BOSTON UNIVERSITY

Deep Learning for Data Science
DS 542

https://dl4ds.github.io/fa2025/

Diffusion Models

Original slides by Tom Gardos,
other content from Understanding Deep Learning unless otherwise cited

Plan for Today

- Project 4
- Denoising autoencoders
- Error diffusion process
- Diffusion models

Next time

More math

Latent diffusion (faster!)

Project 4 Inputs

11 classes

dragon
dog
cat
frog
⋮

https://github.com/DL4DS/synth-cute

Project 4

ETA Wednesday

Build a model

- Synthetic data set
  - Built with Stable Diffusion 3.
- Build your own image diffusion model based on this data set.

Grading criteria

Auto-grader (not live yet)

- Inception score
- Fréchet Inception Distance

Manual-grading (subjective)

- 5% our chosen seeds
- 5% your choice of best output

Will share our favorites in Piazza

Quantifying Performance - Inception Score

Grading via another model

- Usually the Inception model for ImageNet
- Want generated images to have a single very likely classification.
- But average flat classification across generated images.
- Formal formula checking KL-divergence between those on a per-generated image basis...

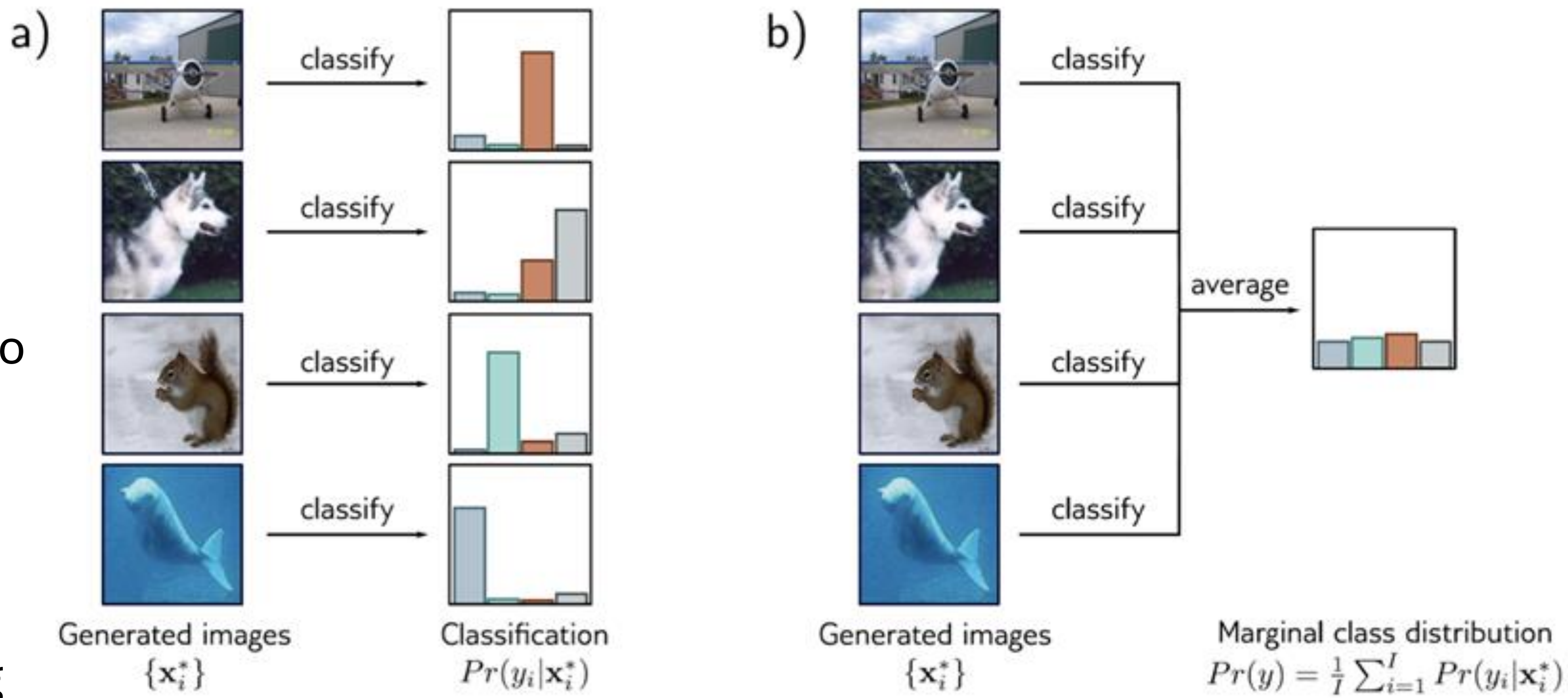


Figure 14.4 Inception score. a) A pretrained network classifies the generated images. If the images are realistic, the resulting class probabilities $Pr(y_i|\mathbf{x}_i^*)$ should be peaked at the correct class. b) If the model generates all classes equally frequently, the marginal (average) class probabilities should be flat. The inception score measures the average distance between the distributions in (a) and the distribution in (b). Images from Deng et al. (2009).

Inception Score Math

Inception score

Expectation over samples

$$e^{\mathbb{E}_x[KL(p(y|x)||p(y))]}$$

class dist. from image x (made from)

overall distribution

Why exponentiate the whole thing?

Decoder ring

- $p(y)$ = probability of class y
- $p(y|x)$ = conditional probability of class y
- $KL(P(x)||Q(x)) = \sum_{x \in X} P(x) \log \frac{P(x)}{Q(x)} =$ Kullback-Leibler divergence.
  - Interpretation is comparing approximate $Q(x)$ to true $P(x)$.

Improved Techniques for Training GANs (2016)

Interpretation of Inception Score

$$e^{\mathbb{E}_x[KL(p(y|x)||p(y))]}$$

- Range of values is $[1, n]$ for n classes.

- Value of 1 implies $\mathbb{E}_x[KL(p(y|x)||p(y))] = 0$
  - So, average KL divergence is 0.
  - But KL divergences is always ≥ 0.
  - So, this implies that the classifier just predicts original class distribution.

classifier failed!

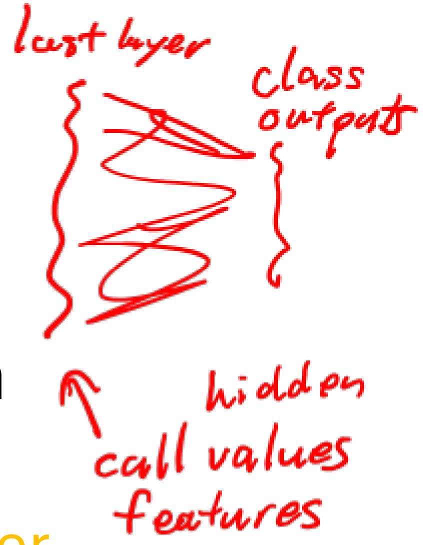
- High values correspond to classifier being able to distinguish classes of generated images.

Quantifying Performance – Fréchet Inception Distance

Another visual similarity metric based on Inception model (others can be used).

- Map generated images to distribution of Inception features.
- Model the distribution of Inception features as a multivariate normal distribution.
- Compare two such distributions with the Wasserstein distance.
  - Also called “earth mover’s distance”
  - Smaller is better.
  - Closed form solution from multivariate normal assumption.

Fréchet Inception Distance Math



- Let f map images to the features (last hidden outputs) of a classification model.
  - Originally used Inception model. Project 4 will use a new classifier.
- Apply f to real data set and generated data set.
  - Compute mean μ and covariance Σ of f outputs for each data set.
  - Use these statistics to specify multivariate normal distribution approximating the distribution of the features of each data set.
- Compute Fréchet distance d between these distributions.

$$d^2 = |\mu_G - \mu_R|^2 + \mathrm{tr}\left(\Sigma_G + \Sigma_R - 2(\Sigma_G \Sigma_R)^{1/2}\right)$$

GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium (2017)

Any Questions?

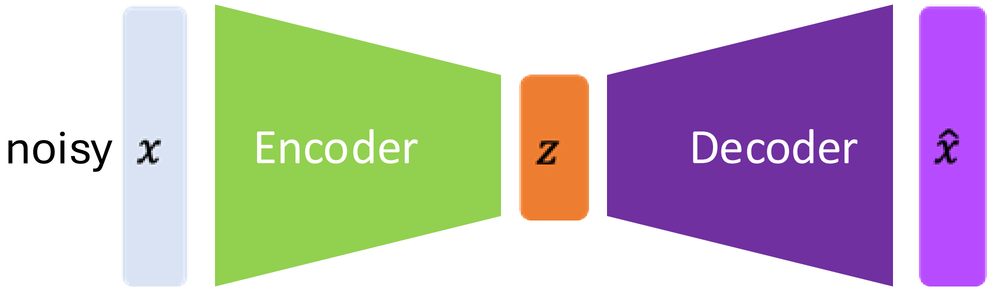
???

Moving on

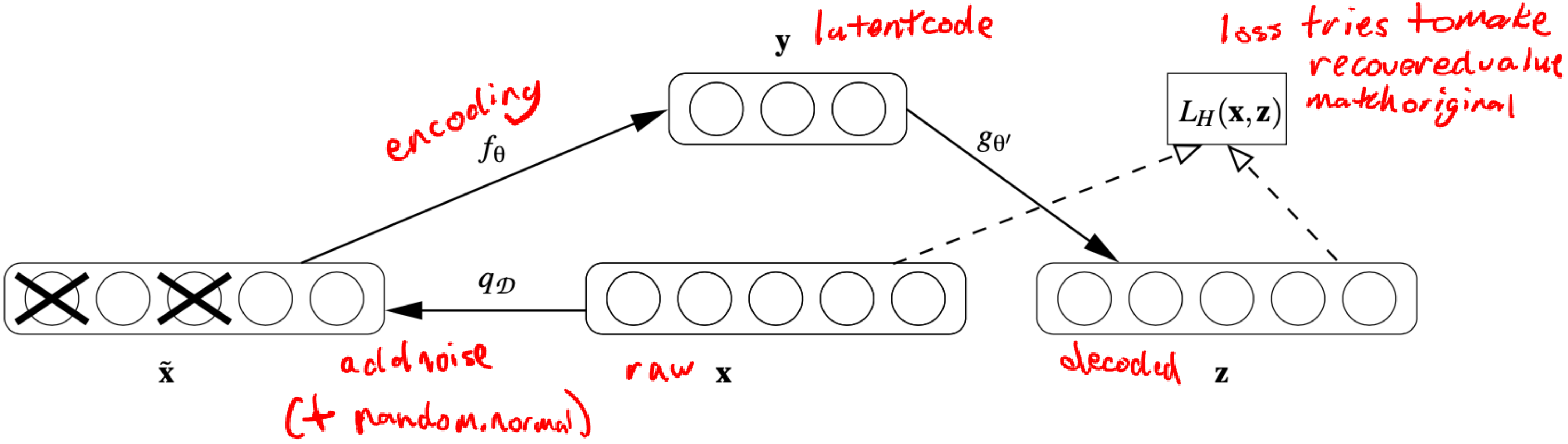
- Project 4
- Denoising autoencoders
- Error diffusion process
- Diffusion models

Denoising Autoencoder Idea

- Train an autoencoder but feed noisy data into the encoder.
- Still try to recover the clean data.



Denoising Autoencoder Training



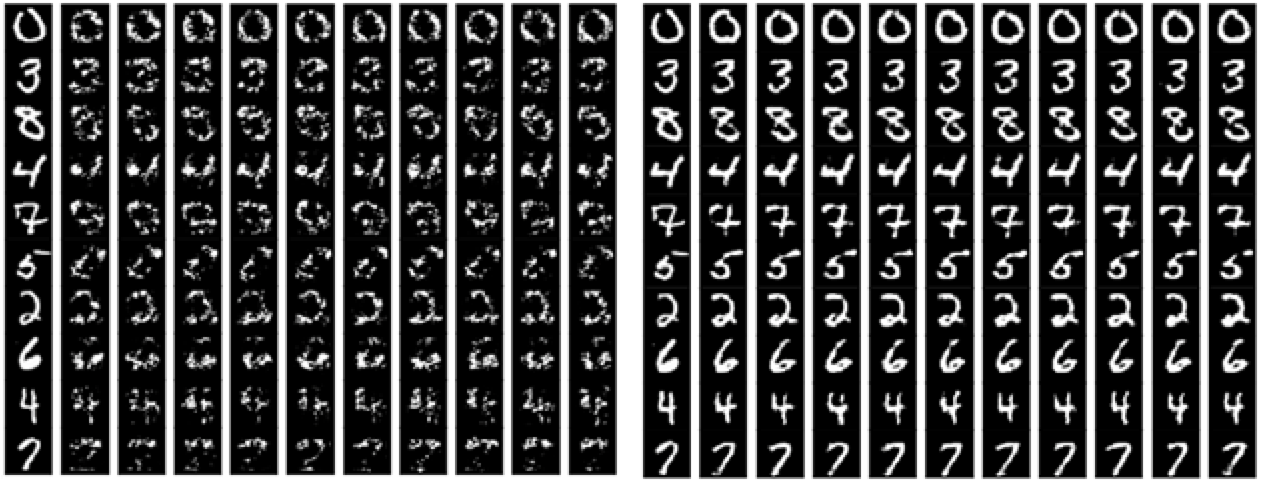
"Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion" by Vincent et al (2010)

Denoising Autoencoders

Early predecessors, but could not handle nearly as much noise.

“Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion” by Vincent et al (2010)

pre deep learning, didn't work w/ mostly noise images



(a) SAE

Stacked autoencoder

(b) SDAE

stacked denoising autoencoder

reconstructs noisy image much better.

Any Questions?

???

Moving on

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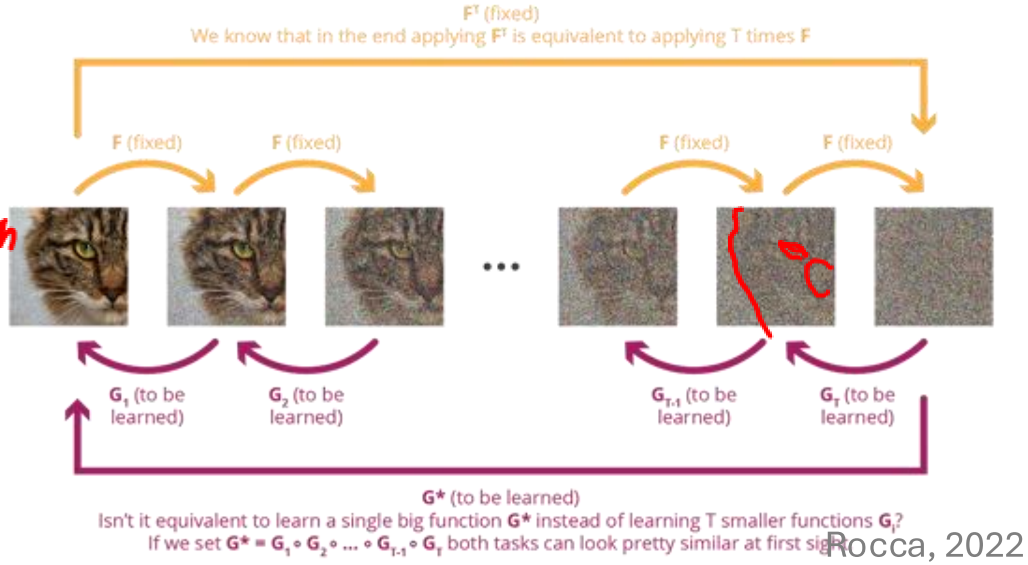
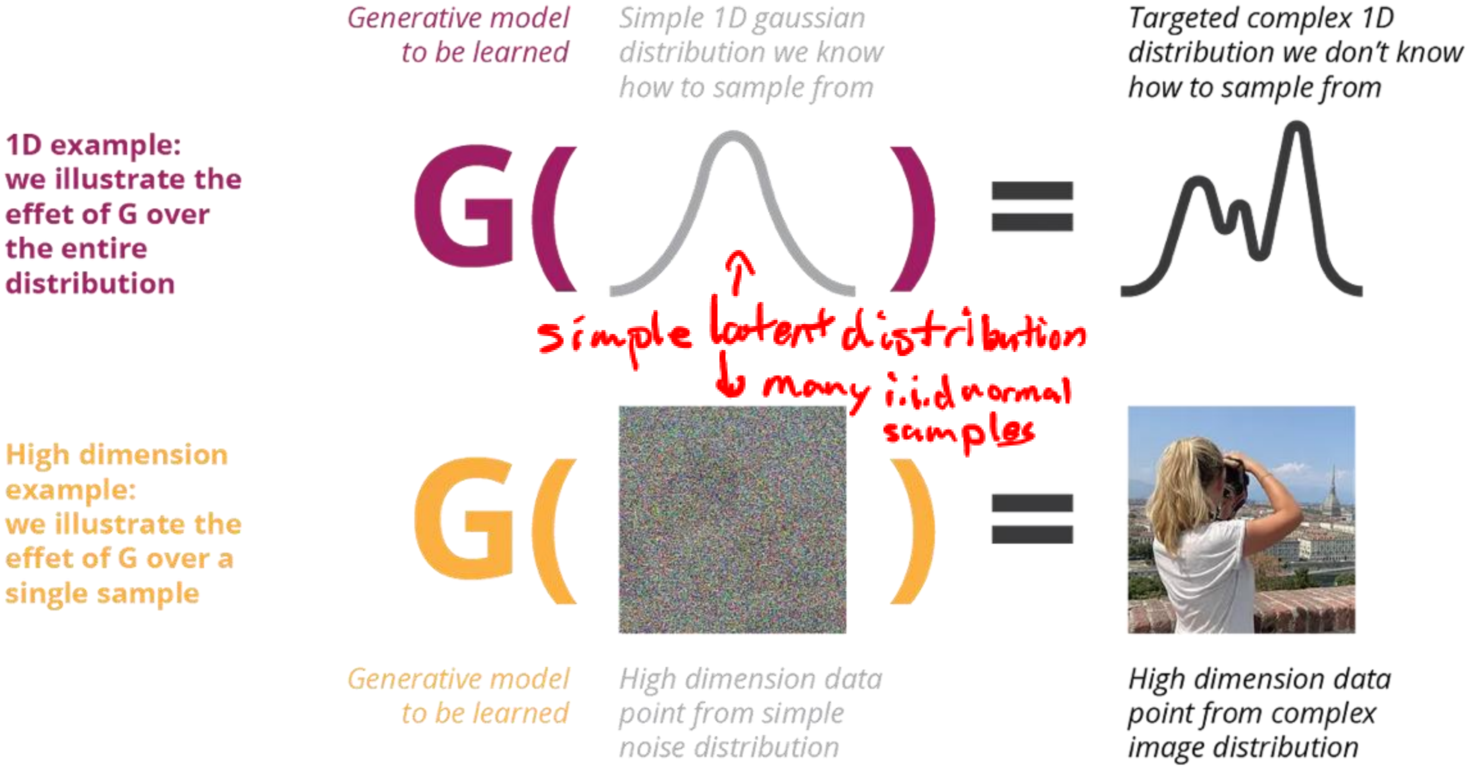
Basic idea of Diffusion Probabilistic Models

- 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.



Rocca, 2022

Simple Latent Distribution to Complex Output Distribution



simple latent distribution

many i.i.d normal samples

both examples preserve signal shape

scalar

+

$H \times W \times C$

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

Rocca, 2022, "Understanding Diffusion Probabilistic Models (DPMs)"

Stochastic process

Stochastic Processes

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

time series analysis too

Realization of a random variable → sample

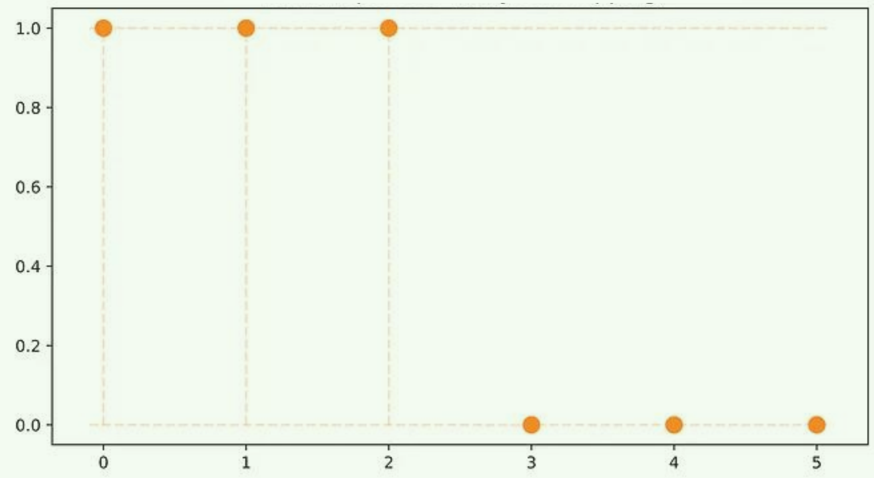
Realization of a stochastic process → sample path or trajectory

sequence of images w/ increasing noise

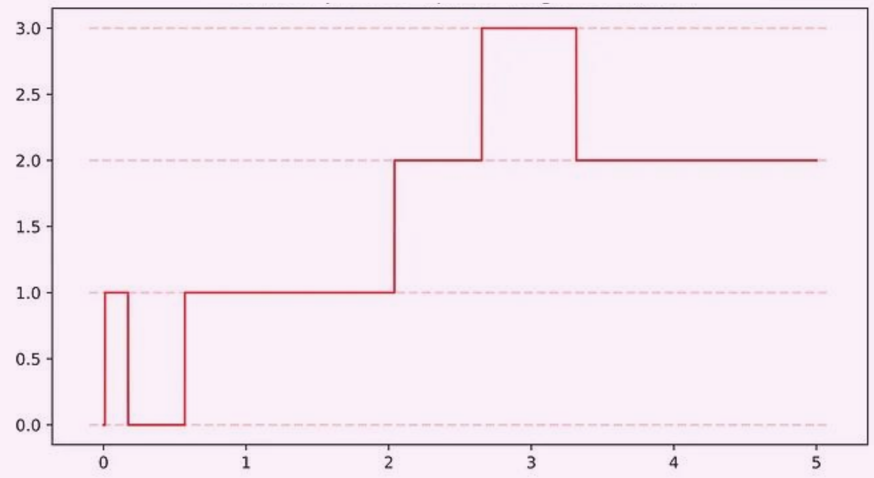
Different types of stochastic processes

Discrete Value

Coin Flipping

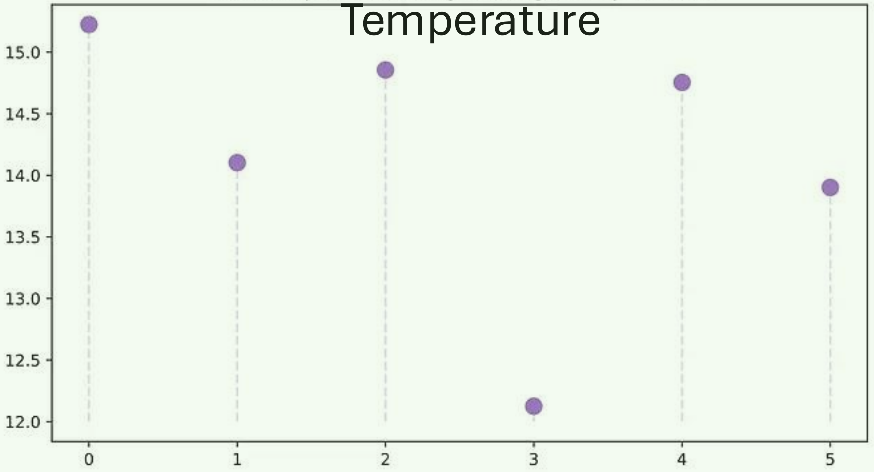


Queue Length Over Time

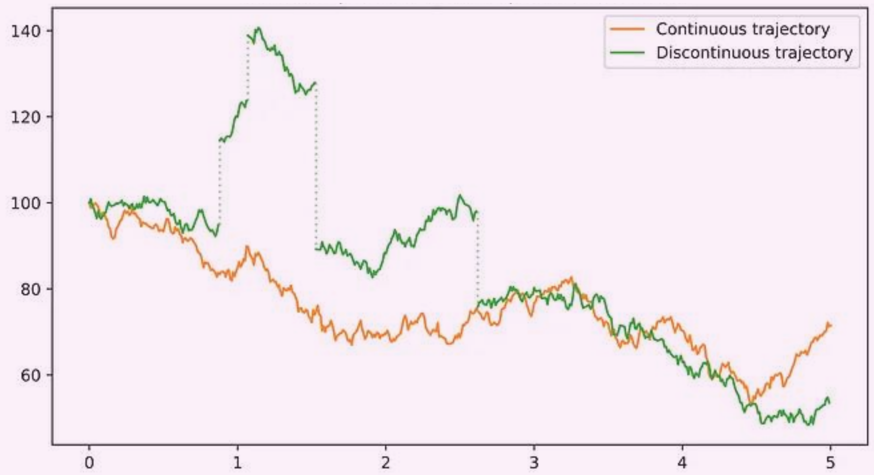


Continuous Value

Daily Average Temperature



Stock Price



Discrete Time

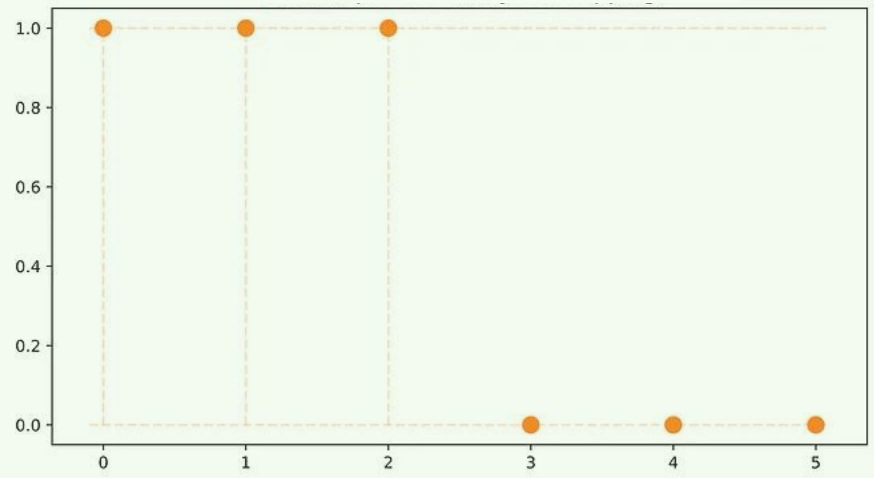
Continuous Time

Rocca, 2022

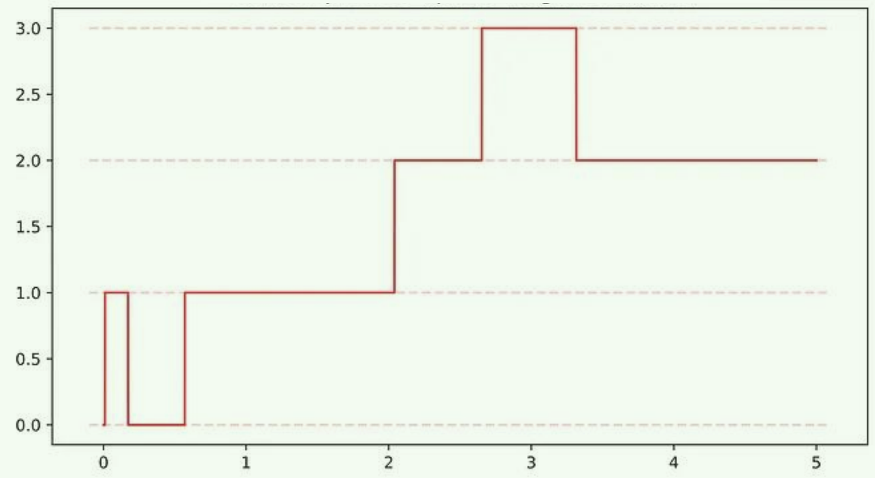
Different types of stochastic processes

Discrete Value

Coin Flipping

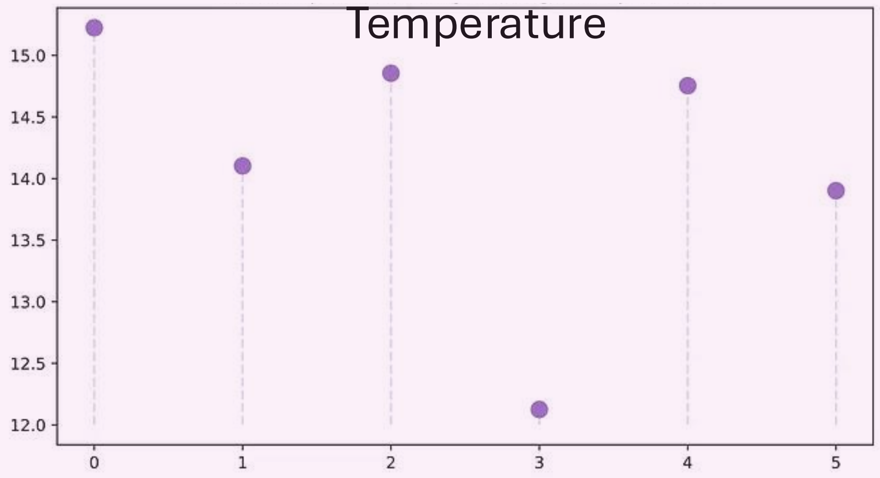


Queue Length Over Time

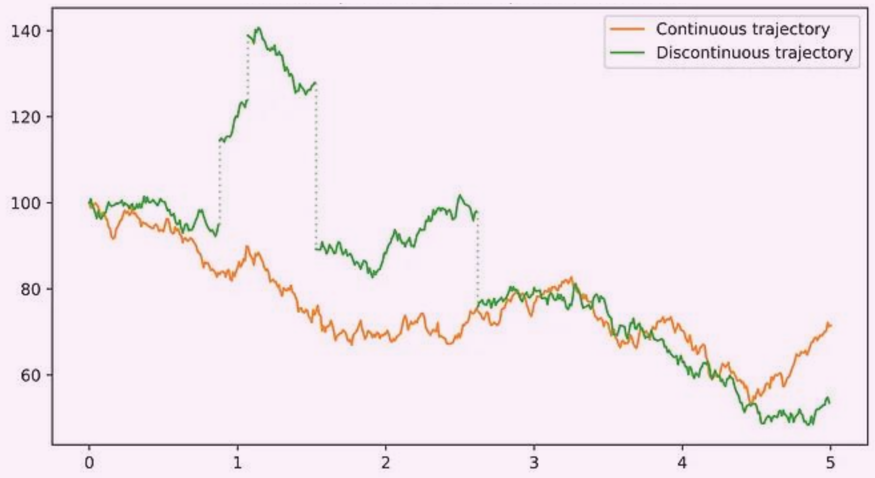


Continuous Value

Daily Average Temperature



Stock Price



Discrete Time

Continuous Time

Rocca, 2022

Markov (Stochastic) Process

"memoryless"

A *Markov process* is a *stochastic process* with no memory; only the current state matters.

Future behavior only depends on the present, or

Present only depends on the previous sample.

$$P\left(X_{t_n} \middle| \underbrace{X_{t_{n-1}}, \dots, X_{t_0}}_{\text{known conditions}}\right) = P\left(X_{t_n} \middle| X_{t_{n-1}}\right) \ \forall \underbrace{t_0 < t_1 < \ \dots}_{\text{don't matter if}} < \underset{\uparrow \text{ is known}}{t_{n-1}} < t_n$$

focus here

→ Markov Chains observing/inferring states

Markov Reward Process + rewards

Markov Decision Processes + actions

MDPs are umbrella problem for sequential decision making problems

Diffusion Process

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

$$\underbrace{dX_t}_{\text{how does X evolve?}} = \overbrace{a(X_t, t)dt}^{\text{expected rate of change}} + \underbrace{\sigma(X_t, t)}_{\text{how does uncertainty grow}} dW_t$$

source of noise

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)

pollen on water
stock prices
Einstein + small particles

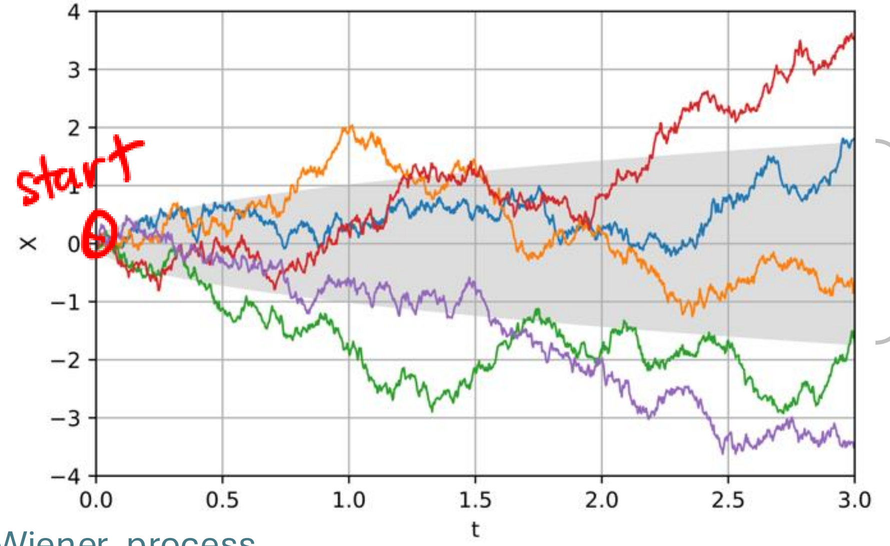
Continuous time stochastic process

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, $\boxed{W_{t+u} - W_t \sim \mathcal{N}(0, u).}$
4. W has almost surely continuous paths: W_t is almost surely continuous in t.

0 centered because a predictable mean would go into drift (a(·))

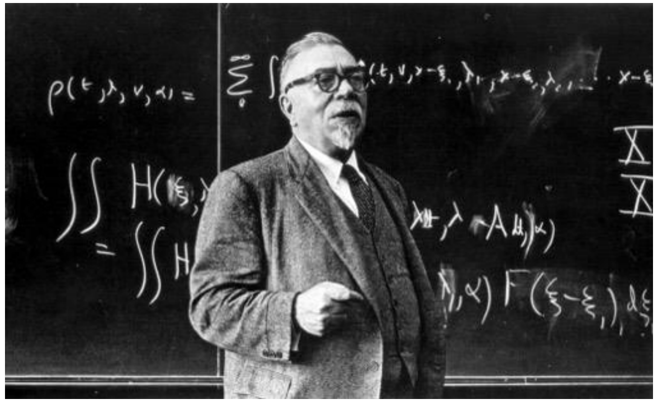
Five sampled processes



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).

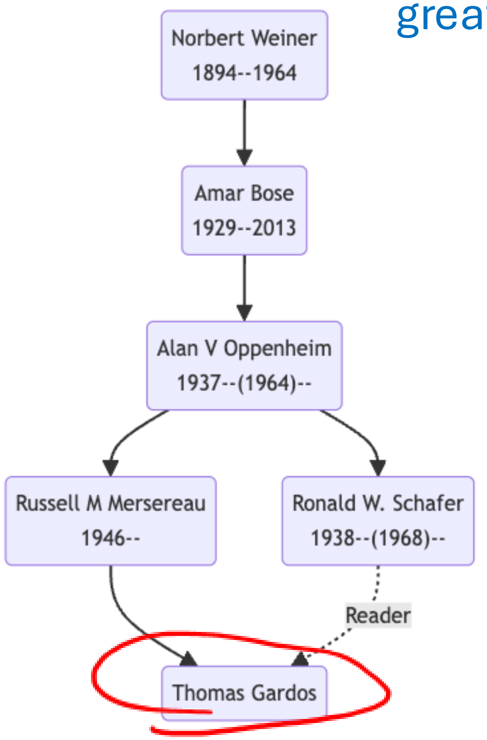
A child prodigy, Wiener later became *an early researcher in stochastic and mathematical noise processes*, contributing work relevant to electronic engineering, electronic communication, and control systems.

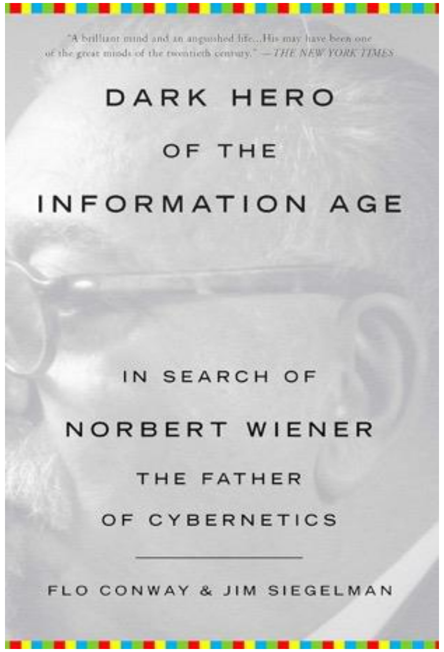
Wiener is considered the originator of cybernetics, the science of communication as it relates to living things and machines.

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 dev is equal to the time step.

difference b/w these is normally distributed.

Exact/ True if continuous process + measured @ fixed interval

Discretizing the SDE

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

back to more general diffusion process

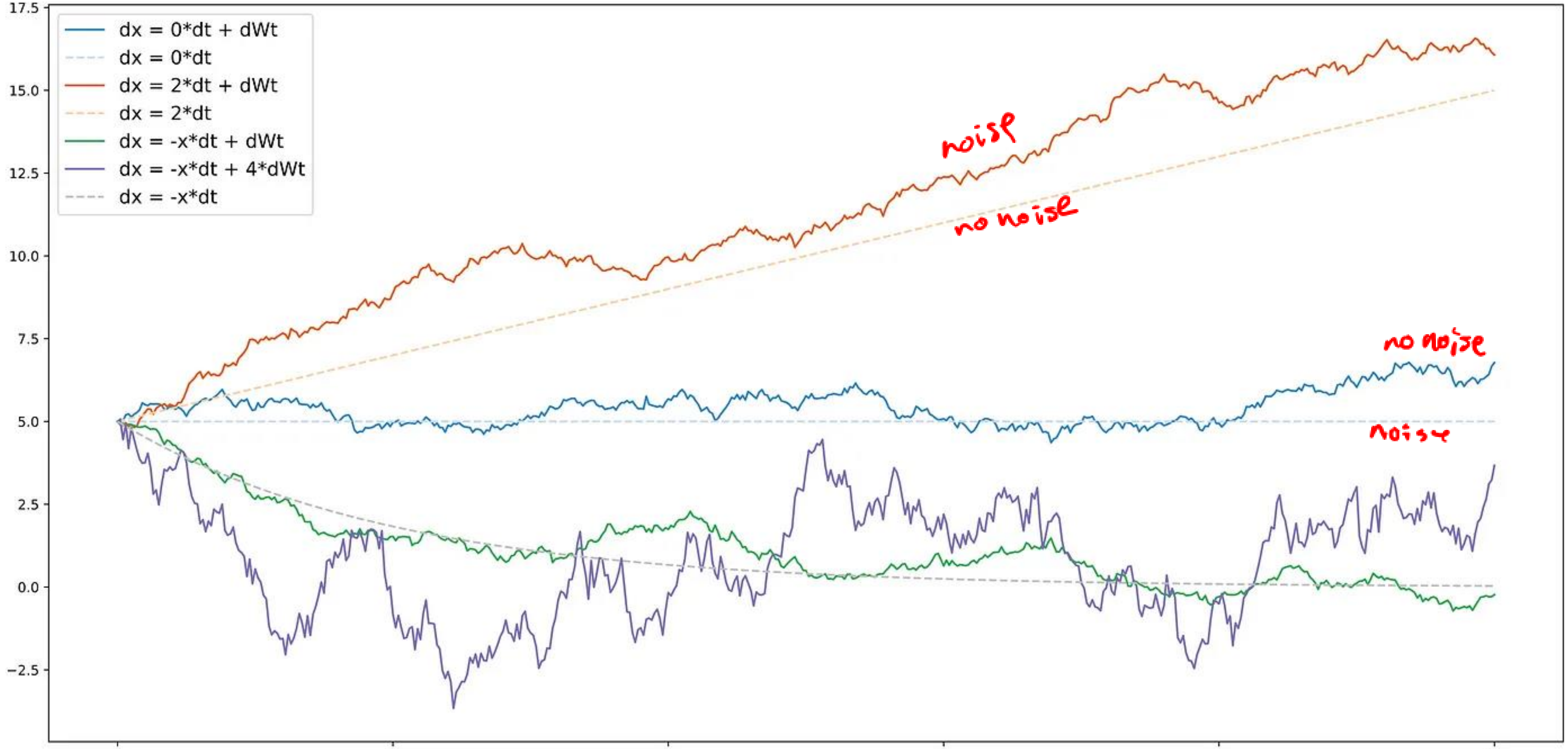
Which can also be rewritten

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

Deterministic drift term

Normal RV with std proportional to diffusion term

Diffusion process samples



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Reversed time process

If X_t is a diffusion process such that

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

← continuous time diffusion

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

backwards/reverse order

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

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

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

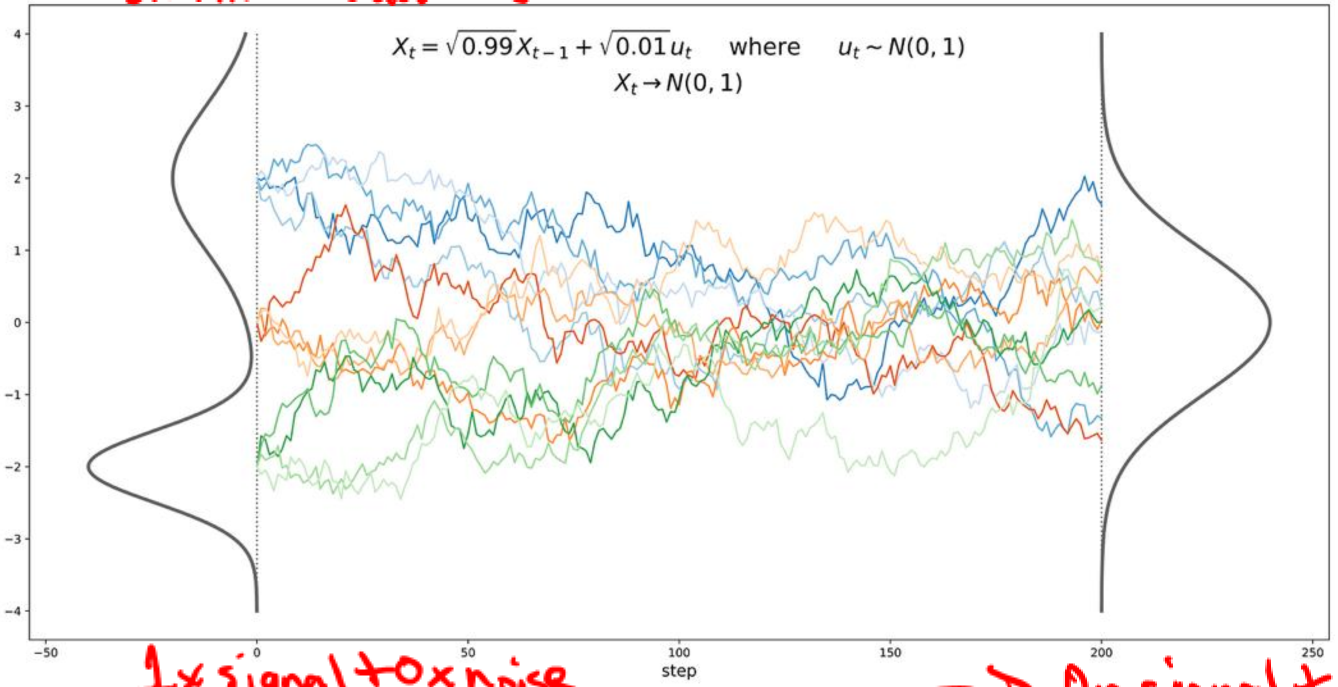
and $p(X_t)$ is the *marginal probability* of X_t

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

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

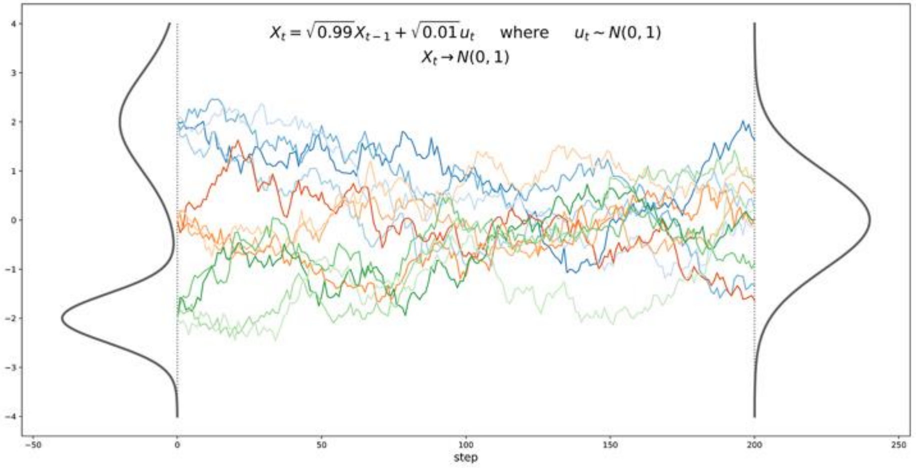


1x signal + 0x noise

→ 0x signal + 1x noise

usually $\mathcal{N}(0, I)$

Intuition behind diffusion processes



Towards Gaussian

For the diffusion process

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

After a given number of steps T we can write

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

substitute for X_{T-1}

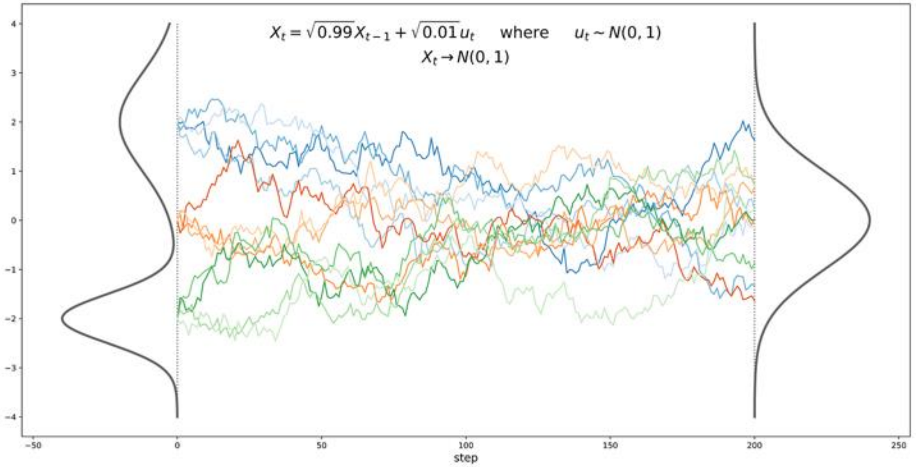
substitute for X_{T-2}

⋮

really just one normal distribution

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

After a given number of steps T we can write

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

after T steps

For number of steps T large enough, we have

$$\underbrace{(\sqrt{1-p})}_{0<\dots<1}{}^T \xrightarrow[T\to\infty]{} 0 \quad \text{and} \quad \overbrace{\underbrace{\sum_{i=0}^{T-1}\left(\sqrt{p}(\sqrt{1-p})^i\right)^2}_{\text{Variance of the gaussian}}}^{\text{Geometric series}} = p\frac{1-(1-p)^T}{1-(1-p)} \xrightarrow[T\to\infty]{} 1$$

parameters chosen to get 1 from Σ

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

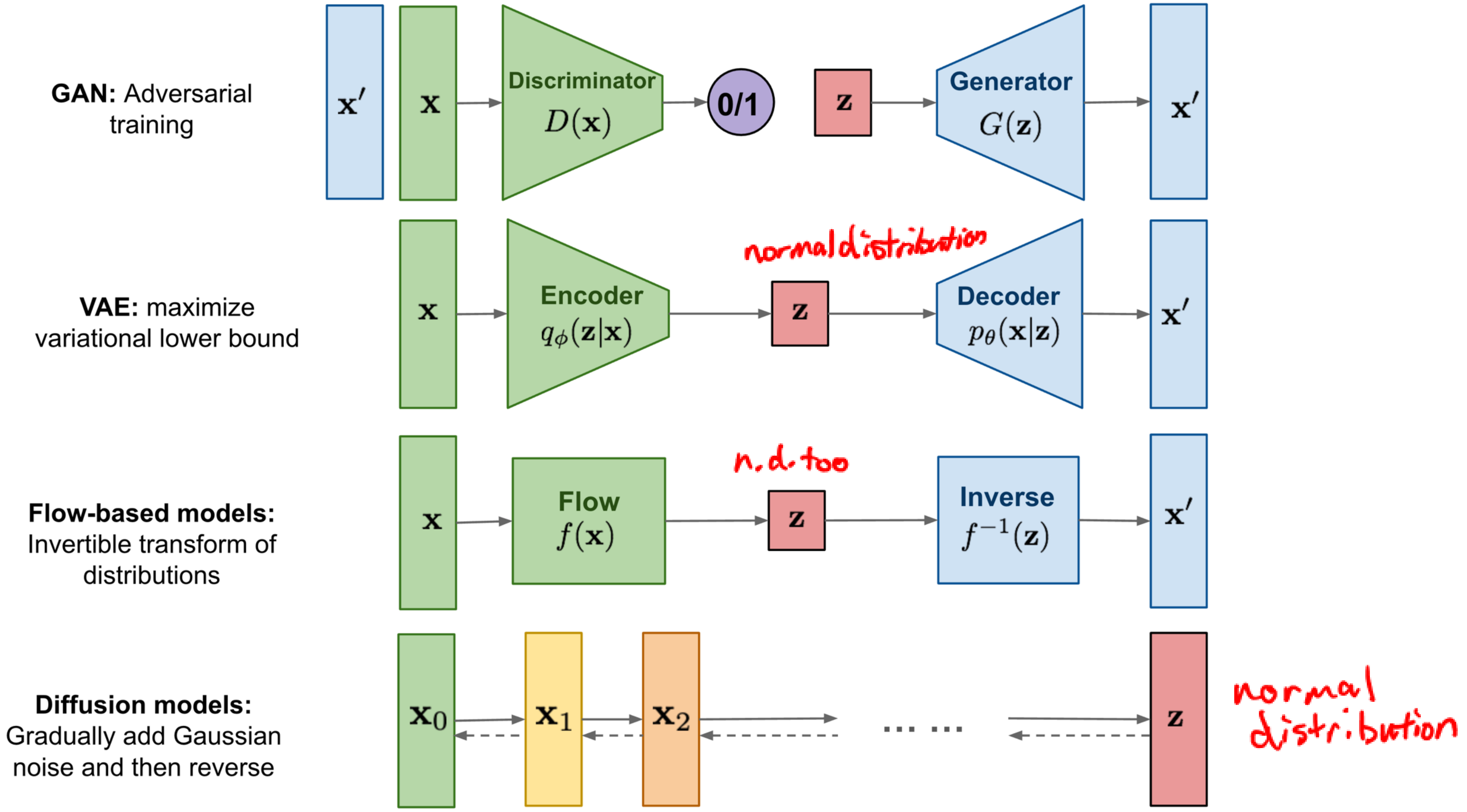
Any Questions?

???

Moving on

- Project 4
- VAE math wrap up
- Denoising autoencoders
- Error diffusion process
- Diffusion models

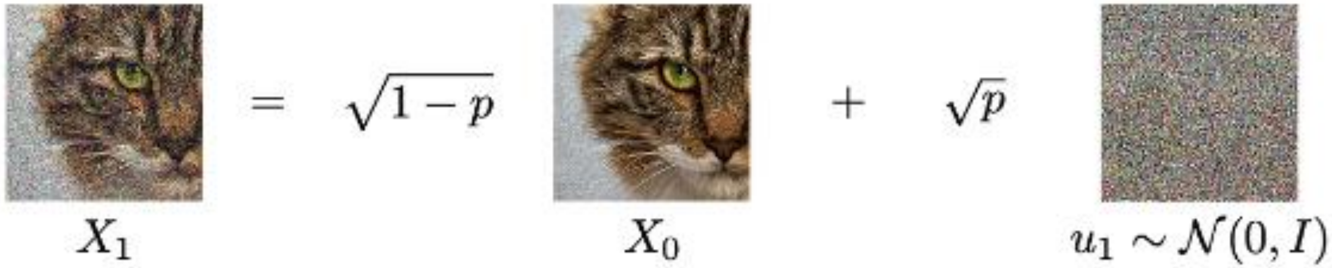
Different Generative Models



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

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



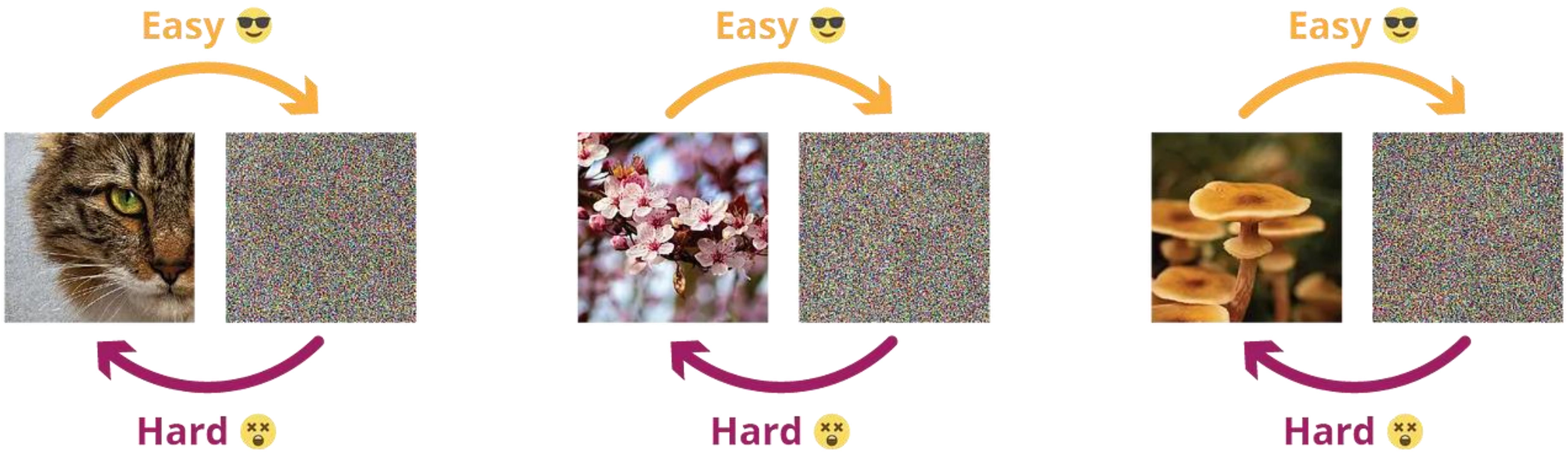
Why use diffusion?

Answer:

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

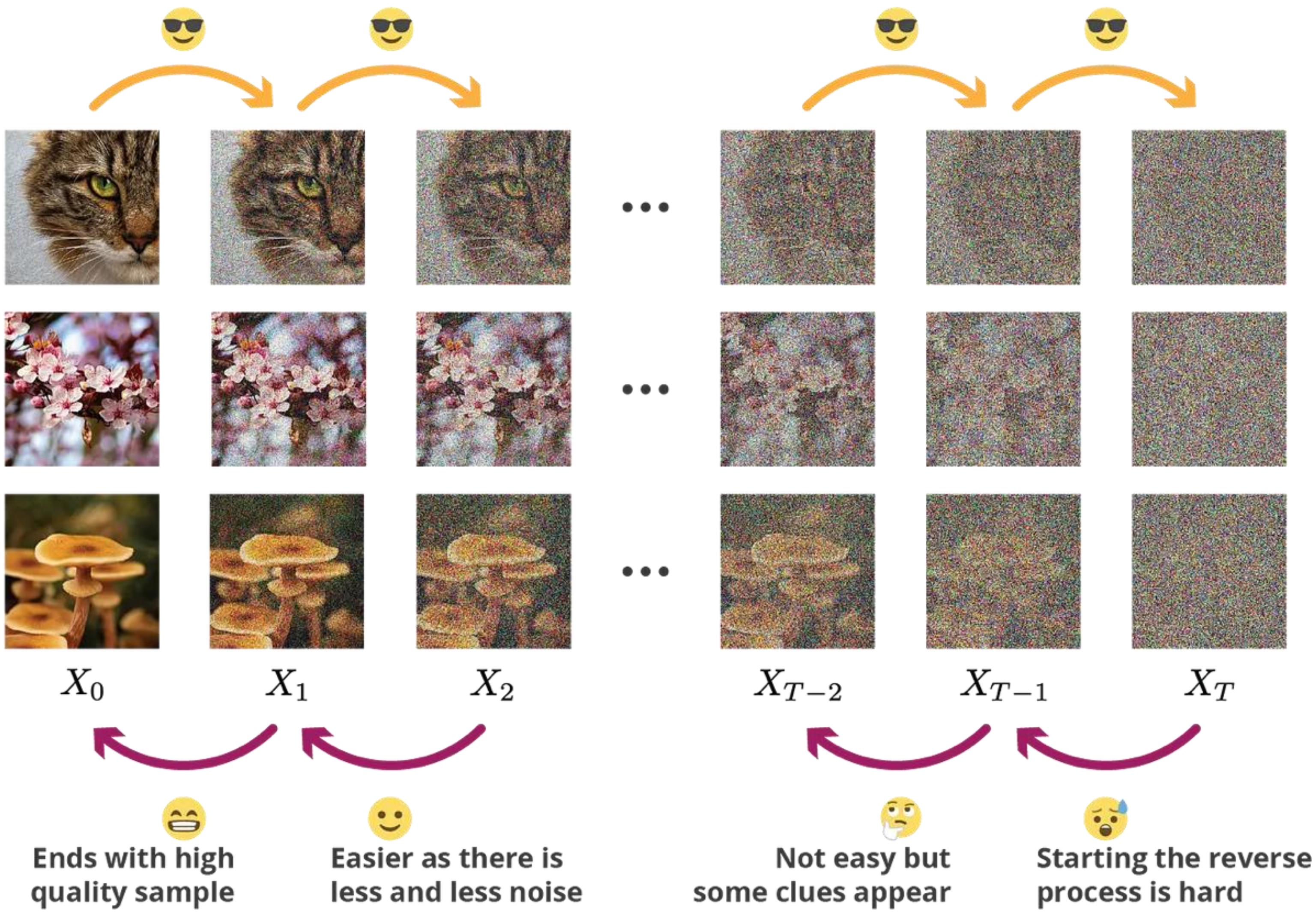
that will enable the learning of the reverse process

Intuition behind learning the reverse process



Reversing process in one step is extremely difficult.

Doing it in steps gives us some clues



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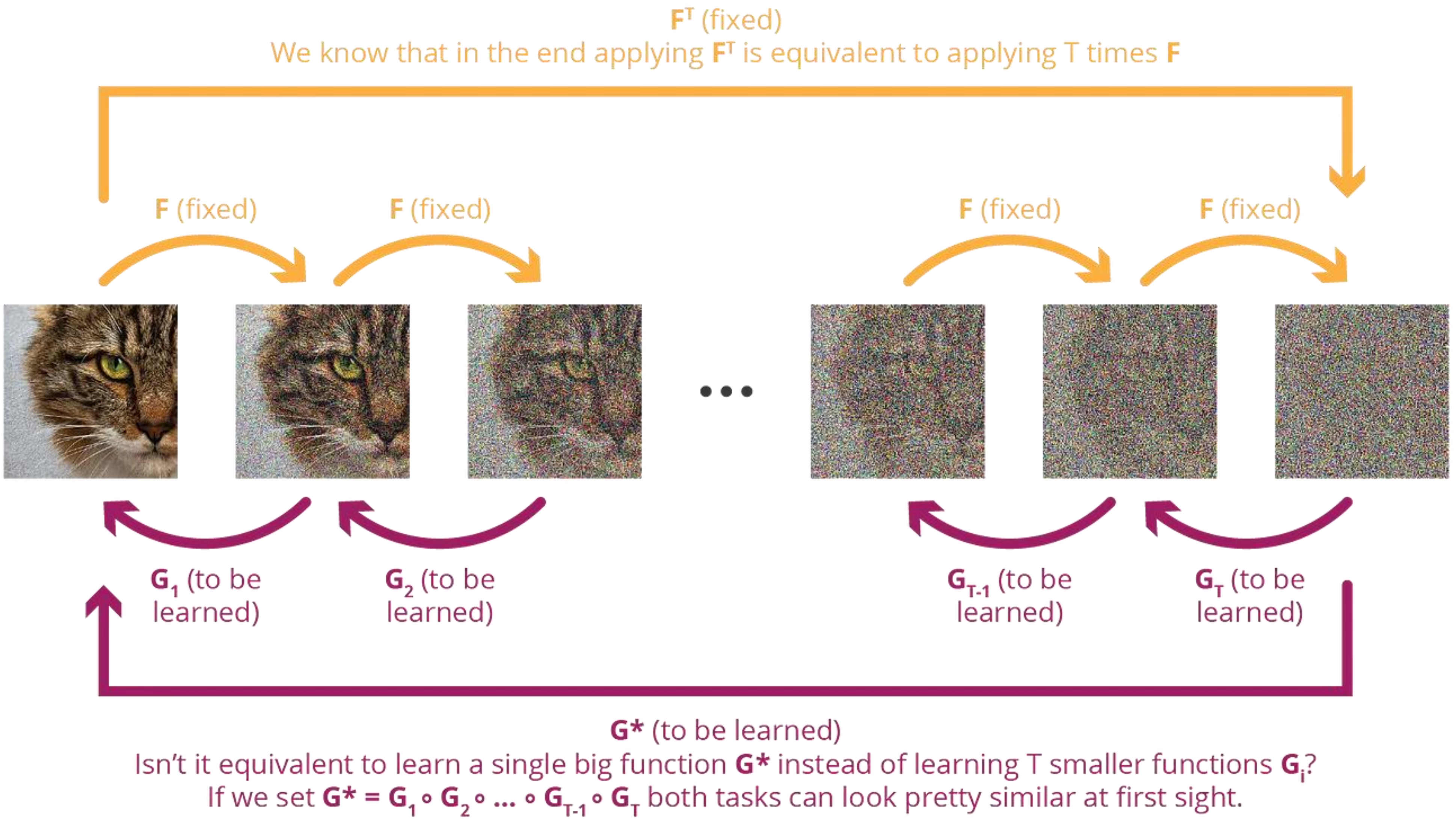
One step versus multi-step



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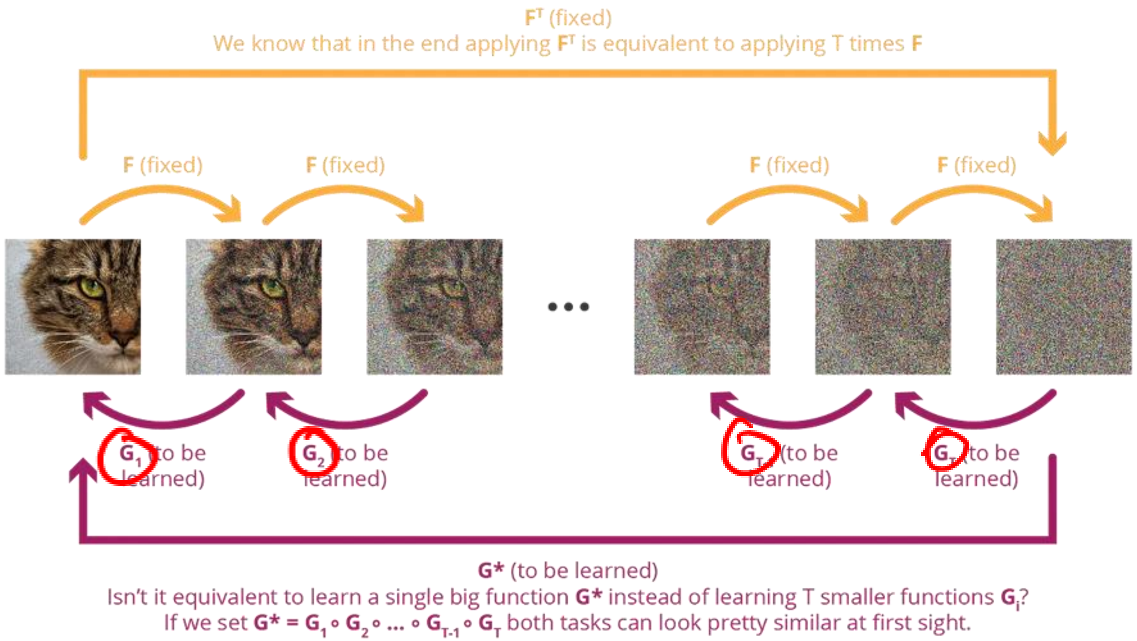
Advantage of multi-step reverse process



Learn $G_1, G_2, \dots, G_T$ vs G_T

a lot

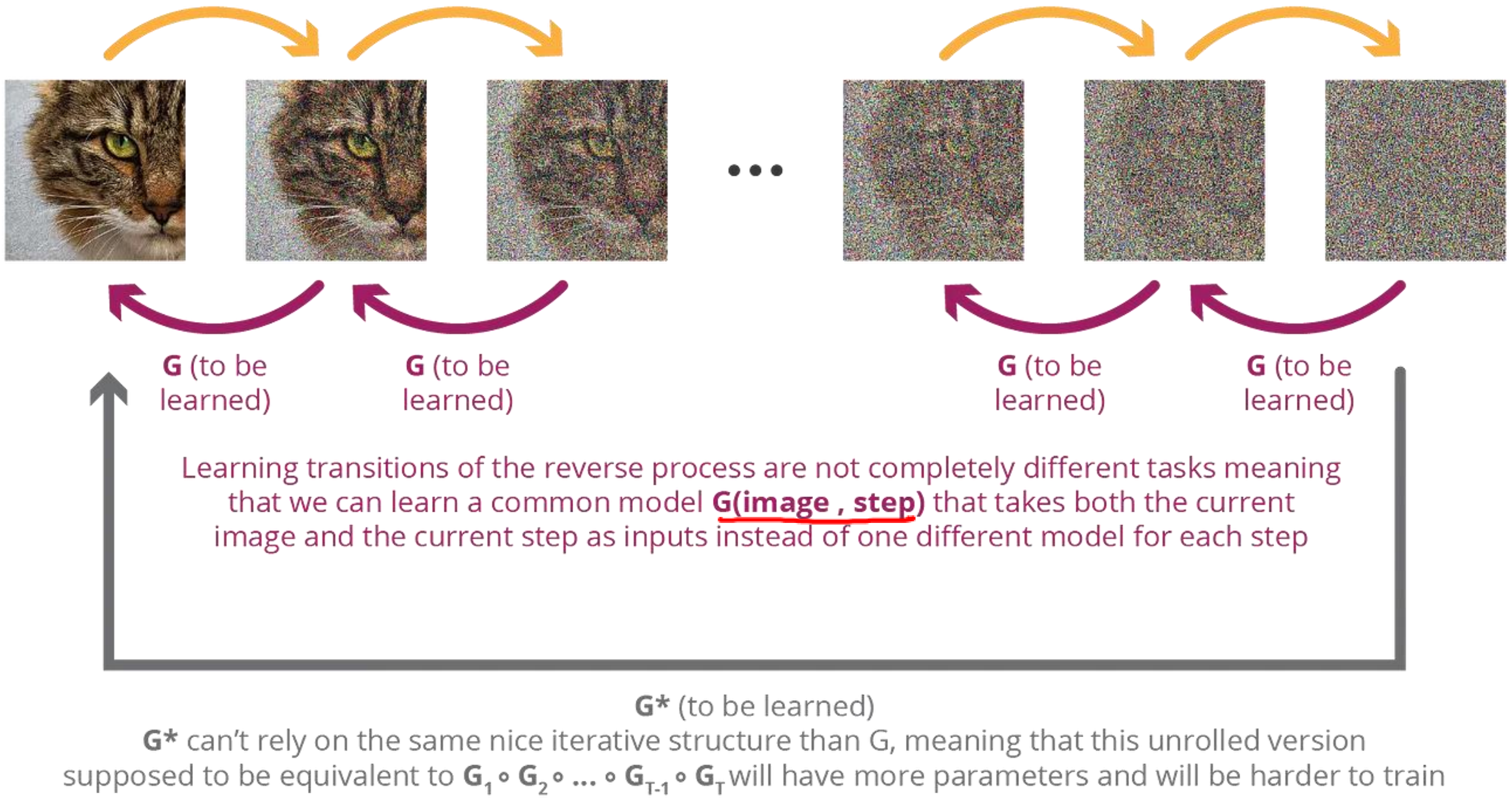
hard

Can we implement as $G(x_t, t)$?

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 the Backward Process

can vary noise per step

$(\beta_t = p)$

previous image scaled down

multivariate

x_t is normally distributed w/ mean $\sqrt{1-\beta_t}\, x_{t-1}$

+ standard deviation β_t

FIXED FORWARD PROCESS

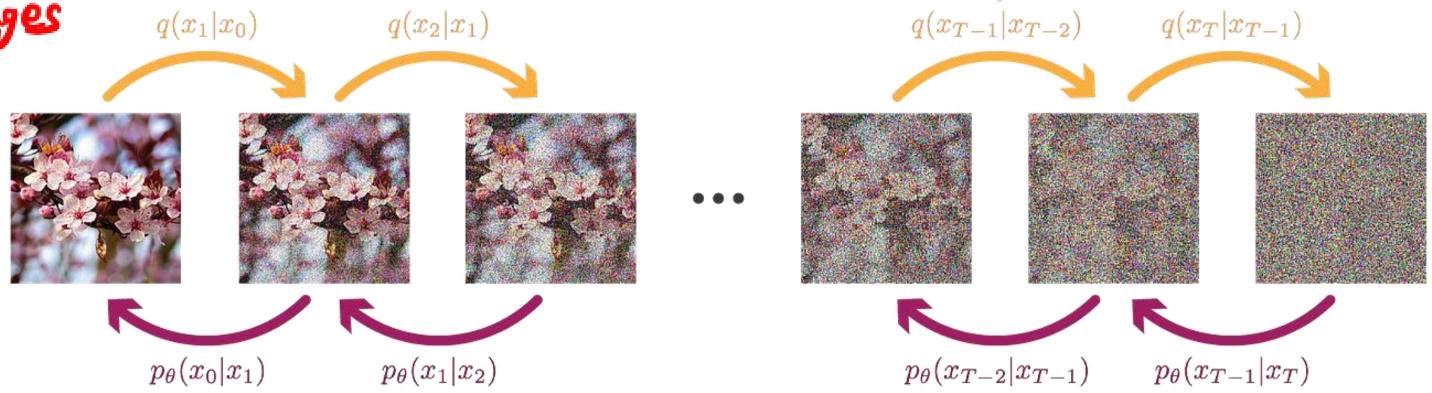
Initial distribution

$q(x_0)$

distribution of real images

Gaussian transition kernel

$$\underbrace{q(x_t|x_{t-1})}_{\text{conditional distribution based on previous step}} = \mathcal{N}(x_t; \sqrt{1-\beta_t}x_{t-1}, \beta_t I)$$



final distribution of x_T is $N(x_T;0,I)$

Approximation of

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

Gaussian transition kernel with parameters to be learned

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

noise

mean of previous x_{t-1}

conditional distribution going backwards

Initial distribution

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

LEARNED BACKWARD PROCESS

θ = model parameters

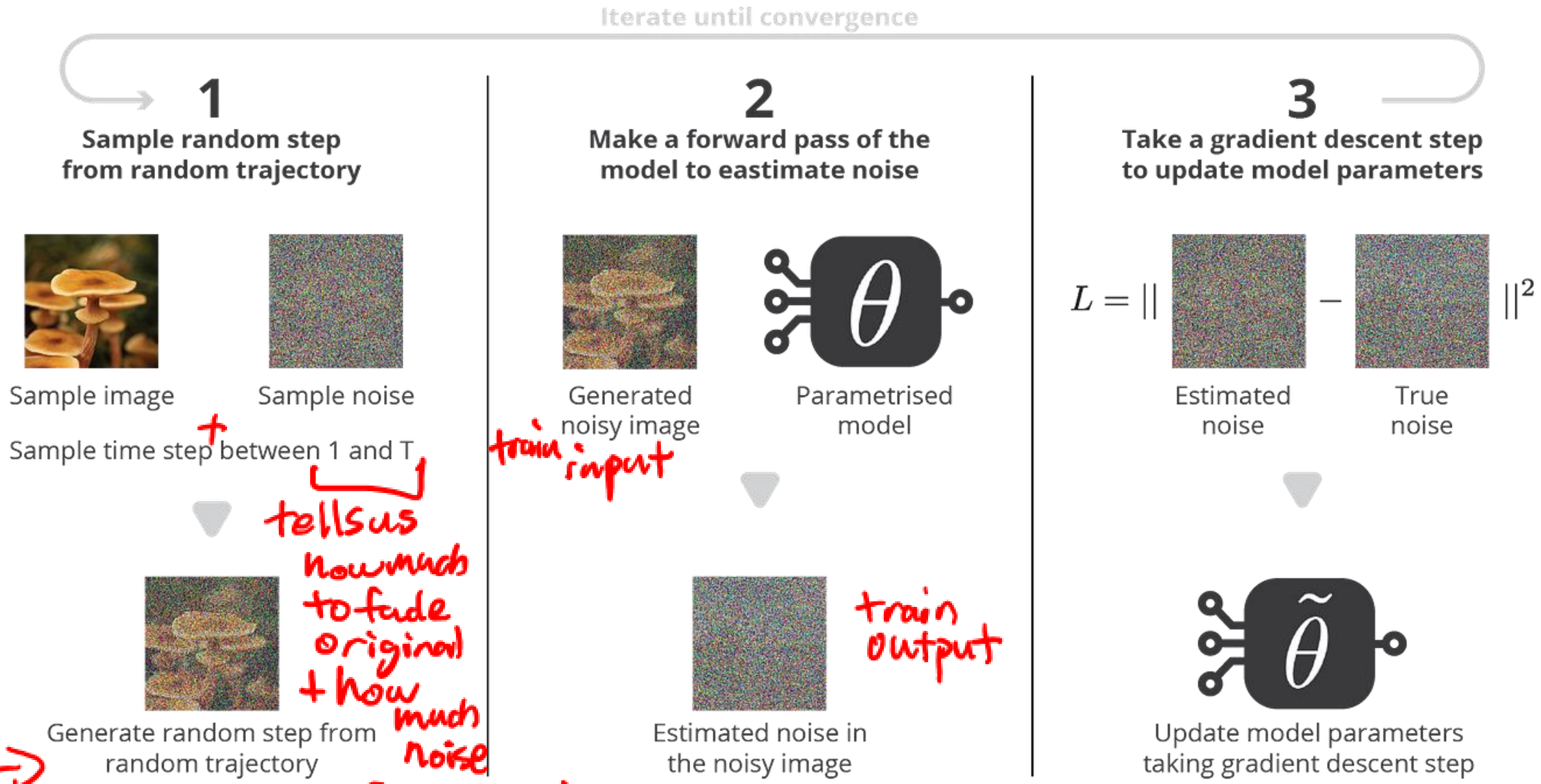
Rocca, 2022

blog walks through math

Skipping a Lot of Math…

Will sketch it next time.

Focus on Estimating the Noise



+ tells us how much to fade original + how much noise (magnitude)

train input

train output

loss function pushes noise mis-estimate to zero

Sample + steps of forward diffusion from sample image →

Rocca, 2022

Training

Algorithm 1 Training

repeat

$x_0 \sim q(x_0)$ training image ▷*Sample random initial data*

$t \sim \text{Uniform}(\{1, ..., T\})$ ▷*Sample random step*

$\epsilon \sim \mathcal{N}(0, I)$ ▷*Sample random noise*

$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon$ fast forward t steps ▷*Rand. step of rand. trajectory*

Take gradient descent step on $\nabla_\theta || \epsilon - \underbrace{\epsilon_\theta(x_t, t)}_{\text{estimate noise}} ||^2$ ▷*Optimisation*

until converged

calculate gradient of loss from noise estimate

precalculated from β_t's

Output: noise estimator taking in (x_t, t)

Sampling

Algorithm 2 Sampling

1: $x_T \sim \mathcal{N}(0, I)$ final noise distribution ▷*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: $\tilde{\epsilon} = \epsilon_\theta(x_t, t)$ estimate noise ▷*Estimated noise in current noisy data*
5: $\tilde{x_0} = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1 - \bar{\alpha}_t}\tilde{\epsilon})$ estimate original x ▷*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: $x_{t-1} = \boxed{\tilde{\mu}} + \sigma_t z$ ▷*Previous step sampling*
8: **end for**
move toward estimate, but not all the way.
9: **return** x_0

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Why Not One Step Reversal?

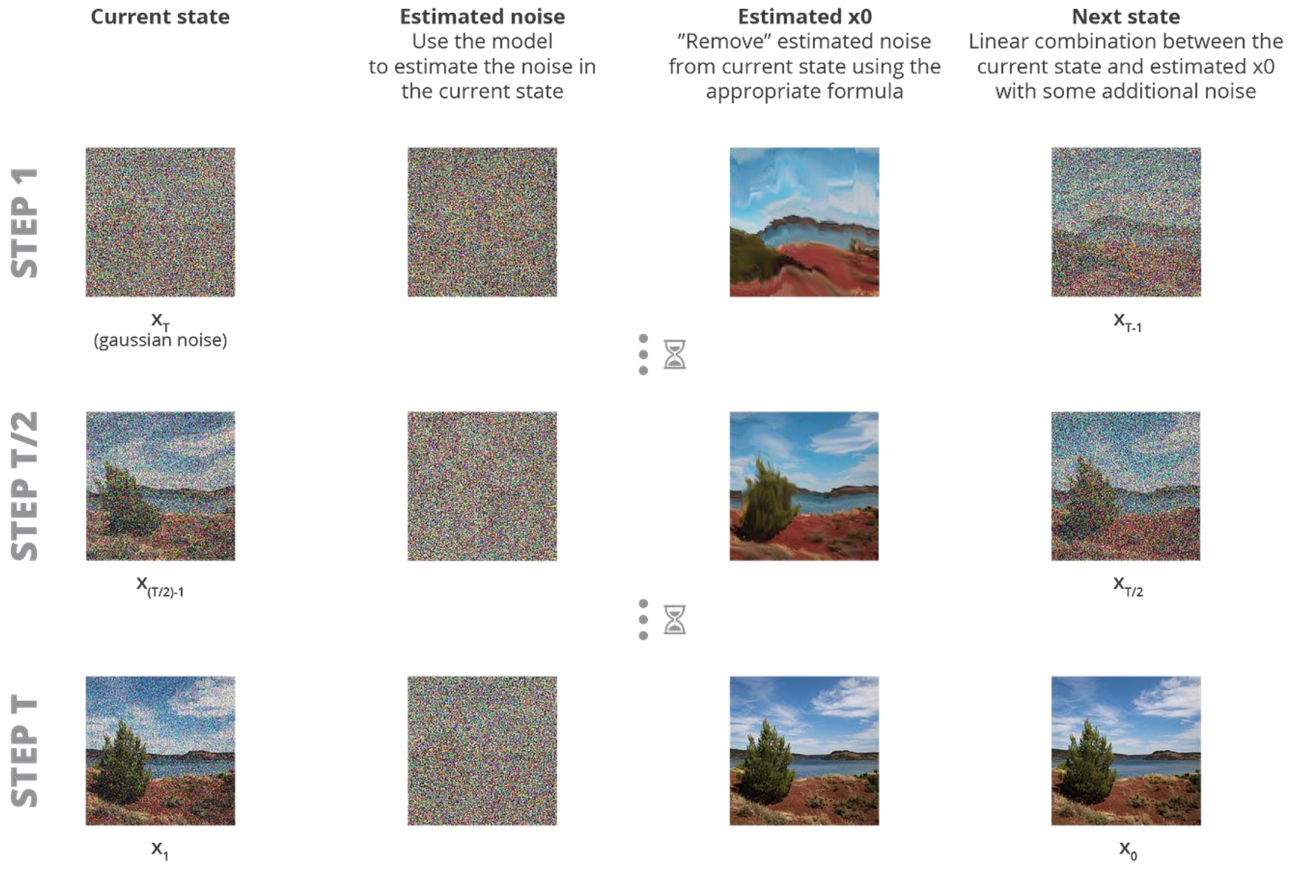
- Because we don't think that our model was actually good enough to reverse the whole thing at once.

hubris –
can't map pure noise
to clean image directly.

- Remember, the noise terms are larger than the signal terms when we start this process!

Sampling Example

start



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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 size as input, as opposed to VAE which reduces dimensionality

next improvement is ~~diffusions~~ diffusion in small latent space.

Diffusion Model from Scratch

- HuggingFace Notebook
- https://github.com/huggingface/diffusion-models-class

Any Questions?

???

Moving on

- Project 4
- VAE math wrap up
- Denoising autoencoders
- Error diffusion process
- Diffusion models