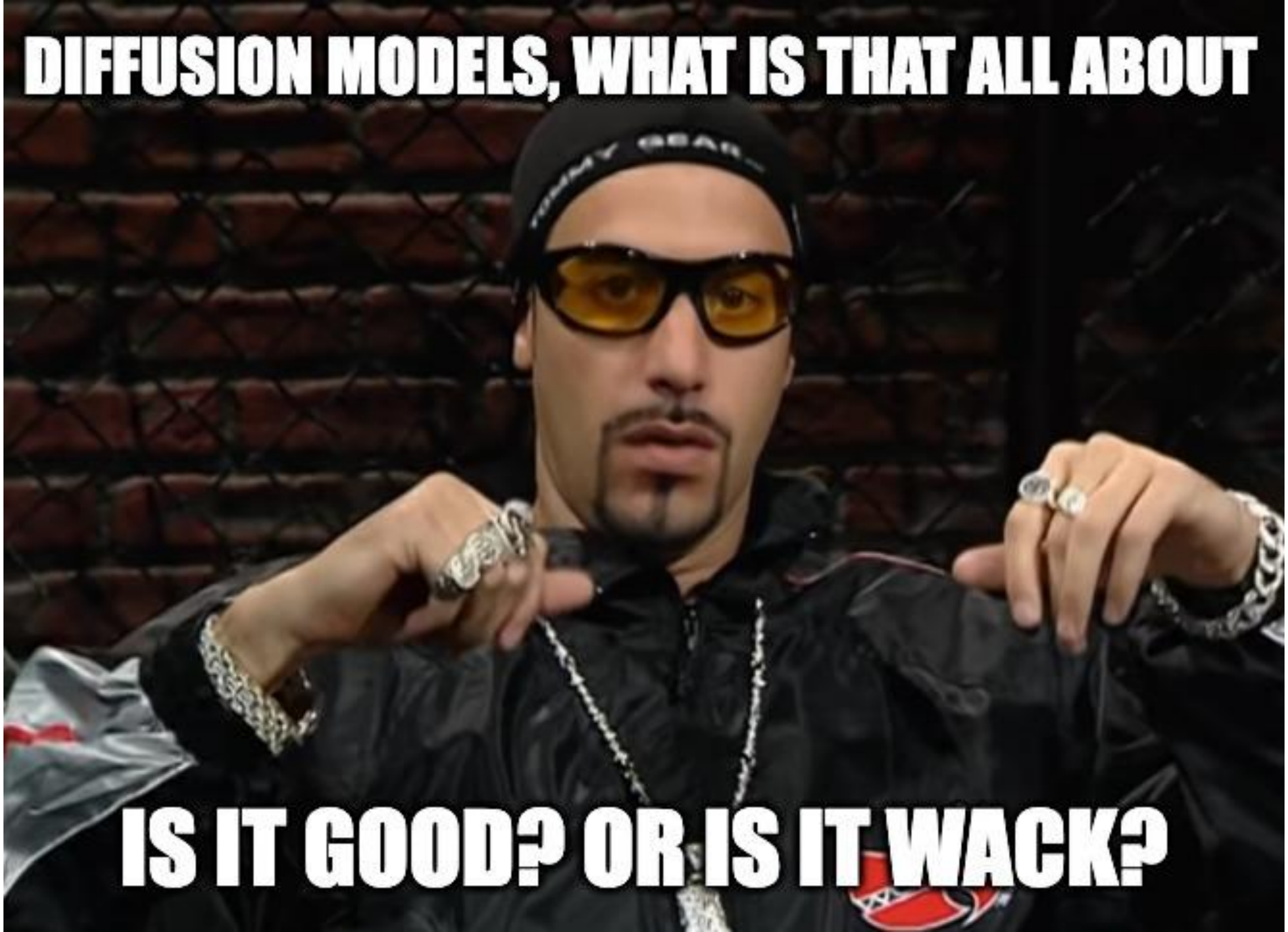

DIFFUSION MODELS, WHAT IS THAT ALL ABOUT
IS IT GOOD? OR IS IT WACK?

About Me

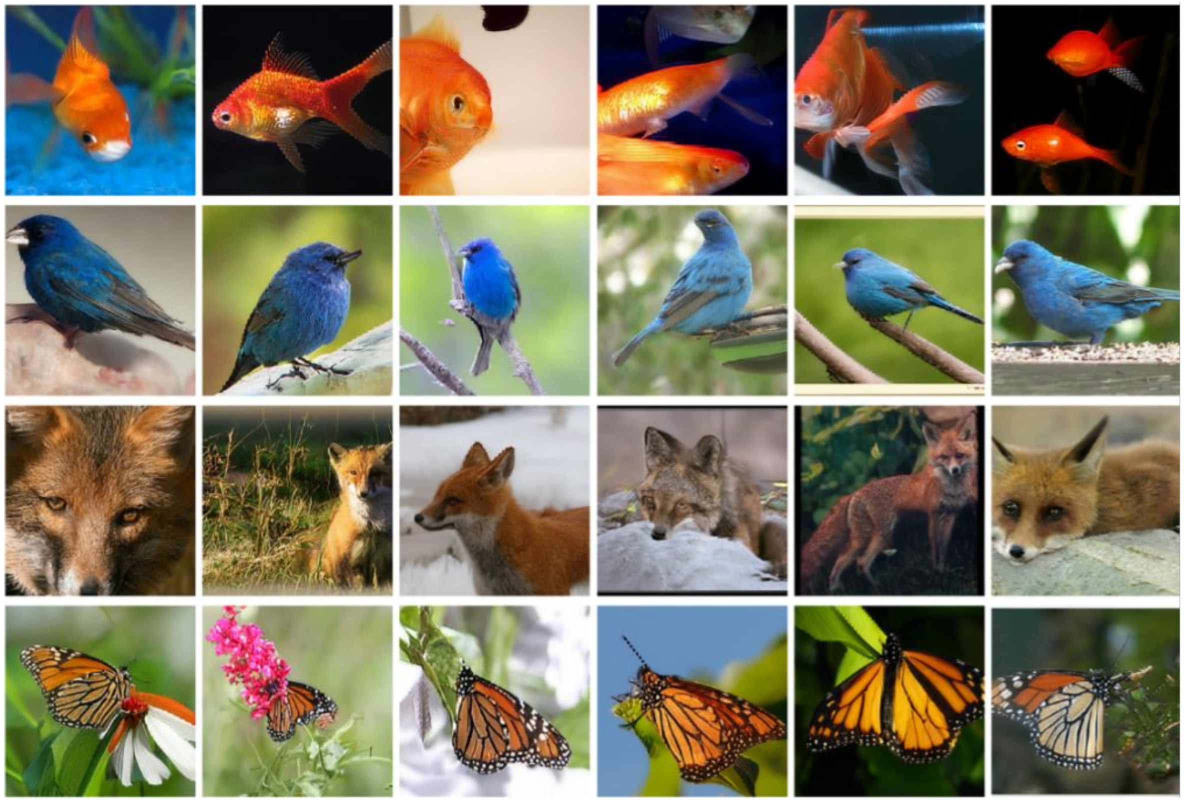
I'm Calvin, a 3rd year PhD student here at Brown, advised by Chen Sun

- I work on Diffusion Modeling and Reinforcement Learning

Diffusion models are really good at learning conditional distributions.

$$p(x \mid y)$$

Use Case: Class-Conditioned Generation $p(image \mid class\_label)$



source: [Image Super-Resolution via Iterative Refinement]

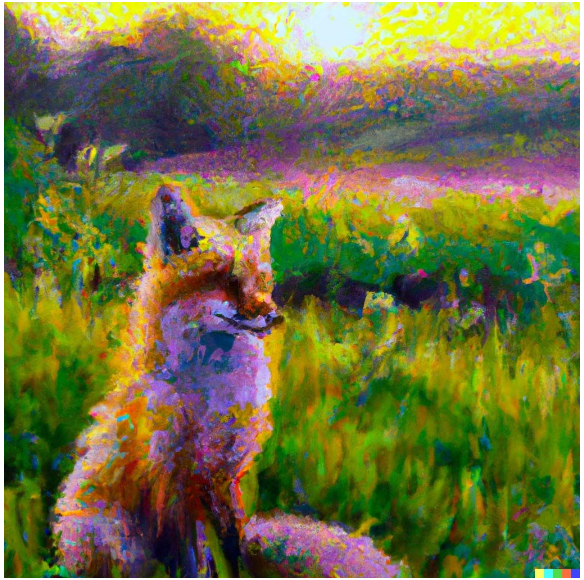
Use Case: Text-to-Image Generation

$p(image \mid text\_caption)$

"a painting of a fox sitting in a field at sunrise in the style of Claude Monet"

Parti (but pretend it is ImageN)

StableDiffusion

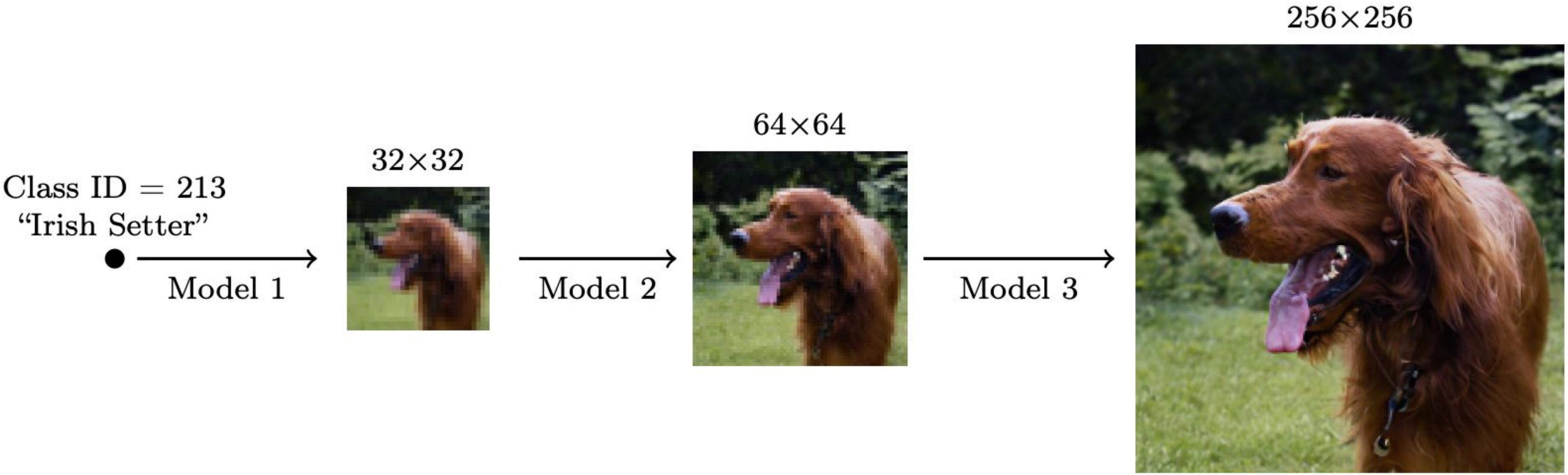


Dall-E 2.0

source: ImageN, StableDiffusion, Dall-E 2.0

Use Case: Super Resolution

$p(image \mid low\_res)$



source: [Cascaded Diffusion Models]()

Recap: Generative Modeling

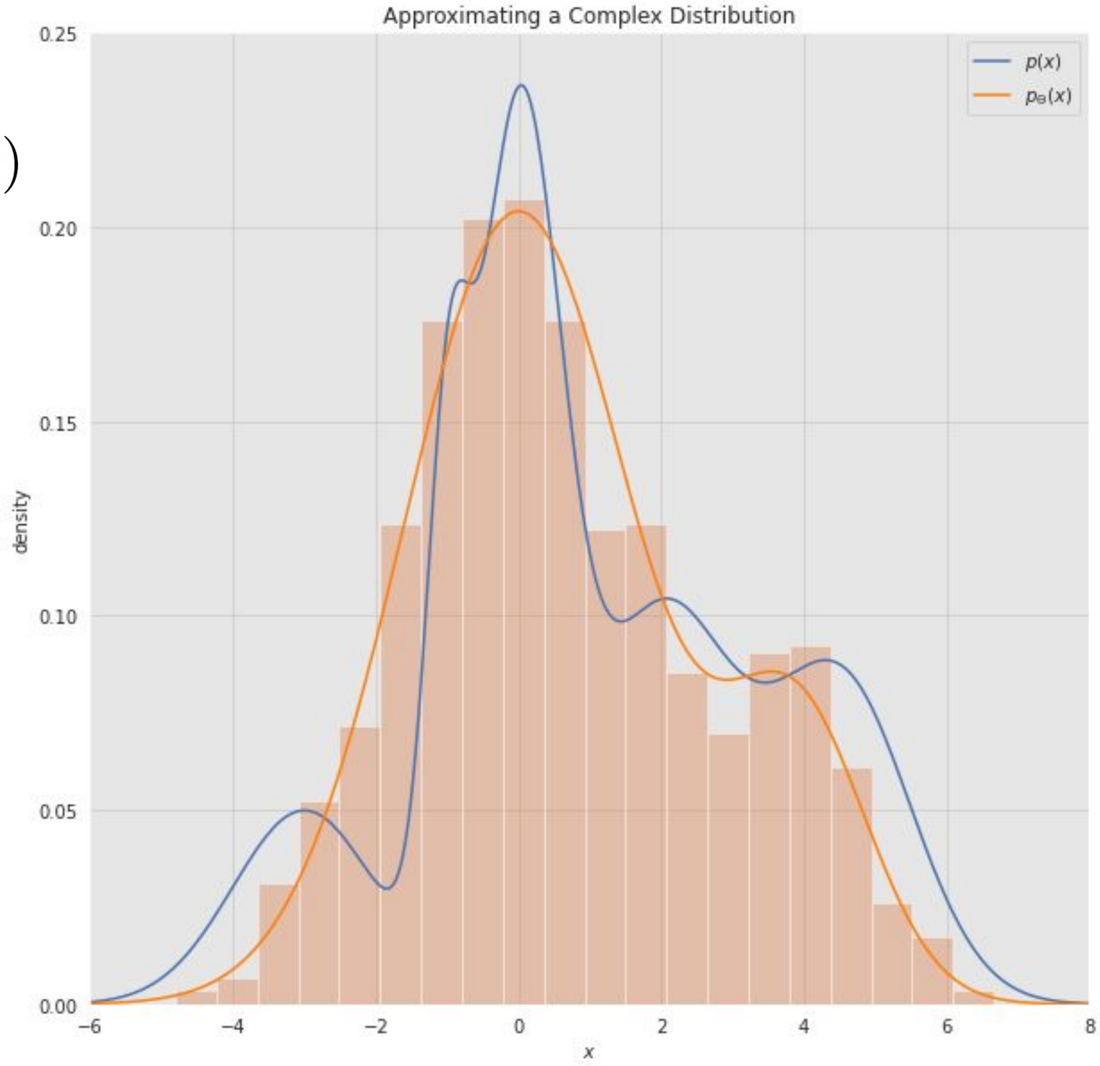
Recall the goal of generative modeling - learning a *model* of a distribution from which we can *generate* new samples.

Given $\boldsymbol{x} \sim p(\boldsymbol{x})$ we might want to learn $p_\theta(\boldsymbol{x}) \approx p(\boldsymbol{x})$ (*modeling*)

Then, we can generate new samples $\boldsymbol{x}^* \sim p_\theta(\boldsymbol{x})$ (*generation*)

Why is this useful?

Given $\boldsymbol{x} \sim p(\boldsymbol{x})$



Generative Modeling: Themes

What are some common themes of generative modeling?

- We want to learn some **complex** distribution $p_\theta(\boldsymbol{x}) \approx p(\boldsymbol{x})$
- But we only have access to some **simple** distributions (such as Gaussians)

Generative Modeling: Themes

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Idea: Let's learn a complex function (aka a neural network) to transform a simple distribution sample into a complex one!

- Gaussian Sample ==(neural net)==> Data Sample

Generative Modeling: Themes

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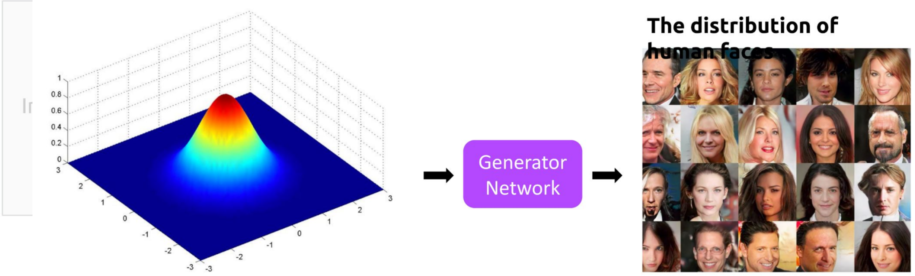
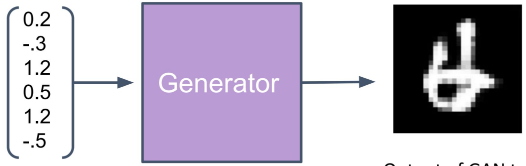
- Gaussian Sample ==(neural net)==> Data Sample

You have seen this before in:





Random Vector (sampled from unit normal distribution)

Output of GAN trained on MNIST images

Diffusion Models: a TLDR

An observation: adding steady amounts of Gaussian noise eventually corrupts an image into something indistinguishable from a random Gaussian sample.

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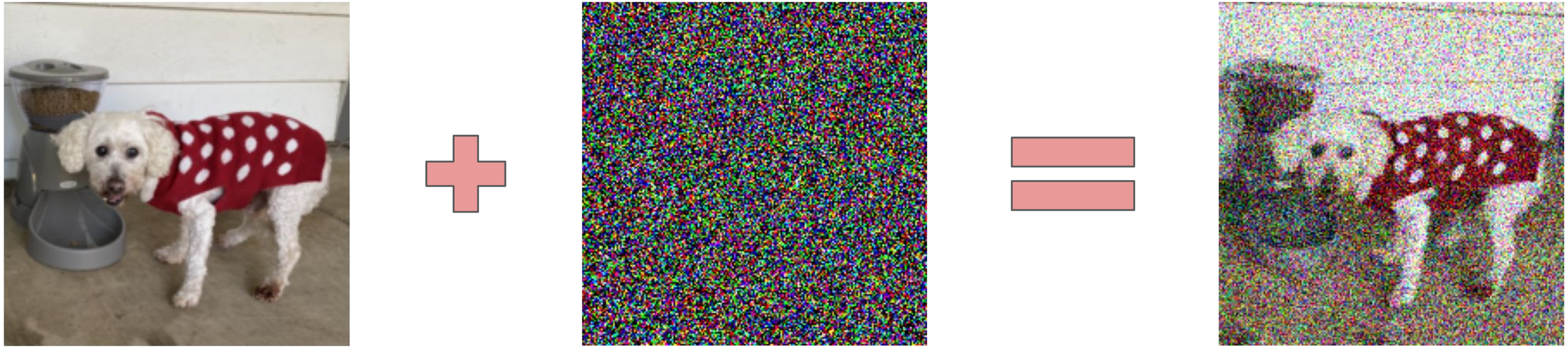

One Step

Diffusion Models: a TLDR

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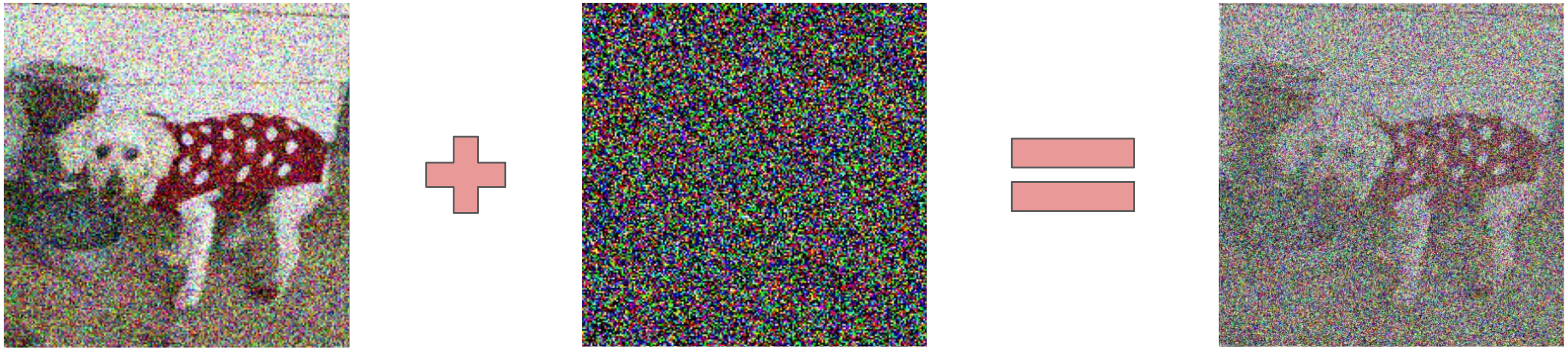


Another Step

Diffusion Models: a TLDR

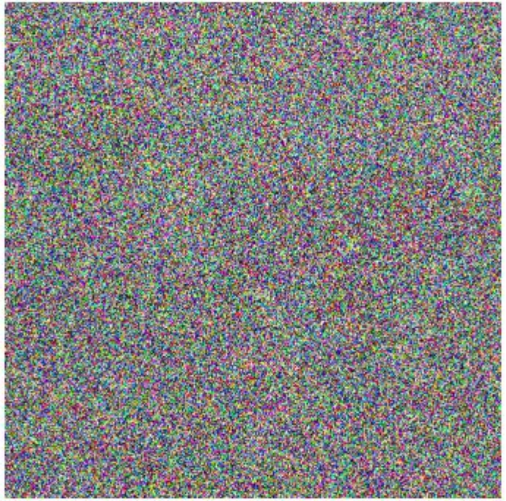
An observation: adding steady amounts of Gaussian noise eventually corrupts an image into something indistinguishable from a random Gaussian sample.

Many Steps

Diffusion Models: a TLDR

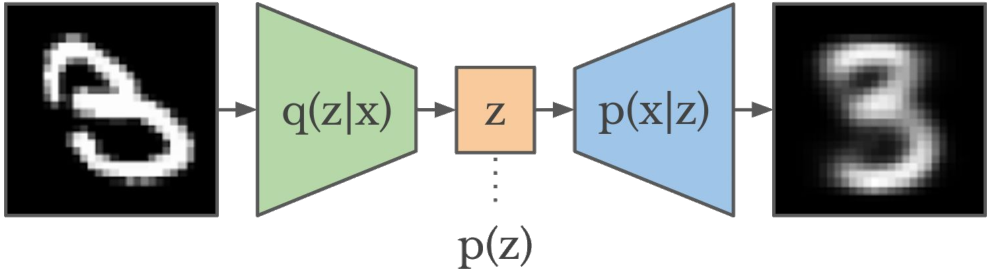
An observation: adding steady amounts of Gaussian noise eventually corrupts an image into something indistinguishable from a random Gaussian sample.

- Diffusion models simply learn to **reverse** this procedure over many timesteps



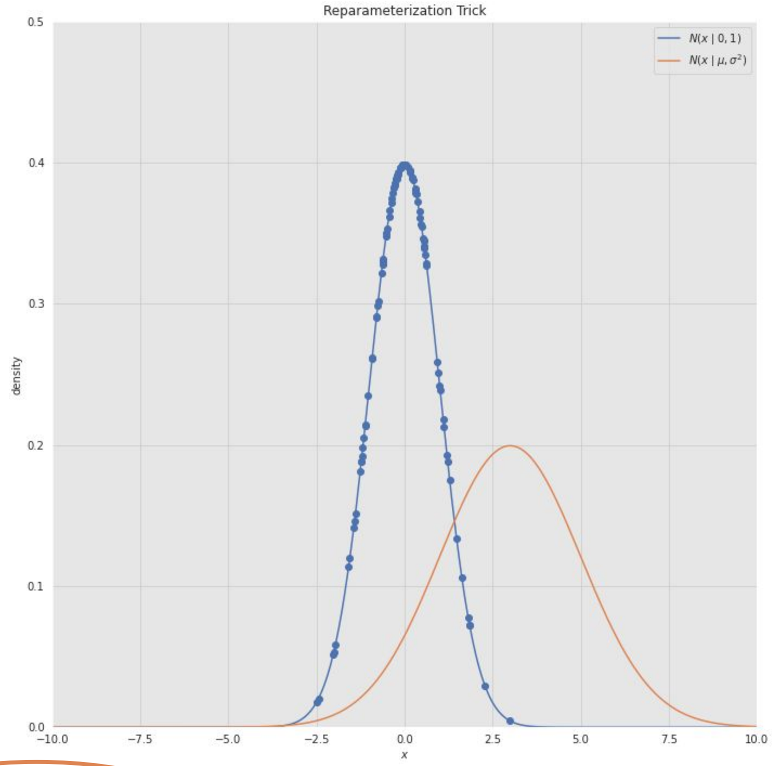
Recap: Variational Autoencoders

Visually, we often see a VAE as:



How do we perform backpropagation through samples?

Recap: Reparameterization Trick



For $x \sim \mathcal{N}(x \mid \mu, \sigma^2)$, ϵ , where $\epsilon \sim \mathcal{N}(x \mid 0, \mathrm{I})$

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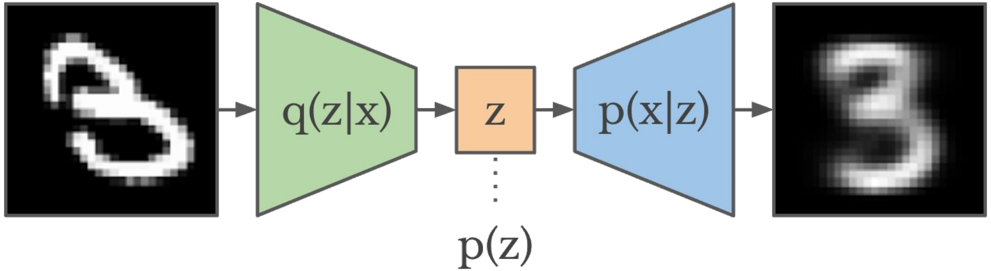
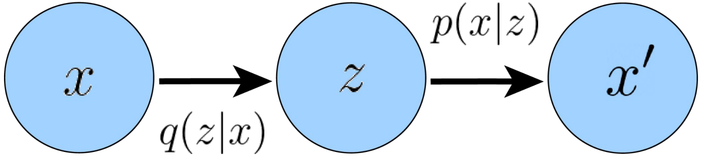


Or as:



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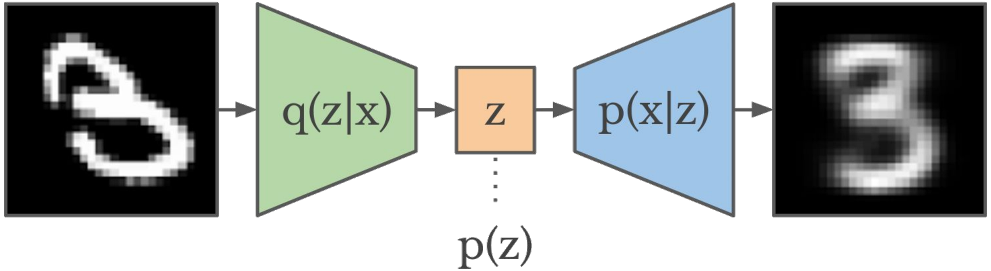

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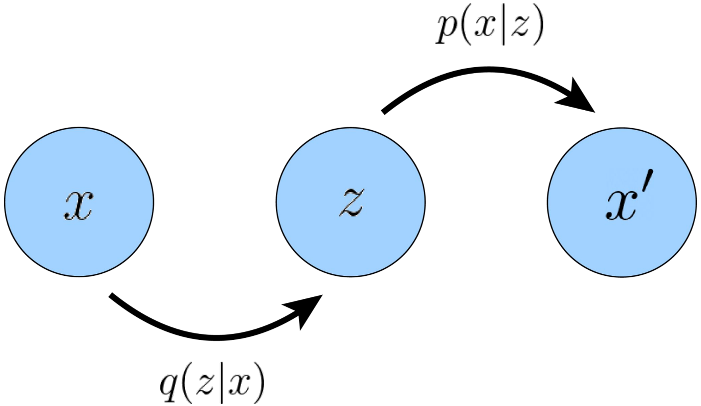

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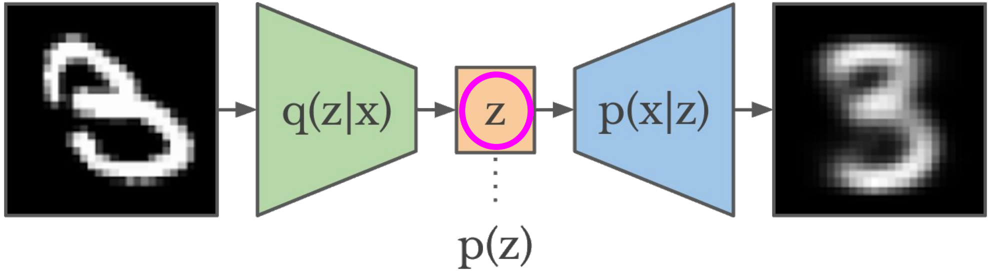

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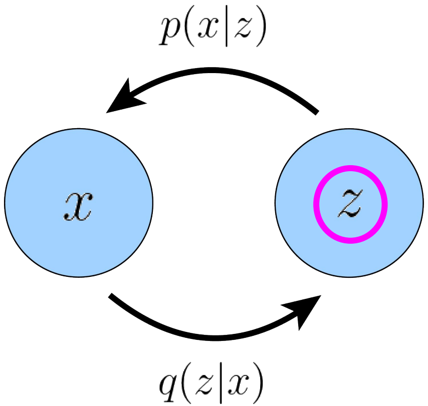
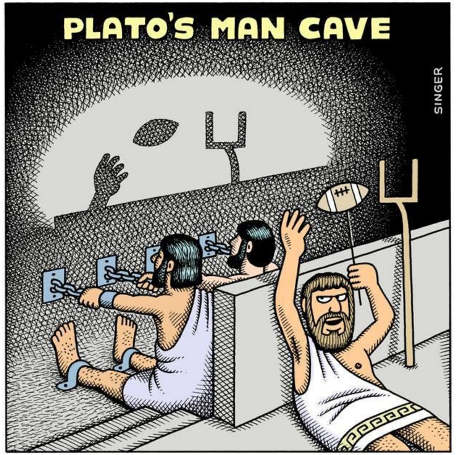


…but what's the intuition behind what is learned?

Generative Modeling with Latent Variables

Given $\boldsymbol{x} \sim p(\boldsymbol{x})$ we might want to learn $p_\theta(\boldsymbol{x}) \approx p(\boldsymbol{x})$ (*modeling*)

What if we assume latent variables $\boldsymbol{z}$ exist?



Elon has an idea…

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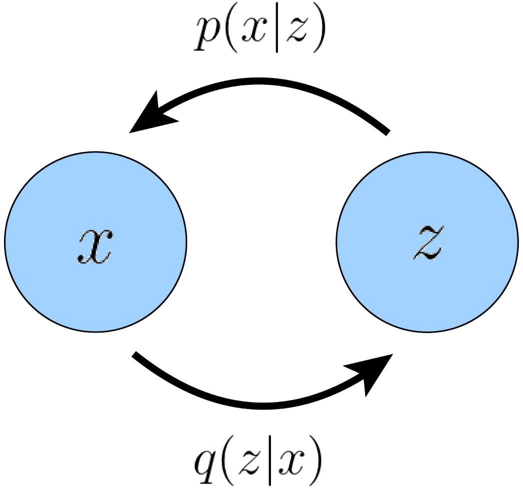
Hierarchical VAEs

Generalize VAEs by enabling a hierarchy of latents $z = z_1, ...z_T$

This is essentially learning a bunch of stacked VAEs



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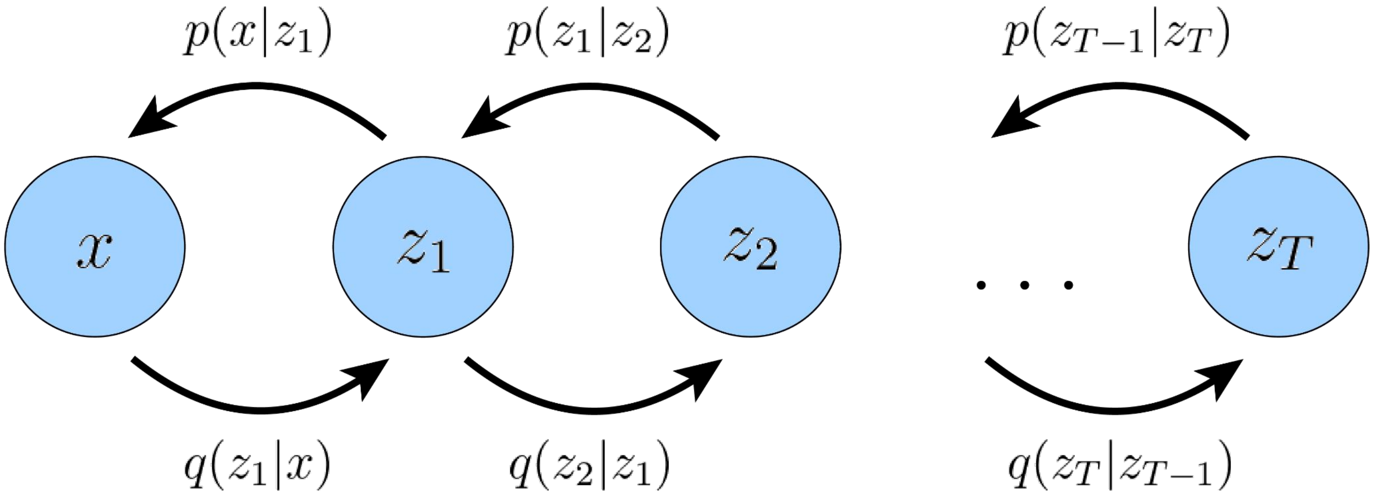
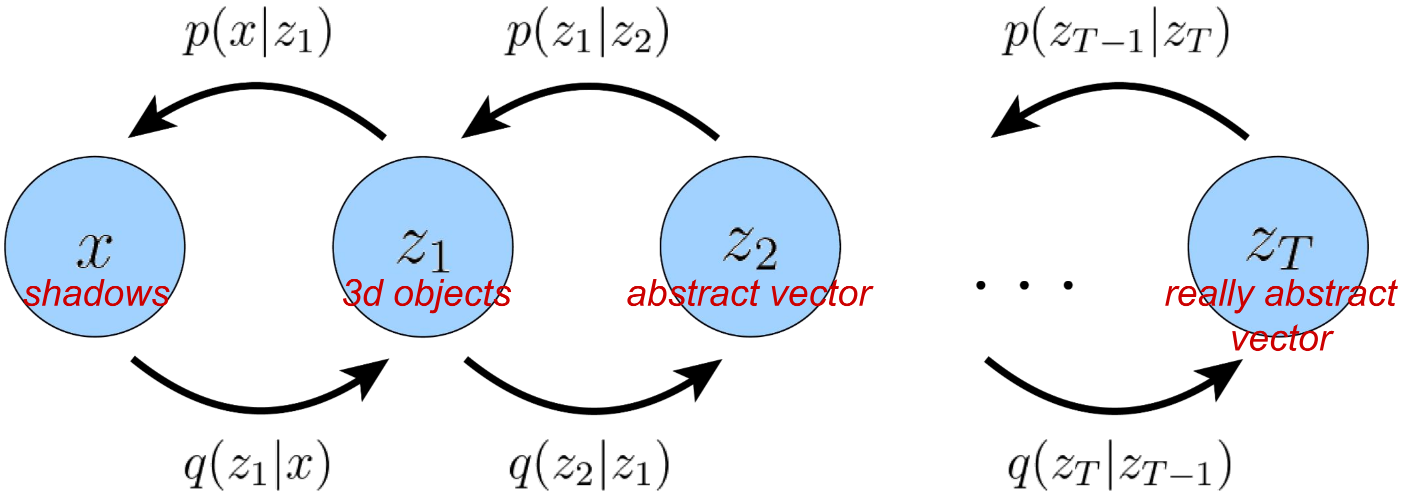


Disclaimer: Elon did not actually come up with this idea.

Hierarchical VAEs

Let's think like a caveman…



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- In a VAE we learn two networks: an encoder and a decoder.
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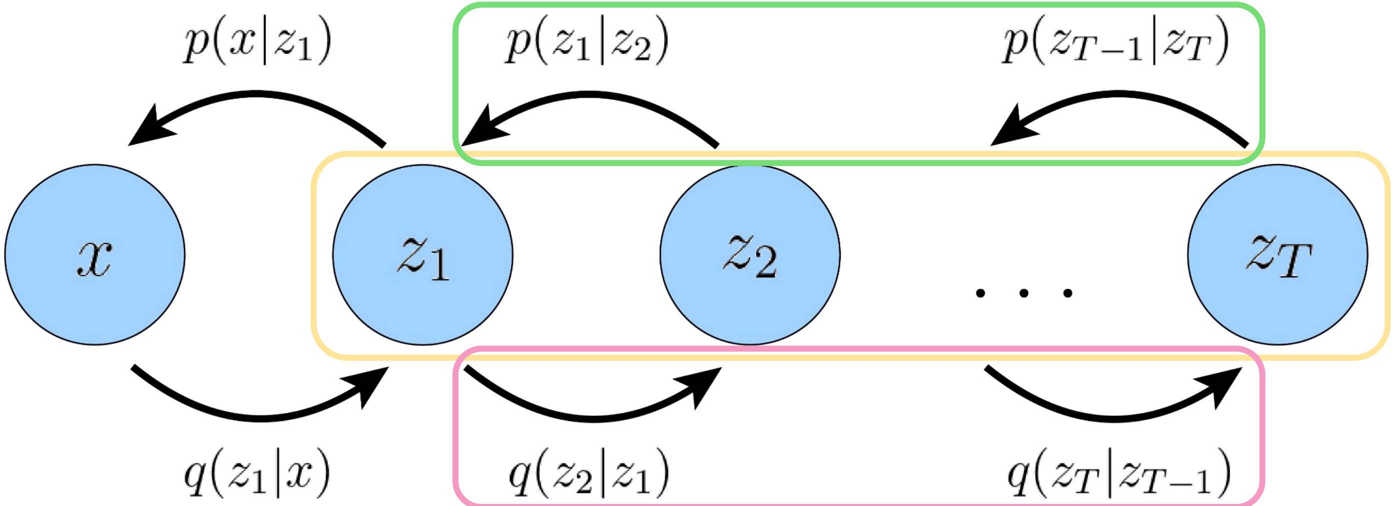
…what if we assume all latent dimensions are the same?



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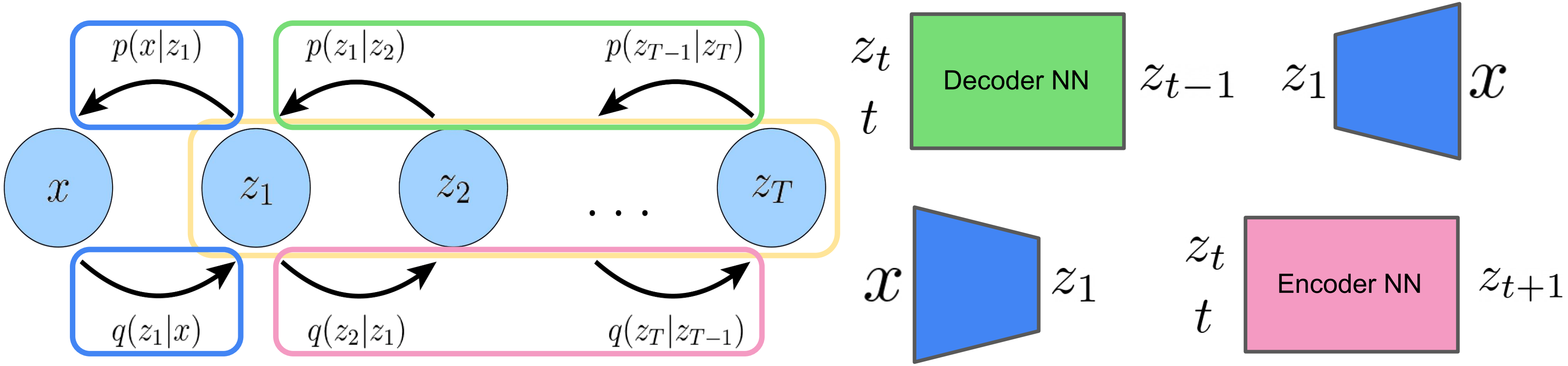

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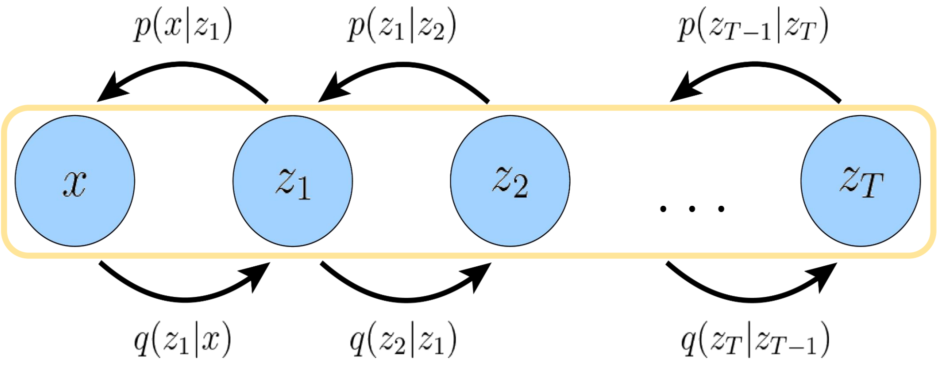

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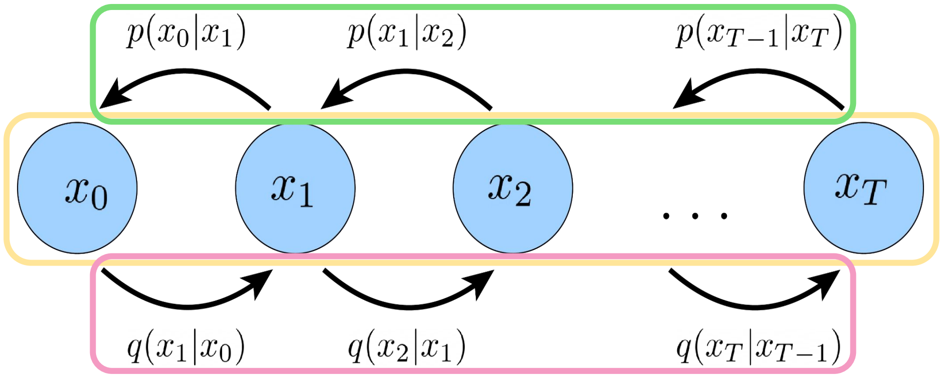

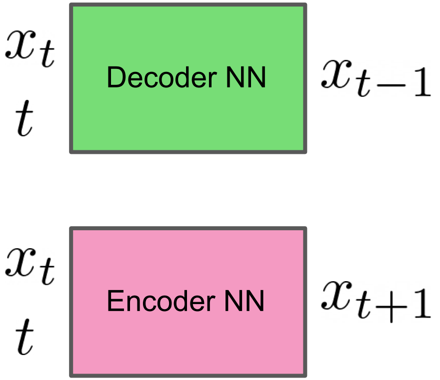

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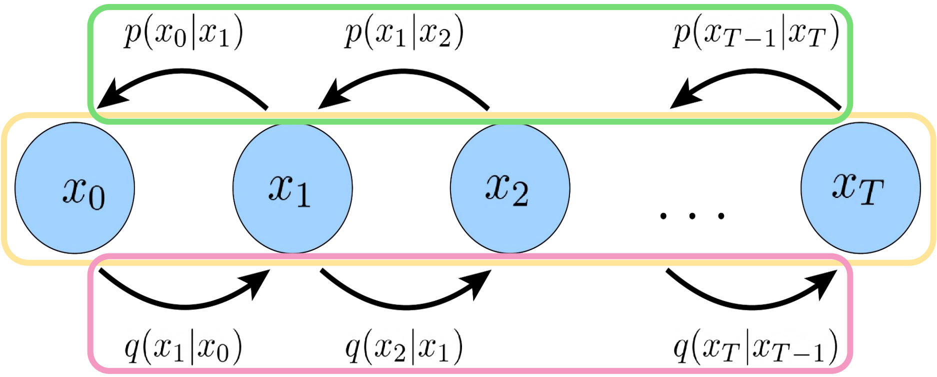

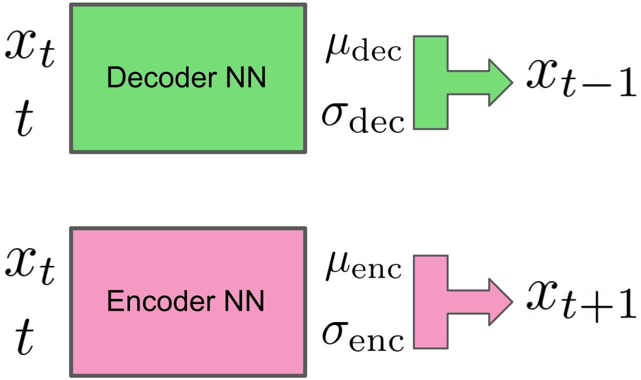

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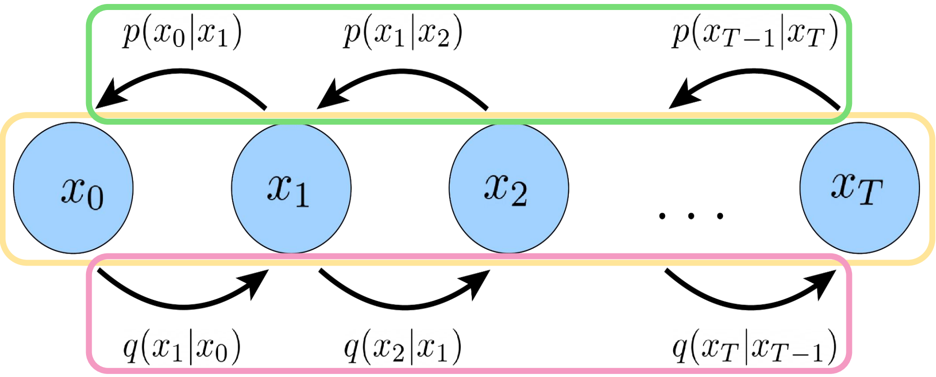
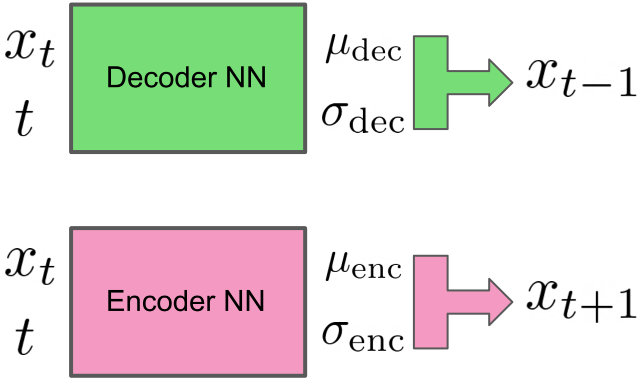
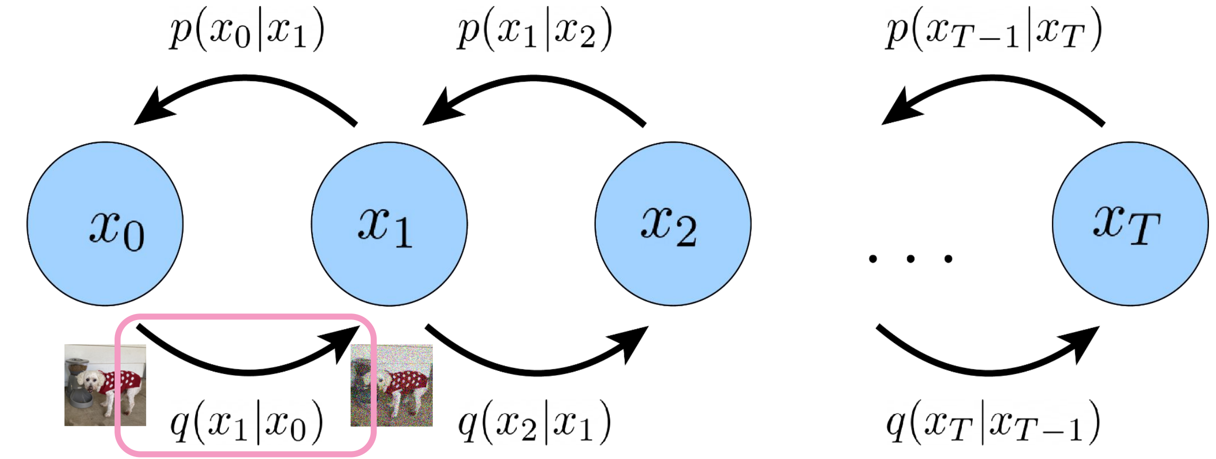




Let's take a look at one encoding



$$q(x_1|x_0) = \mathcal{N}(x_1|x_0, \sigma_1^2\mathrm{I})$$

$x_1 \sim q(x_1|x_0)$ $\boldsymbol{x}_0$ $\boldsymbol{\epsilon}_0$

reparam. trick!

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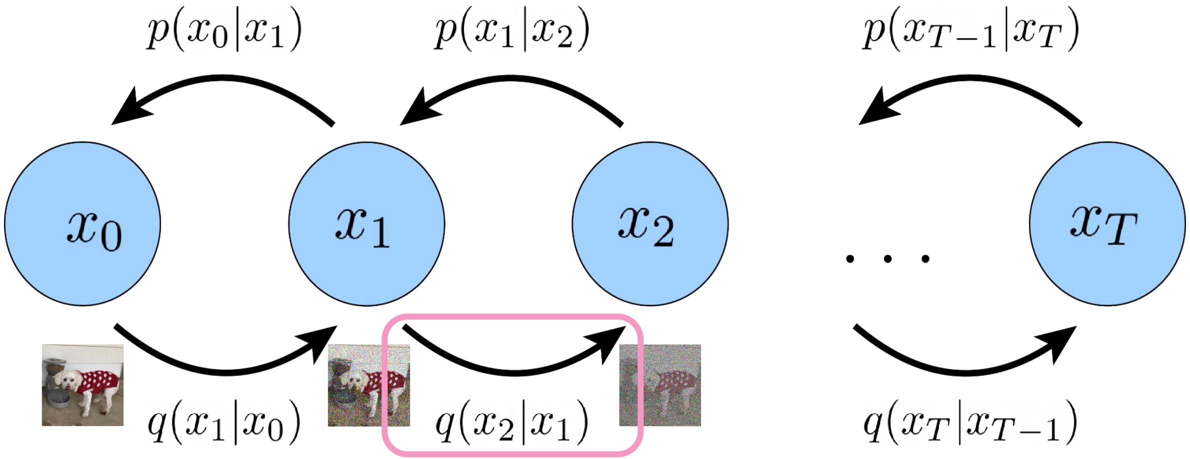

$$q(x_2|x_1) = \mathcal{N}(x_2|x_1, \sigma_2^2 \mathrm{I})$$

$x_2 \sim q(x_2|x_1)$ $\quad$ x_1 $\quad$ $\boldsymbol{\epsilon}_0$

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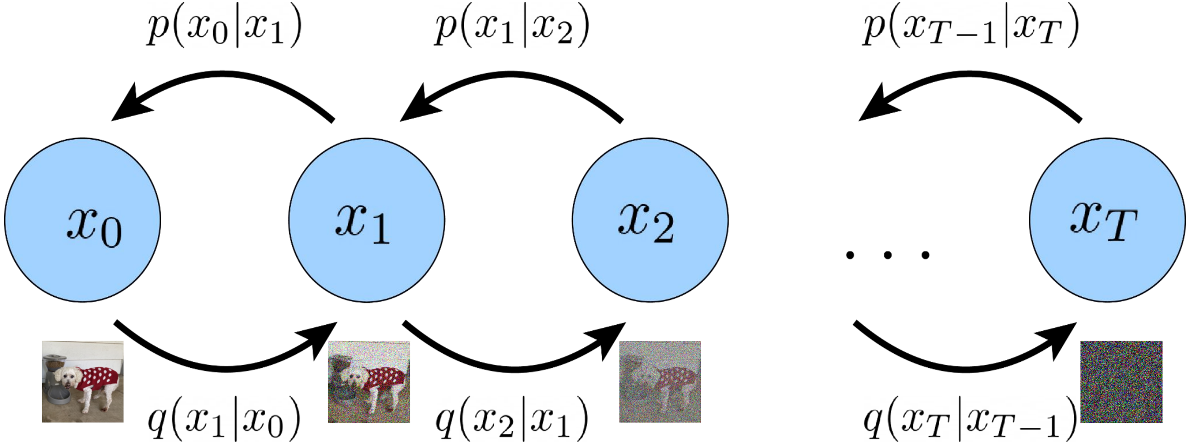

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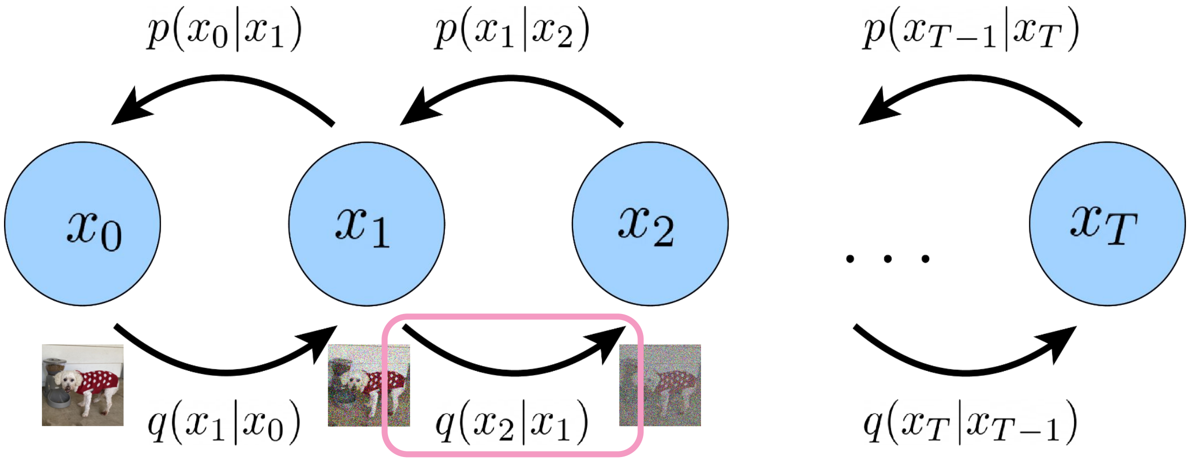

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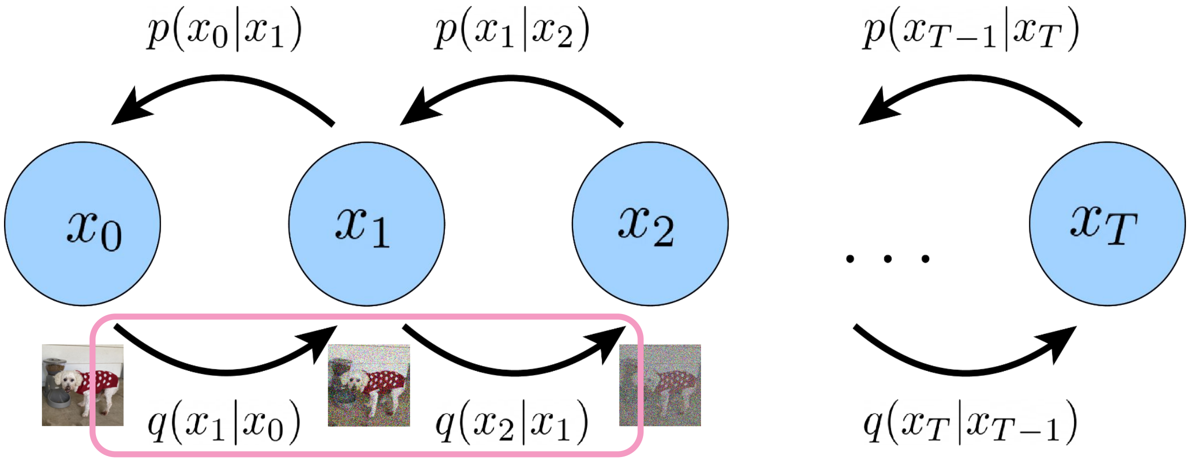

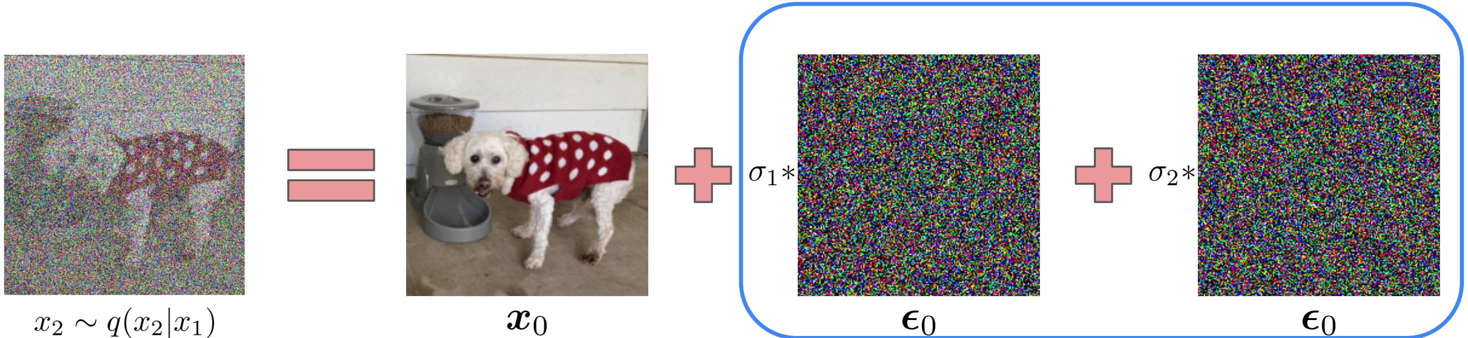

Aggregate into 1 sample!

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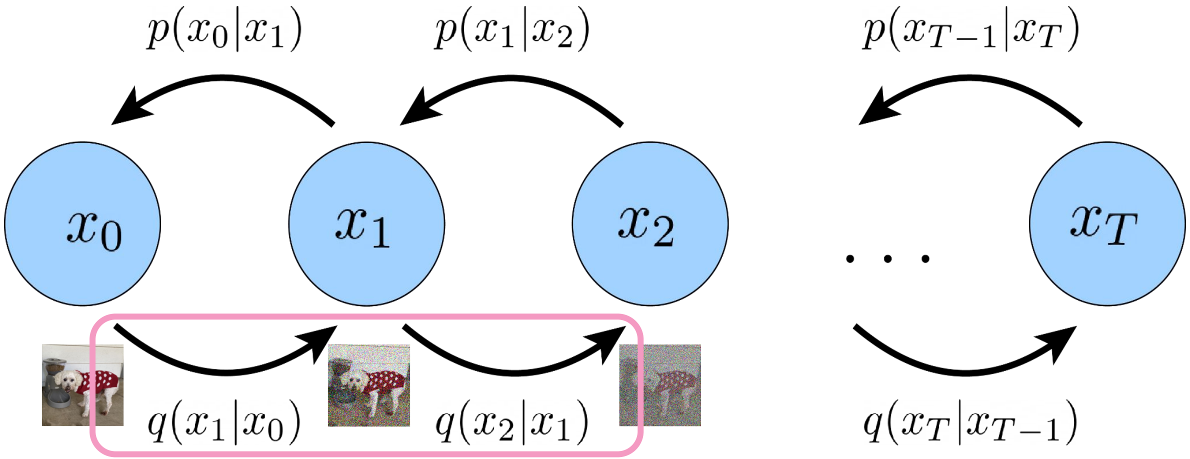


where,

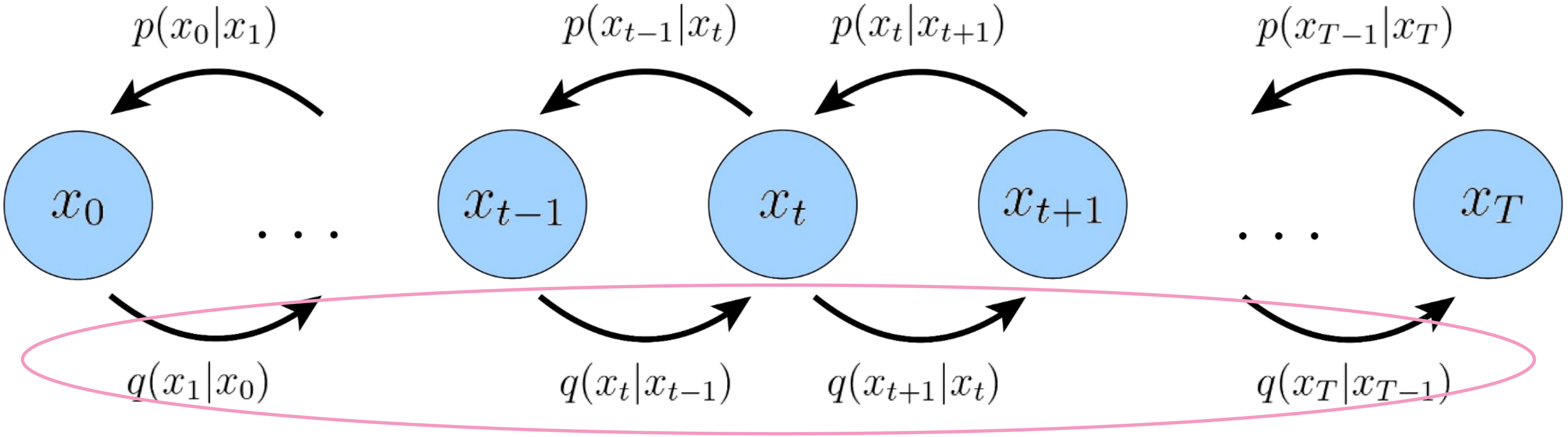
$$\alpha_2 = \sqrt{\sigma_1^2 + \sigma_2^2}$$

and,

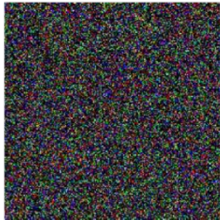
$$q(x_2|x_0) = \mathcal{N}(x_2|x_0, \alpha_2^2)$$

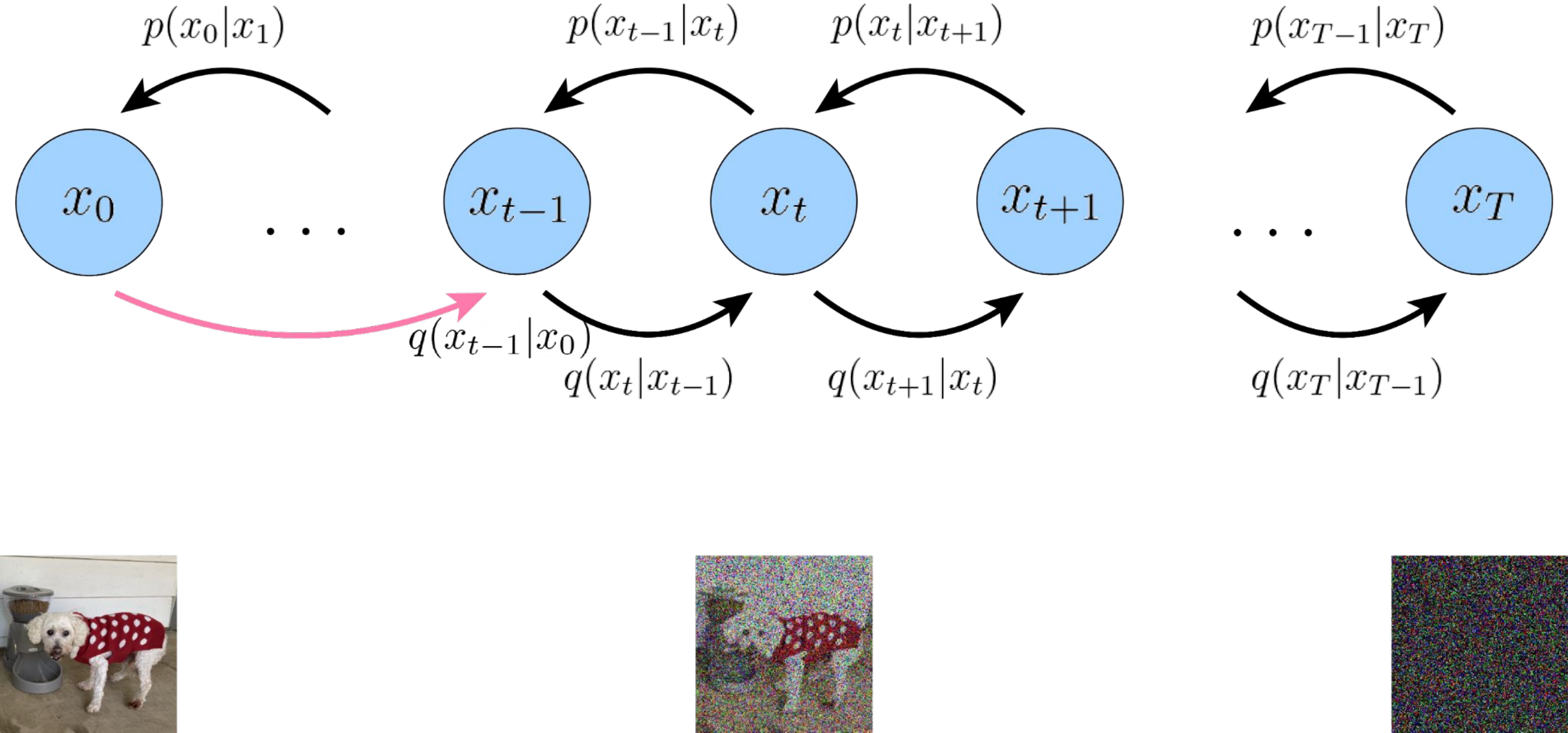
Aggregate into 1 sample!

reparam. trick!



Individual (known) Gaussians!




$p(x_0|x_1)$
$p(x_{t-1}|x_t)$
$p(x_t|x_{t+1})$
$p(x_{T-1}|x_T)$
x_0
$\dots$
x_{t-1}
x_t
x_{t+1}
$\dots$
x_T
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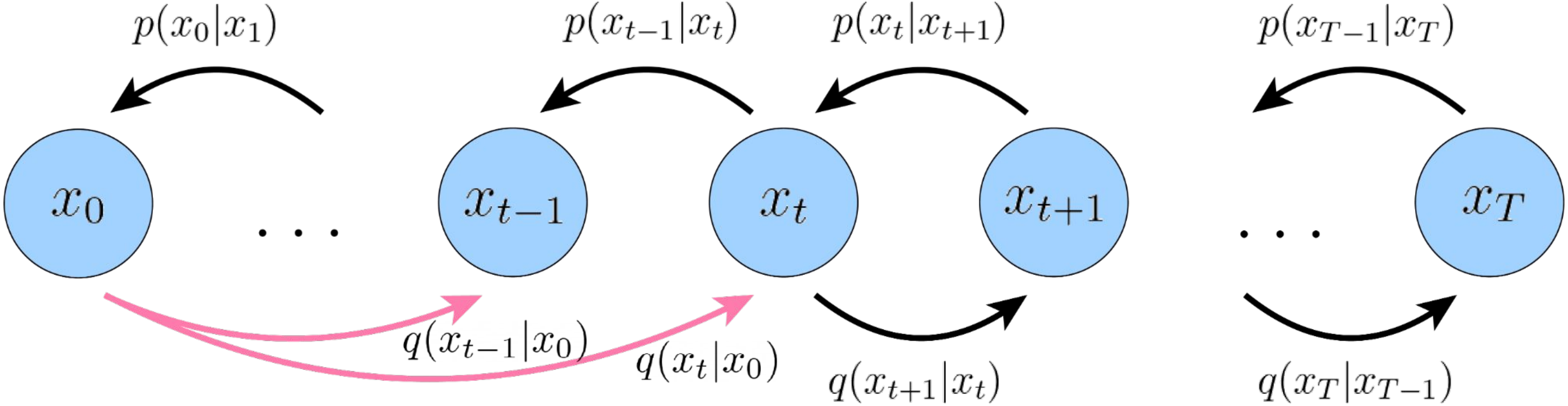
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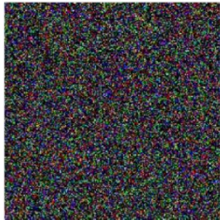

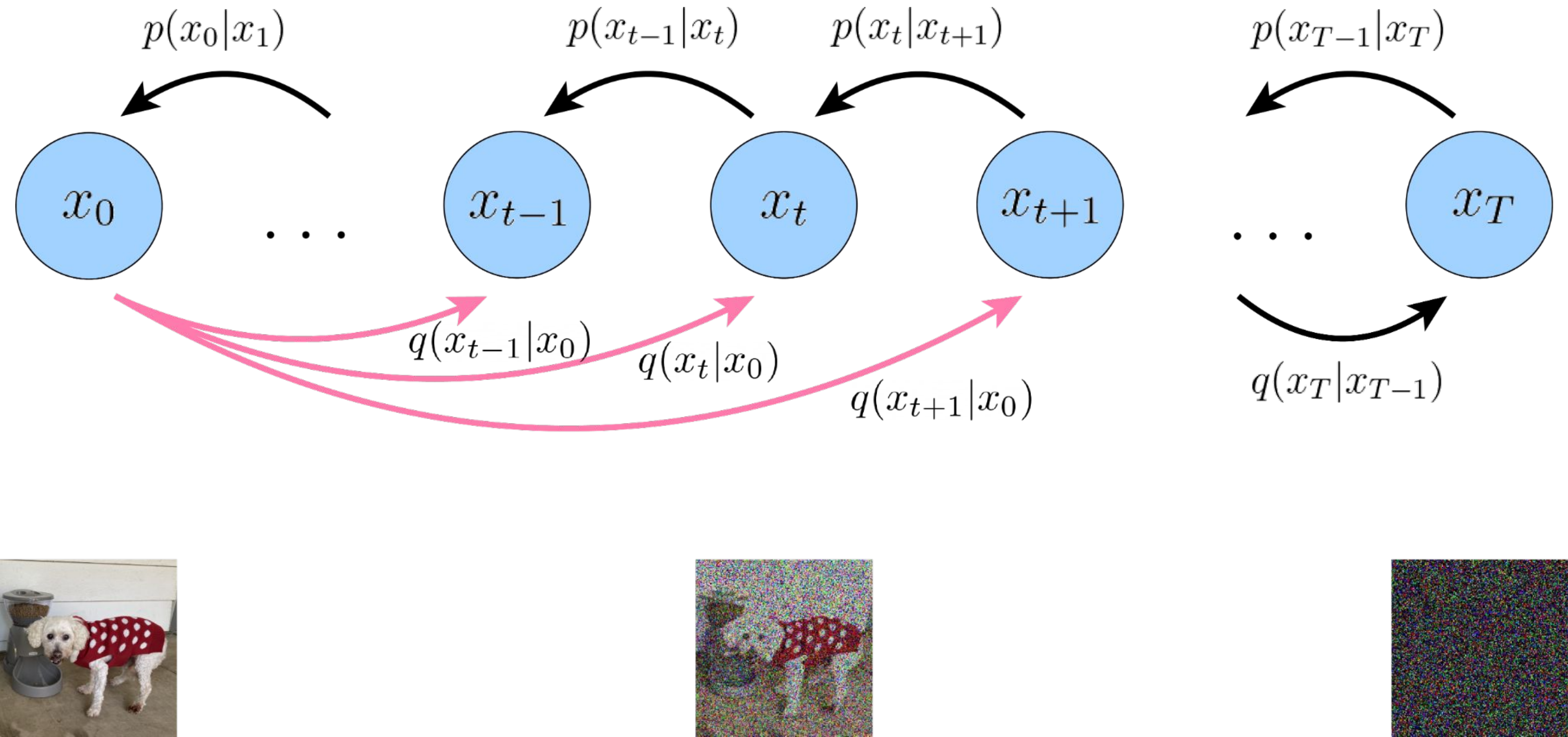

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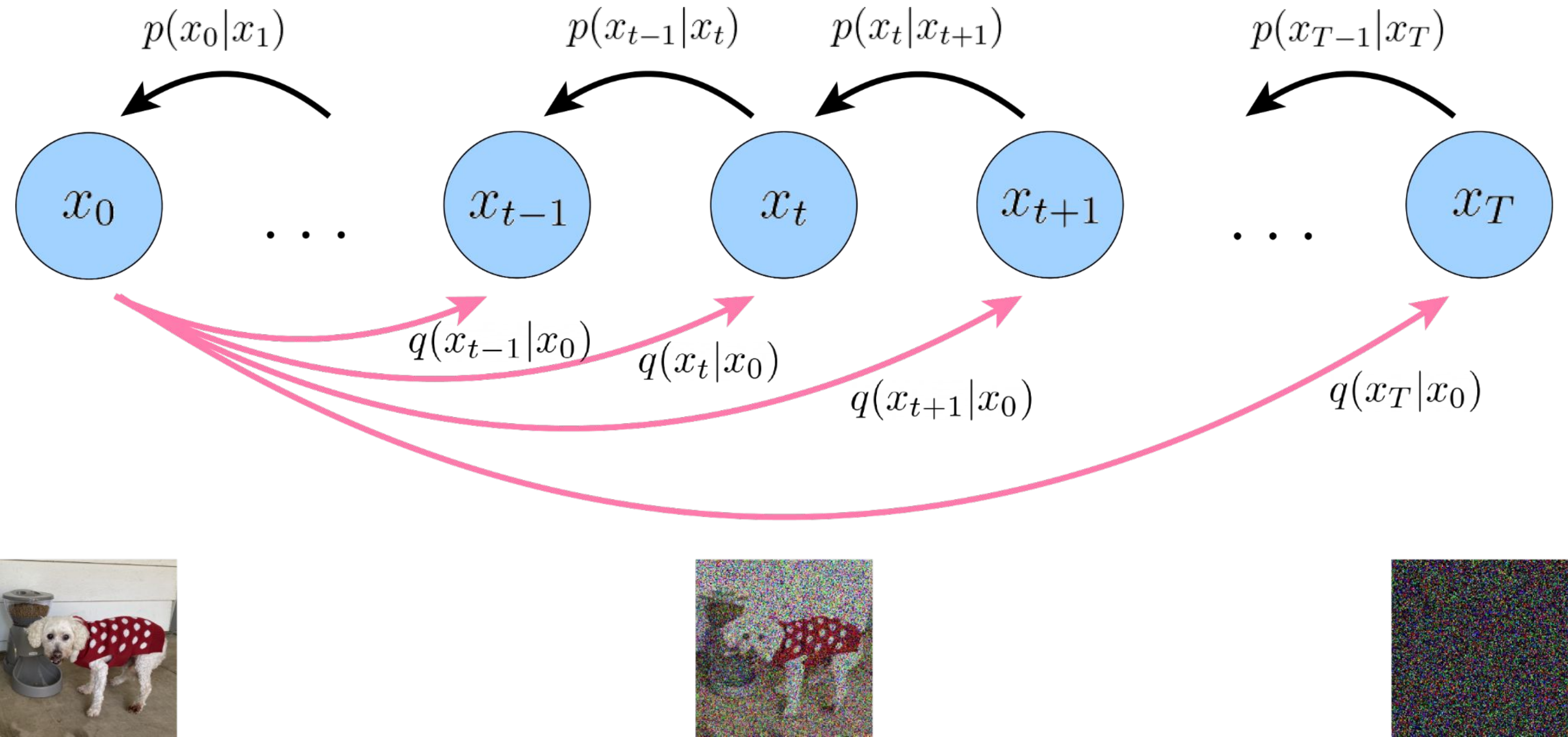
$q(x_T|x_{T-1})$

$q(x_t|x_0)$ is a Gaussian, for arbitrary t!

$q(x_t|x_0) = \mathcal{N}(x_t|x_0, \alpha_t^2 \mathrm{I})$, where $\alpha_0, \alpha_1, \ldots \alpha_T$ are all known/fixed.



Hierarchical VAEs

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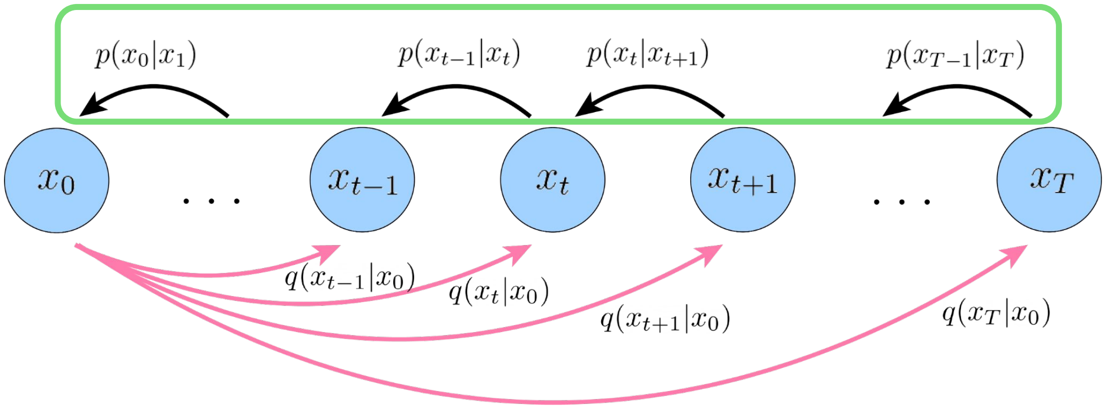

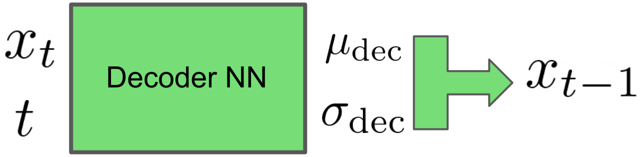

…then we can aggregate and simplify the distribution of each intermediate “latent”!

Diffusion Models

It turns out, that this is exactly what a diffusion model is!

- A Hierarchical VAE with these assumptions:

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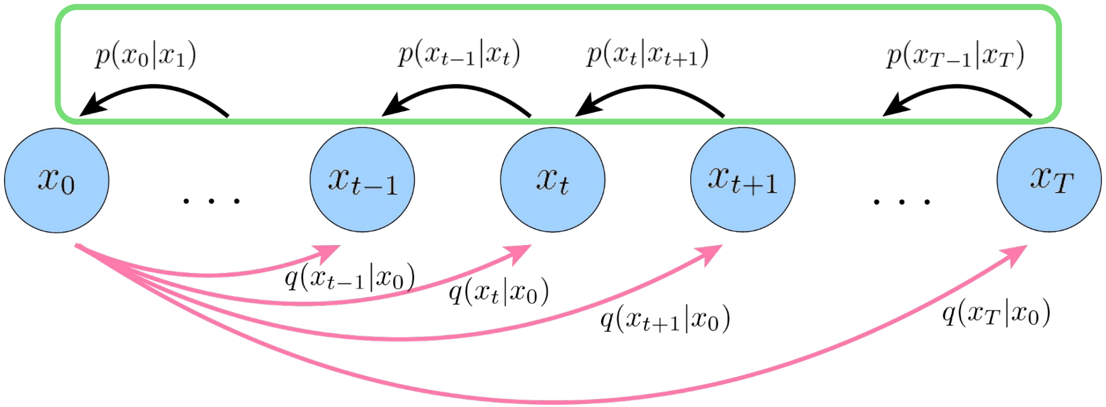
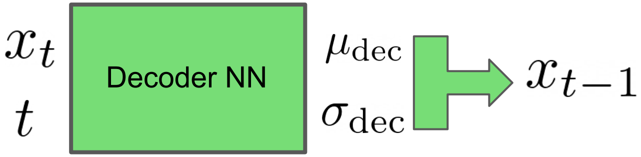
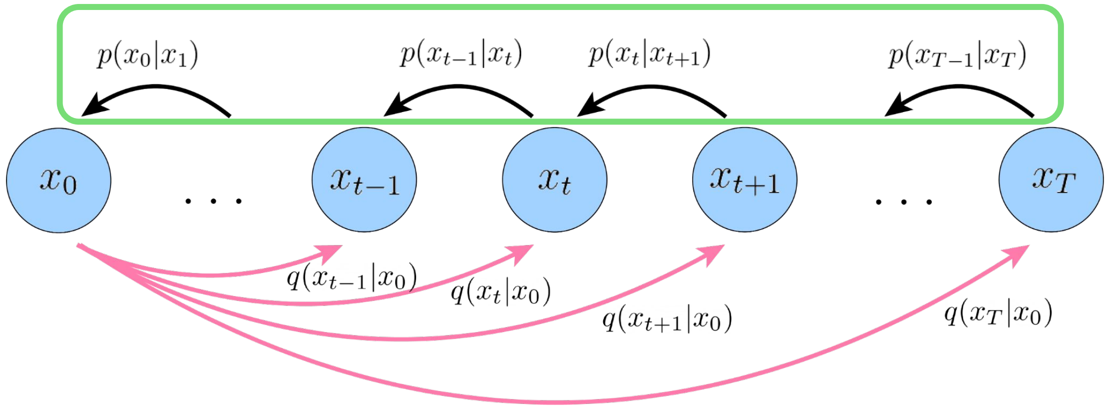
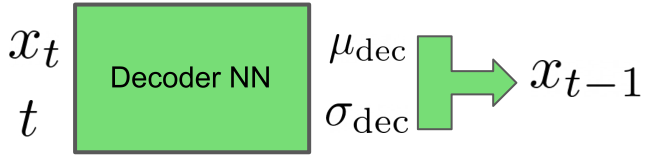




Diffusion Models

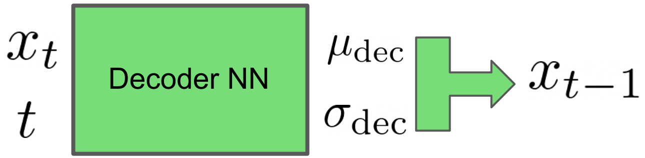
A diffusion model is implemented as a single neural network (the decoder)





Optimization?

We want to learn a denoising decoder:

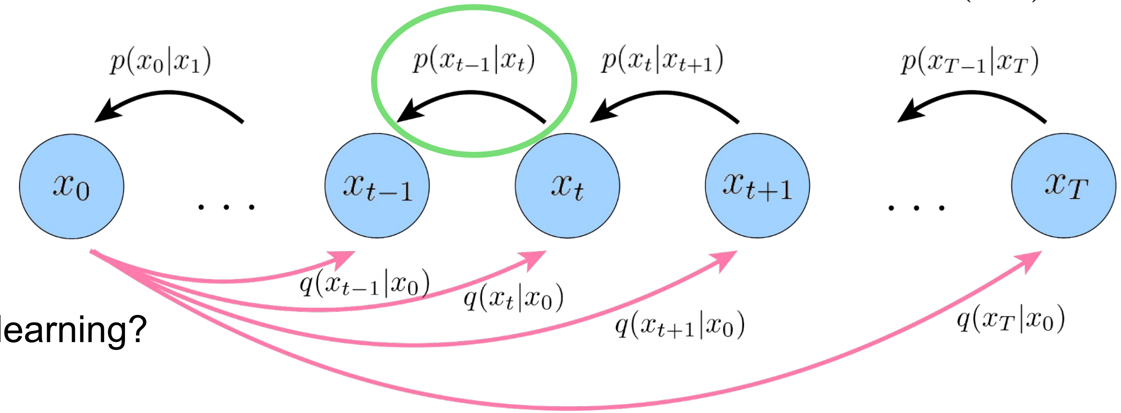


$$\hat{x}_{t-1} = \mu_{\text{dec}} + \sigma_{\text{dec}} * \epsilon$$

reparam. trick!

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

But what is the form of x_{t-1}?



…can we formulate this as supervised learning?

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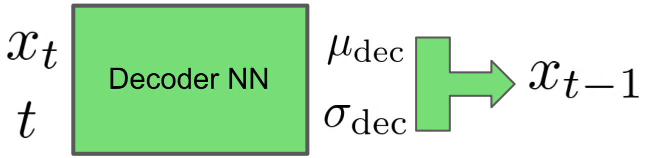

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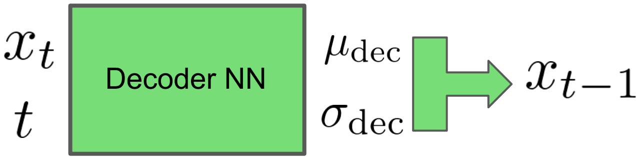

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$$\boxed{\begin{gathered} q(x_{t-1}|x_0) = \mathcal{N}(x_{t-1}|x_0, \alpha_{t-1}^2 \mathrm{I}) \\ \therefore x_{t-1} = x_0 + \alpha_{t-1} * \epsilon \end{gathered}}$$

reparam. trick!

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

Do we really need to predict σ_{dec}*?*

What is the ground truth signal for μ_{dec}*?*

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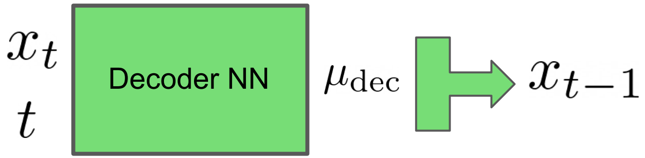

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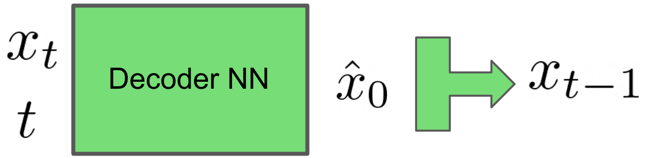

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Do we really need to predict σ_{dec}?

What is the ground truth signal for μ_{dec}?

Optimization?

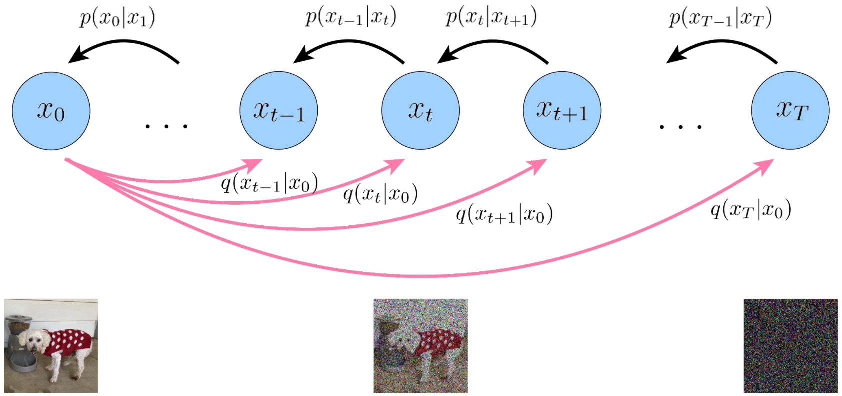
We want to learn a denoising decoder:

So in the end, a diffusion model is simply *one* Neural Network that predicts a clean image x_0 from arbitrary noisified image x_t.

Diffusion Models: A Summary

A Diffusion Model is:

- One NN that predicts a clean image from a noisy version of the image



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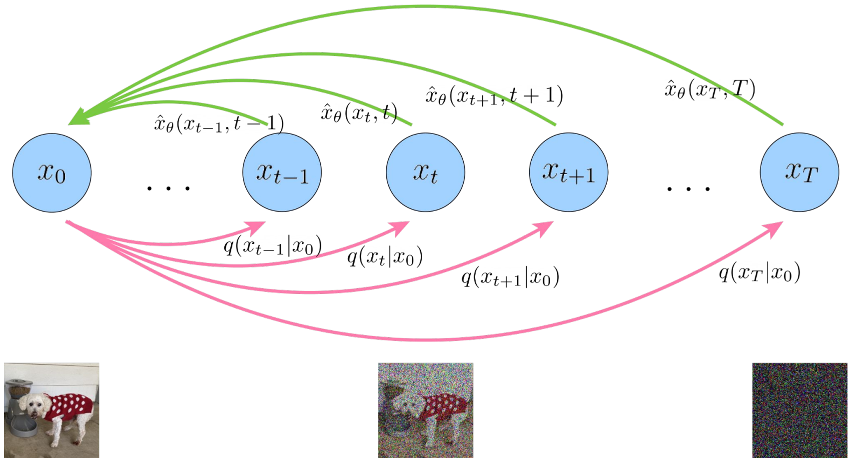
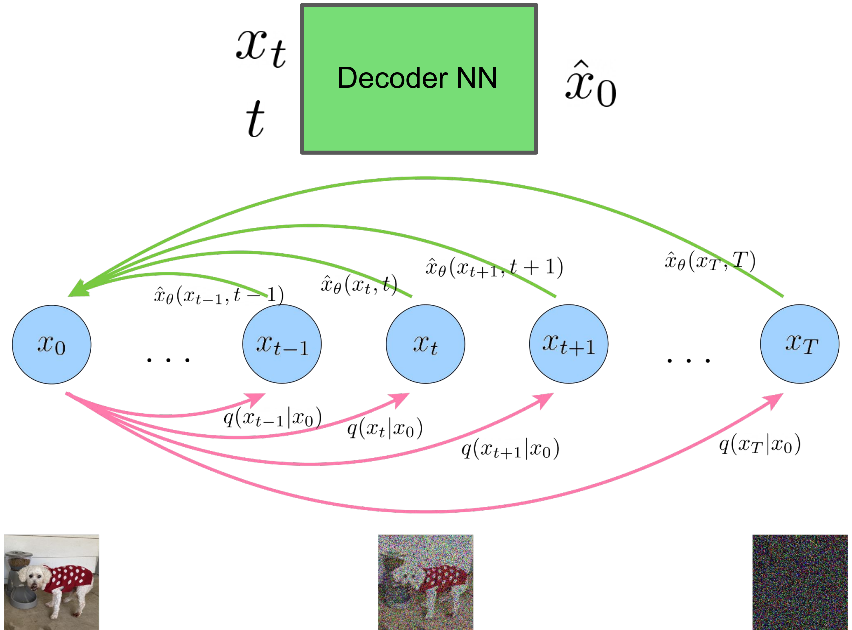
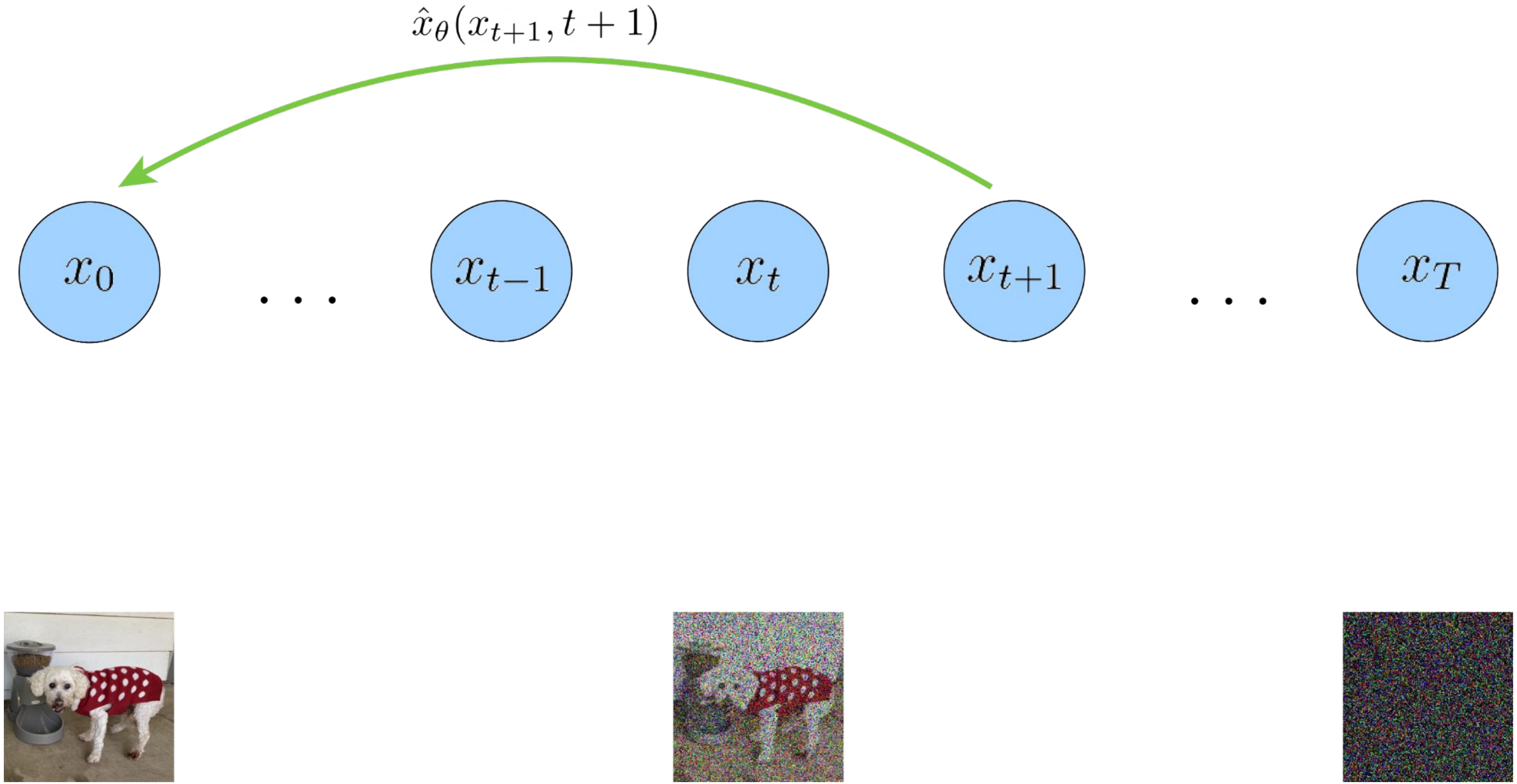


Diffusion Models: A Summary

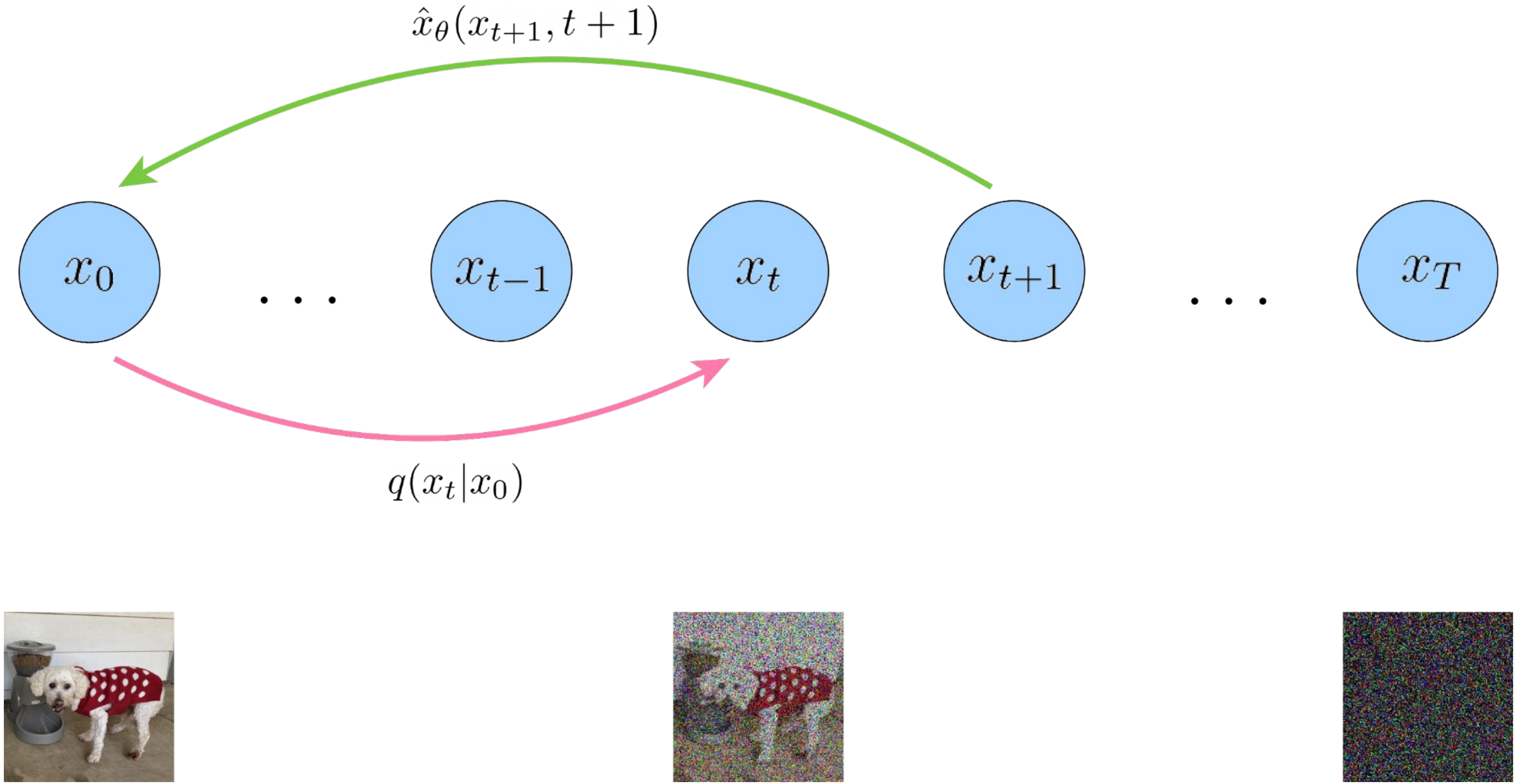
How do we perform sampling?



Sampling



Sampling



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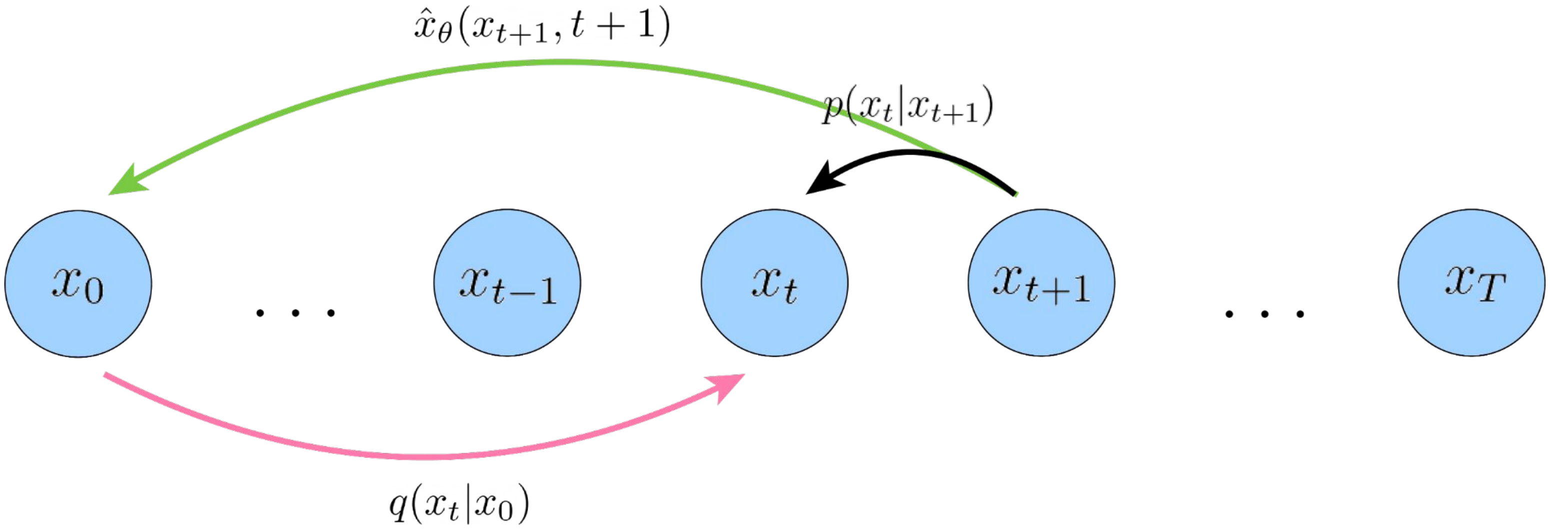

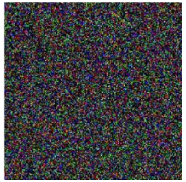

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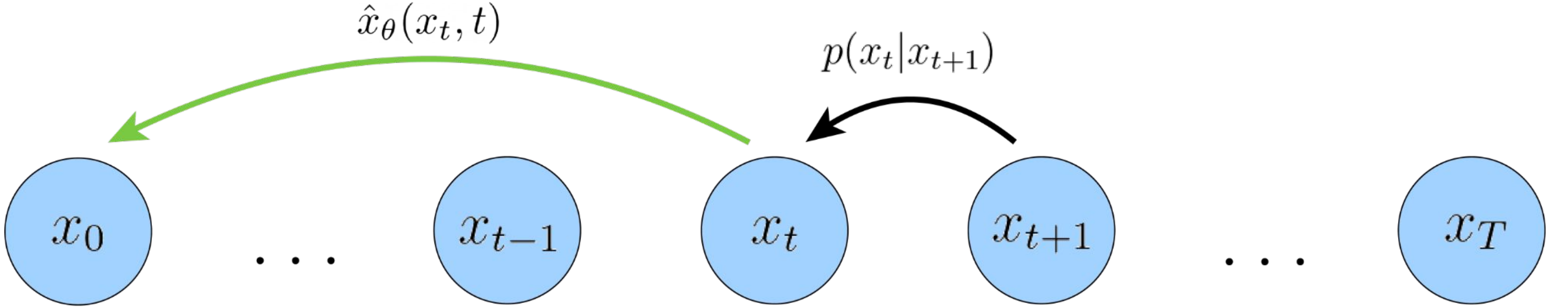
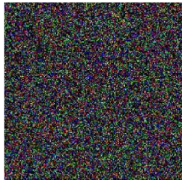
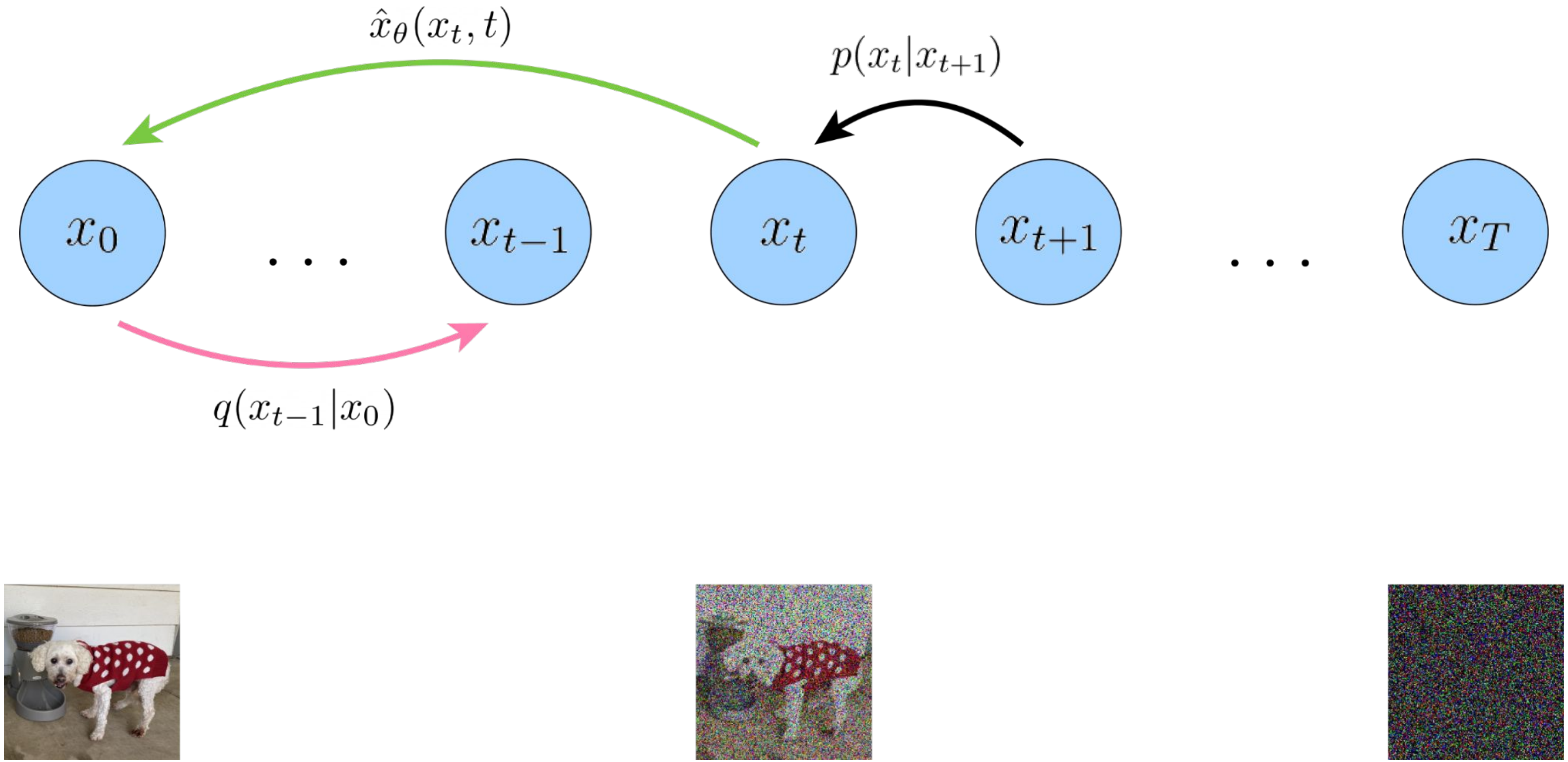




Sampling



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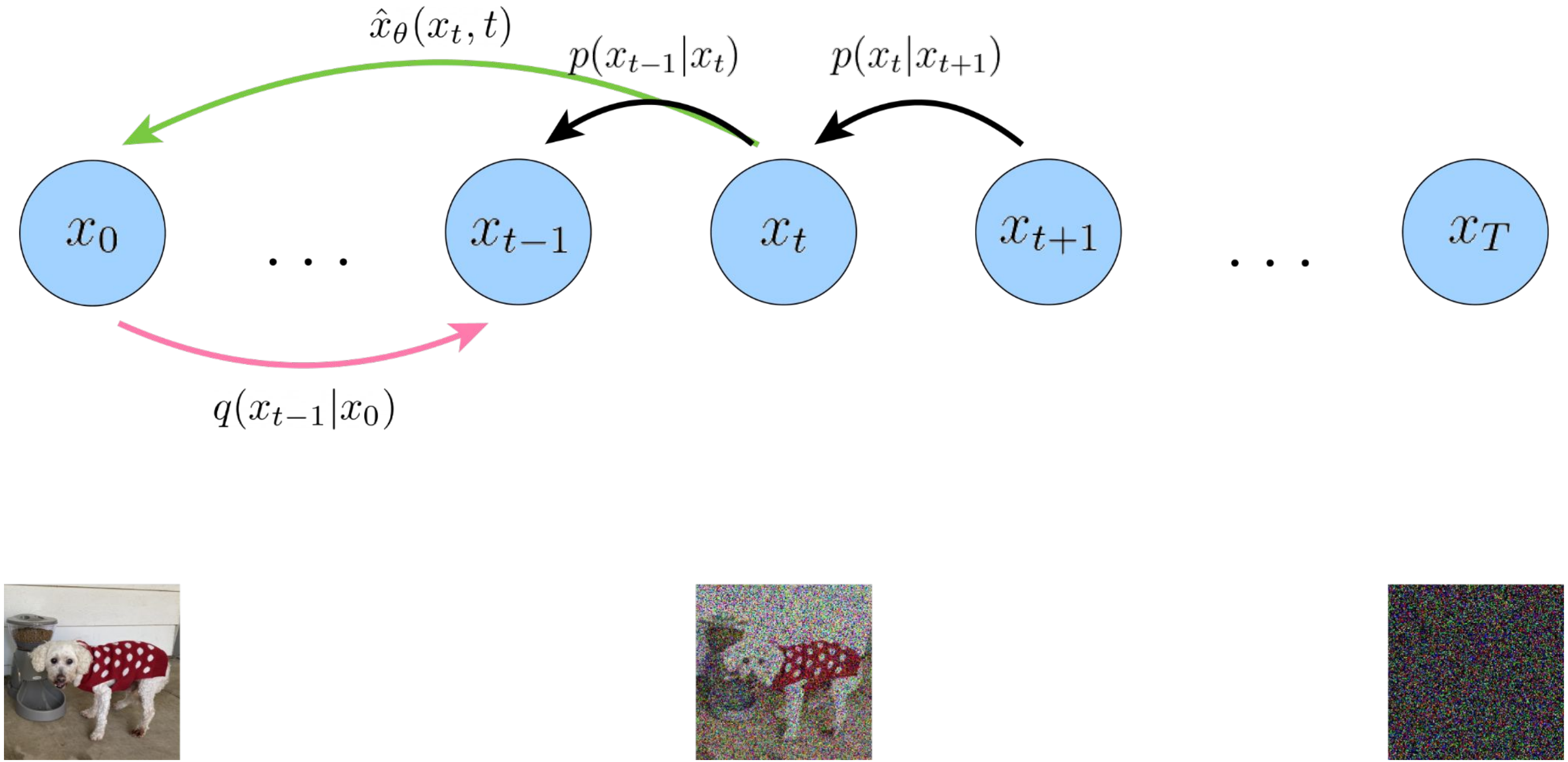
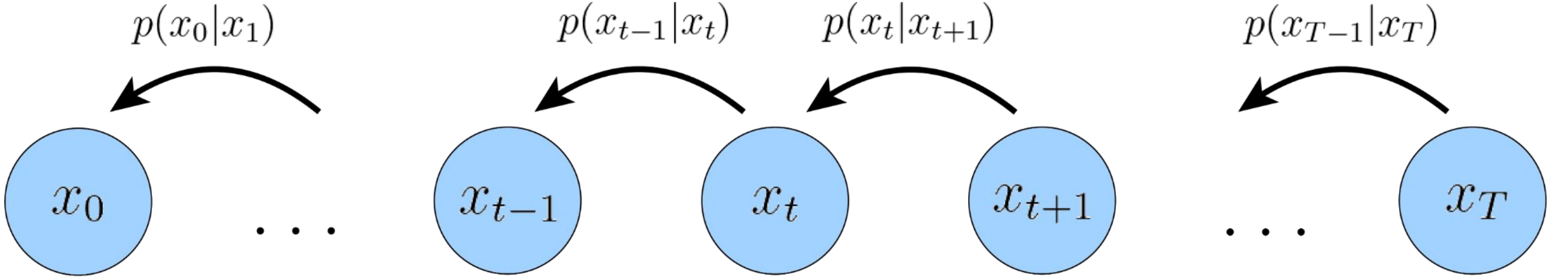
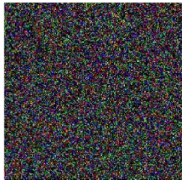


$\hat{x}_\theta(x_t, t)$
$p(x_{t-1}|x_t)$
$p(x_t|x_{t+1})$
x_0
$\ldots$
x_{t-1}
x_t
x_{t+1}
$\ldots$
x_T
$q(x_{t-1}|x_0)$

Sampling





Pseudocode

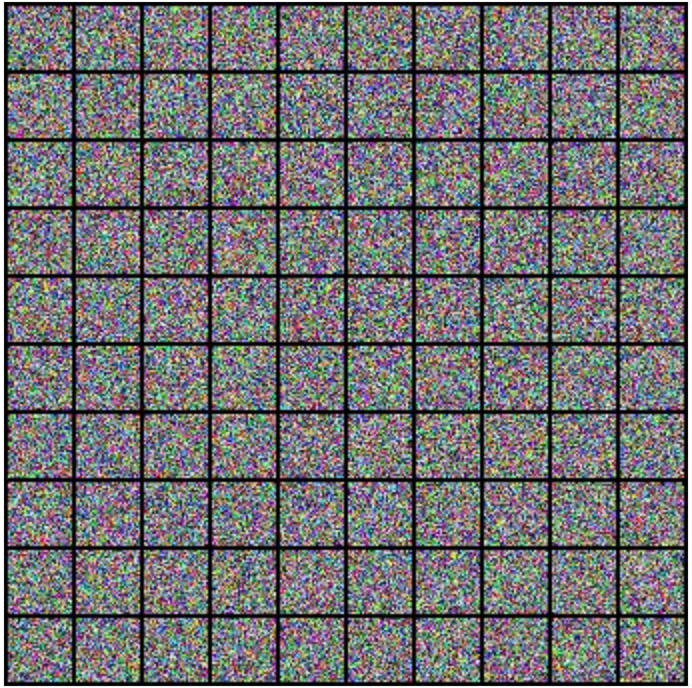
Algorithm 1 Training

repeat
  $\boldsymbol{x}_0 \sim q(\boldsymbol{x}_0)$
  $t \sim \texttt{Uniform}(1, ..., T)$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
    $\nabla_\theta ||\boldsymbol{x}_0 - \hat{\boldsymbol{x}}_\theta(\boldsymbol{x}_0 + \alpha_t \boldsymbol{\epsilon}, t)||^2$
until converged

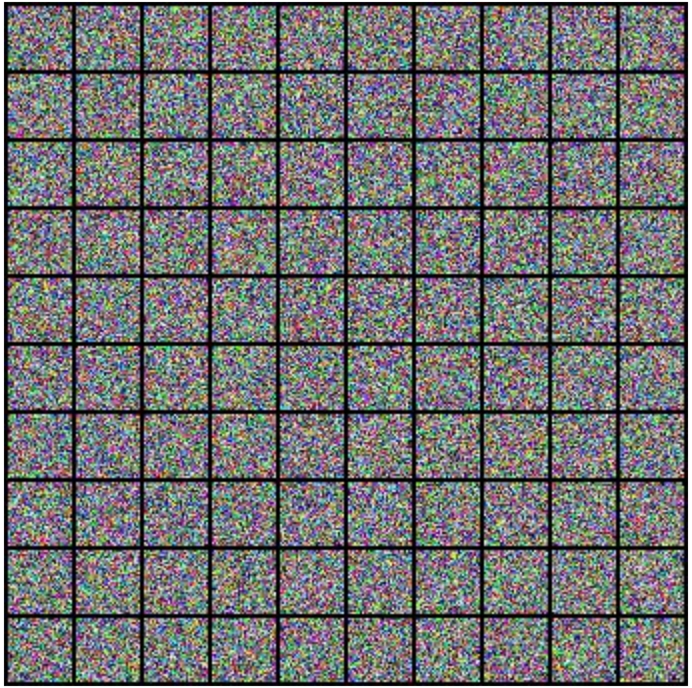
Algorithm 2 Sampling

$\boldsymbol{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, ..., 1$:
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\boldsymbol{\epsilon} = 0$
  $\boldsymbol{x}_{t-1} = \hat{\boldsymbol{x}}_\theta(\boldsymbol{x}_t, t) + \alpha_{t-1}\epsilon$
end for
return $\boldsymbol{x}_0$

Examples!



Celeb-A



CIFAR-10

source: [Generative Modeling by Estimating Gradients of the Data Distribution]

Examples!

1024x1024 samples

source: *Generative Modeling by Estimating Gradients of the Data Distribution*

Three Different Interpretations

It turns out, training a DiffModel can be done using three different interpretations:

- Predicting original image 🖼️ (we just did this)
- Predicting noise 🔊 (coming up!)
- Predicting score function 💯 (coming up!)

Diffusion Models as a Noise Predictor 🔊

Recall that our objective is to predict $\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) \approx \boldsymbol{x}_0$

Image 🖼️ and Noise 🔊? They are the same!

What does it mean intuitively?

For arbitrary $\boldsymbol{x}_t \sim q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)$, we can rewrite it as $\boldsymbol{x}_t = \boldsymbol{x}_0 + \alpha_t \boldsymbol{\epsilon}_0$

Predicting $\boldsymbol{x}_0$ *determines* $\boldsymbol{\epsilon}_0$ and vice-versa, since they sum to the same thing!

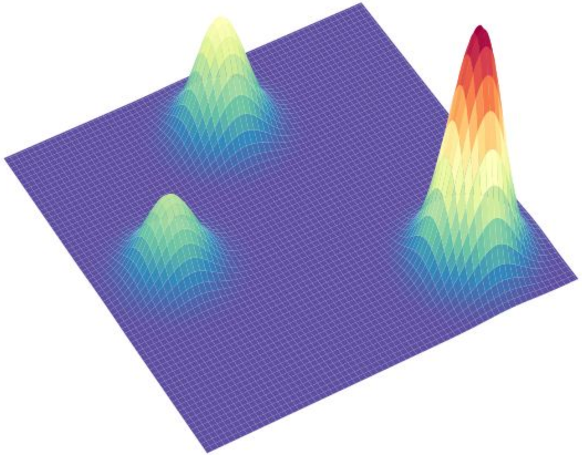
$\boldsymbol{x}_t \sim q(\boldsymbol{x}_t \mid \boldsymbol{x}_0)$ $\boldsymbol{x}_0$ $\boldsymbol{\epsilon}_0$

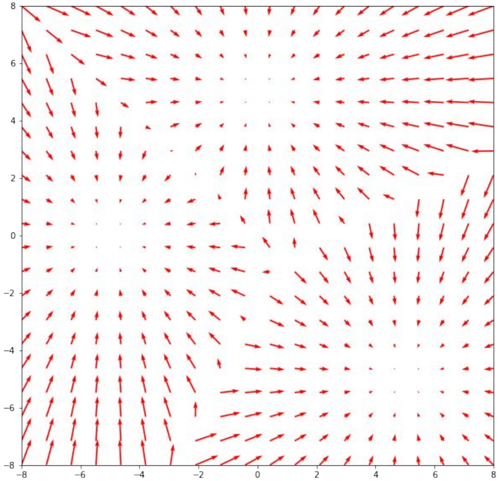
Score Functions 💯

What are score functions?

$$\nabla_{\boldsymbol{x}} \log p(\boldsymbol{x})$$

Intuitively, they describe how to move in data space to improve the (log) likelihood.





Tweedie's Formula

Mathematically, for a Gaussian variable $\boldsymbol{z} \sim \mathcal{N}(\boldsymbol{z}; \boldsymbol{\mu}_z, \boldsymbol{\Sigma}_z)$Tweedie's formula states:

$$\mathbb{E}\left[\boldsymbol{\mu}_z \mid \boldsymbol{z}\right] = \boldsymbol{z} + \boldsymbol{\Sigma}_z \nabla_{\boldsymbol{z}} \log p(\boldsymbol{z})$$

Then, since we have previously shown that:

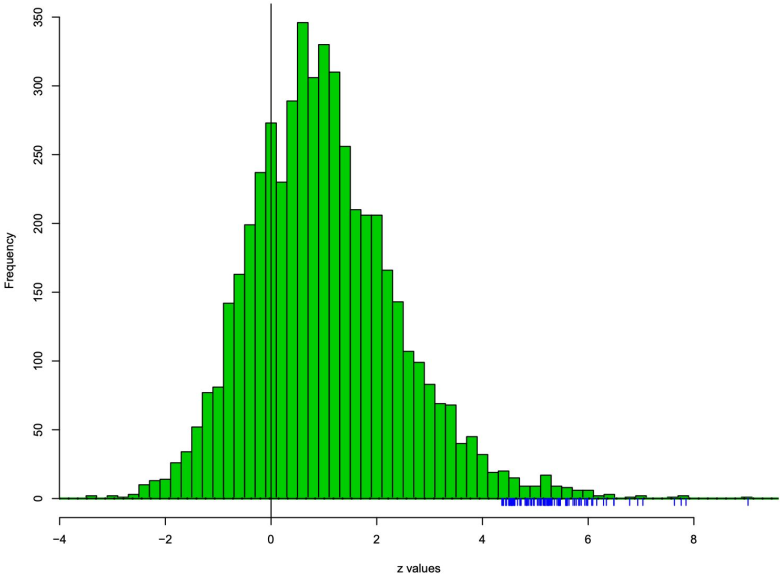
$$q(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t; \boldsymbol{x}_0, \alpha_t^2\mathbf{I})$$

By Tweedie's Formula, we derive:

$$\mathbb{E}[\boldsymbol{\mu}_{\boldsymbol{x}_t} \mid \boldsymbol{x}_t] = \boldsymbol{x}_t + \alpha_t^2 \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$$

The best estimate for the true mean is $\boldsymbol{\mu}_{\boldsymbol{x}_t} = \boldsymbol{x}_0$

$$\boldsymbol{x}_0 = \boldsymbol{x}_t + \alpha_t^2 \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$$



Tweedie's Formula

There exists a mathematical formula that states that:

$$\boldsymbol{x}_0 \approx \boldsymbol{x}_t + \alpha_t^2 \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$$

Due to the fact that the distribution is Gaussian:

$$q(\boldsymbol{x}_t|\boldsymbol{x}_0) = \mathcal{N}(\boldsymbol{x}_t \mid \boldsymbol{x}_0, \alpha_t^2 \mathbf{I})$$

Diffusion Models as a Score Predictor 💯

Recall that our objective is to predict $\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) \approx \boldsymbol{x}_0$

Score 💯 and Noise 🔊?

There is a relationship between the score and the noise, which we can derive by equating Tweedie's formula with the Reparameterization Trick.

$$\begin{aligned}\boldsymbol{x}_0 = \boldsymbol{x}_t + \alpha_t^2 \nabla \log p(\boldsymbol{x}_t) &= \boldsymbol{x}_t - \alpha_t \boldsymbol{\epsilon}_0 \\ \therefore\ \alpha_t^2 \nabla \log p(\boldsymbol{x}_t) &= -\alpha_t \boldsymbol{\epsilon}_0 \\ \nabla \log p(\boldsymbol{x}_t) &= -\frac{1}{\alpha_t} \boldsymbol{\epsilon}_0\end{aligned}$$

Intuitively, the direction to move in data space towards a natural image is the negative noise term that was added.

Three Different Interpretations

It turns out, training a DiffModel can be implemented as a neural net that:

- 🖼️ Predicts original image $\hat{\boldsymbol{x}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) \approx \boldsymbol{x}_0$
- 🔊 Predicts noise epsilon $\hat{\boldsymbol{\epsilon}}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) \approx \boldsymbol{\epsilon}_0$
- 💯 Predicts score function $\boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{x}_t, t) \approx \nabla_{\boldsymbol{x}_t} \log p(\boldsymbol{x}_t)$

A Summary

We have learned that a diffusion model is simply one neural network that predicts a clean image from a noisy image.

Objective: $\arg\min_{\boldsymbol{\theta}} \; ||x_0 - \hat{x}_\theta(x_t, t)||^2$

Sampling: