BOSTON UNIVERSITY

Diffusion Models

DL4DS – Spring 2025

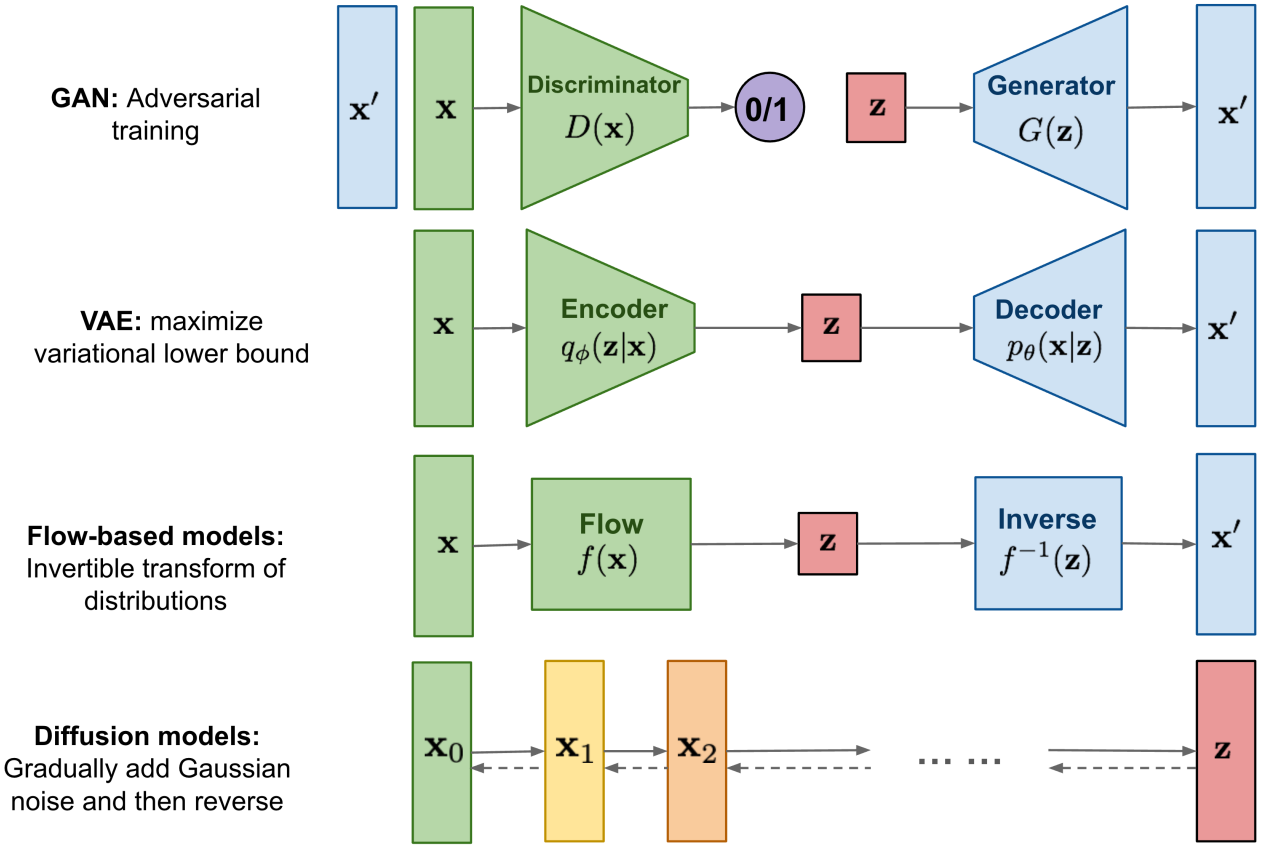
Based on Rocca, 2022, "Understanding Diffusion Probabilistic Models (DPMs)", Towards Data Science and other references…

DS542 Gardos
Prince, *Understanding Deep Learning*,
Other Content Cited

Outline

- Contextualizing Diffusion Models
- Theory behind diffusion models
- Architectures and Training
- Applications

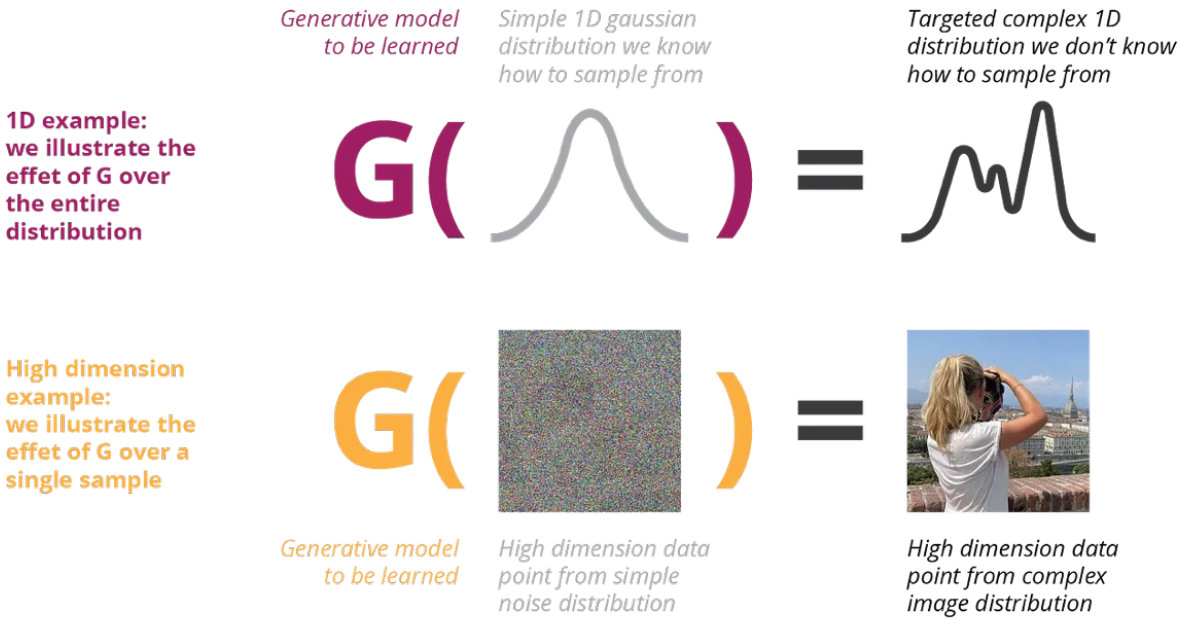
Different Generative Models



L. Weng, "What are Diffusion Models?", blog post, 2021

Given a probability distribution only described by some available samples, how can one generate a new sample?

Introduction



Generative models aims at learning a function that takes data from a simple distribution and transform it into data from a complex distribution.

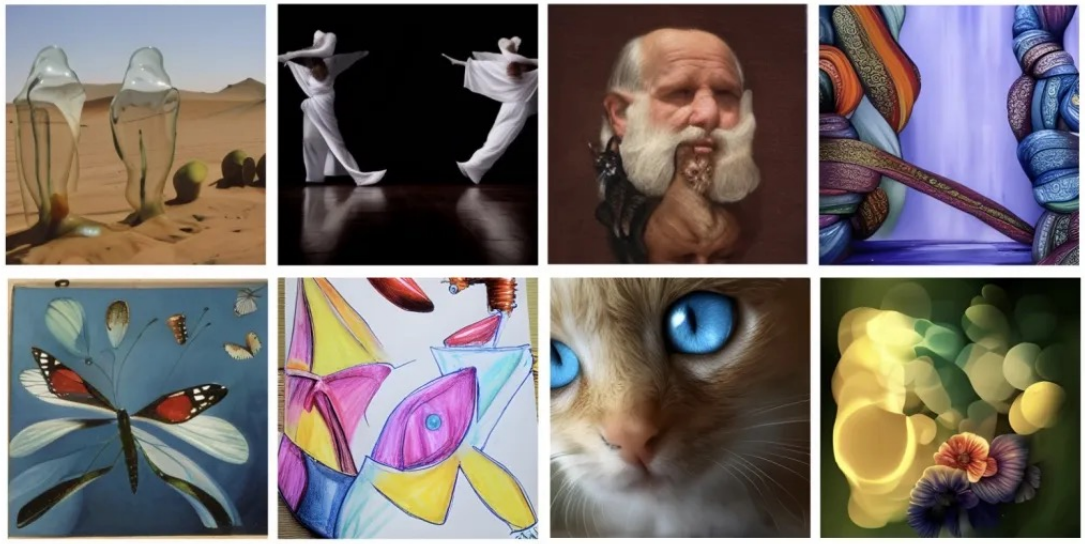
Retrospective

- 2013: Kingma and Welling introduce Variational AutoEncoder.
- 2014: Goodfellow et al introduced Generative Adversarial Networks (GANs).
- 2015: Sohl-Dickstein “Deep Unsupervised Learning using Nonequilibrium Thermodynamics”
- 2020 (DDPM): J. Ho, A. Jain, and P. Abbeel, “Denoising Diffusion Probabilistic Models”
- 2022 (DDIM): J. Song, C. Meng, and S. Ermon, “Denoising Diffusion Implicit Models” – more efficient
- 2022 (Stable Diffusion): R. Rombach, A. Blattmann, D. Lorenz, P. Esser, and B. Ommer, “High-Resolution Image Synthesis with Latent Diffusion Models”
- 2023 (Diffusion Transformer): W. Peebles and S. Xie, “Scalable Diffusion Models with Transformers”

UDL Chapter 18 – Diffusion Models

- 18.2 Encoder (forward process)
  - Defines the noise diffusion process
- 18.3 Decoder model (reverse process)
  - Derives the denoising steps based on neural networks
- 18.4 Training
  - Derives a lower bound (ELBO) on the loss function
  - Initial diffusion loss function
- 18.5 Reparameterization of loss function
  - Shown to work better empirically
- 18.6 Implementaiton
  - Training and sampling algorithms

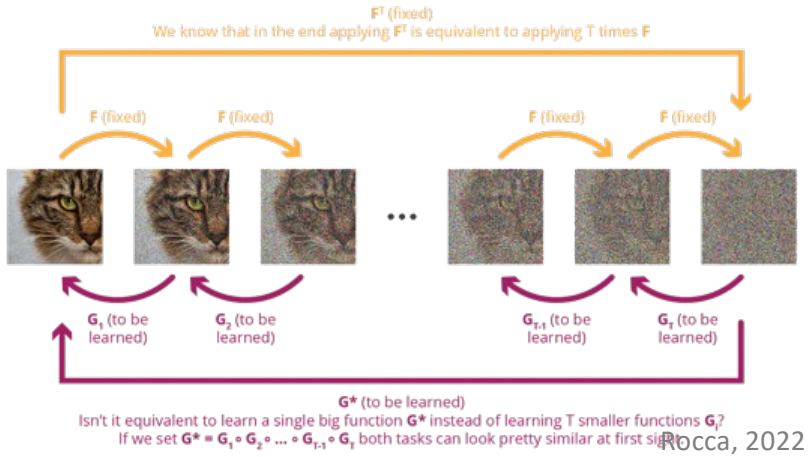
Examples



Examples above have been generated by Meta Make-A-Scene model, that generates images from both a text prompt and a basic sketch for greater level of creative control.

Basic idea of Diffusion Probabilistic Models

- learn the *reverse process* of
- a well defined *stochastic forward process* that progressively destroys information, taking data from our complex target distribution and bringing them to a simple gaussian distribution.
- *reverse process* is then expected to take the path in the opposite direction, taking gaussian noise as an input and generating data from the distribution of interest.



Outline

First:

- Stochastic Process
- Diffusion Process

Then intuition behind DPMs

Then some math basis

Then how trained in practice

Stochastic Process

Stochastic Processes

- Discrete: $X_n, \quad \forall\, n \in \mathbb{N}$
- Continuous: $X_t, \quad \forall t \geq 0$

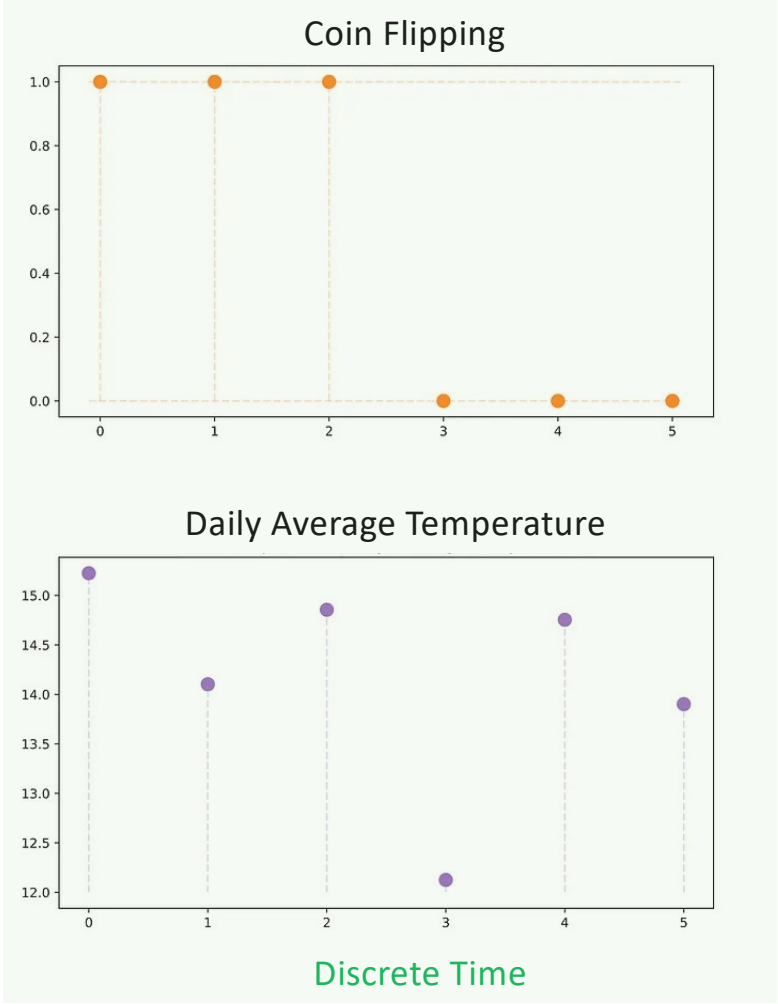
Realization of a random variable → sample

Realization of a stochastic process → sample path or trajectory

Different types of stochastic processes

Discrete Value

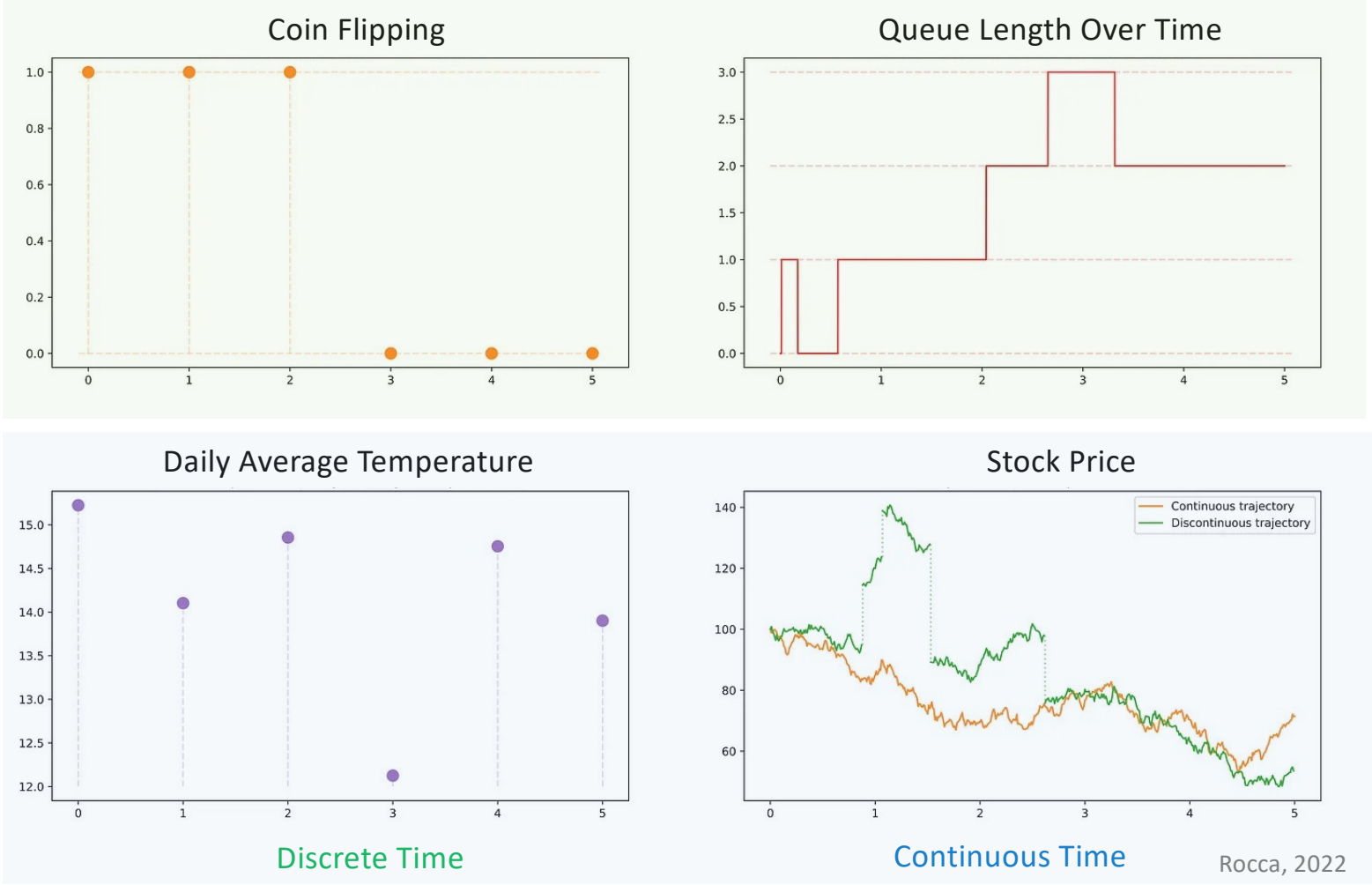
Continuous Value



Different types of stochastic processes

Discrete Value

Continuous Value



Markov Process

A *Markov process* is a *stochastic process* with no memory of past.

Future behavior depends on (at most) the present, or

Present depends on (at most) the previous sample.

$$P\left(X_{t_n}\middle|X_{t_{n-1}},\dots,X_{t_0}\right)=P\left(X_{t_n}\middle|X_{t_{n-1}}\right)\quad\forall t_0<t_1<\ \dots<t_{n-1}<t_n$$

Btw, i.i.d. coin flips are trivially Markov – next coin toss not dependent on current outcome.

Which of these are Markov Processes?

Diffusion Process

Any *diffusion process* can be described by a *stochastic differential equation* (SDE)

$$dX_t = a(X_t, t)dt + \sigma(X_t, t)dW_t$$

This means that an infinitesimal change in the value of the random variable, X, is equal to a times an infinitesimal change in time plus σ times an infinitesimal change in a Weiner process at that time.

Diffusion Process

Any *diffusion process* can be described by a *stochastic differential equation* (SDE)

$$dX_t = a(X_t, t)dt + \sigma(X_t, t)dW_t$$

where:

- $a(\cdot)$ is called the drift coefficient
- $\sigma(\cdot)$ is called the diffusion coefficient
- W is the Wiener process

Both a and σ are a function of the value and time

Diffusion Process

Any *diffusion process* can be described by a *stochastic differential equation* (SDE)

$$\underbrace{dX_t = a(X_t, t)dt}_{\text{Simple differential equation}} + \underbrace{\sigma(X_t, t)dW_t}_{\text{Stochastic part}}$$

where:

- $a(\cdot)$ is called the drift coefficient
- $\sigma(\cdot)$ is called the diffusion coefficient
- W is the Wiener process

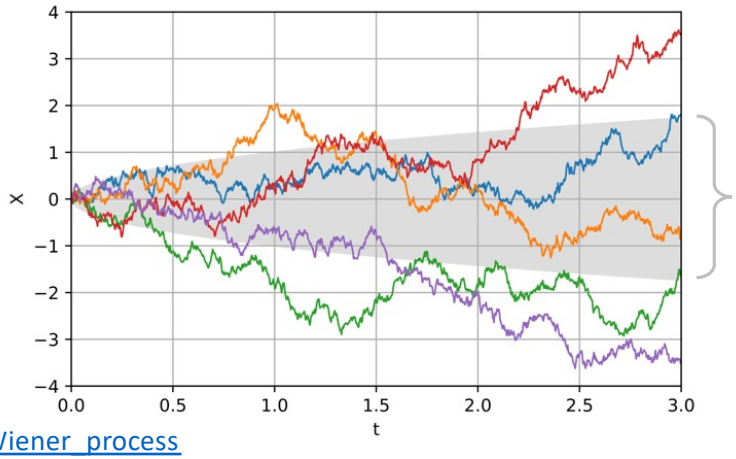
Wiener Process (Brownian Motion)

Continuous time stochastic process

The Wiener process W_t is characterised by the following properties:[2]

1. $W_0 = 0$ almost surely
2. W has independent increments: for every $t > 0$, the future increments $W_{t+u} - W_t$, $u \geq 0$, are independent of the past values W_s, $s < t$.
3. W has Gaussian increments: $W_{t+u} - W_t$ is normally distributed with mean 0 and variance u, $W_{t+u} - W_t \sim \mathcal{N}(0, u)$.
4. W has almost surely continuous paths: W_t is almost surely continuous in t.

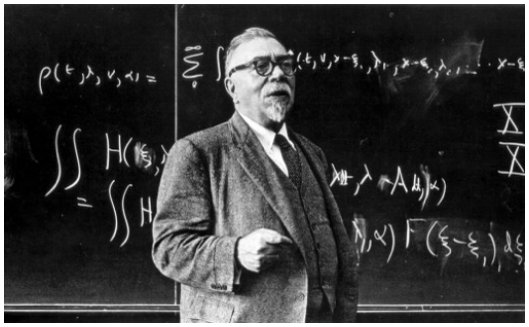
Five sampled processes



Expected standard deviation

https://en.wikipedia.org/wiki/Wiener_process

Norbert Weiner



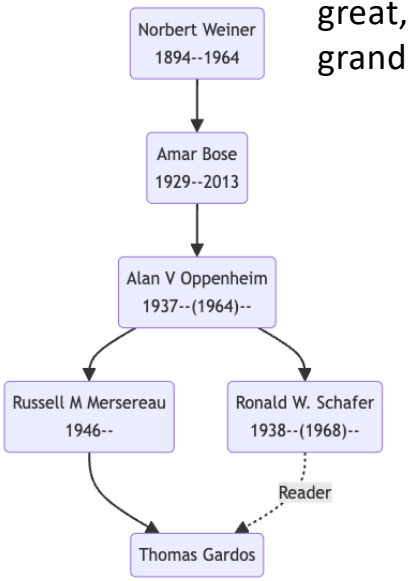
Norbert Wiener (November 26, 1894 – March 18, 1964) was an American computer scientist, mathematician and philosopher. He became a professor of mathematics at the Massachusetts Institute of Technology (MIT).

A child prodigy, Wiener later became *an early researcher in stochastic and mathematical noise processes*, contributing work relevant to electronic engineering, electronic communication, and control systems.

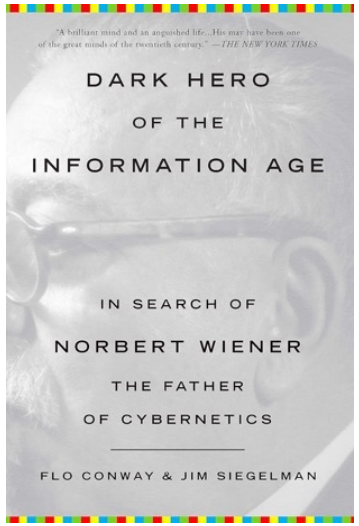
Wiener is considered the originator of cybernetics, the science of communication as it relates to living things and machines.

Heavily influenced John von Neumann, Claude Shannon, etc…

Wrote "The Machine Age" in 1949 anticipating robots, etc.



great, great
grand advisor ☺



https://en.wikipedia.org/wiki/Norbert_Wiener
https://www.nytimes.com/2013/05/21/science/mit-scholars-1949-essay-on-machine-age-is-found.html

Discretizing

So

$$dW_t \approx W_{t+dt} - W_t \sim \mathcal{N}(0, dt)$$

Property of Weiner Process: The std is equal to the time step.

Discretizing the SDE

$$X_{t+dt} - X_t \approx a(X_t, t)dt + \sigma(X_t, t)U \quad \text{where} \quad U \sim \mathcal{N}(0, dt)$$

Which can also be rewritten

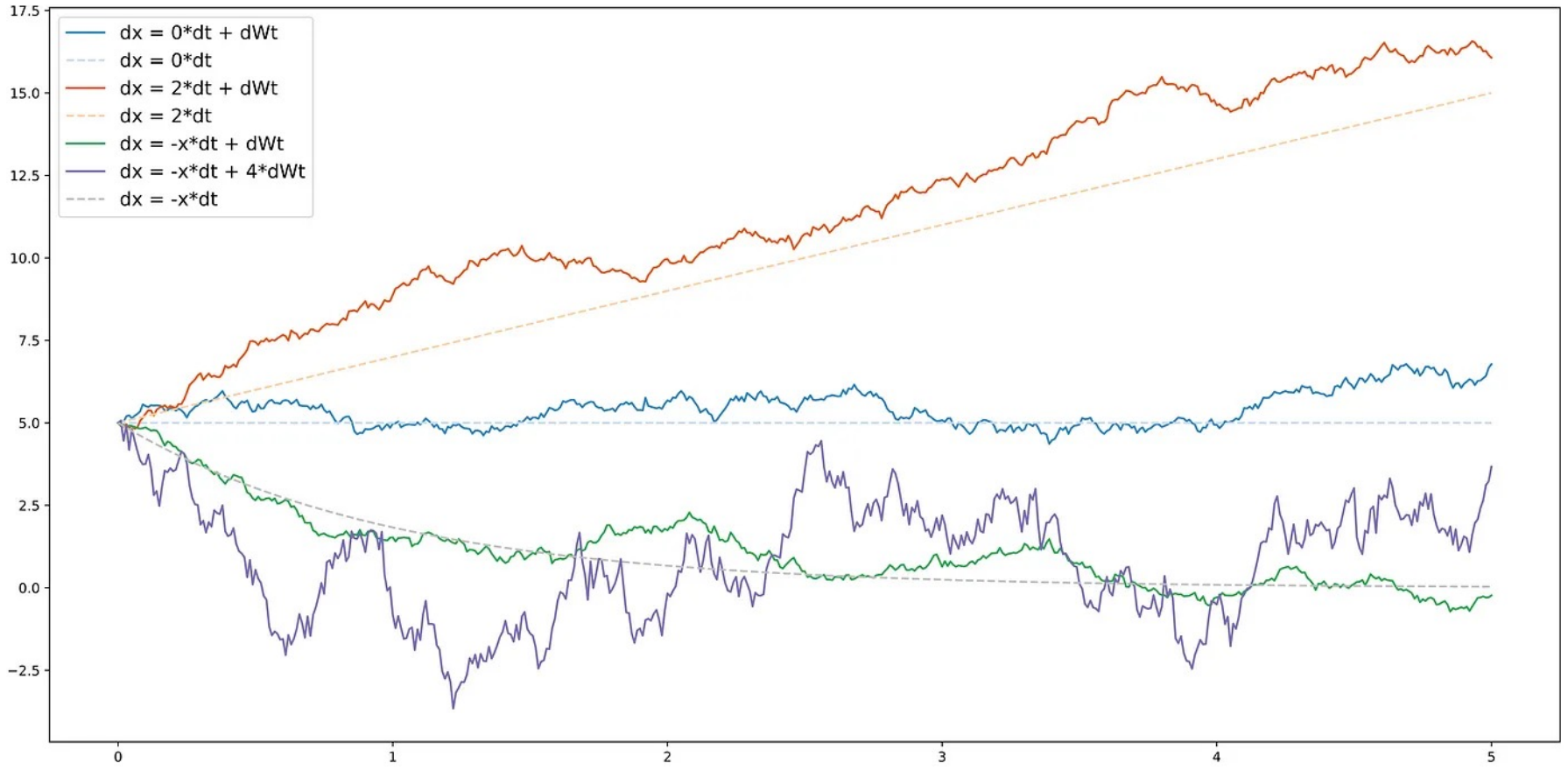
$$X_{t+dt} \approx X_t + a(X_t, t)dt + U' \quad \text{where} \quad U' \sim \mathcal{N}(0, \sigma(X_t, t)dt)$$

Deterministic drift term

Normal RV with std proportional to diffusion term

Diffusion process samples

Stochastic and Non-stochastic



Reversed time process

If X_t is a diffusion process such that

$$dX_t = a(X_t, t)dt + \sigma(t)dW_t$$

then the reversed-time process, $\bar{X}_t = X_{T-t}$ is also a diffusion process

$$d\bar{X}_t = \left[a(\bar{X}_t, t) - \sigma^2(t)\nabla_{X_t} \log p(X_t)\right]dt + \sigma(t)dW_t$$

$$= \bar{a}(\bar{X}_t, t)dt + \sigma(t)dW_t$$

where $\nabla_{X_t} \log p(X_t)$ is called the *score function* and $p(X_t)$ is the *marginal probability* of X_t

Reversed time process

$$d\bar{X}_t = \left[a(\bar{X}_t, t) - \sigma^2(t)\nabla_{X_t} \log p(X_t)\right]dt + \sigma(t)dW_t$$

$$= \bar{a}(\bar{X}_t, t)dt + \sigma(t)dW_t$$

where $\nabla_{X_t} \log p(X_t)$ is called the *score function* and $p(X_t)$ is the *marginal probability* of X_t

But we don't know $p(X_t)$ or $\nabla_{X_t} \log p(X_t)$ and will have to estimate it with a neural network.

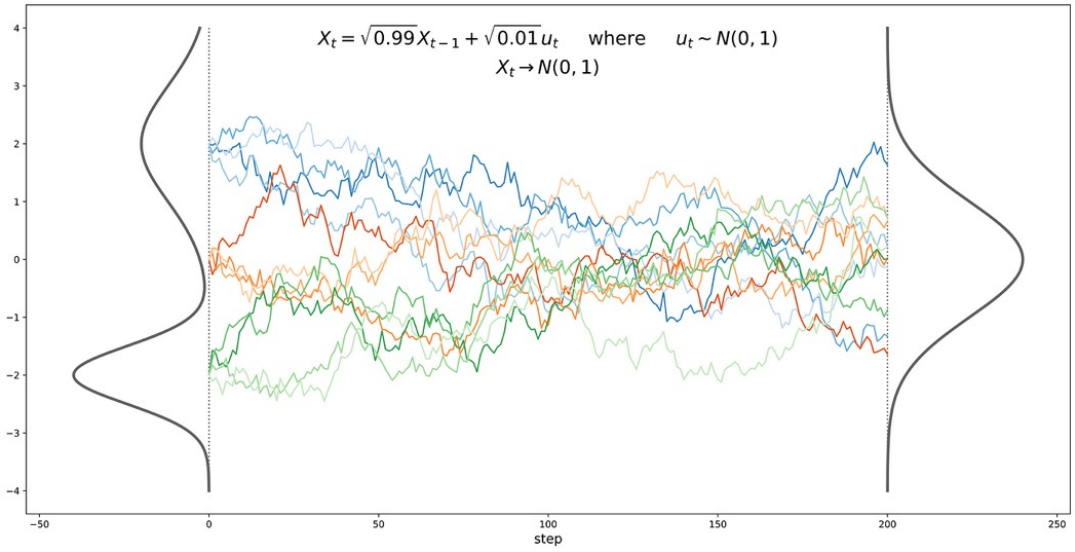
In practice, $\nabla_{X_t} \log p(X_t)$ is easier to estimate than $p(X_t)$ (it has to integrate to 1 – global normalization constraint)

Intuition behind diffusion processes

Progressively destroys relevant information

E.g. with shrinking ($|a| < 1$) *drift coefficient* and non-zero *diffusion coefficient* will turn complex distribution into isotropic gaussian

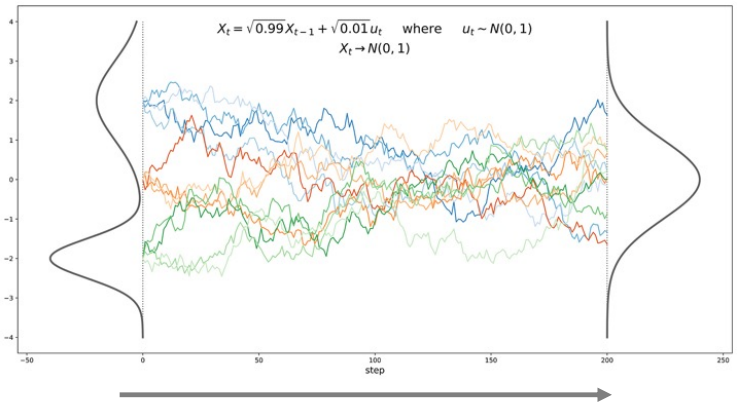
$$X_t = \sqrt{1-p}X_{t-1} + \sqrt{p}u_t \qquad \text{where} \qquad u_t \sim \mathcal{N}(0,1) \quad \text{and} \quad p = 0.01$$



Intuition behind diffusion processes

For the diffusion process

$$X_t = \sqrt{1-p}X_{t-1} + \sqrt{p}u_t \qquad \text{where} \qquad u_t \sim \mathcal{N}(0,1) \quad \text{and} \quad p = 0.01$$



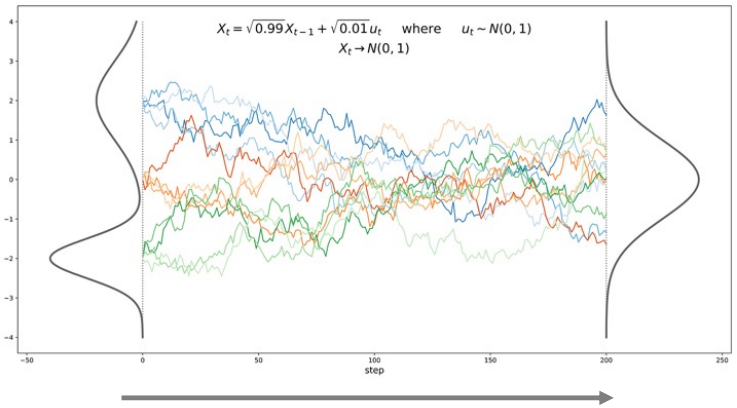
Towards Gaussian

After a given number of steps T we can write

$$\begin{aligned} X_T &= \sqrt{1-p}X_{T-1} + \sqrt{p}u_T \\ &= (\sqrt{1-p})^2 X_{T-2} + \sqrt{1-p}\sqrt{p}u_{T-1} + \sqrt{p}u_T \\ &= \dots \\ &= (\sqrt{1-p})^T X_0 + \underbrace{\sum_{i=0}^{T-1} \sqrt{p}(\sqrt{1-p})^i u_{T-i}} \end{aligned}$$

This is a sum of independent gaussians, so can express as single gaussian with variance the sum of the variances.

Intuition behind diffusion processes



Towards Gaussian

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For number of steps T large enough, we have

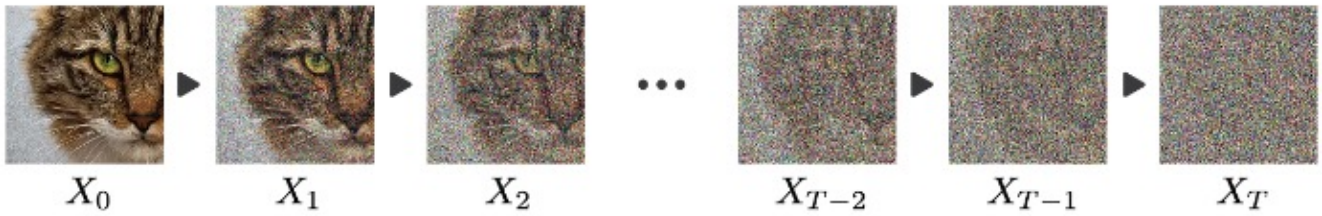
$$(\sqrt{1-p})^T \underset{T\to\infty}{\longrightarrow} 0 \qquad \text{and} \qquad \sum_{i=0}^{T-1} \underbrace{\left(\sqrt{p}(\sqrt{1-p})^i\right)^2}_{\text{Variance of the gaussian}} = p\frac{1-(1-p)^T}{1-(1-p)} \underset{T\to\infty}{\longrightarrow} 1$$

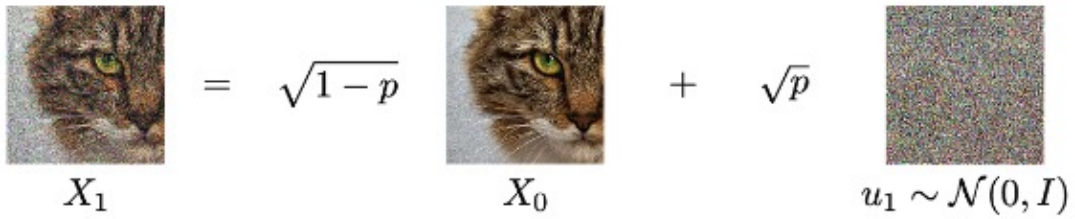
Geometric series

So for any starting point, we tend to a normal gaussian.

Same idea but for images

But in $H \times W \times C$ dimensions, e.g. $100 \times 100 \times 3$ for 100×100 resolution RGB images





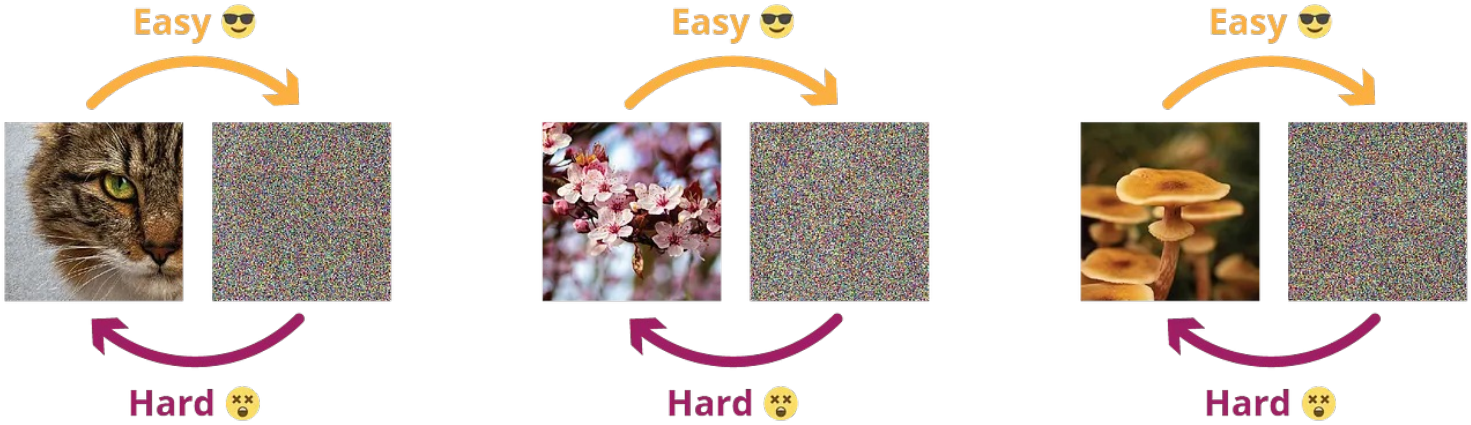
Why use diffusion?

Answer:

Gives us a progressive and structured way to go from a complex distribution to an isotropic gaussian noise

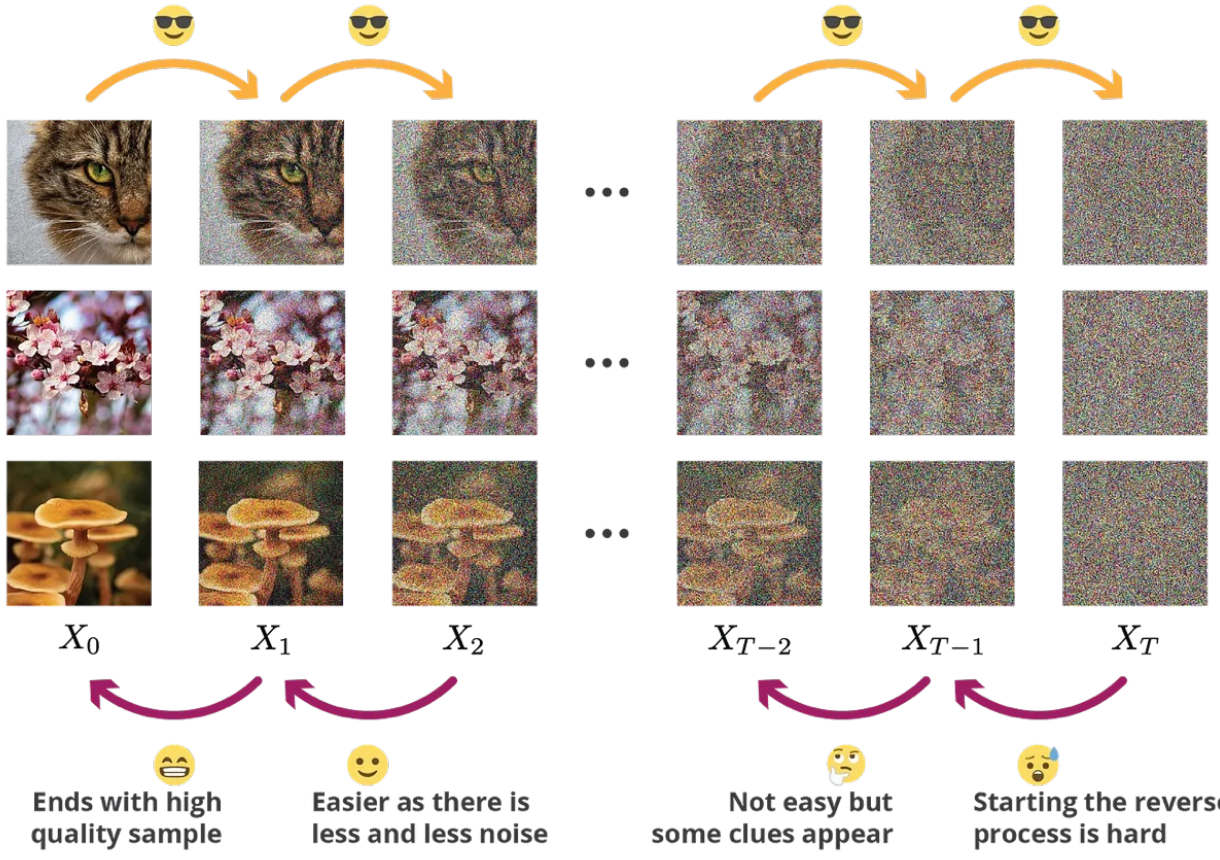
that will enable the learning of the reverse process

Intuition behind learning the reverse process

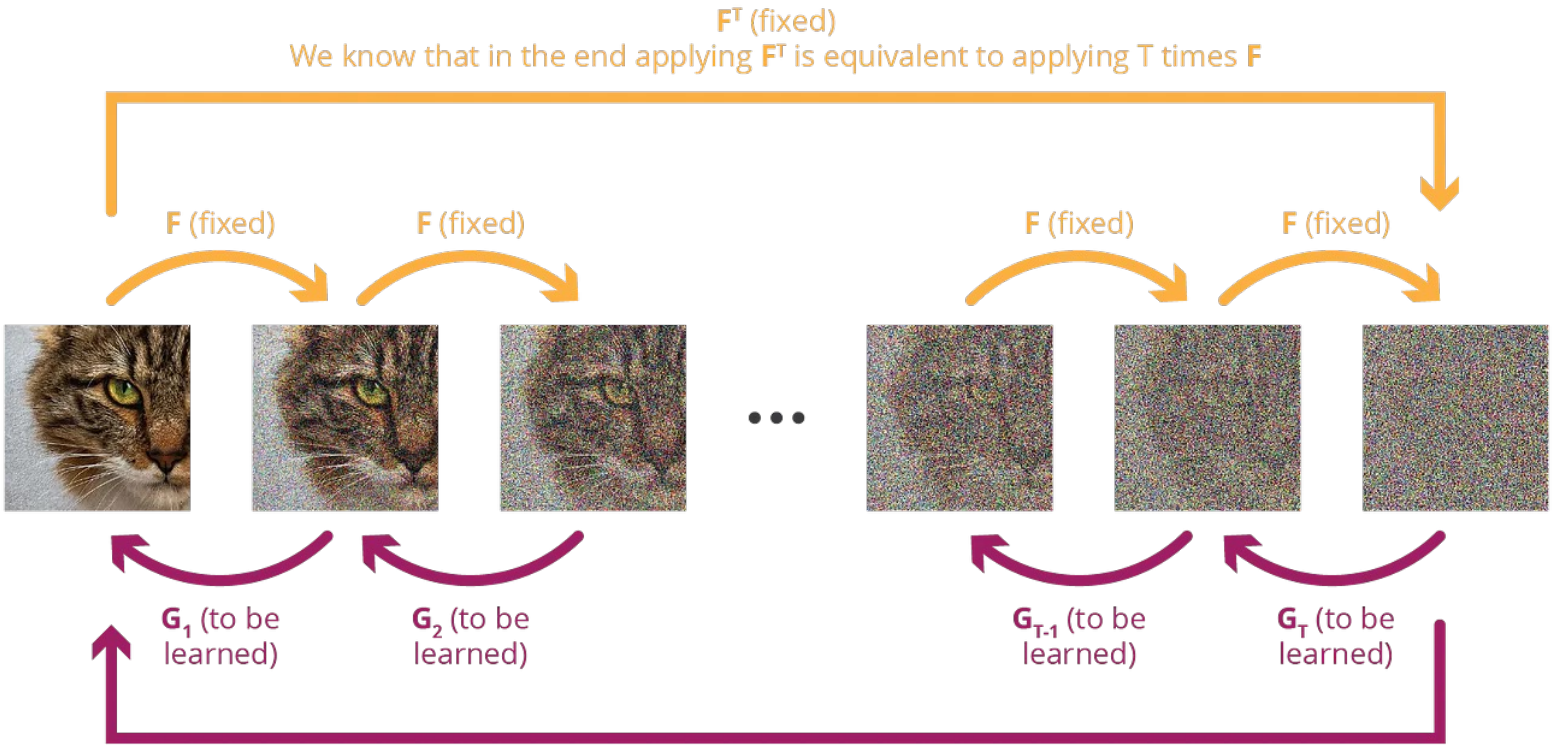


Reversing process in one step is extremely difficult

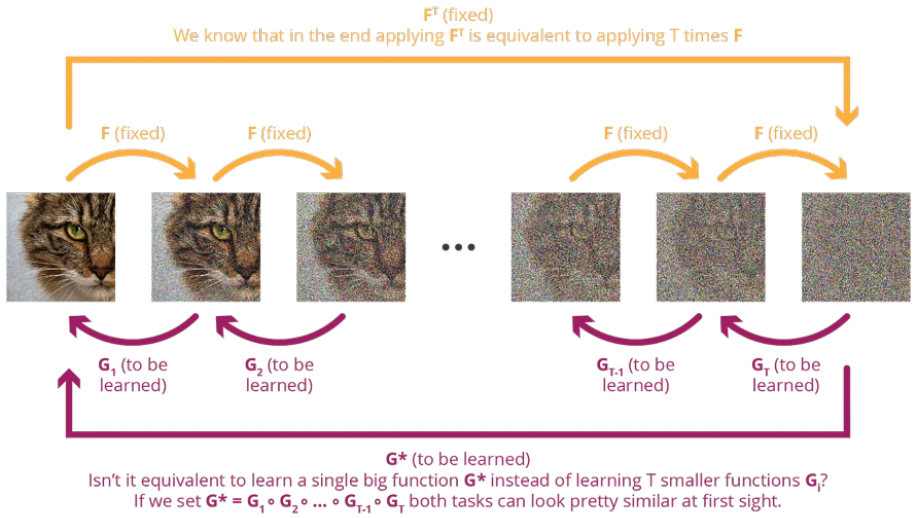
Doing it in steps gives us some clues



One step versus multi-step



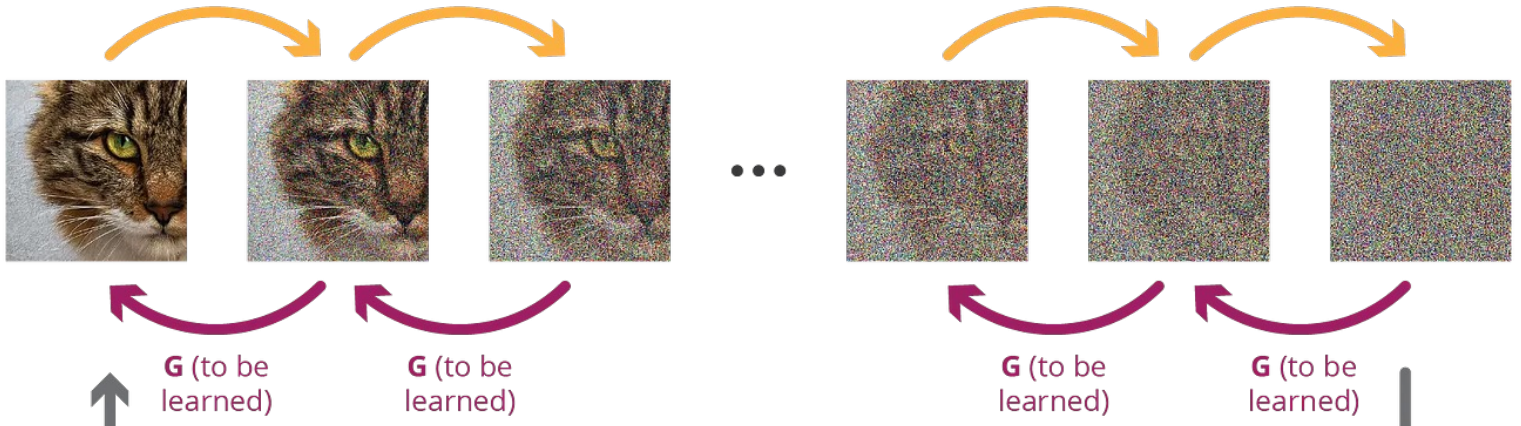
Advantage of multi-step reverse process



1. Don't have to learn a unique transform G_i for each step, but rather a single transform that is a function of the index step. Drastically reduces size of the model.

2. Gradient descent is much more difficult in one step and can exploit coarse to fine adjustments in multiple steps,.

Iterative versus one step



Learning transitions of the reverse process are not completely different tasks meaning that we can learn a common model **G(image , step)** that takes both the current image and the current step as inputs instead of one different model for each step

G* (to be learned)

G* can't rely on the same nice iterative structure than G, meaning that this unrolled version supposed to be equivalent to $\mathbf{G_1 \circ G_2 \circ \ldots \circ G_{T-1} \circ G_T}$ will have more parameters and will be harder to train

Similarities and differences to VAEs

Similarities:

- An encoder transforms a complex distribution into a simple distribution in a structured way to learn a decoder that produces a similar sample

Differences:

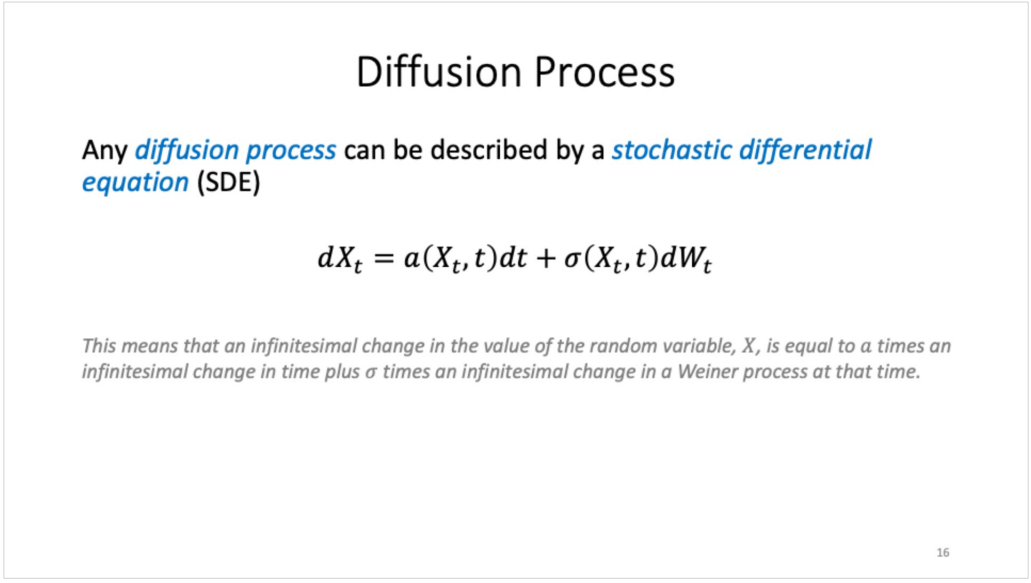
- DPM is multi-step, versus one step for VAE
- DPM encoder is fixed and does not get trained
- DPM will be trained based on the structure of the diffusion process
- DPM latent space is exactly same as input, as opposed to VAE which reduces dimensionality


Dall-E 3
DETOUR
CAUTION:
MATHEMATICS
AHEAD

Mathematics of Diffusion Models

Assume the forward and reverse process operate in T steps.

Both forward and reverse process are discrete so becomes a *Markov chain* with *gaussian transition probability*.



$\mathcal{N}(\mu, \sigma^2)$

Mathematics of Diffusion Models

Denote x_0 as a sample from a distribution $q(x_0)$.

Forward process: gaussian transition probability

$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{(1-\beta_t)}\, x_{t-1}, \beta_t I) \quad \text{where} \quad t \in \mathbb{N}$$

and where β_t indicates trade-off between info to be kept from previous step and new noise added.

$\mathcal{N}(\mu, \sigma^2)$

Mathematics of Diffusion Models

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and where β_t indicates trade-off between info to be kept from previous step and new noise added.

We can equivalently write

$$x_t = \sqrt{(1-\beta_t)}\, x_{t-1} + \sqrt{\beta_t}\, \epsilon_t \qquad \epsilon_t \sim \mathcal{N}(0, I)$$

Discretized diffusion process

$\mathcal{N}(\mu, \sigma^2)$

Mathematics of Diffusion Models

Through recurrence, we can represent any step in the chain as directly represented from x_0:

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

where

$$\alpha_t = (1 - \beta_t) \quad \text{and} \quad \bar{\alpha}_t = \prod_{i=1}^{t} \alpha_i = \prod_{i=1}^{t} (1 - \beta_i)$$

and from the Markov property, the entire forward trajectory is

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

The reverse process

With the assumption on the drift and diffusion coefficients, the reverse of the diffusion process takes the same form.

Reverse gaussian transition probability

$$q(x_{t-1}|x_t)$$

can then be approximated by

$$p_\theta(x_{t-1} \mid x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$$

where μ_θ and Σ_θ are two functions parameterized by θ and learned.

The reverse process

Using the Markov property, the probability of a given backward trajectory can be approximated by

$$\mathrm{p}_\theta(x_{0:T}) = p(x_T) \prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)$$

where $p(x_T)$ is an isotropic gaussian distribution that does not depend on θ

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

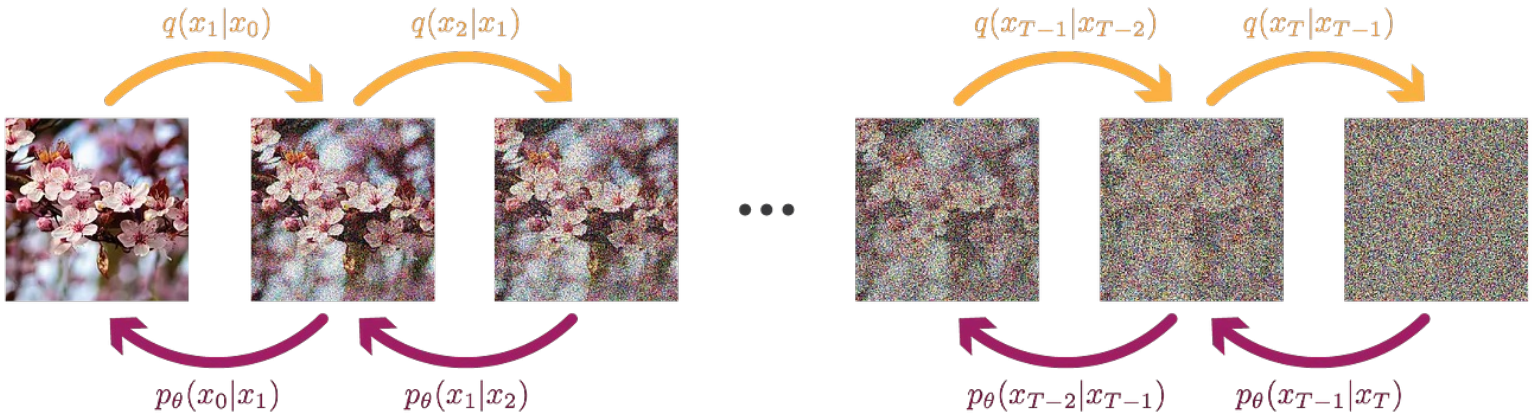
FIXED FORWARD PROCESS

Initial distribution

$q(x_0)$

Gaussian transition kernel

$q(x_t|x_{t-1}) = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$



Approximation of

$q(x_{t-1}|x_t)$

Gaussian transition kernel with parameters to be learned

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

Initial distribution

$p(x_T) = \mathcal{N}(x_t; 0, I)$

LEARNED BACKWARD PROCESS

Questions

How do we learn the parameters θ for μ_θ and Σ_θ?

What is the loss to be optimized?

- We hope that $p_\theta(x_0)$, the distribution of the last step of the reverse process, will be close to $q(x_0)$

Optimization Objective

$$
\begin{aligned}
\mu_\theta^*, \Sigma_\theta^* &= \arg\min_{\mu_\theta, \Sigma_\theta} \left(D_{KL}(q(x_0)||p_\theta(x_0))\right) \\
&= \arg\min_{\mu_\theta, \Sigma_\theta} \left(-\int q(x_0) \log\left(\frac{p_\theta(x_0)}{q(x_0)}\right) dx_0\right) \\
&= \arg\min_{\mu_\theta, \Sigma_\theta} \left(-\int q(x_0) \log(p_\theta(x_0)) dx_0\right)
\end{aligned}
$$

Skipping a lot more math

- Expand p-theta as marginalization integral
- Use Jensen's inequality to define a slightly simpler upper bound to the loss
- Some manipulations with Bayes' Theorem
- Properties of KL divergence of two gaussian distributions
- An additional simplification suggested by [Ho et al 2020]

Diffusion models in practice

We have the forward process

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

and our reverse process

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

and we want to train to minimize this simplified upper bound

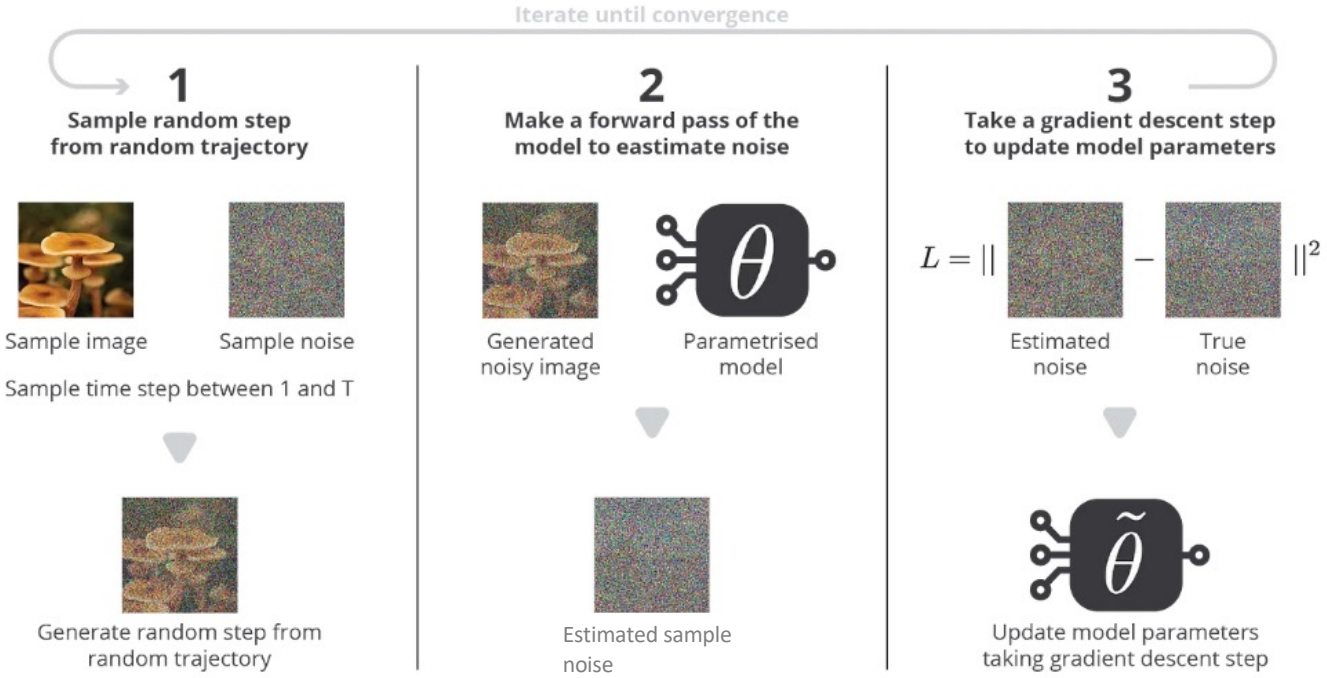
$$\mathbb{E}_{x_0,t,\epsilon}\left(||\epsilon - \epsilon_\theta(x_t, t)||^2\right) = \mathbb{E}_{x_0,t,\epsilon}\left(||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2\right)$$

Dall-E 3

Training Process

Algorithm 1 Training

1: **repeat**
2: $x_0 \sim q(x_0)$ ▷*Sample random initial data*
3: $t \sim \text{Uniform}(\{1, ..., T\})$ ▷*Sample random step*
4: $\epsilon \sim \mathcal{N}(0, I)$ ▷*Sample random noise*
5: $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t}\epsilon$ ▷*Rand. step of rand. trajectory*
6: Take gradient descent step on $\nabla_\theta ||\epsilon - \epsilon_\theta(x_t, t)||^2$ ▷*Optimisation*
7: **until** converged



To sample/generate

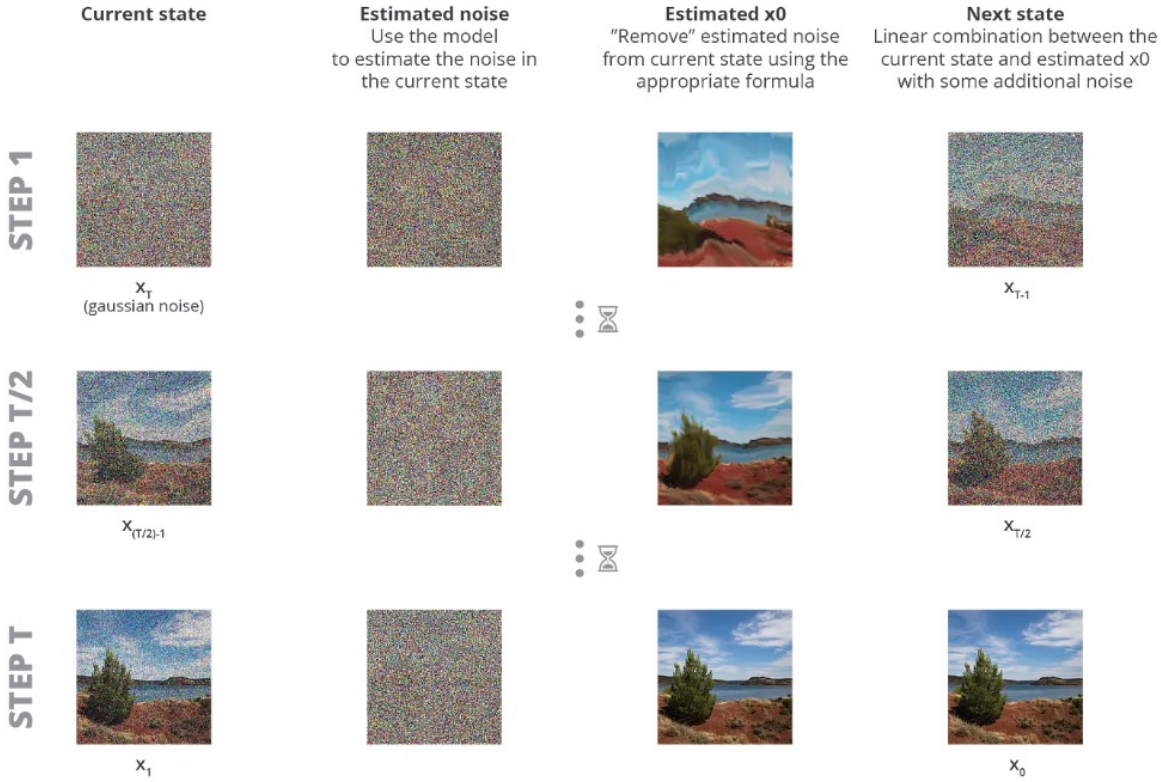


Illustration of the sampling process of a denoising diffusion probabilistic model.

To sample/generate (unconditional generation)

will generate plausible looking members of the training set

Algorithm 2 Sampling

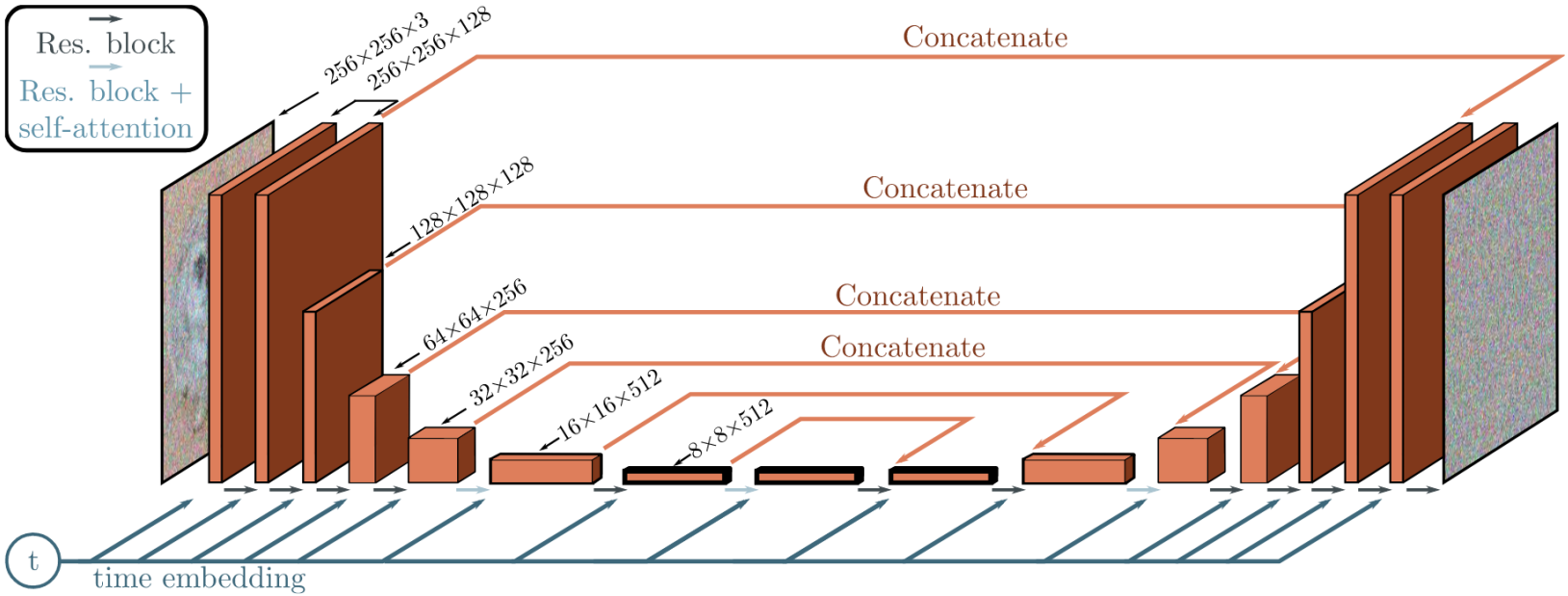
1: $x_T \sim \mathcal{N}(0, I)$ ▷ *Initial isotropic gaussian noise sampling*
2: **for** t = T, ..., 1 **do**
3: $z \sim \mathcal{N}(0, I)$ if $t > 1$ else $z = 0$ ▷ *Sample random noise (if not last step)*
4: $\tilde{\epsilon} = \epsilon_\theta(x_t, t)$ ▷ *Estimated noise in current noisy data*
5: $\tilde{x_0} = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\tilde{\epsilon})$ ▷ *Estimated x_0 from estimated noise*
6: $\tilde{\mu} = \mu_t(x_t, \tilde{x_0}) \left(= \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right)\right)$ ▷ *Mean for previous step sampling*
7: $x_{t-1} = \tilde{\mu} + \sigma_t z$ ▷ *Previous step sampling*
8: **end for**
9: **return** x_0

$\epsilon_\theta(x_t, t)$ is our trained neural network model
σ_t is a variance based on a predefined noise schedule

U-Net (2016) as the Noise Estimation Model

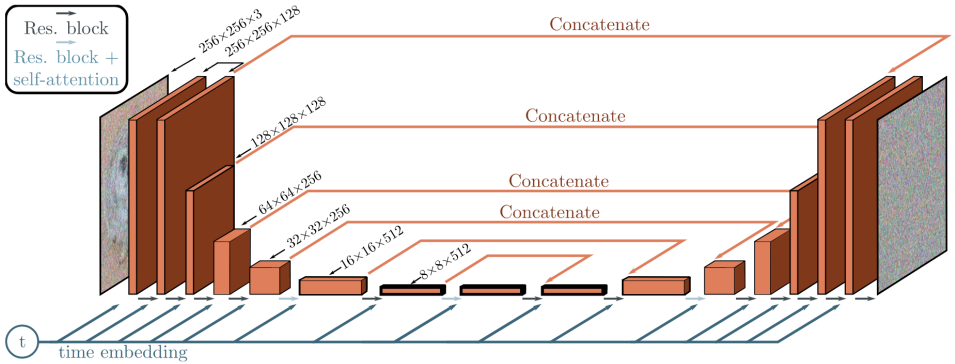
Output is same size as the input.

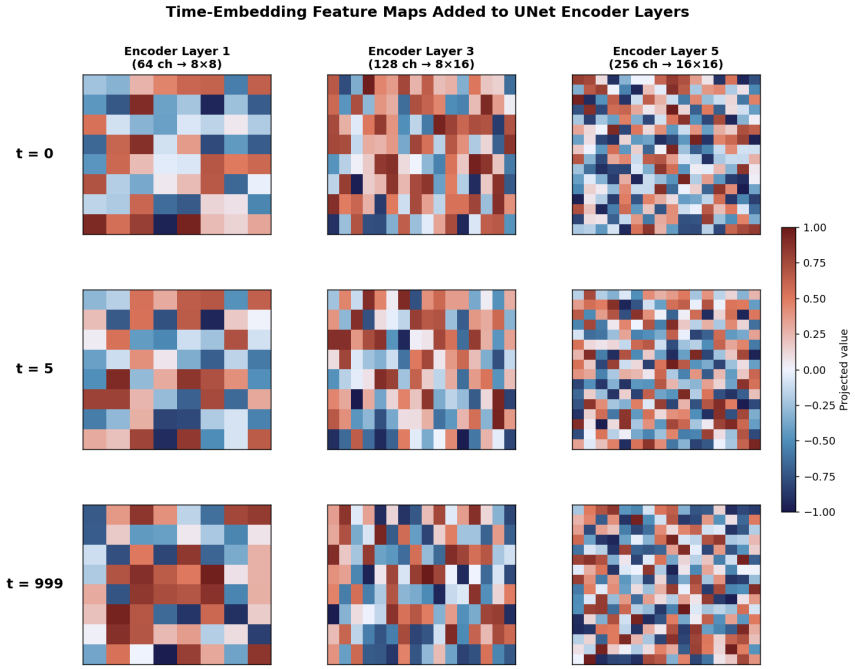
Addition of a time embedding to incorporate time step.



U-Net (2016) Time Embedding

tells U-Net which time step it is dealing with





Step 1: Sinusoidal positional encoding (like in Transformers)

- Mapped to high-dimensional vector

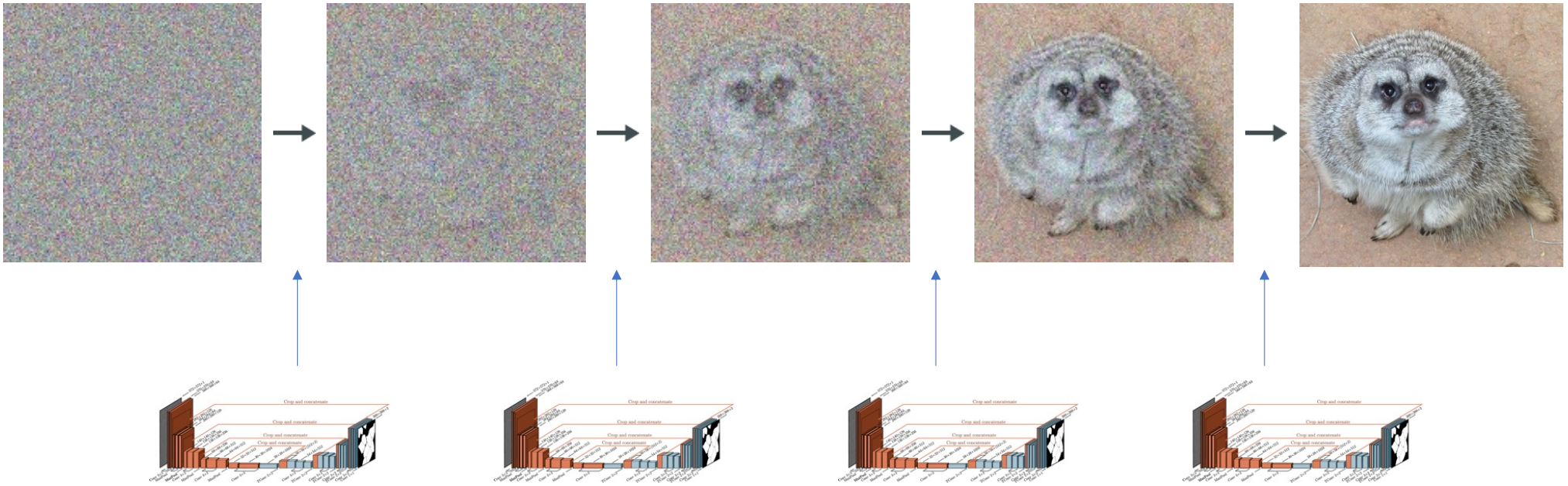
Step 2: MLP Projection

- Pass through 2-layer FCN to produce final embedding vector

Projected into each residual block (via own linear layer) and added to feature map

U-Net for reverse diffusion

Estimate the original noise and remove it from current image.



Diffusion Model Code Examples

- 🤗 Hugging Face Diffusers basic_training.ipynb

- https://huggingface.co/learn/diffusion-course
  - 02_diffusion_models_from_scratch.ipynb

Conditional (Guided) Diffusion

Conditional generation

Classifier Guidance

- Modify the denoising update from z_t to z_{t-1} to incorporate class information, c.

Guidance from text

- Condition on a sentence embedding computed from a language model

Classifier Guidance

Goal

- Steer generation toward a desired class ***c*** (e.g. “cat”, “car”, “face”)
- Need the **conditional** score: $\nabla \log p(x_t \mid \boldsymbol{c})$

Bayes’ Rule Trick

$\nabla \log p(x_t \mid \boldsymbol{c}) = \nabla \log p(x_t) + \nabla \log p(\boldsymbol{c} \mid x_t)$

Note: $\nabla \log p(\boldsymbol{c}) = 0$ (w.r.t x)

How It Works

- Train a **separate classifier** $p(\boldsymbol{c} \mid x_t)$ on noisy images at all noise levels 
- At each denoising step, add the classifier’s gradient to the score
- Scale by **s** (guidance scale) to control how strongly class info steers generation

Dhariwal and Nichol, “Diffusion Models Beat GANs on Image Synthesis.” 2021.

Conditional generation using classifier guidance

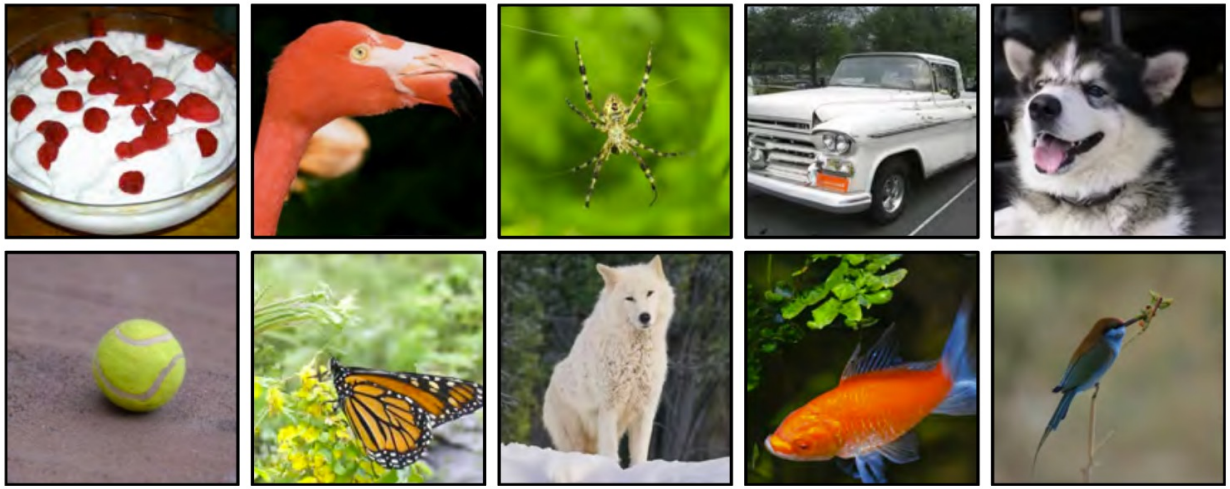


Figure 18.12 Conditional generation using classifier guidance. Image samples conditioned on different ImageNet classes. The same model produces high quality samples of highly varied image classes. Adapted from Dhariwal & Nichol (2021).

Dhariwal and Nichol, "Diffusion Models Beat GANs on Image Synthesis." 2021.

Classifier-Free Guidance

Key Idea (Ho & Salimans, 2022)

- No separate classifier needed — one model does everything
- During **training**: randomly drop conditioning *c* ~10–20% of the time (replace with ∅)
- Same network learns both conditional and unconditional denoising

Sampling (guided noise estimate)

$$\tilde{\varepsilon} = \varepsilon_\theta(x_t, t, \emptyset) + \mathbf{s} \cdot [\, \varepsilon_\theta(x_t, t, \mathbf{c}) - \varepsilon_\theta(x_t, t, \emptyset) \,]$$

- **s** = guidance scale: higher **s** → stronger conditioning (typical: 3–15)
- Works with any conditioning: class labels, text, images
- Powers Stable Diffusion, DALL·E 2, Imagen, Midjourney

Cascaded conditional generation based on a text prompt

- Encode the test via a pre-trained language model
- Inject via cross attention in U-Net blocks
- Higher res images conditioned on lower-res images

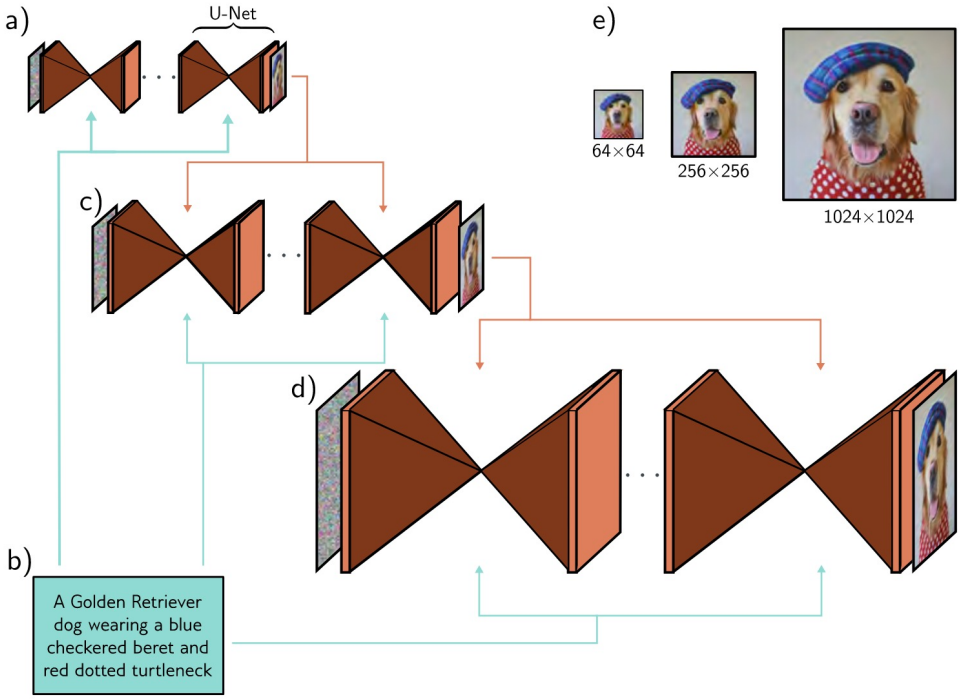


Figure 18.11 Cascaded conditional generation based on a text prompt. a) A diffusion model consisting of a series of U-Nets is used to generate a 64×64 image. b) This generation is conditioned on a sentence embedding computed by a language model. c) A higher resolution 256×256 image is generated and conditioned on the smaller image *and* the text encoding. d) This is repeated to create a 1024×1024 image. e) Final image sequence. Adapted from Saharia et al. (2022b).

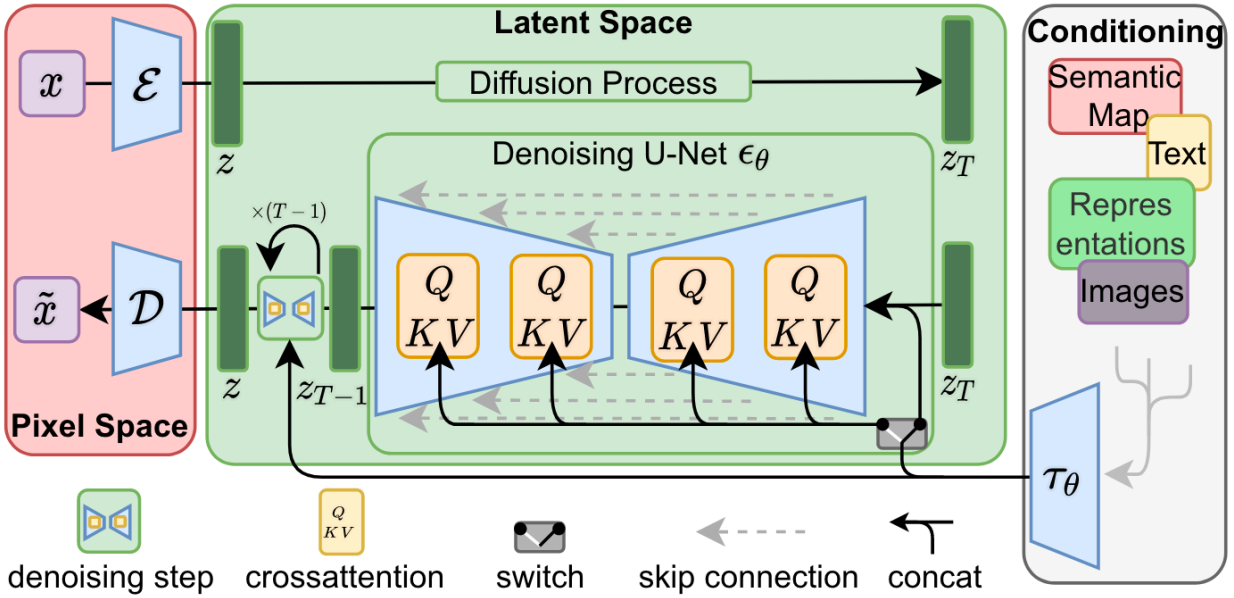
Conditional generation using text prompts

Figure 18.13 Conditional generation using text prompts. Synthesized images from a cascaded generation framework, conditioned on a text prompt encoded by a large language model. The stochastic model can produce many different images compatible with the prompt. The model can count objects and incorporate text into images. Adapted from Saharia et al. (2022b).

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

Stable Diffusion – Latent Diffusion Models

Project the original data to a smaller latent space using a conventional autoencoder and then run the diffusion process in the smaller space.

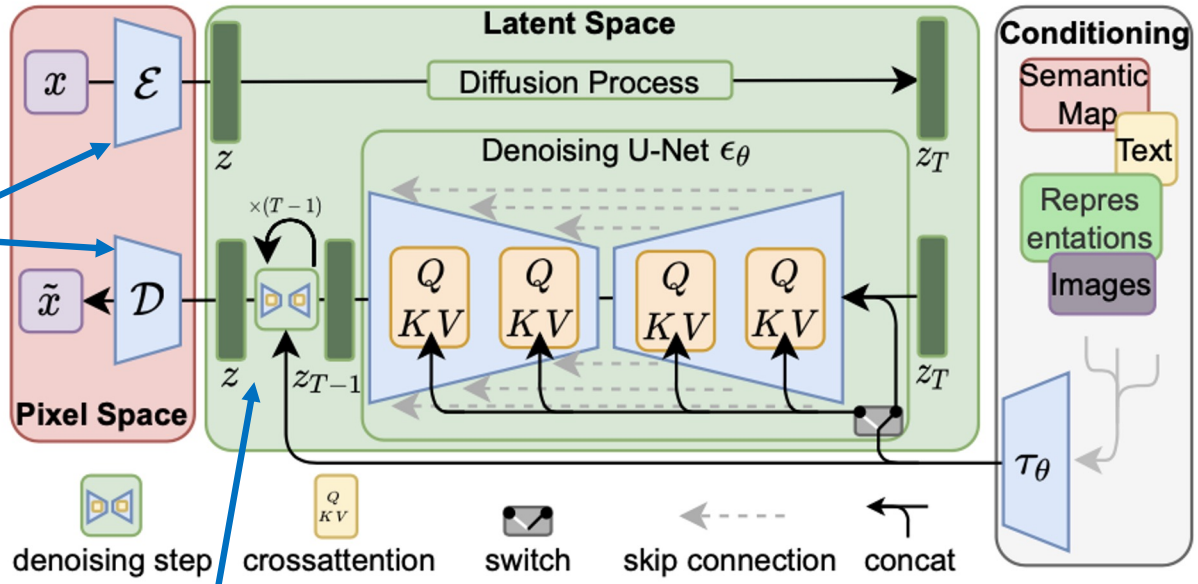


Rombach et al, "High-Resolution Image Synthesis with Latent Diffusion Models," 2022

Conditioning in Latent Space

Conditioning takes over all of latent sampling.

Pick your favorite autoencoder with a small latent space.



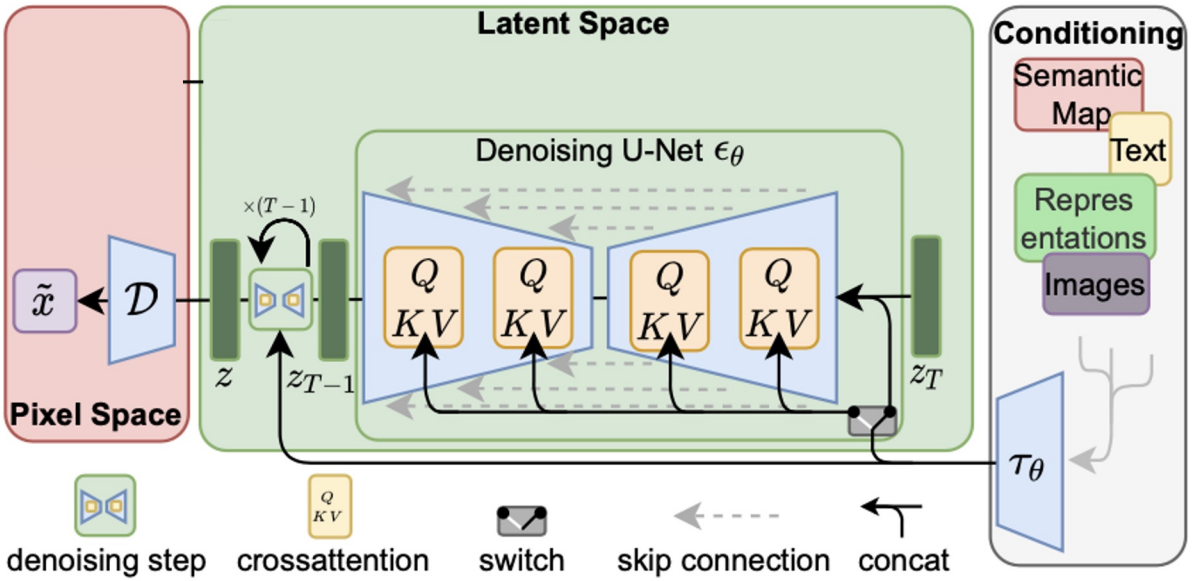
T total repetitions of denoising with conditioning.

Conditioning affects each denoising step.

Rombach et al, "High-Resolution Image Synthesis with Latent Diffusion Models," 2022

Conditioning in Latent Space – Sampling/Generation

Denoising process in latent space and the decoding from latent space to pixel space.



Rombach et al, "High-Resolution Image Synthesis with Latent Diffusion Models," 2022

Super Resolution

- Downsample training images 4x
- Upsample with bicubic interpolation.
- Train latent diffusion model to recover the finer-grained details.

"High-Resolution Image Synthesis with Latent Diffusion Models"
By Rombach, Blattman, Lorenz, Esser and Ommer (2021)

Figure 9. ImageNet 64→256 super-resolution on ImageNet-Val. *LDM-SR* has advantages at rendering realistic textures but SR3 can synthesize more coherent fine structures. See appendix for additional samples and cropouts. SR3 results from [70].

In Painting

Mask some of the image and reconstruct rest of the image to be consistent.

- Don’t change the unmasked part!
- Keeping unmasked part mostly easy because latent code has spatial structure.

“High-Resolution Image Synthesis with Latent Diffusion Models”
By Rombach, Blattman, Lorenz, Esser and Ommer (2021)

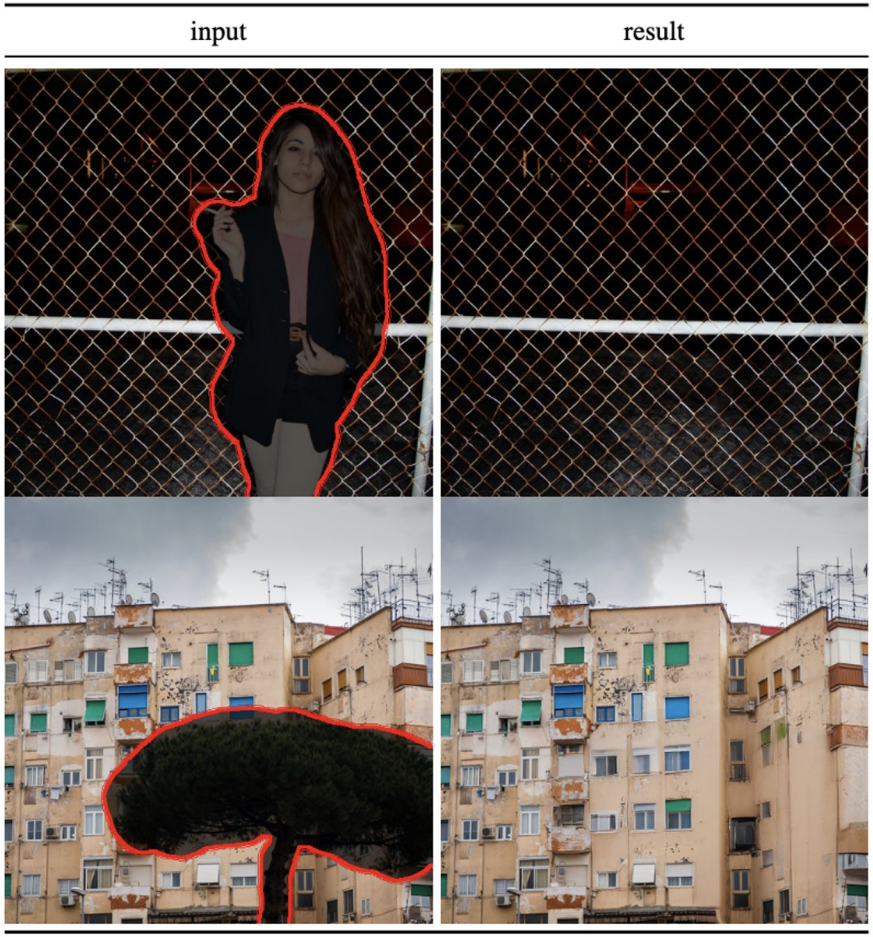


Figure 10. Qualitative results on object removal with our *big, w/ ft* inpainting model. For more results, see Fig. 21.

Protein Design & Drug Discovery

Protein Structure Generation

- RFdiffusion: fine-tune protein structure prediction network on denoising tasks
- Generates novel protein backbones for binder design, enzyme scaffolding

Molecular Docking (Drug Discovery)

- DiffDock: treats docking as diffusion over ligand poses (not sampling-and-scoring)
- Generates 3D drug molecules conditioned on target protein binding sites

Watson et al., "De novo design of protein structure and function with RFdiffusion," Nature 2023;

Corso, Stärk et al., "DiffDock," ICLR 2023

Finance & Synthetic Data

Financial Time Series Forecasting

- TimeGrad: autoregressive denoising diffusion for probabilistic multivariate forecasting
- Captures complex cross-sectional dependencies in asset returns

Synthetic Tabular Data Generation

- TabDDPM / MTabGen: generate realistic tabular data preserving statistical properties
- Privacy-preserving data sharing in healthcare & finance (differential privacy integration)

Rasul et al., "Autoregressive Denoising Diffusion Models for Multivariate Probabilistic Time Series Forecasting," ICML 2021; Villaizan-Vallelado et al., "MTabGen," ACM TKDD 2025

For additional practice

- Notebook 18.1 – Diffusion Encoder in 1D  
- Notebook 18.2 – Training Decoder  
- Notebook 18.3 – 1D Reparameterized Model (more robust)  
- Notebook 18.4 – Families of Diffusion Models (DDIM)  

Resources

- UDL, Chapter 18, Diffusion Models
- Rocca, "Understanding Diffusion Probabilistic Models (DPMs)", Medium.com, 2022
- HuggingFace Diffusion Models Class
- CVPR 2023 Tutorial: Denoising Diffusion Models: A Generative Learning Big Bang, https://cvpr.thecvf.com/virtual/2023/tutorial/18546

Feedback

https://forms.gle/pXHM5nx1Ti9aFmpw6