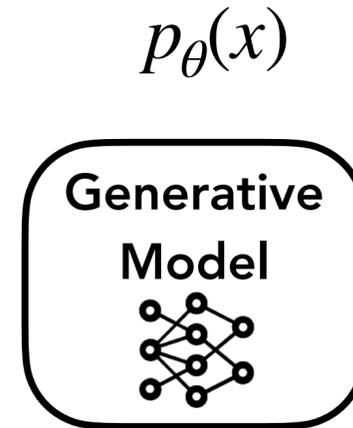
Generative modeling



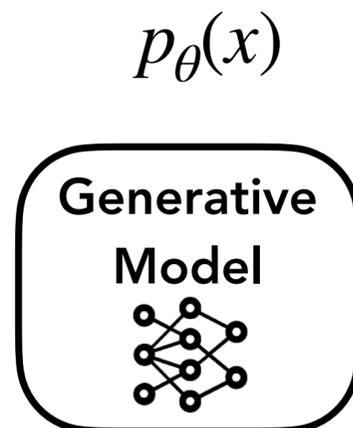
Generative modeling



Train



- Autoregressive
- Variational auto encoder (VAE)
- Generative adversarial networks (GAN)
- Denoising Diffusion models



Sample



Diffusion models

Emerging as powerful generative models

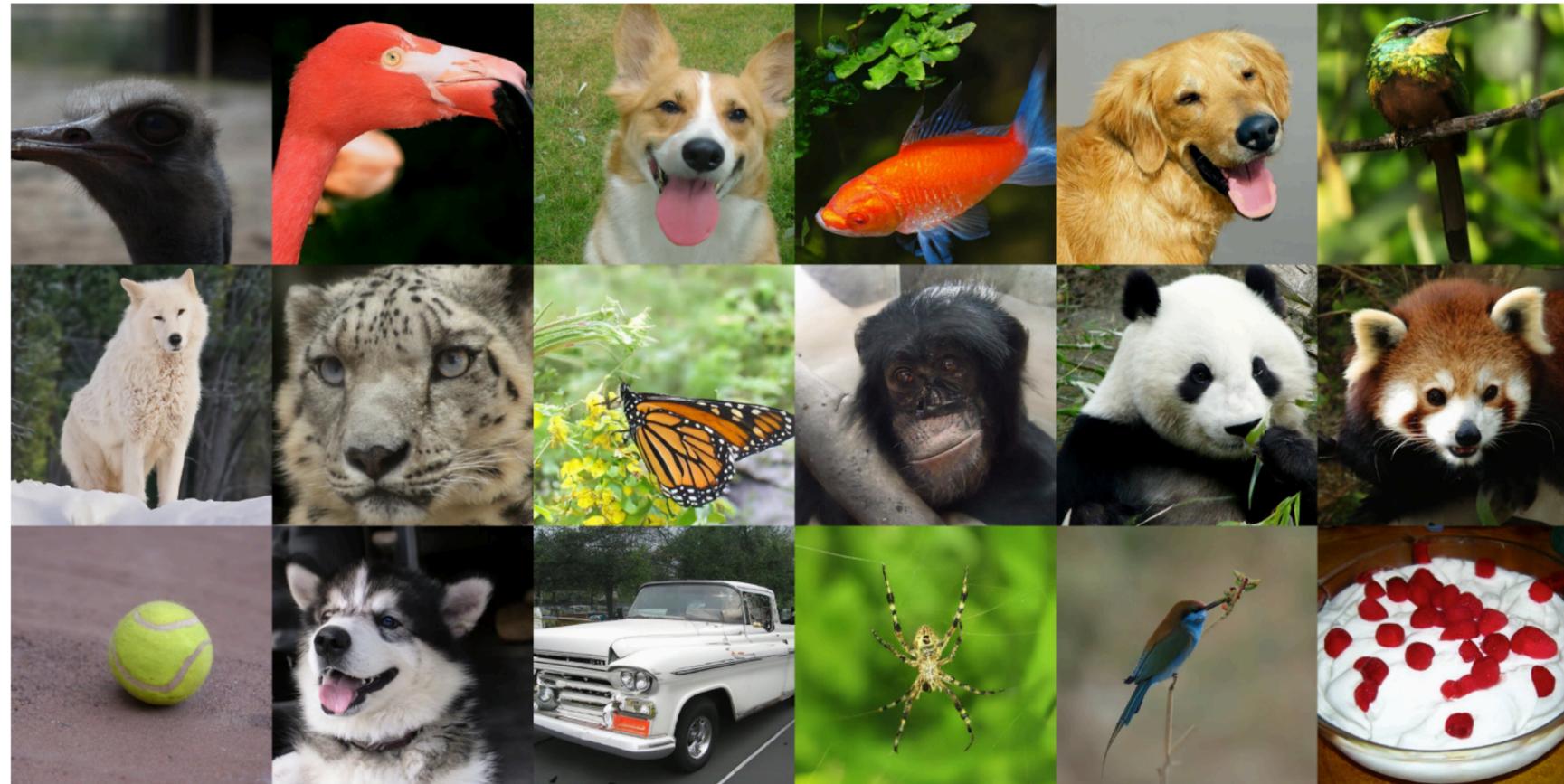
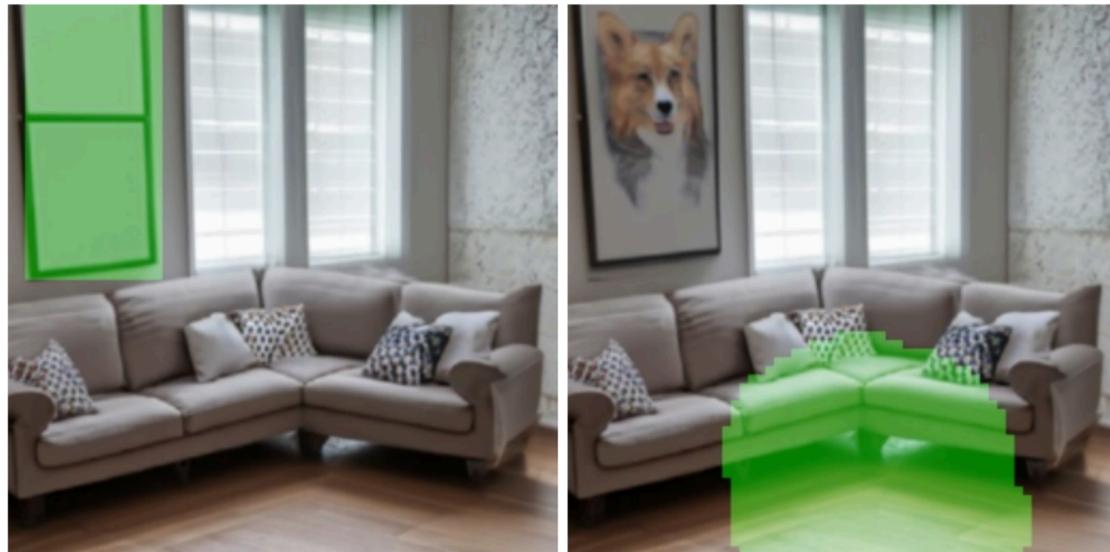


Figure 1: Selected samples from our best ImageNet 512×512 model (FID 3.85)

Diffusion models



“a cozy living room”

“a painting of a corgi
on the wall above
a couch”

Figure 3. Iteratively creating a complex scene using GLIDE.



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

Diffusion models

huggingface / [diffusers](#) Public



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🤖 Diffusers provides pretrained diffusion models across multiple modalities, such as vision and audio, and serves as a modular toolbox for inference and training of diffusion models.

🤖 Diffusers: State-of-the-art diffusion models for image and audio generation in PyTorch

[deep-learning](#) [pytorch](#)
[image-generation](#) [diffusion](#)
[score-based-generative-modeling](#)

📖 [Readme](#)
📄 [Apache-2.0 license](#)
★ 1.2k stars
👁 42 watching
🍴 61 forks

 **Jack Hessel** @jmhessel · Jun 11

"Oil painting of a group of confused people wondering what to do with the most complicated machine in the world" [#dalle2](#)



ALT

Outline

- History
- Method
 - In theory → in practice
 - “Diffusion as gradients”
- Controllable generation
- Examples: GLIDE, Dalle-2, Imagen

Diffusion probabilistic models
[Sohl-Dickstein et al, ICML 2015]

Deep Unsupervised Learning using Nonequilibrium Thermodynamics

Jascha Sohl-Dickstein
Stanford University
Eric A. Weiss
University of California, Berkeley
Niru Maheswaranathan
Stanford University
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Denoising diffusion probabilistic models (DDPM)
[Ho et al, Neurips 2020]

Denoising Diffusion Probabilistic Models

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Improvements & Applications, e.g.

Improved Denoising Diffusion Probabilistic Models

Alex Nichol^{*1} Prafulla Dhariwal^{*1}

ICML 2021

GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models

Alex Nichol^{*} Prafulla Dhariwal^{*} Aditya Ramesh^{*} Pranav Shyam Pamela Mishkin Bob McGrew
Ilya Sutskever Mark Chen

ICML 2022

A Connection Between Score Matching
and Denoising Autoencoders

Pascal Vincent
vincentp@iro.umontreal.ca
Dept. IRO, Université de Montréal,
CP 6128, Succ. Centre-Ville, Montréal (QC) H3C 3J7, Canada.

Denoising score matching
[Vincent, 2010]

Generative Modeling by Estimating Gradients of the Data Distribution

Yang Song
Stanford University
yangsong@cs.stanford.edu

Stefano Ermon
Stanford University
ermon@cs.stanford.edu

Noise-conditioned score networks
[Song & Ermon, Neurips 2019]

Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding

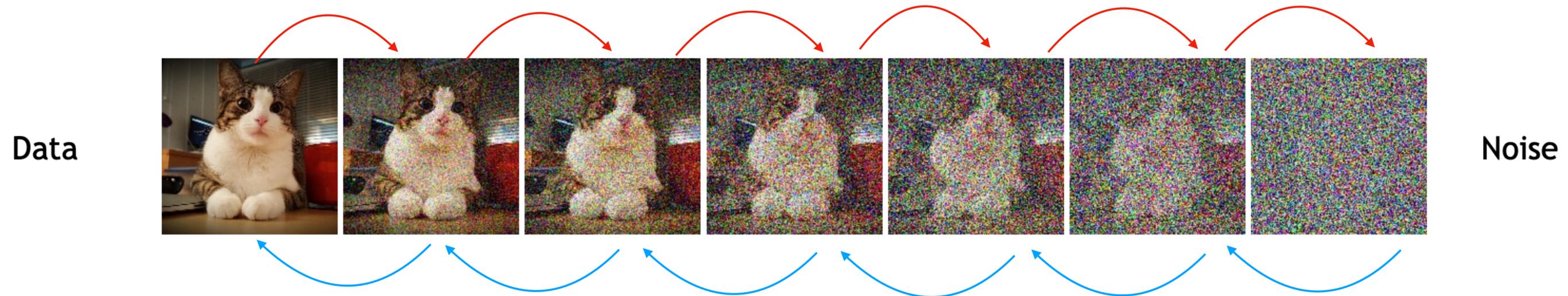
Chitwan Saharia*, William Chan*, Saurabh Saxena†, Lala Li‡, Jay Whang‡, Emily Denton, Seyed Kamyar Seyed Ghasemipour, Burcu Karagol Ayan, S. Sara Mahdavi, Rapha Gontijo Lopes, Tim Salimans, Jonathan Ho†, David J Fleet†, Mohammad Norouzi*
{sahariac,williamchan,mnorouzi}@google.com
{srbs,lala,jwhang,jonathanho,davidfleet}@google.com
Google Research, Brain Team
Toronto, Ontario, Canada

Arxiv May 2022

MANY more in [CVPR 2022 Tutorial]!!

Denoising diffusion models

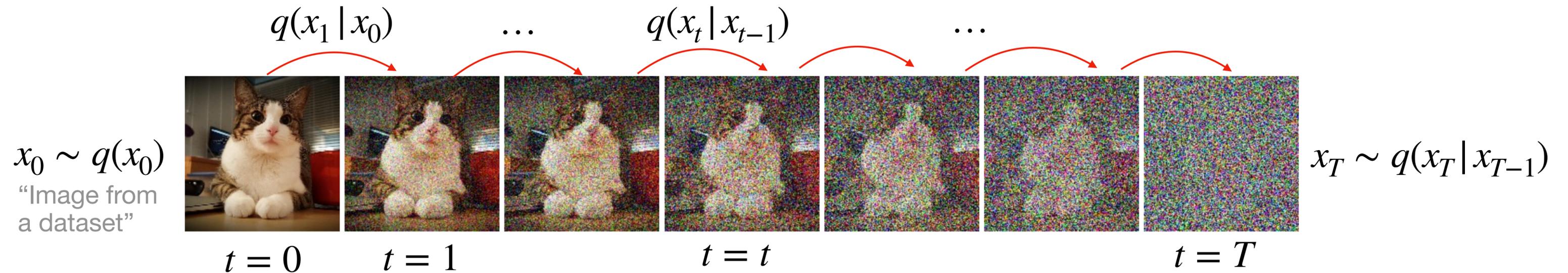
- Destroy structure in data by progressively adding noise (“**diffusion**”)



- Learn to reverse the diffusion process (“**denoising**”)
 - This gives us a model of the data & a way to generate
- *Intuition: modeling small changes is easier than directly modeling the data*

Denoising diffusion models

- **Forward diffusion process:** adds noise to data



- $q(x_t | x_{t-1}) = \mathcal{N}(x_t ; \text{mean}_t, \text{variance}_t)$

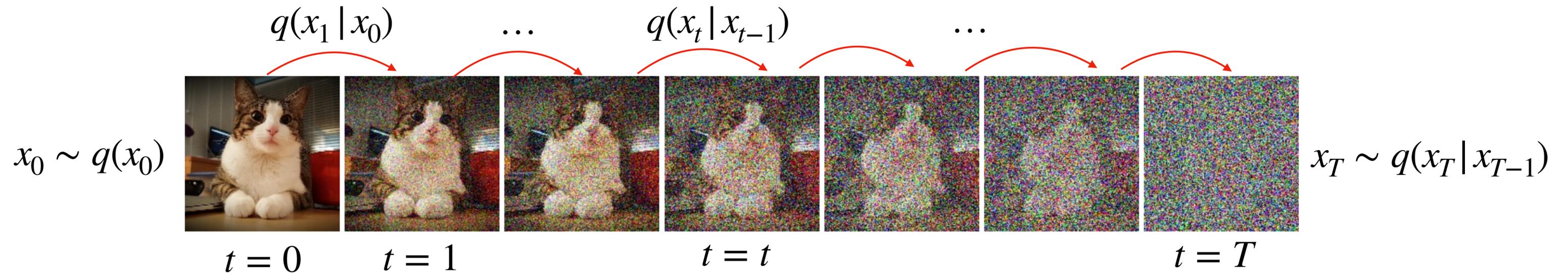
- $\text{mean}_t = \sqrt{(1 - \beta_t)} x_{t-1}$

- $\text{variance}_t = \beta_t I$

Forward process variances β_t , determined by a schedule β_1, \dots, β_T , e.g. linear from $\beta_1 = 10^{-4}$ to $\beta_T = 0.02$ in [Ho et al 2022].

Denoising diffusion models

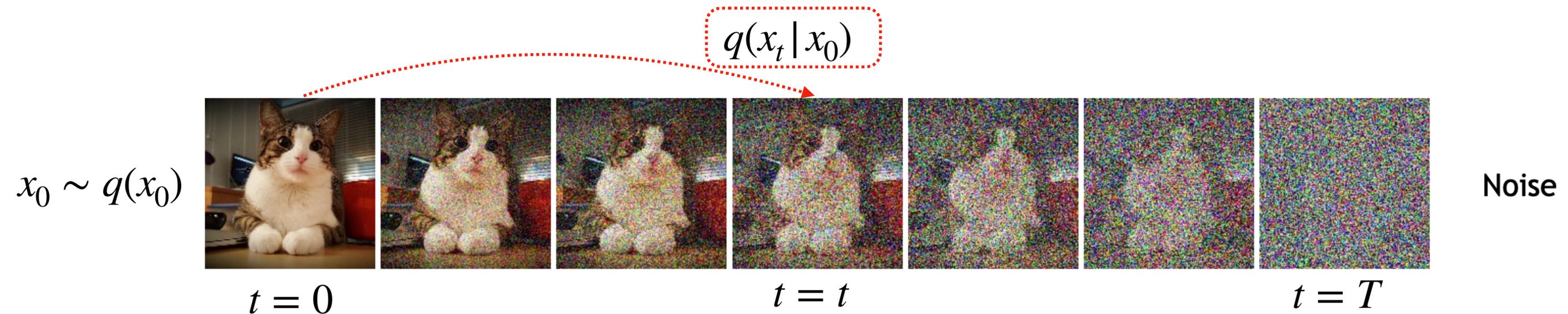
- **Forward diffusion process:** adds noise to data



- $$q(x_{0:T}) = q(x_0) \prod_{t=1}^T q(x_t|x_{t-1})$$

Denoising diffusion models

- **Forward diffusion process:** adds noise to data



- $q(x_t | x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t}x_0, \sqrt{(1 - \bar{\alpha}_t)}I)$

- $\bar{\alpha}_t = \prod_{t'=1}^t (1 - \beta_{t'})$

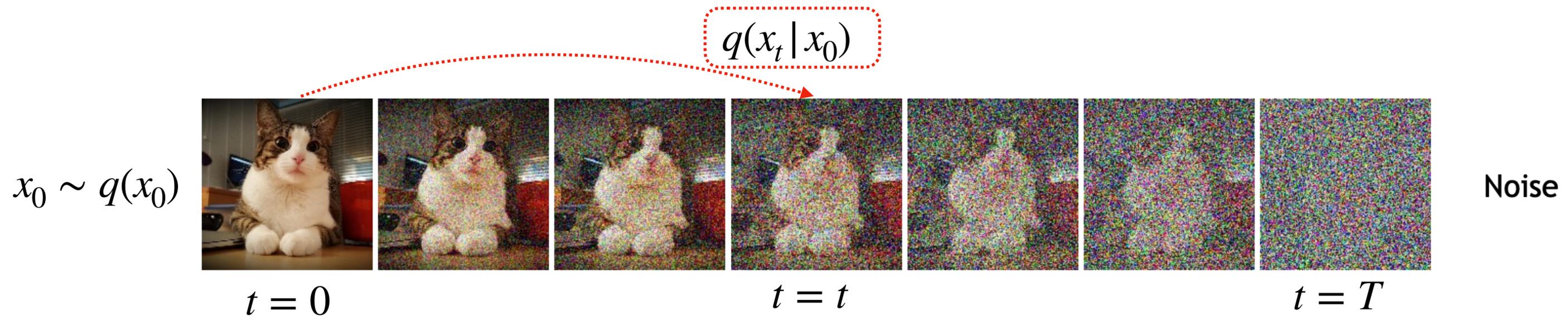
- This lets us sample x_t given x_0 and noise schedule:

$$x_t = \sqrt{\bar{\alpha}_t}x_0 + \sqrt{(1 - \bar{\alpha}_t)}\epsilon,$$

where $\epsilon \sim \mathcal{N}(0, I)$. “the re-parameterization trick”

Denoising diffusion models

- **Forward diffusion process:** adds noise to data



- $q(x_t | x_0) = \mathcal{N}(x_t ; \sqrt{\bar{\alpha}_t}x_0, \sqrt{(1 - \bar{\alpha}_t)}I)$

- Noise schedule (choice of β_t , which determines $\bar{\alpha}_t$) designed so that:

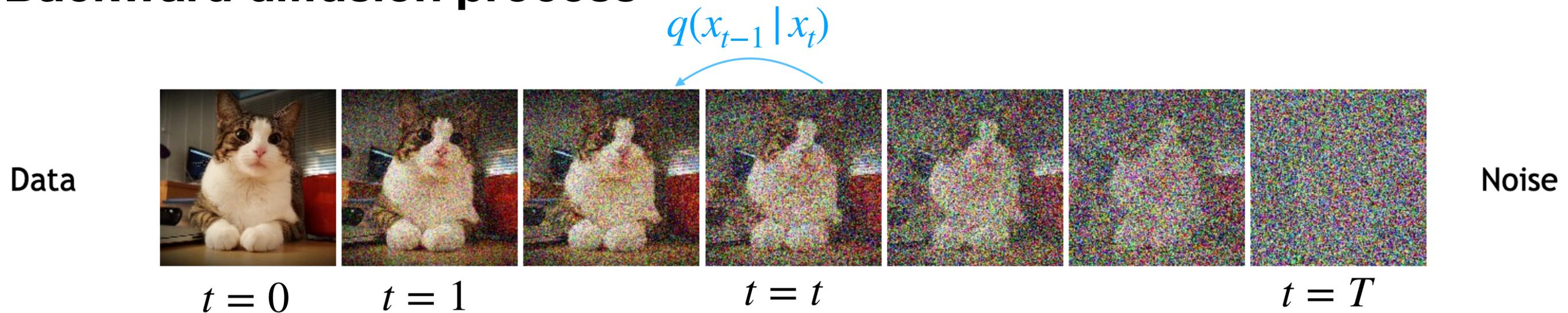
- $\sqrt{\bar{\alpha}_t}$ decreases towards zero

Example: linear from $\beta_1 = 10^{-4}$ to $\beta_T = 0.02$ in [Ho et al 2022].

- Final step is standard Gaussian noise, $q(x_T | x_0) \approx \mathcal{N}(x_T; 0, I)$

Denoising diffusion models

- **Backward diffusion process**

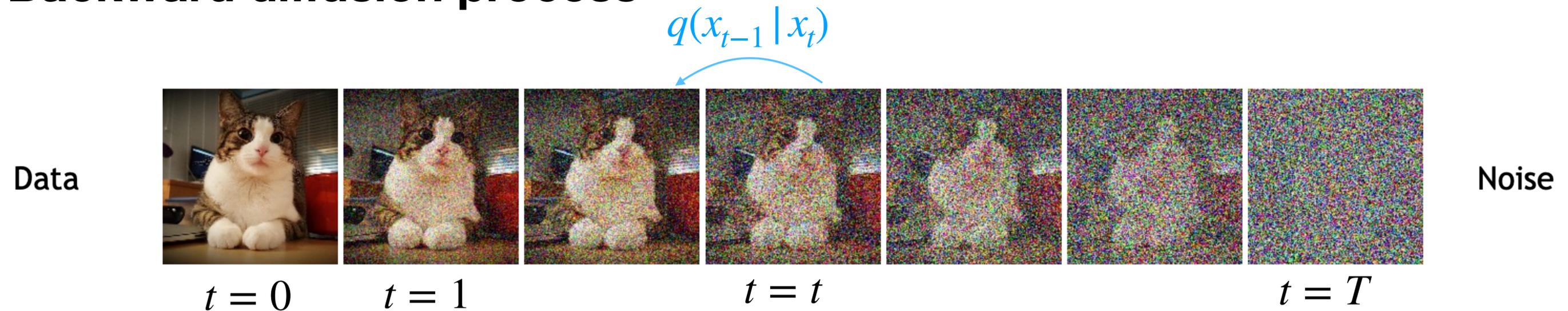


- If we knew how to “reverse time”, we could generate data:

- $x_T \sim N(0, I)$
- Iteratively sample $x_{t-1} \sim q(x_{t-1} | x_t)$

Denoising diffusion models

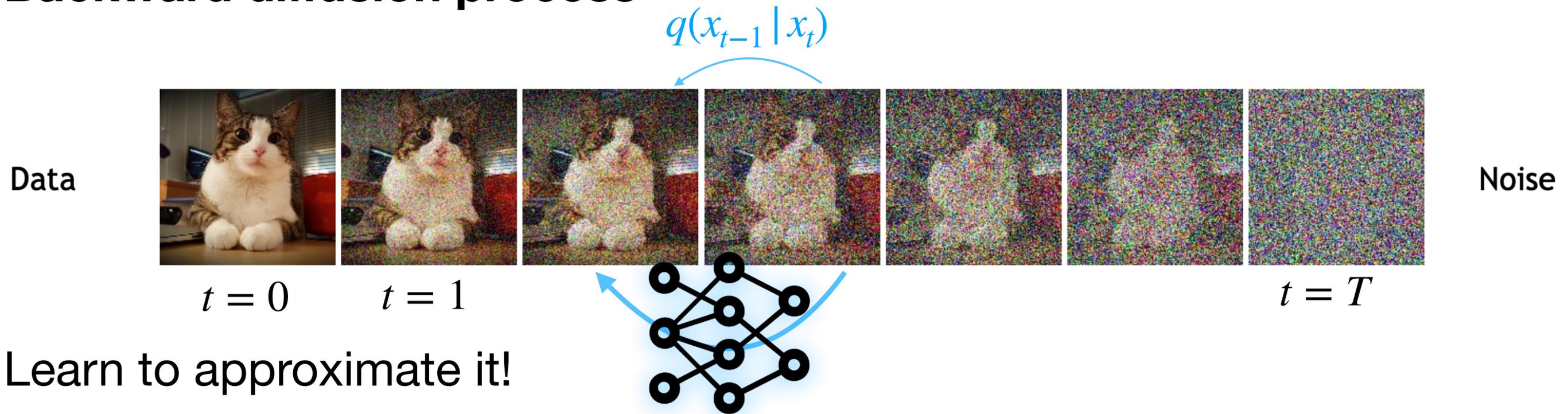
- **Backward diffusion process**



- Adding noise is easy, but we don't know how to “reverse time”
 - $q(x_{t-1} | x_t) \propto q(x_{t-1})q(x_t | x_{t-1})$

Denoising diffusion models

- **Backward diffusion process**

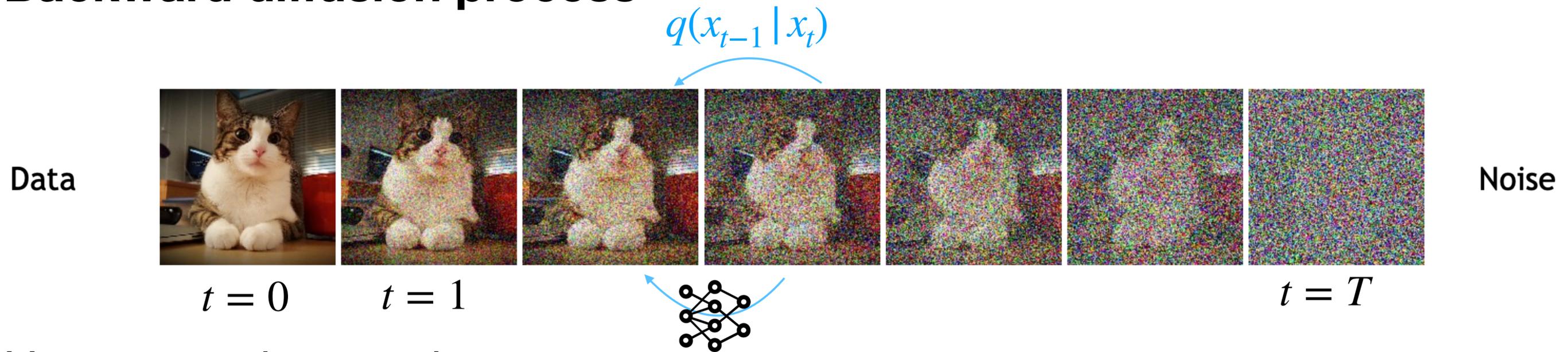


- Learn to approximate it!

- $q(x_{t-1} | x_t) \approx p_{\theta}(x_{t-1} | x_t)$

Denoising diffusion models

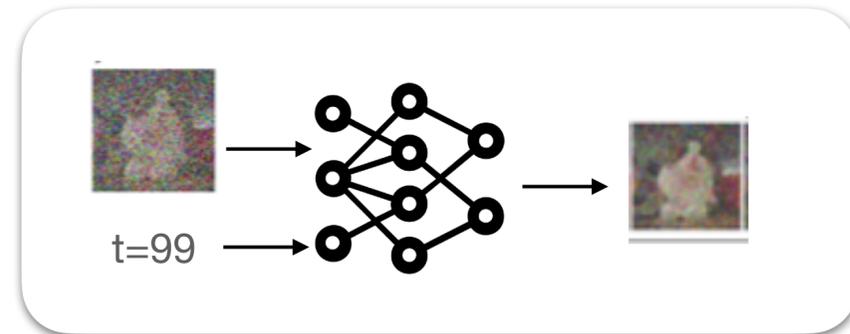
- **Backward diffusion process**



- Use a neural network:

- $p_{\theta}(x_{t-1} | x_t) = \mathcal{N}(x_{t-1} ; \mu_{\theta}(x_t, t), \sigma_t^2 I)$

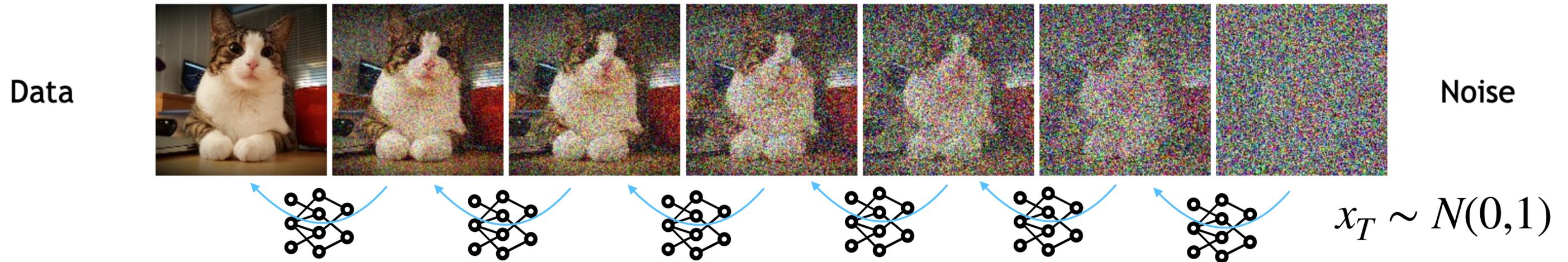
Reverse process variance (“reverse noise schedule”)
E.g set to β_t [Ho et al 2020], learned [Nichol & Dhariwal 2021]



often a U-Net architecture

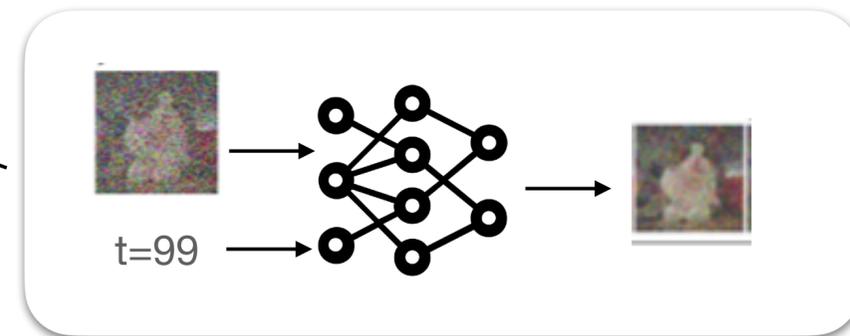
Denoising diffusion models

- **Backward diffusion process**



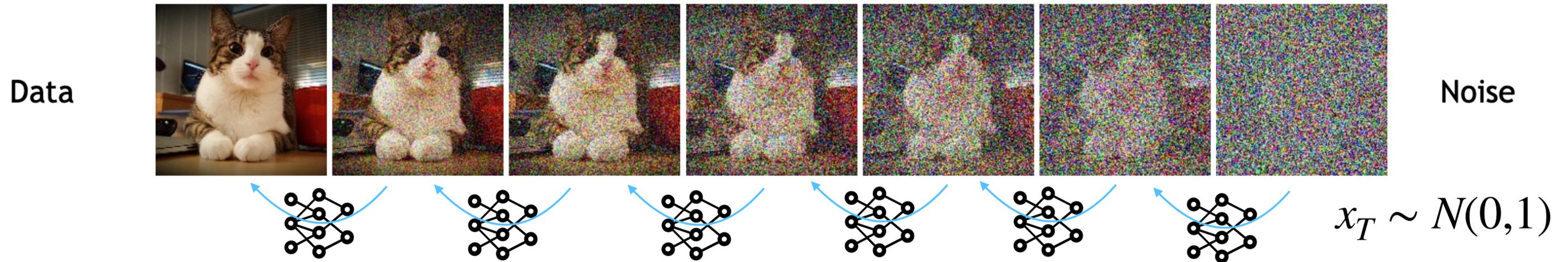
- Iteratively sample $x_{t-1} \sim p_{\theta}(x_{t-1} | x_t)$

- $\rightarrow x_0$ is a cat image



Denoising diffusion models

- **Backward diffusion process**



- Gives us a model of the process:

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

How do we learn such a network?

- Maximize marginal log-likelihood:

$$\bullet \mathbb{E}_{x_0 \sim q(x_0)} -\log p_\theta(x_0) \leq \mathbb{E}_{q(x_0)q(x_{1:T}|x_0)} \left[-\log \frac{p_\theta(x_{0:T})}{q(x_{1:T}|x_0)} \right]$$

Variational bound
(similar to VAEs)

- ... derivation ...

See Appendix A of [Ho et al 2020]

$$\bullet \implies L = \mathbb{E} \left[\text{KL}(q(x_{t-1} | x_t, x_0) || p_\theta(x_{t-1} | x_t)) \right]$$

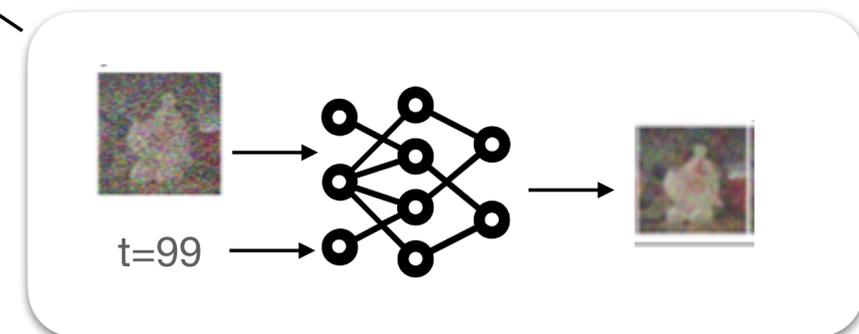
$$\bullet \propto \mathbb{E}_t \left[\|\mu_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2 \right]$$

Gaussian \rightarrow MSE Loss!!

The “target” mean can be computed given x_0, x_t and noise schedule:

$$q(x_{t-1} | x_t, x_0) = \mathcal{N}(\mu_t(x_t, x_0), \tilde{\beta}_t I), \text{ where}$$

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



How do we learn such a network?

In practice

- $L = \mathbb{E} \left[\|\mu_t(x_t, x_0) - \mu_\theta(x_t, t)\|^2 \right]$. First, [Ho et al 2020] observe that μ_t can be rewritten as:

See eqn. (10) in [Ho et al 2020]

$$\mu_t(x_t, x_0) = \underbrace{\frac{1}{\sqrt{\alpha_t}}}_{a_t} \left(x_t - \underbrace{\frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t}}}_{b_t} \epsilon \right).$$

- Since x_t, a_t, b_t are given, [Ho et al 2020] predict noise $\epsilon \approx e_\theta(x_t, t)$:

- $\mu_\theta(x_t, t) = a_t(x_t - b_t e_\theta(x_t, t))$

- The objective simplifies to:

- $\tilde{L} = \mathbb{E} \left[\lambda_t \|\epsilon - e_\theta(x_t, t)\|^2 \right]$, where $\lambda_t = \frac{\beta_t^2}{2\sigma_t^2 \alpha_t (1 - \bar{\alpha}_t)}$

eqn. (12) in [Ho et al 2020]

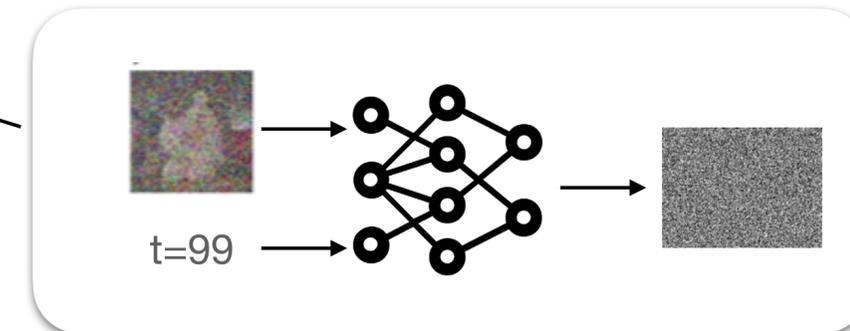
- Finally, [Ho et al 2020] drop the weighting term λ_t :

- $\mathcal{L}_{\text{simple}} = \mathbb{E}_{t, x_0, \epsilon} \left[\|\epsilon - e_\theta(x_t, t)\|^2 \right]$

eqn. (14) in [Ho et al 2020]

Recall that $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon$,

Intuitively, the network only predicts the “unknown” part



We will see later that there is a connection between predicting the noise and predicting a gradient

Algorithm summary

Training

Algorithm 1 Training

1: **repeat**

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

3: $t \sim \text{Uniform}(\{1, \dots, T\})$

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

5: Take gradient descent step on

$\nabla_{\theta} \left\| \epsilon - \epsilon_{\theta} \left(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t \right) \right\|^2$ MSE loss on
(actual noise, predicted noise)

6: **until** converged

$x_t \sim q(x_t | x_0)$

Recall that:

$$q(x_t | x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}_t} x_0, \sqrt{(1 - \bar{\alpha}_t)} I)$$

This lets us sample x_t using the re-parameterization trick:

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{(1 - \bar{\alpha}_t)} \epsilon, \text{ where } \epsilon \sim \mathcal{N}(0, I)$$

Algorithm summary

Show me the code!

 [huggingface / diffusers](#) Public

Algorithm 1 Training

- 1: **repeat**
 - 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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 - 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
 - 5: Take gradient descent step on
$$\nabla_{\theta} \|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2$$
 - 6: **until** converged
-

```
# Sample noise that we'll add to the images
noise = torch.randn(clean_images.shape).to(clean_images.device)
bsz = clean_images.shape[0]
```

Algorithm summary

Show me the code!

Algorithm 1 Training

- 1: **repeat**
 - 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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bsz = clean_images.shape[0]
# Sample a random timestep for each image
timesteps = torch.randint(
    0, noise_scheduler.num_train_timesteps, (bsz,), device=clean_images.device
).long()
```

Algorithm summary

Show me the code!

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 - 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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 $\nabla_{\theta} \|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon; t)\|^2$
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$$x_t \sim q(x_t | x_0)$$

```
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bsz = clean_images.shape[0]
# Sample a random timestep for each image
timesteps = torch.randint(
    0, noise_scheduler.num_train_timesteps, (bsz,), device=clean_images.device
).long()

# Add noise to the clean images according to the noise magnitude at each timestep
# (this is the forward diffusion process)
noisy_images = noise_scheduler.add_noise(clean_images, noise, timesteps)
```

Algorithm summary

Show me the code!

Algorithm 1 Training

- 1: **repeat**
 - 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
 - 3: $t \sim \text{Uniform}(\{1, \dots, T\})$
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noisy_images = noise_scheduler.add_noise(clean_images, noise, timesteps)
```

```
# Predict the noise residual
noise_pred = model(noisy_images, timesteps)["sample"]
loss = F.mse_loss(noise_pred, noise)
accelerator.backward(loss)
```

Algorithm summary

Show me the code!

Algorithm 1 Training

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 - 2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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 - 4: $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
 - 5: Take gradient descent step on
 $\nabla_{\theta} \|\epsilon - \epsilon_{\theta}(\sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon, t)\|^2$
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-

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Algorithm summary

Sampling

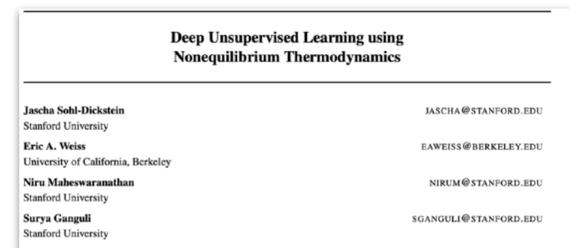
Algorithm 2 Sampling

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

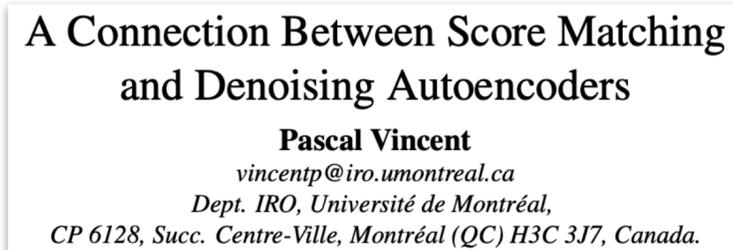
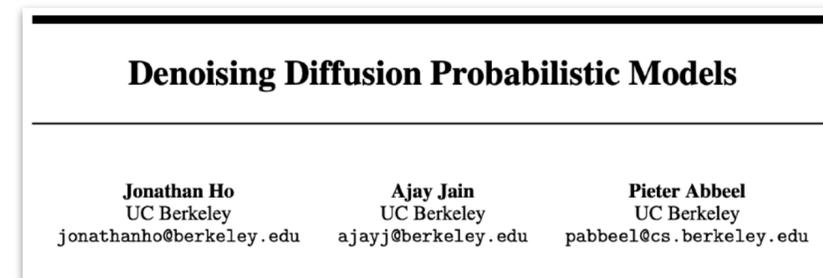
$$\mu_{\theta}(x_t, x_0) = a_t(x_t - b_t \epsilon_{\theta}(x_t, x_0))$$

Diffusion \approx gradients

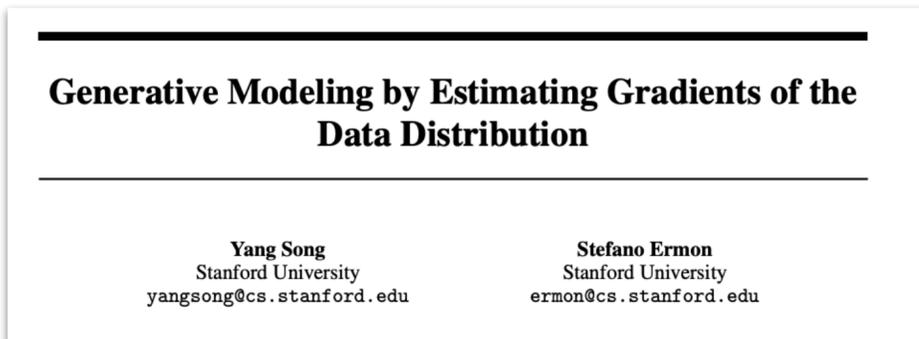
Diffusion probabilistic models
[Sohl-Dickstein et al, ICML 2015]



Denoising diffusion probabilistic models (DDPM)
[Ho et al, Neurips 2020]



Denoising score matching
[Vincent, 2010]



Noise-conditioned score networks
[Song & Ermon, Neurips 2019]

Diffusion \approx gradients

$$\mathcal{L}_{\text{simple}} = \mathbb{E}_{t, x_0, \epsilon} [\|\epsilon - \epsilon_{\theta}(x_t, t)\|^2]$$

Denoising Diffusion Probabilistic Model

$$\mathcal{L}_{\text{score}} = \mathbb{E}_{t, x} [\|\nabla_x \log p_t(x) - s_{\theta}(x, t)\|^2]$$

Noise-Conditional Score-networks

[Ho et al 2020] show:

$$\nabla_{x_t} \log p_t(x_t) \propto \epsilon_{\theta}(x_t, t)$$

(also see 2.2 of [Song et al 2021])

- Noise \approx gradient of log-prob (“score”)
- Noise predictor \approx score predictor
- Intuition: both things learn to predict small changes to noisy data

Diffusion sampling \approx Langevin dynamics

$$x_t = x_{t-1} - \frac{\lambda}{2} \nabla_x E_\theta(x_{t-1}) + \sigma z$$

Langevin Dynamics [Welling & Teh 2011]

Denoising Diffusion Probabilistic Model

$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \epsilon_\theta(x_t, t) \right) + \sigma_t z$$

NCSN Annealed Langevin Dynamics

$$\tilde{x}_t \leftarrow \tilde{x}_{t-1} + \frac{\alpha_i}{2} s_\theta(\tilde{x}_{t-1}, \sigma_i) + \sqrt{\alpha_i} z_t$$

- Diffusion sampling \approx annealed Langevin dynamics with learned gradient

Method Recap

- Diffusion models: learn to iteratively denoise data, $p_{\theta}(x_{t-1} | x_t)$
 - Original formulation: variational inference
 - Practical formulation: similar to denoising score matching
- Intuitively, both learn small changes to noisy data at various noise scales

Guided generation

- Goal: conditional generation

e.g. $p(x | y)$ where y is a class label (e.g. cat) or a text prompt

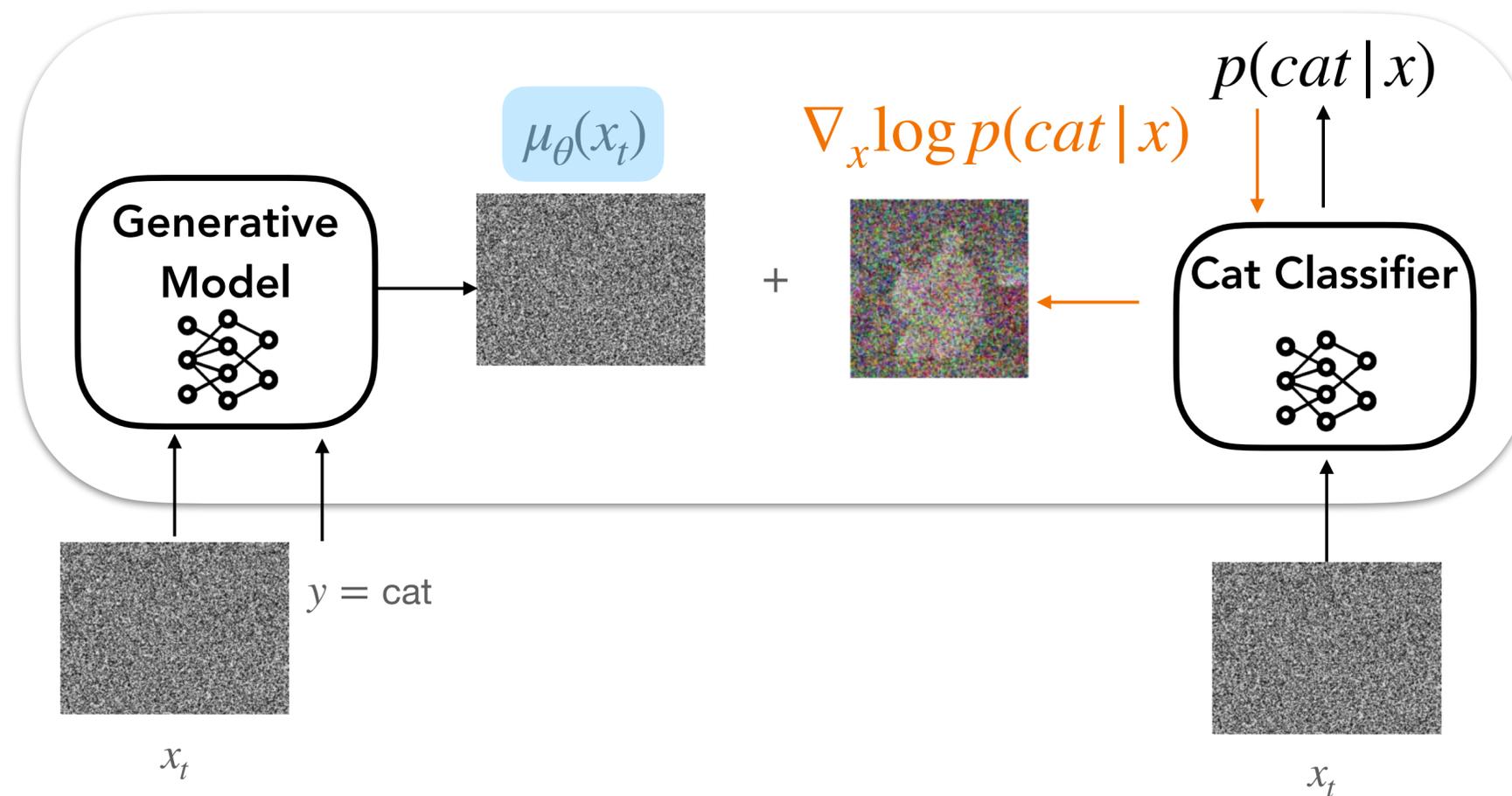
Classifier guidance

At each step of sampling:

$$x_{t-1} \leftarrow \text{sample from } \mathcal{N}(\mu_{\theta}(x_t) + s \cdot \nabla_{x_t} \log p_{\phi}(y | x_t), \sigma_t^2)$$

Classifier is trained on noisy images x_t

Approximates $\propto p(x_t | y)p(y | x_t)^s$



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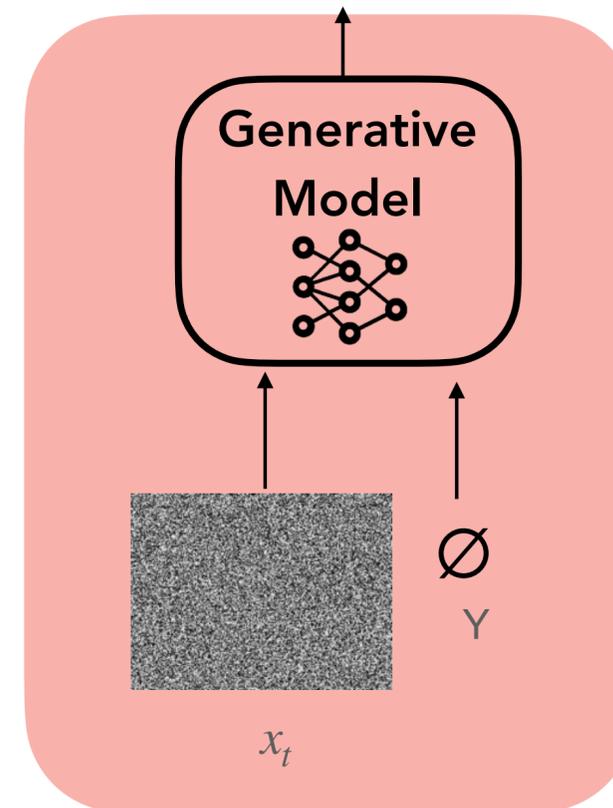
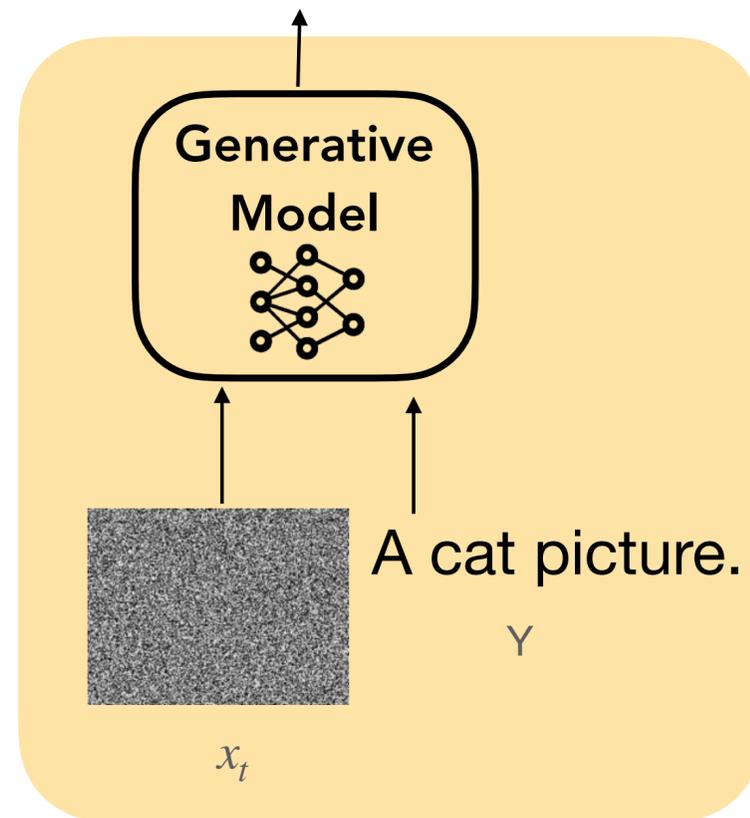


Classifier-free guidance

At each step of sampling use:

$$\epsilon_{\theta}(x_t) + s \cdot \underbrace{(\epsilon_{\theta}(x_t | y) - \epsilon_{\theta}(x_t))}_{\text{'class relevant direction'}}$$

Generative model trained with & without conditioning info



Classifier-free guidance



Figure 1: Unconditional guidance on the malamute class for a 64x64 ImageNet diffusion model. Left to right: increasing amounts of unconditional guidance, starting from non-guided samples on the left.

Case study: GLIDE

- 3.5B text-conditional diffusion model
- Trained on DALL-E dataset

Guidance	Photorealism	Caption
Unguided	-88.6	-106.2
CLIP guidance	-73.2	29.3
Classifier-free guidance	82.7	110.9

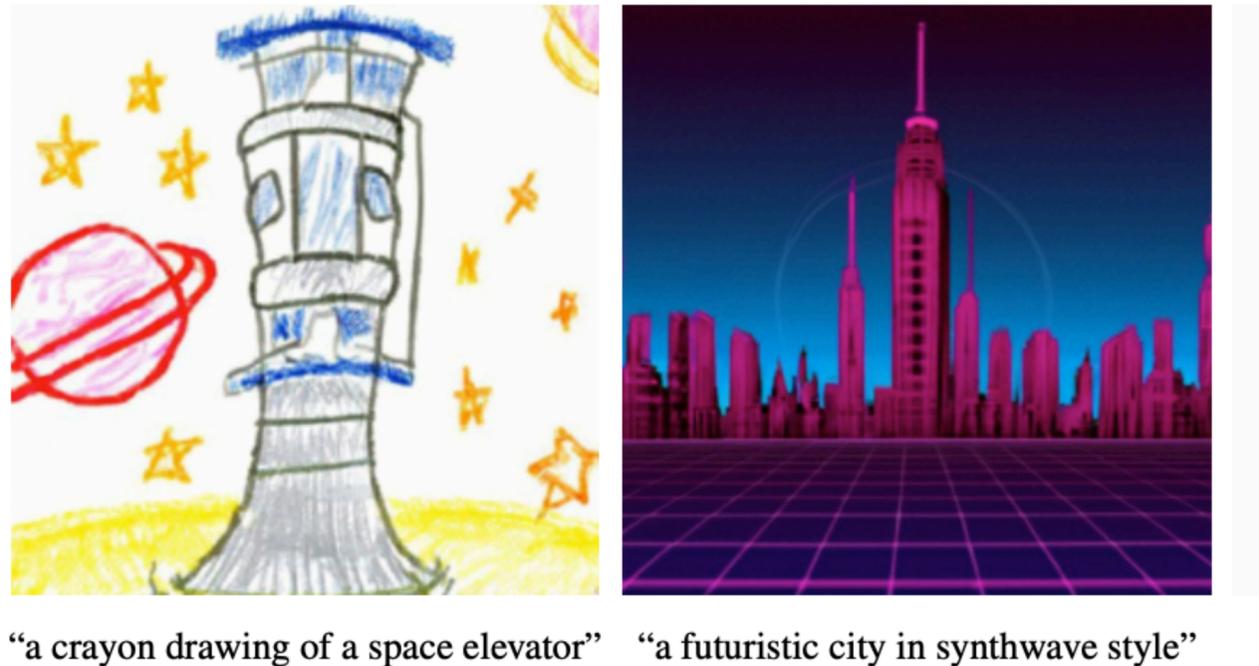


Figure 3. Iteratively creating a complex scene using GLIDE. First, we generate an image for the prompt “a cozy living room”, then use the shown inpainting masks and follow-up text prompts to add a painting to the wall, a coffee table, and a vase of flowers on the coffee table, and finally to move the wall up to the couch.

Figure 1. Selected samples from GLIDE using classifier-free guidance.

Case study: Dall-e 2

- Classifier-free guidance
- Prior: diffusion
- Decoder: diffusion
 - + 2 diffusion upsamplers

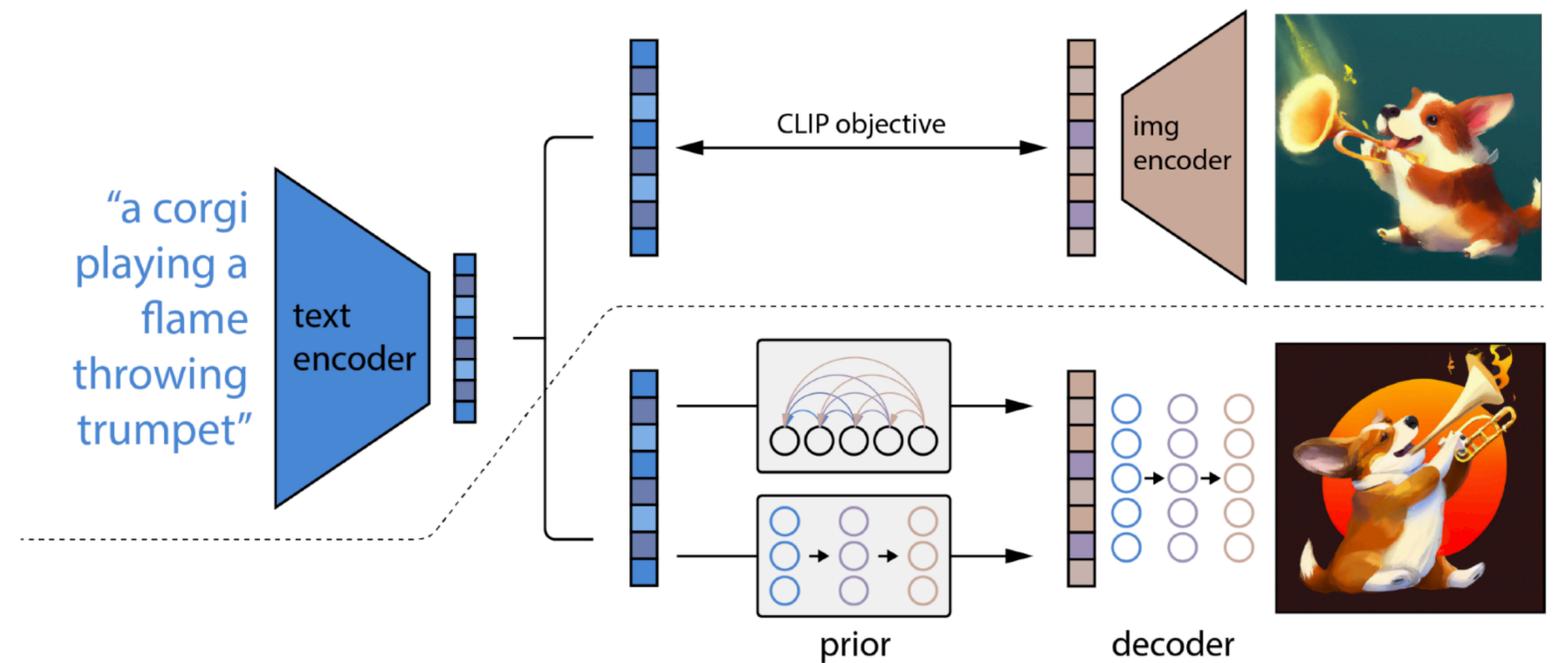


Figure 2: A high-level overview of unCLIP. Above the dotted line, we depict the CLIP training process, through which we learn a joint representation space for text and images. Below the dotted line, we depict our text-to-image generation process: a CLIP text embedding is first fed to an autoregressive or diffusion prior to produce an image embedding, and then this embedding is used to condition a diffusion decoder which produces a final image. Note that the CLIP model is frozen during training of the prior and decoder.

Case study: Dall-e 2



an espresso machine that makes coffee from human souls, artstation



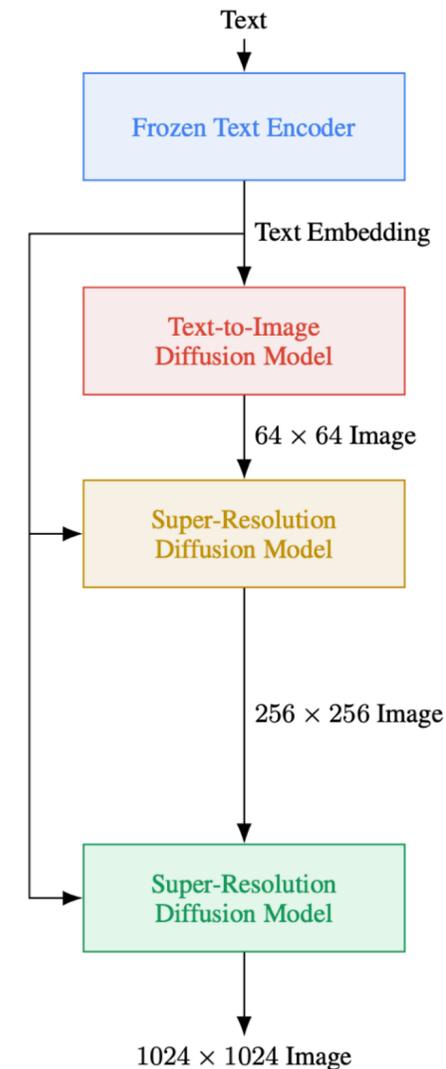
panda mad scientist mixing sparkling chemicals, artstation



a corgi's head depicted as an explosion of a nebula

Case study: Imagen

- Classifier-free guidance
- Frozen T5-XXL text encoder
- Cascaded diffusion
- 2B model
- ~460M internal image-text pairs
- ~400M public image-text pairs



“A Golden Retriever dog wearing a blue checkered beret and red dotted turtleneck.”

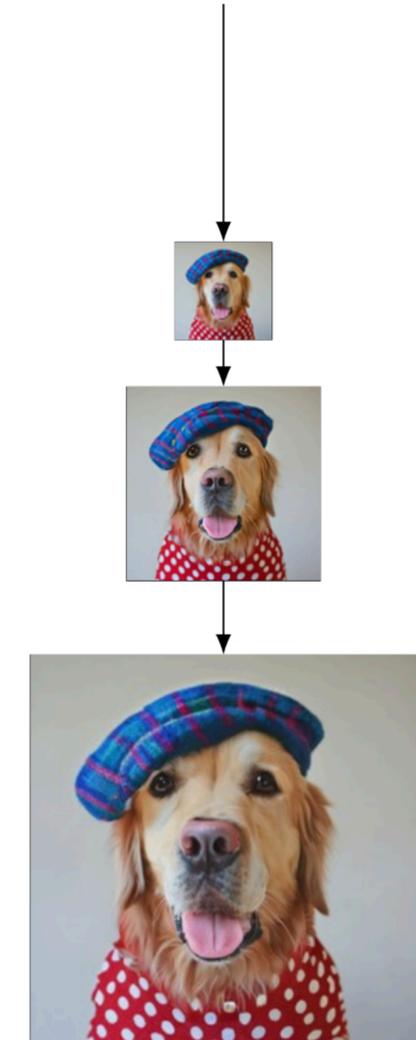


Figure A.4: Visualization of Imagen. Imagen uses a frozen text encoder to encode the input text into text embeddings. A conditional diffusion model maps the text embedding into a 64×64 image. Imagen further utilizes text-conditional super-resolution diffusion models to upsample the image, first $64 \times 64 \rightarrow 256 \times 256$, and then $256 \times 256 \rightarrow 1024 \times 1024$.

Case study: Imagen



A wall in a royal castle. There are two paintings on the wall. The one on the left a detailed oil painting of the royal raccoon king. The one on the right a detailed oil painting of the royal raccoon queen.



A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk.



A chrome-plated duck with a golden beak arguing with an angry turtle in a forest.

Case study: Imagen

Model	COCO FID ↓
Trained on COCO	
AttnGAN (Xu et al., 2017)	35.49
DM-GAN (Zhu et al., 2019)	32.64
DF-GAN (Tao et al., 2020)	21.42
DM-GAN + CL (Ye et al., 2021)	20.79
XMC-GAN (Zhang et al., 2021)	9.33
LAFITE (Zhou et al., 2021)	8.12
Make-A-Scene (Gafni et al., 2022)	7.55
Not trained on COCO	
DALL-E (Ramesh et al., 2021)	17.89
GLIDE (Nichol et al., 2021)	12.24
DALL-E 2 (Ramesh et al., 2022)	10.39
Imagen (Our Work)	7.27

Imagen attains a new state-of-the-art COCO FID.

The end