CS 4644-DL / 7643-A: Lecture 18
Danfei xu

Generative Models:

Denoising Diffusion Probabilistic Models (DDPMs)

Taxonomy of Generative Models

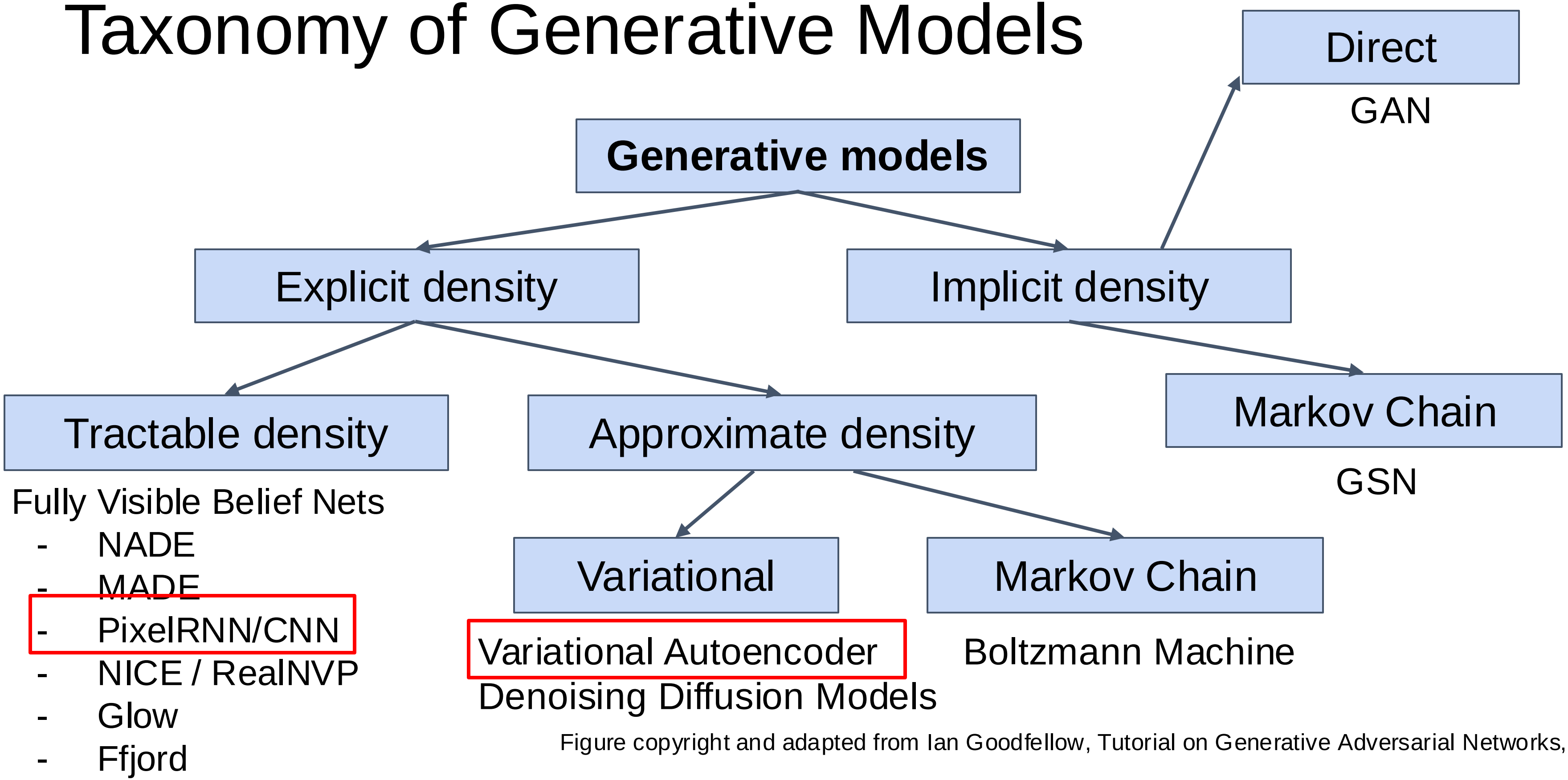


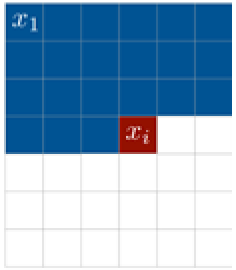
Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Fully visible belief network (FVBN)

Explicit density model

Use probability chain rule to decompose likelihood of an image x into product of 1-d distributions:

$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

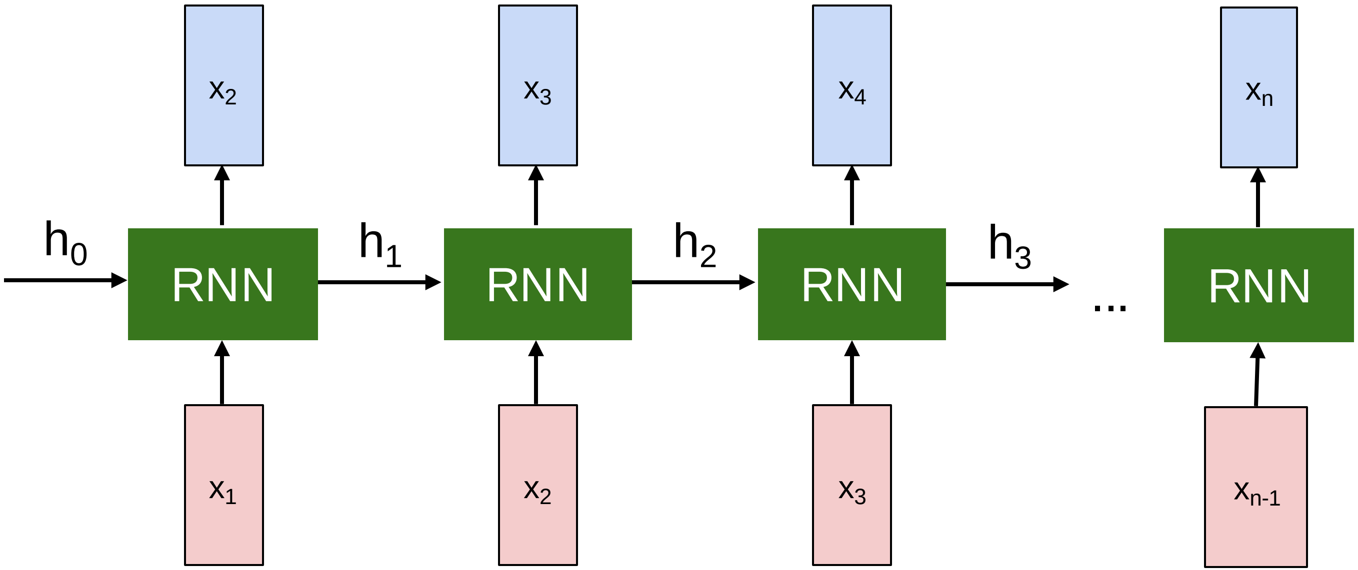


Likelihood of image x

Probability of i'th pixel value given all previous pixels

Then maximize likelihood of training data

Recurrent Neural Network



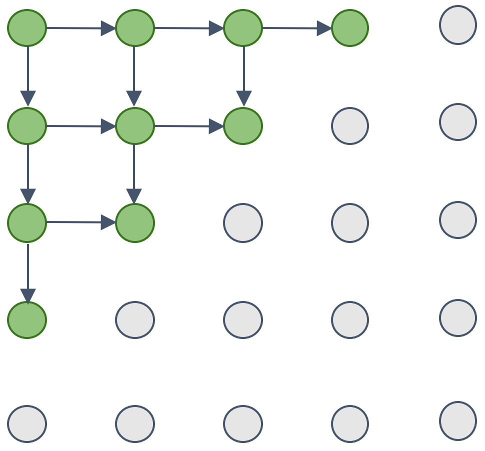
$$p(x_i|x_1, ..., x_{i-1})$$

PixelRNN *[van der Oord et al. 2016]*

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

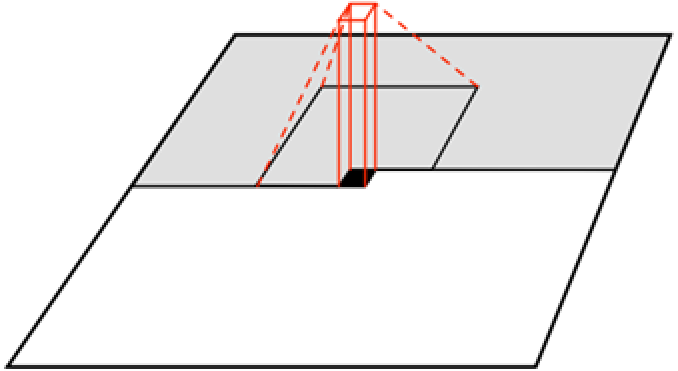
Drawback: sequential generation is slow in both training and inference!



PixelCNN *[van der Oord et al. 2016]*

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region (**masked convolution**)



Taxonomy of Generative Models

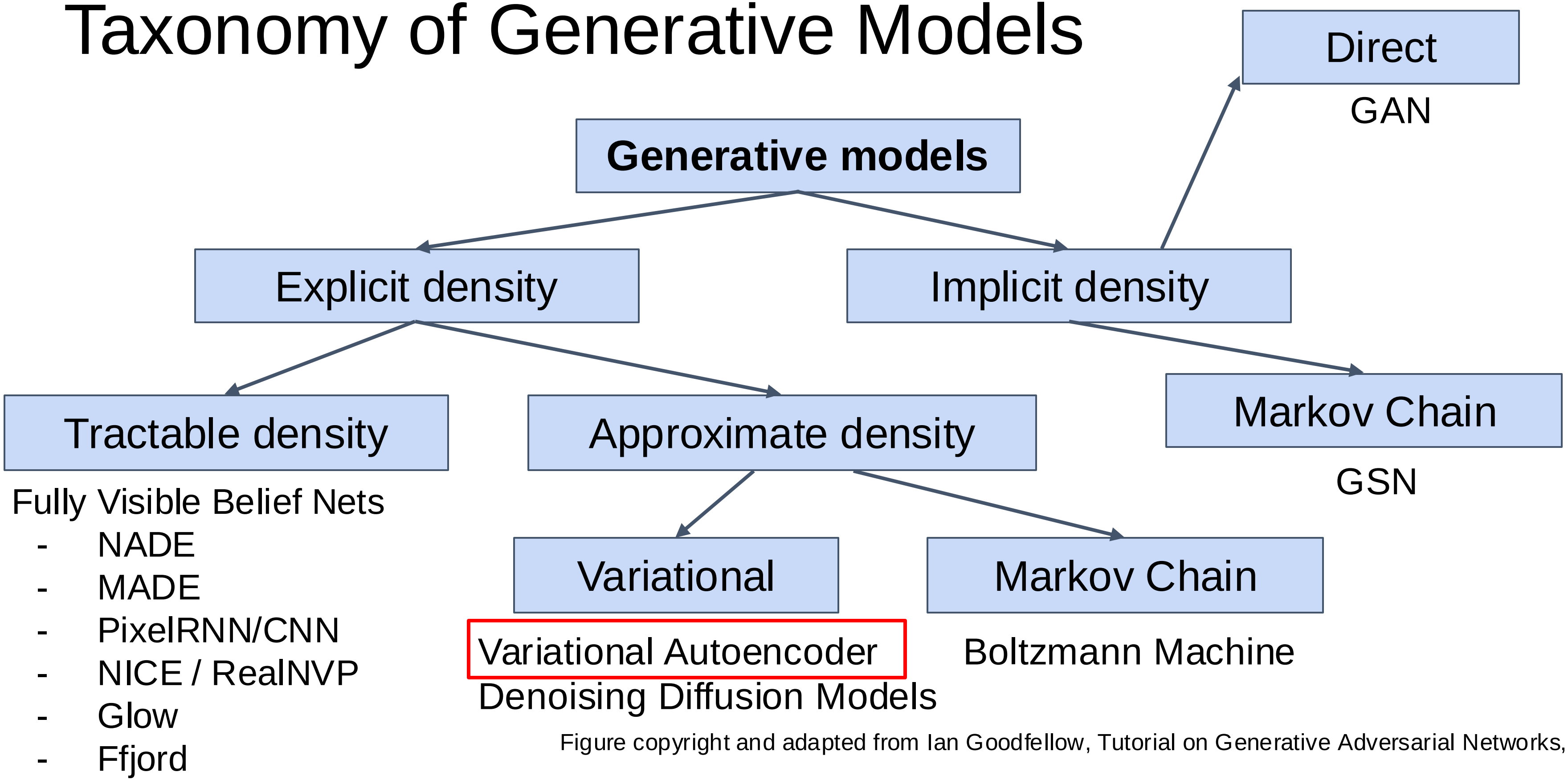


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

So far...

PixelR/CNNs define tractable density function, optimize likelihood of training data:

$$p_\theta(x) = \prod_{i=1}^{n} p_\theta(x_i | x_1, ..., x_{i-1})$$

Variational Autoencoders (VAEs) define intractable density function with latent **z**:

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

No dependencies among pixels, can generate all pixels at the same time!

Latent variable z that captures important *factors of variations* in dataset

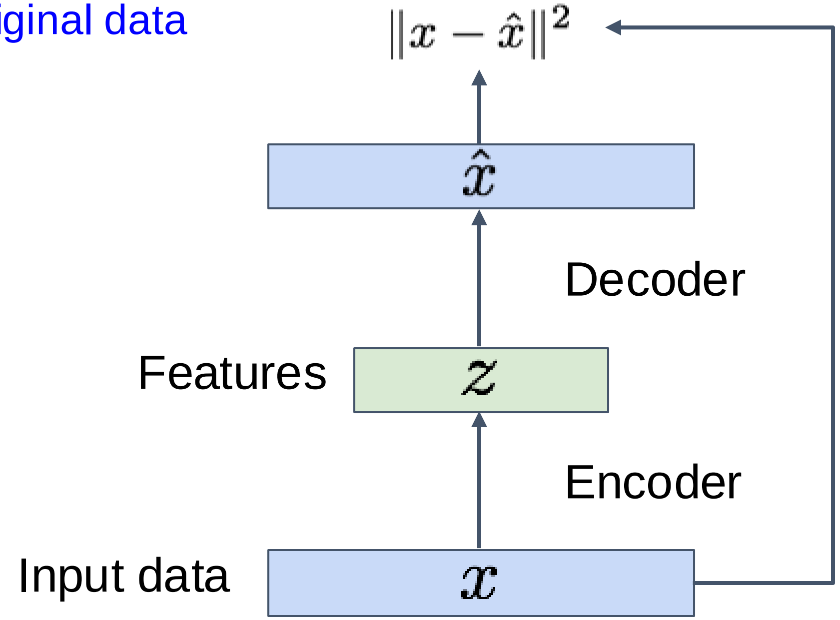
Cannot optimize (maximum likelihood estimation) directly, derive and optimize lower bound on likelihood instead

Some background first: Autoencoders

Train such that features can be used to reconstruct original data

L2 Loss function:

Doesn't use labels!



Reconstructed data

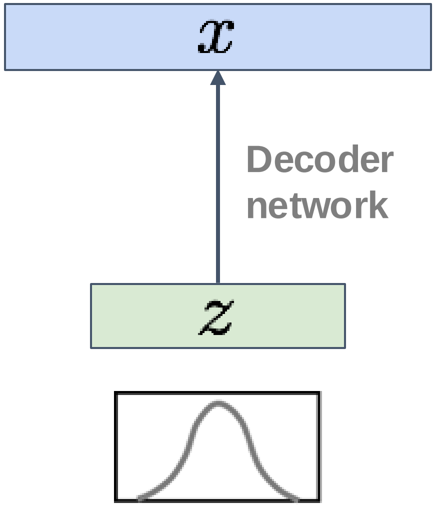
Encoder: 4-layer conv
Decoder: 4-layer upconv

Input data

Variational Autoencoders

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$



Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

We want to estimate the true parameters θ^* of this generative model given training data x.

How should we represent this model?

Assume p(z) is *known* and ***simple***, e.g. isotropic Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

Conditional p(x|z) is ***complex*** (generates image) => represent with neural network

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Intractability

😢 ✓ ✓

Data likelihood: $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$

Can we do Monte Carlo sampling?

$$\log p(x) \approx \log \frac{1}{k} \sum_{i=1}^{k} p(x|z^{(i)}), \text{ where } z^{(i)} \sim p(z)$$

Can we estimate posterior density? Not quite, but …

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

VAE: We can use an approximate posterior $q_\theta(z|x)$ (variational distribution) to form a *tractable lower bound* of the data likelihood p(x).

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Logarithms)}$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,\|\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

Sample z from the learned posterior (encoder) to train the decoder to reconstruct!

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

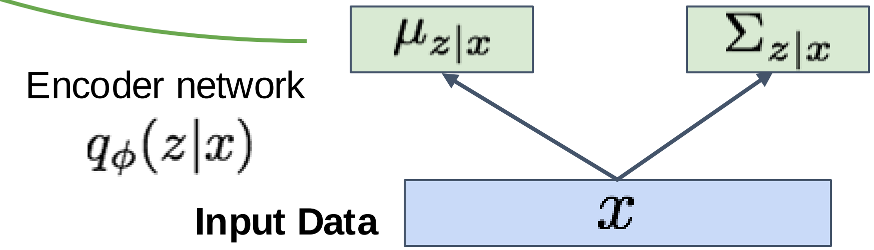
Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \boxed{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x})||\mathcal{N}(0, I))$$

Have analytical solution

Make approximate posterior distribution close to prior



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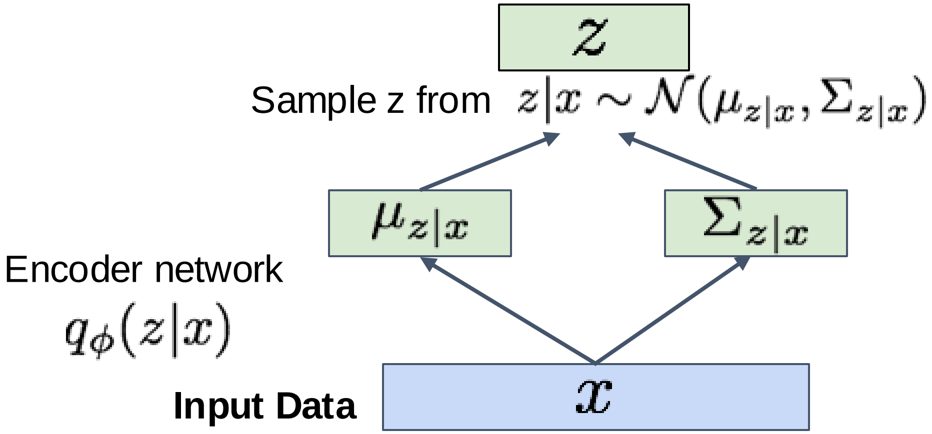
Reparameterization trick to make sampling differentiable:

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

$$z = \mu_{z|x} + \epsilon\sigma_{z|x}$$



Variational Autoencoders

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$$\underbrace{\boxed{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right]} - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Reparameterization trick to make sampling differentiable:

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

Input to the graph

$$z = \mu_{z|x} + \epsilon\sigma_{z|x}$$

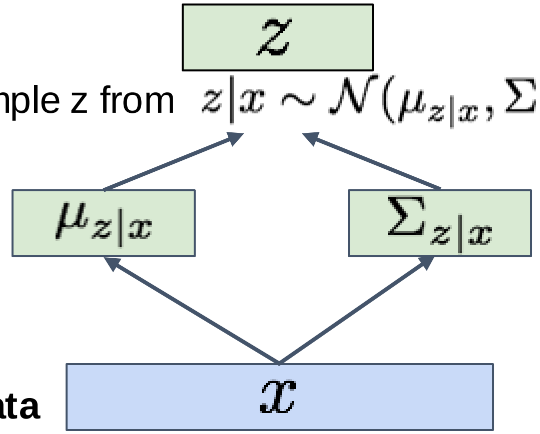
Part of computation graph

Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$

Encoder network

$q_\phi(z|x)$

Input Data

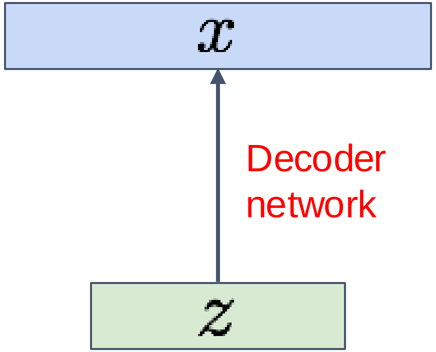


Variational Autoencoders: Generating Data!

Our assumption about data generation process

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

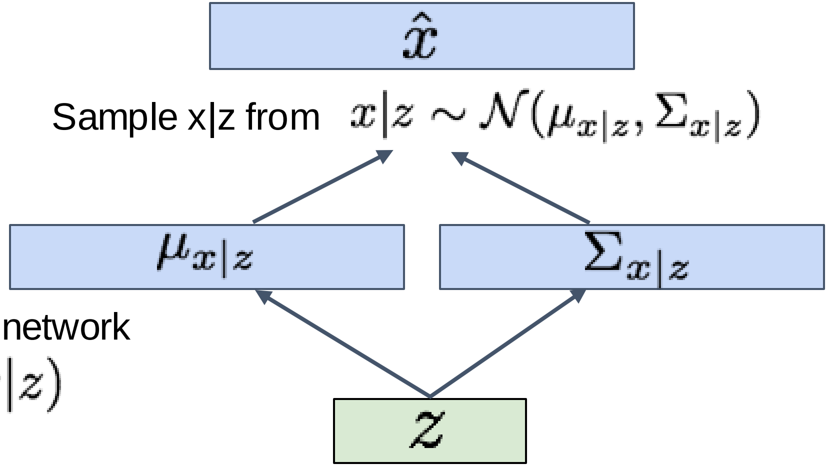


Sample from true prior

$z^{(i)} \sim p_{\theta^*}(z)$

Now given a trained VAE:
use decoder network & sample z from prior!

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$



Decoder network

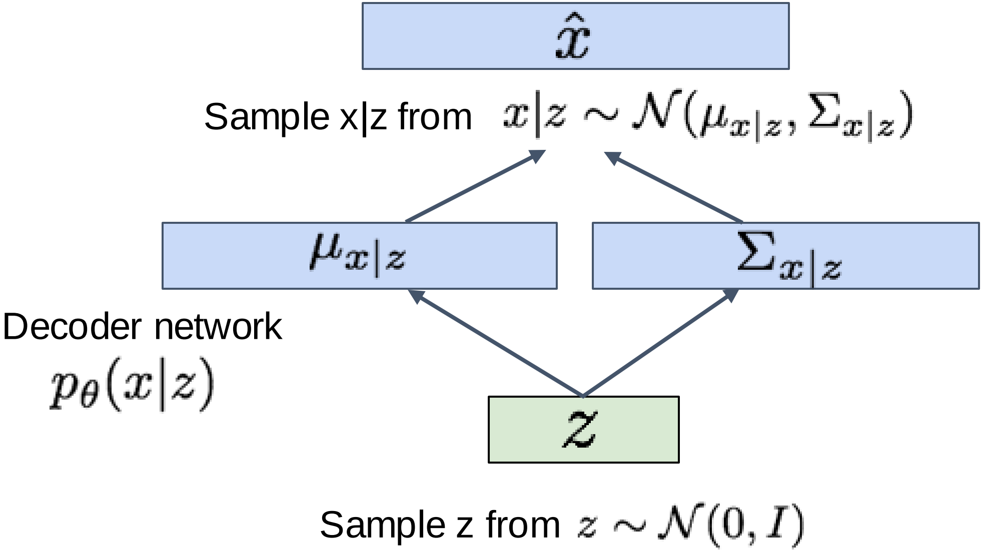
$p_\theta(x|z)$

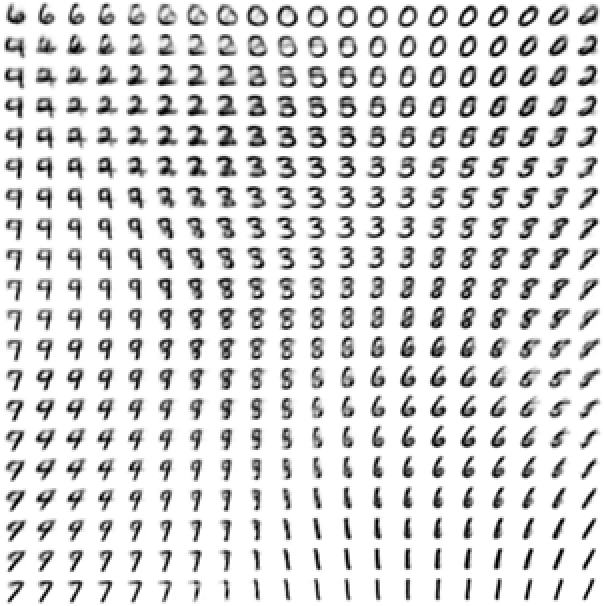
Sample z from $z \sim \mathcal{N}(0, I)$

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!





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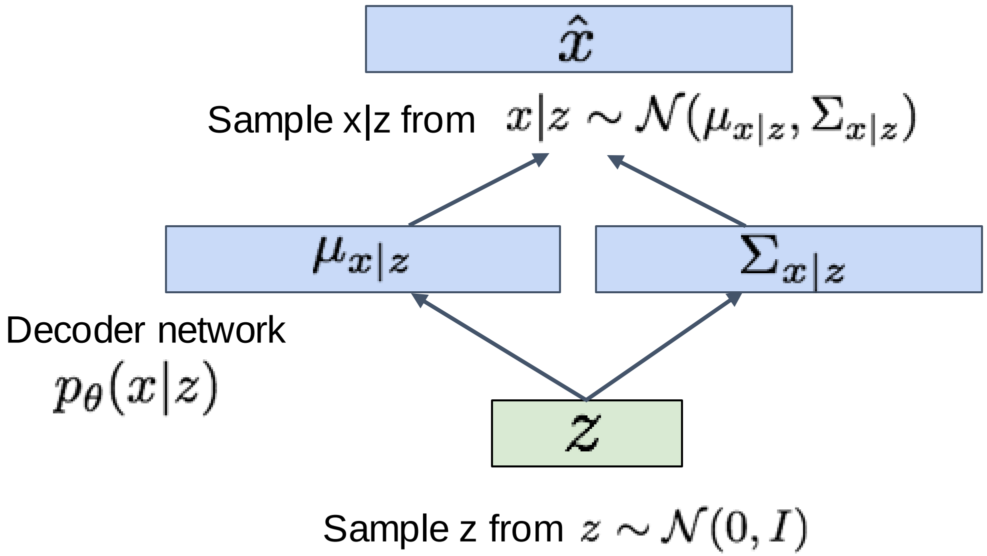
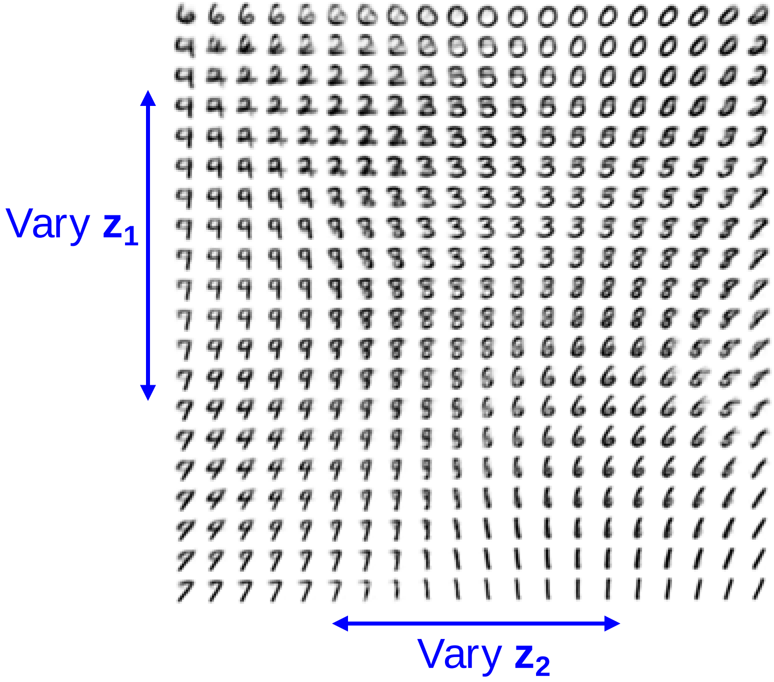


Data manifold for 2-d **z**



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Variational Autoencoders: Generating Data!

Diagonal prior on **z**
=> independent
latent variables

Different
dimensions of **z**
encode
interpretable factors
of variation

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Also good feature representation that can be computed using $q_\phi(z|x)$!

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

32x32 CIFAR-10

Labeled Faces in the Wild

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Latent space z is interpretable and may be useful for other downstream tasks.

Cons:

- Samples are blurry
- KL weights are hard to tune
- Latent distributions are aggressive representation bottlenecks that may limit the expressiveness of the model.

Can be made more powerful by making VAE hierarchical (multiple layers of latents).
Diffusion model (denoising diffusion) can be thought of a type of hierarchical VAE!

Taxonomy of Generative Models

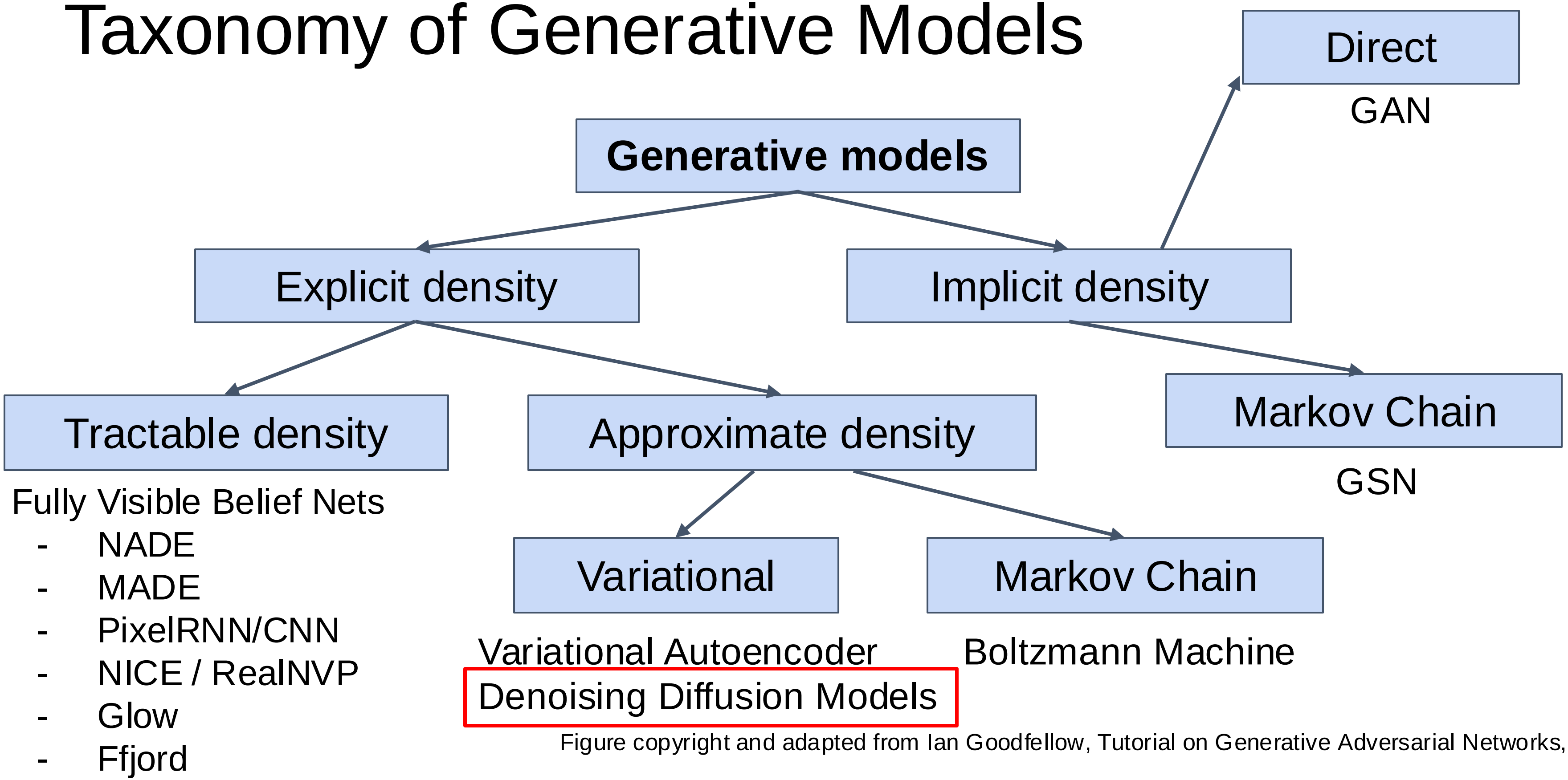

Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Denoising Diffusion Probabilistic Models (DDPMs)

And Conditional Diffusion Models

TEXT DESCRIPTION

An astronaut Teddy bears A bowl of soup

riding a horse lounging in a tropical resort in space playing basketball with cats in space

in a photorealistic style in the style of Andy Warhol as a pencil drawing

→

DALL·E 2

https://openai.com/dall-e-2/

TEXT DESCRIPTION

An astronaut **Teddy bears** A bowl of soup

mixing sparkling chemicals as mad scientists shopping for groceries **working on new AI research**

as kids' crayon art **on the moon in the 1980s** underwater with 1990s technology

→

DALL·E 2

https://openai.com/dall-e-2/

https://openai.com/dall-e-2/

Watch 321 | Fork 5k | Starred 33k

rity | Insights

main | 1 branch | 0 tags | Go to file | Add file | Code

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assets	Release under CreativeML Open RAIL M License	2 months ago
configs	stable diffusion	3 months ago
data	stable diffusion	3 months ago
ldm	stable diffusion	3 months ago
models	add configs for training unconditional/class-conditional ldms	11 months ago
scripts	Release under CreativeML Open RAIL M License	2 months ago
LICENSE	Release under CreativeML Open RAIL M License	2 months ago
README.md	Release under CreativeML Open RAIL M License	2 months ago
Stable_Diffusion_v1_Model_Card.md	Release under CreativeML Open RAIL M License	2 months ago
environment.yaml	Release under CreativeML Open RAIL M License	2 months ago
main.py	add configs for training unconditional/class-conditional ldms	11 months ago
notebook_helpers.py	add code	11 months ago
setup.py	add code	11 months ago

README.md

Stable Diffusion

Stable Diffusion was made possible thanks to a collaboration with Stability AI and Runway and builds upon our previous work:

High-Resolution Image Synthesis with Latent Diffusion Models
Robin Rombach*, Andreas Blattmann*, Dominik Lorenz, Patrick Esser, Björn Ommer
CVPR '22 Oral | *GitHub* | *arXiv* | *Project page*

About

A latent text-to-image diffusion model

ommer-lab.com/research/latent-diffus...

Readme
View license
33k stars
321 watching
5k forks

Releases

No releases published

Packages

No packages published

Contributors 7

Languages

Jupyter Notebook 90.1%
Python 9.8%
Shell 0.1%

https://github.com/CompVis/stable-diffusion

Landscape Highlights of Diffusion Models (Nov 2022)

basic principles

- *Diffusion probabilistic models* (Sohl-Dickstein et al., 2015)
- *Noise-conditioned score network* (**NCSN**; Yang & Ermon, 2019)
- *Denoising diffusion probabilistic models* (**DDPM**; Ho et al. 2020)

conditional & high-res image generation

- *Classifier-guided conditional generation* (Dhariwal and Nichole, 2021)
- *Classifier-free Diffusion Guidance* (Ho and Salimans, 2022)
- *Latent-space Diffusion* (**StableDiffusion**; Rombach and Blattmann et al., 2022)

new applications

- *Planning with Diffusion for Flexible Behavior Synthesis* (**Diffuser**; Janner et al., 2022)
- *DreamFusion: Text-to-3D using 2D Diffusion* (Poole and Jain et al., 2022)
- *Make-A-Video: Text-to-Video Generation without Text-Video Data* (Singer et al., 2022)

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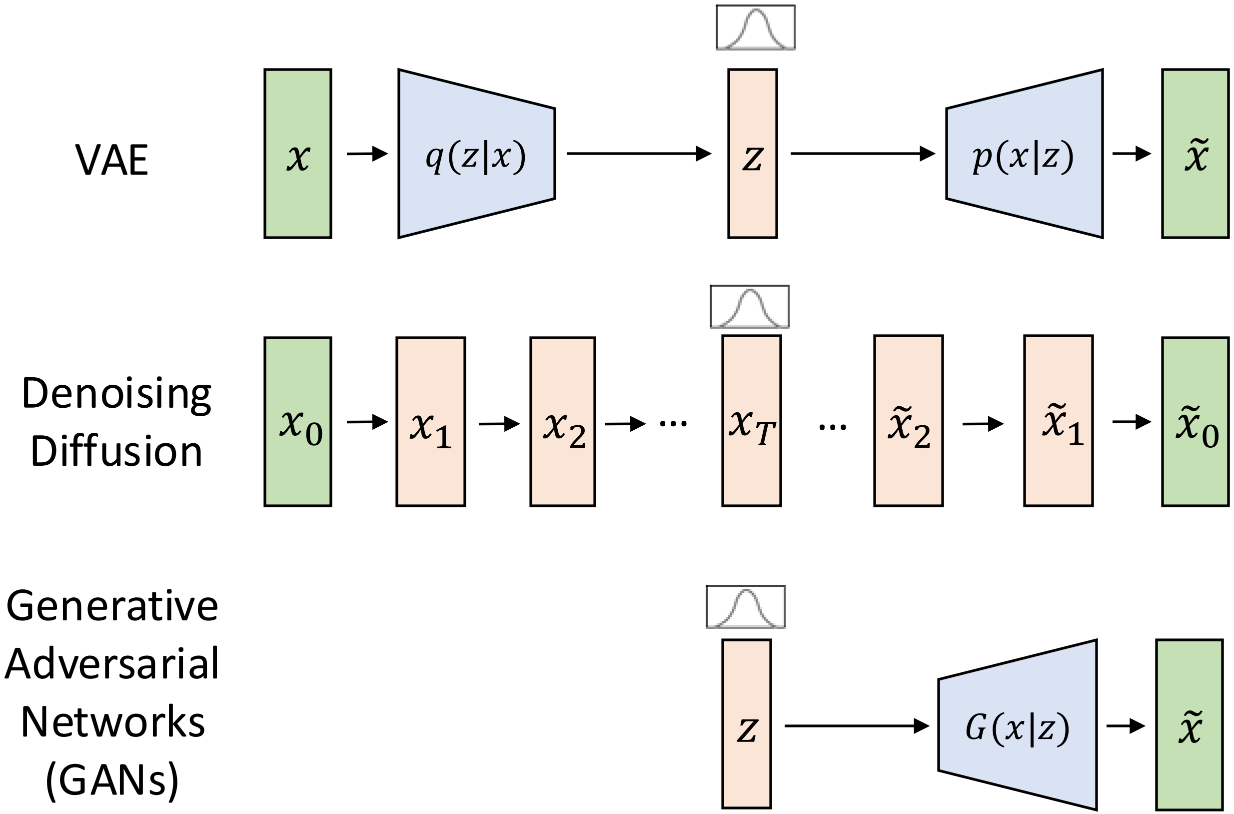
Denoising Diffusion: Image to Noise and Back



The Denoising Diffusion Process

image from
dataset

x_0

The Denoising Diffusion Process

image from dataset

The "forward diffusion" process: add Gaussian noise each step

x_0 → x_1 → ...

The Denoising Diffusion Process

image from dataset

The “forward diffusion” process: add Gaussian noise each step

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

$x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_{T-1} \rightarrow x_T$


…


The Denoising Diffusion Process

image from dataset

The "forward diffusion" process: add Gaussian noise each step

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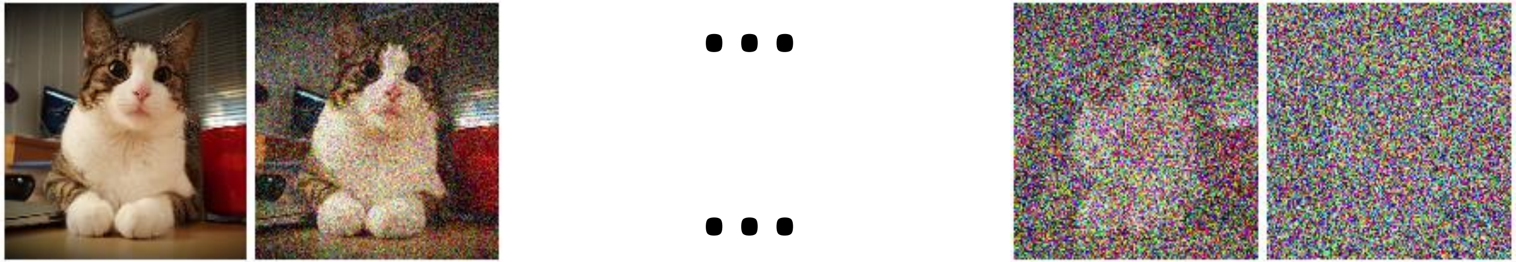
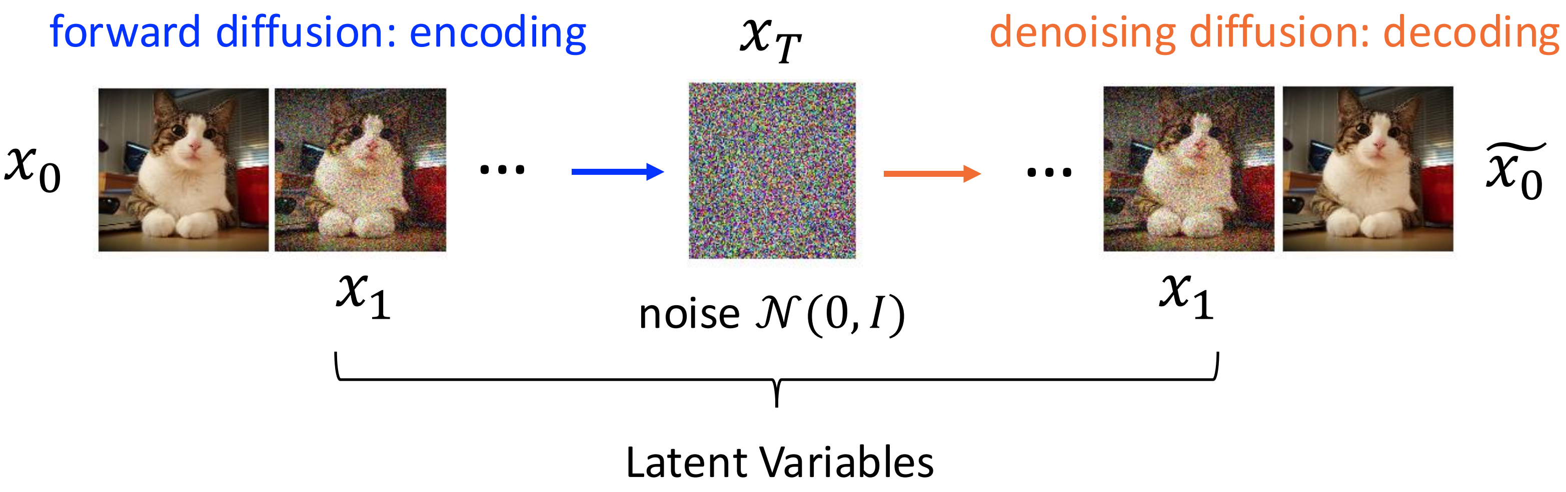
$x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_{T-1} \rightarrow x_T$



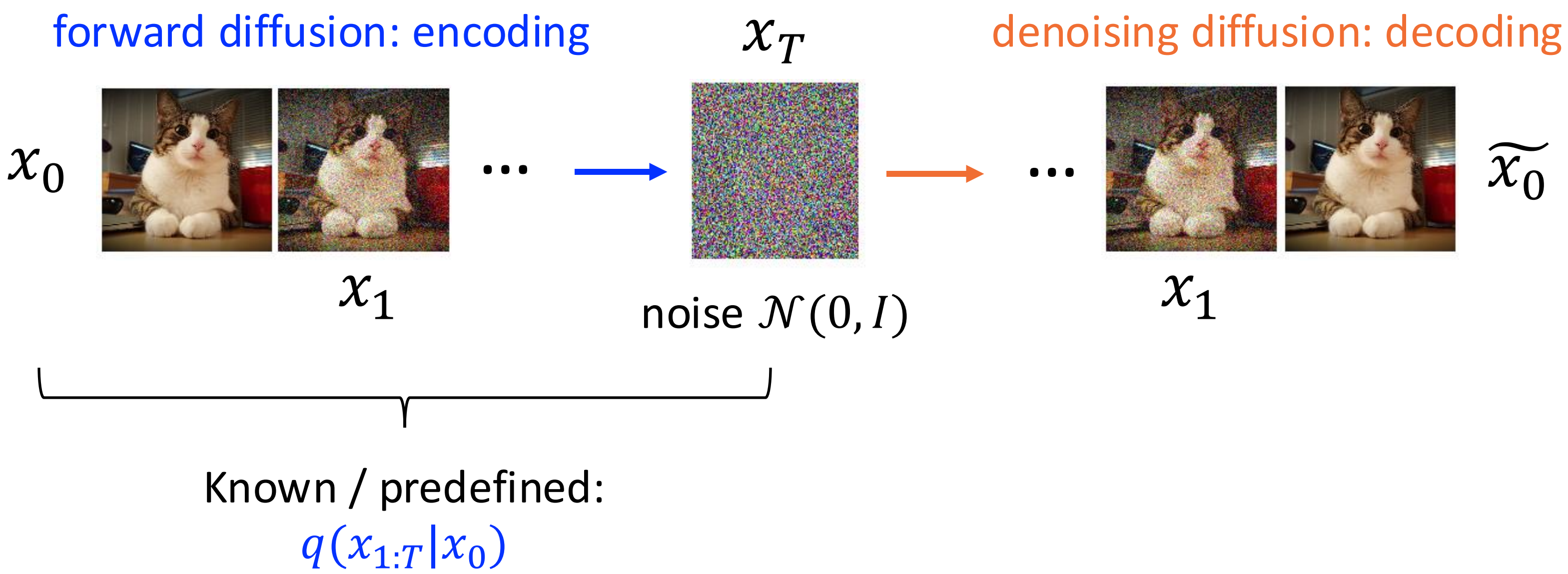
$x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_{T-1} \leftarrow x_T$

The "denoising diffusion" process: generate an image from noise by *denoising* the gaussian noises

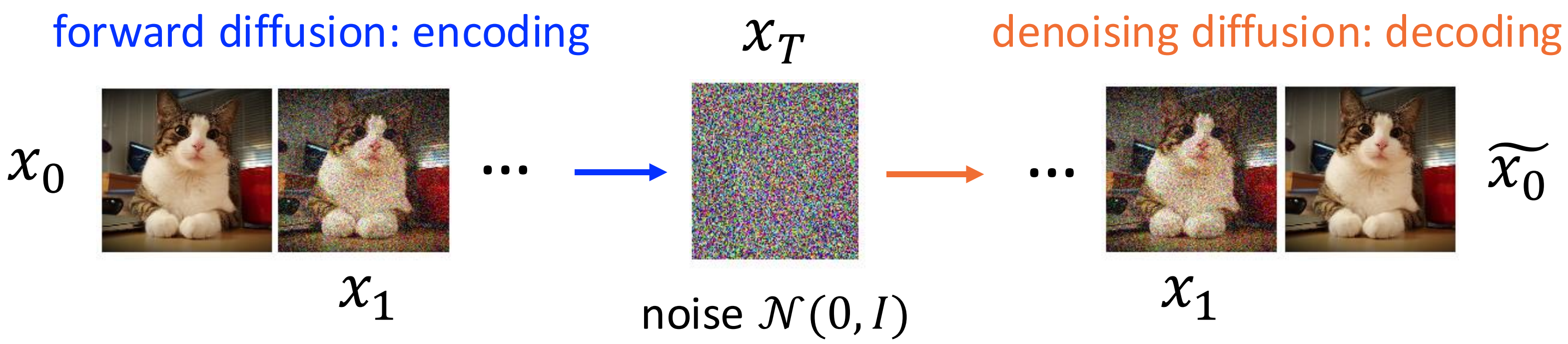
Connection to VAEs



Connection to VAEs



Connection to VAEs



Known / predefined:
$q(x_{1:T}|x_0)$

Unknown / learned:

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

Similar to VAEs, use the denoising decoding process to generate new images.

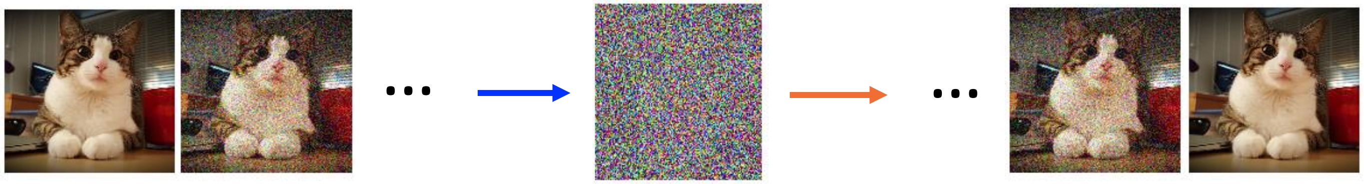
Connection to VAEs

forward diffusion: encoding

x_T

denoising diffusion: decoding

x_0



$\widetilde{x_0}$

x_1

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

x_1

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

Similar to VAEs, use the denoising decoding process to generate new images.

The Diffusion (Encoding) Process

The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$

The Diffusion (Encoding) Process

The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$

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

Probability Chain Rule (Markov Chain)

The Diffusion (Encoding) Process

The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$ Probability Chain Rule (Markov Chain)

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

The Diffusion (Encoding) Process

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Notation: A Gaussian distribution “for” x_t

Plain English: the distribution for x_t is a Gaussian with mean of $(1-\beta_t)x_{t-1}$, where x_{t-1} is a sample from the previous step, and variance of $\beta_t I$

The Diffusion (Encoding) Process

The **known** forward process $x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_T$

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β_t is the *variance schedule* at the diffusion step t

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β_t is the *variance schedule* at the diffusion step t

$0 < \beta_1 < \beta_2 < \cdots < \beta_T < 1$, typical value range $[0.0001, 0.02]$, with $T = 1000$

The Diffusion (Encoding) Process

The **known** forward process $x_0 \longrightarrow x_1 \longrightarrow \cdots \longrightarrow x_T$

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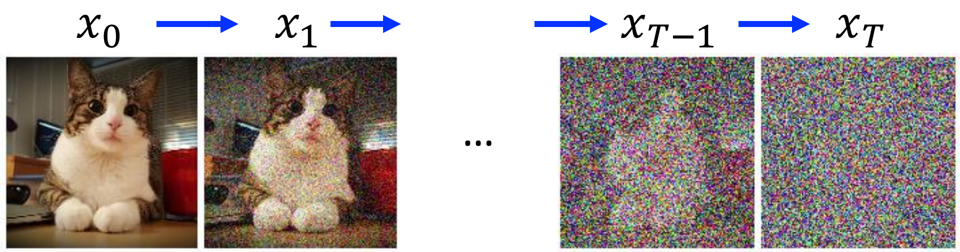

The Diffusion (Encoding) Process

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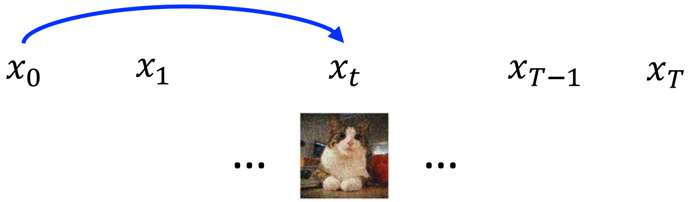
$$q(x_t|x_{t-1}) = \mathcal{N}(x_t; (1-\beta_t)x_{t-1}, \beta_t I)$$ Conditional Gaussian

Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed!

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

, where $a_t = (1-\beta_t)$, $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$



The Diffusion (Encoding) Process

The **known** forward process $x_0 \rightarrow x_1 \rightarrow \cdots \rightarrow x_T$

$$q(x_{1:T}|x_0) = \prod_{t=1}^{T} q(x_t|x_{t-1})$$ Probability Chain Rule (Markov Chain)

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

Nice property: samples from an *arbitrary forward step* are also Gaussian-distributed!

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Gaussian reparameterization trick (recall from VAEs!):

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

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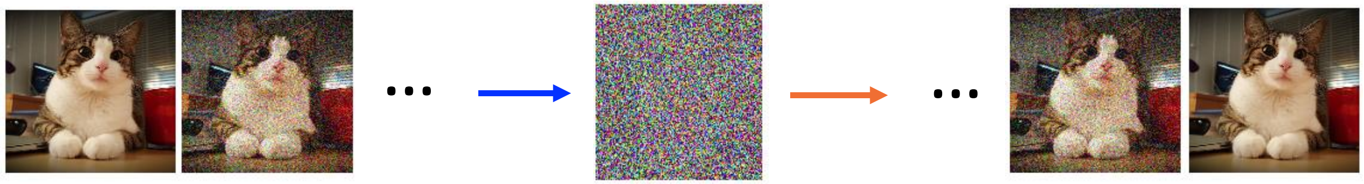
Intuition: We can directly computed noised sample at arbitrary step *t* without going through the Markov chain

The Diffusion and Denoising Process



Known / predefined:

$q(x_{1:T}|x_0)$

Unknown / learned:

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

The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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Probability Chain Rule (Markov Chain)

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

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Conditional Gaussian

Want to learn time-dependent mean

Assume fixed / known variance (simplification)

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How do we form a learning objective?

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High-level intuition: derive a *ground truth denoising distribution* $q(x_{t-1}|x_t, x_0)$ and train a neural net $p_\theta(x_{t-1}|x_t)$ to match the distribution.

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← Recall: Gaussian reparameterization trick

The "ground truth" noise that brought x_{t-1} to x_t . We know this during training because we took this sample during the forward process!

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Assuming identical variance $\Sigma_q(t)$, we have:

$$\text{argmin}_\theta D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) = \text{argmin}_\theta w||\mu_q(t) - \mu_\theta(x_t, t)||$$

Should be variance-dependent, but constant works better in practice

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Intuition: learn to estimate the added noise and remove it!

Should be variance-dependent, but constant works better in practice

The Denoising (Decoding) Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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We know how to learn — Assume fixed / known variance

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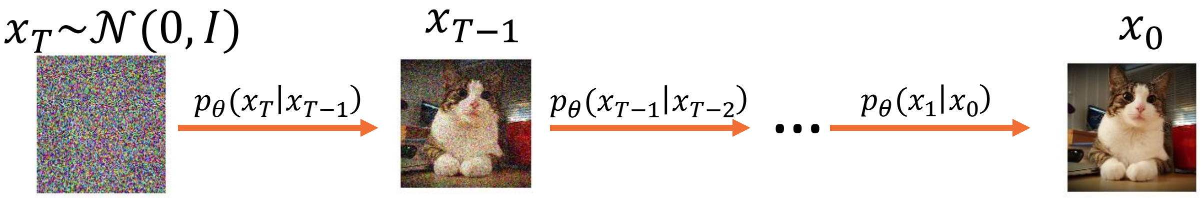

Generate new images!

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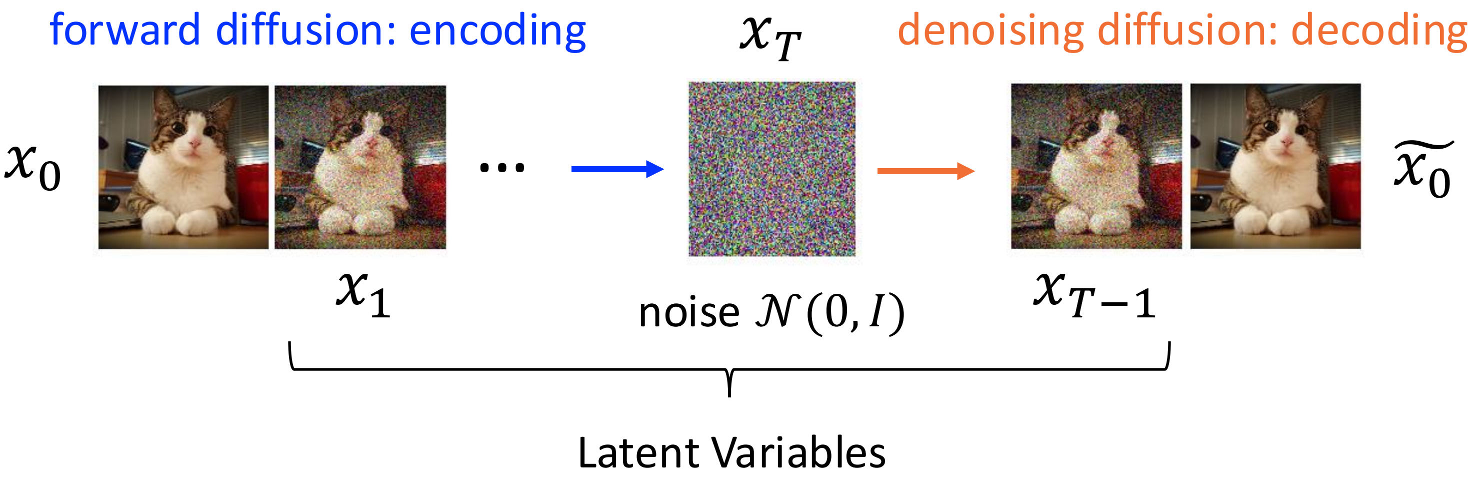
We know how to learn ($\mu_\theta(x_t, t)$)

Assume fixed / known variance ($\Sigma_q(t)$)

How did we arrive at the learning objective? Why is this mathematically correct?

Let's go back to the basics of variational models …

Connection to VAEs



$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

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$$\geq \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

Known forward noise (posterior)

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← reverse denoising

← forward diffusion

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… (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

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known

Easy to optimize / sometimes omitted

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Maximize the agreement between the predicted reverse diffusion distribution p_θ and the "ground truth" reverse diffusion distribution q

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$q(x_{t-1}|x_t) = \boldsymbol{q(x_{t-1}|x_t, x_0)}$ **(markov assumption)**

$$= \frac{q(x_t|x_{t-1}, x_0)q(x_{t-1}|x_0)}{q(x_t|x_0)}$$ (Bayes rule)

$$= \frac{\mathcal{N}(x_t;\sqrt{\alpha_t}x_{t-1},\beta_t I)\mathcal{N}(x_{t-1};\sqrt{\bar{\alpha}_{t-1}}x_{t-1},(1-\bar{\alpha}_{t-1})I)}{\mathcal{N}(x_t;\sqrt{\bar{\alpha}_t}x_0,(1-\bar{\alpha}_{t-1})I)}$$

$$\propto \mathcal{N}\left(x_{t-1};\ \frac{\sqrt{\alpha_t}(1-\bar{\alpha}_{t-1})x_t+\sqrt{\bar{\alpha}_{t-1}}(1-a_t)x_0}{1-\sqrt{\bar{\alpha}_t}}, \Sigma_q(t)\right)$$ (Property of Gaussian)

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Proof using bayes rule and gaussian reparameterization trick

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$$\geq \mathrm{E}_q\left[\log\frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

$$\log p(x_0) \geq \mathrm{E}_q\left[\log\frac{p(x_0|x_{1:T})p(x_{1:T})}{q(x_{1:T}|x_0)}\right]$$ $x = x_0,\ z = x_{1:T}$

$$= \mathrm{E}_q\left[\log\frac{p(x_T)\prod_{t=1}^{T} p_\theta(x_{t-1}|x_t)}{\prod_{t=1}^{T} q(x_t|x_{t-1})}\right]$$

… (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1)$$

$$q(x_{t-1}|x_t, x_0) = \mathcal{N}\left(x_{t-1}; \mu_q(t), \Sigma_q(t)\right)$$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

Proof using bayes rule and gaussian reparameterization trick

The "ground truth" noise that brought x_0 to x_t

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

$p(x) = \int p(x|z)p(z)dz$ Intractable to estimate!

$$\log p(x) = \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right] + D_{KL}(q(z|x)||p(z|x))$$

$$\geq \mathrm{E}_q\left[\log \frac{p(x|z)p(z)}{q(z|x)}\right]$$ Evidence Lower Bound (ELBO)

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... (derivation omitted, see Sohl-Dickstein *et al.,* 2015 Appendix B)

$$= -\mathrm{E}_q[D_{KL}(q(x_T|x_0)||p(x_T))] - \sum_{t=2}^{T} D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t)) + \log p_\theta(x_0|x_1)$$

Minimize the difference of distribution means (assuming identical variance)

$$\mathrm{argmin}_\theta w||\mu_q(t) - \mu_\theta(x_t, t)||$$

Deep Unsupervised Learning using Nonequilibrium Thermodynamics, Sohl-Dickstein *et al.*, 2015

Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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

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

Conditional Gaussian

Learning objective: $\text{argmin}_\theta ||\mu_q(t) - \mu_\theta(x_t, t)||$

$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

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The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

Do we actually need to learn the entire $\mu_\theta(x_t, t)$?

Learning the Denoising Process

The **learned** denoising process $x_0 \leftarrow x_1 \leftarrow \cdots \leftarrow x_T$

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$$\mu_q(t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon\right), \qquad \epsilon \sim \mathcal{N}(0, I)$$

known during inference

Unknown during inference

Recall: this is the "ground truth" noise that brought x_0 to x_t

Learning the Denoising Process

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Learning objective: $\mathrm{argmin}_\theta ||\mu_q(t) - \mu_\theta(x_t, t)||$

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known during inference

Unknown during inference

Recall: this is the "ground truth" noise that brought x_0 to x_t

Idea: just learn ϵ with $\epsilon_\theta(x_t, t)$!

Learning the Denoising Process

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Conditional Gaussian

Simplified learning objective: $\mathrm{argmin}_\theta ||\epsilon - \epsilon_\theta(x_t, t)||$

Learning the Denoising Process

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Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta(x_t, t)||$

Recall: the simplified t-step forward sample:

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

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Conditional Gaussian

Simplified learning objective: $\text{argmin}_\theta ||\epsilon - \epsilon_\theta\left(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t\right)||$

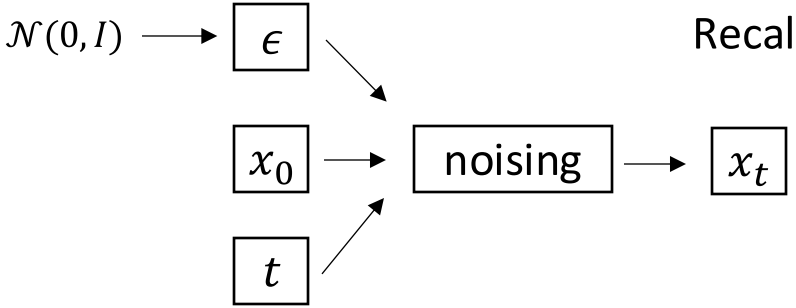
Inference time: $\mu_\theta(x_t, t) = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{\beta_t}{\sqrt{(1-\bar{\alpha}_t)}}\epsilon_\theta(x_t, t)\right)$

Predicted "denoising noise"

The Denoising Diffusion Algorithm

Algorithm 1 Training

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



Recall: the simplified t-step forward sample:

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

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
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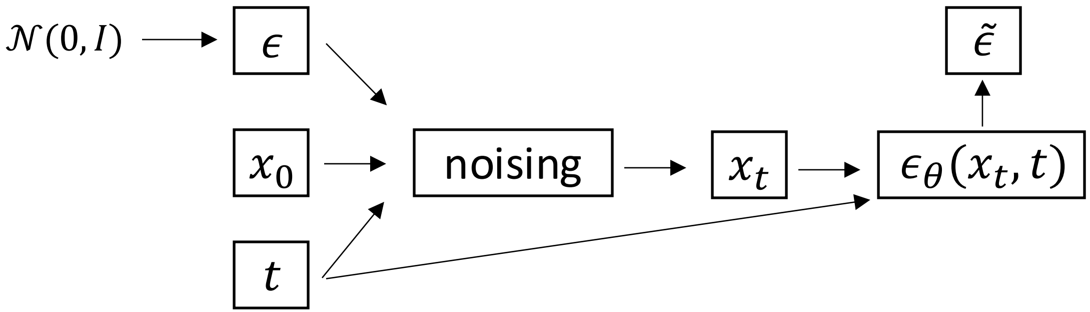

Predict noise with a denoiser network ϵ_θ

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \mathrm{Uniform}(\{1, \ldots, T\})$
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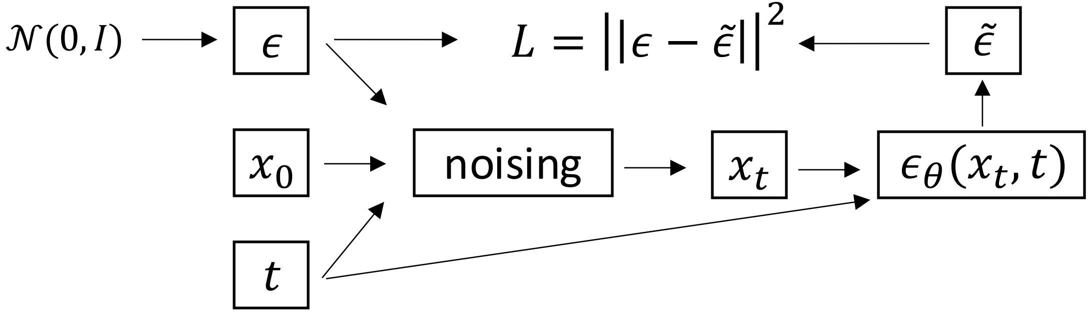

Compute regression loss

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
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$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

Algorithm 2 Sampling

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

The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

The Denoising Diffusion Algorithm

Algorithm 1 Training

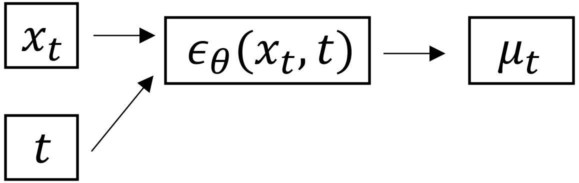
repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \text{Uniform}(\{1, \ldots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \ldots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

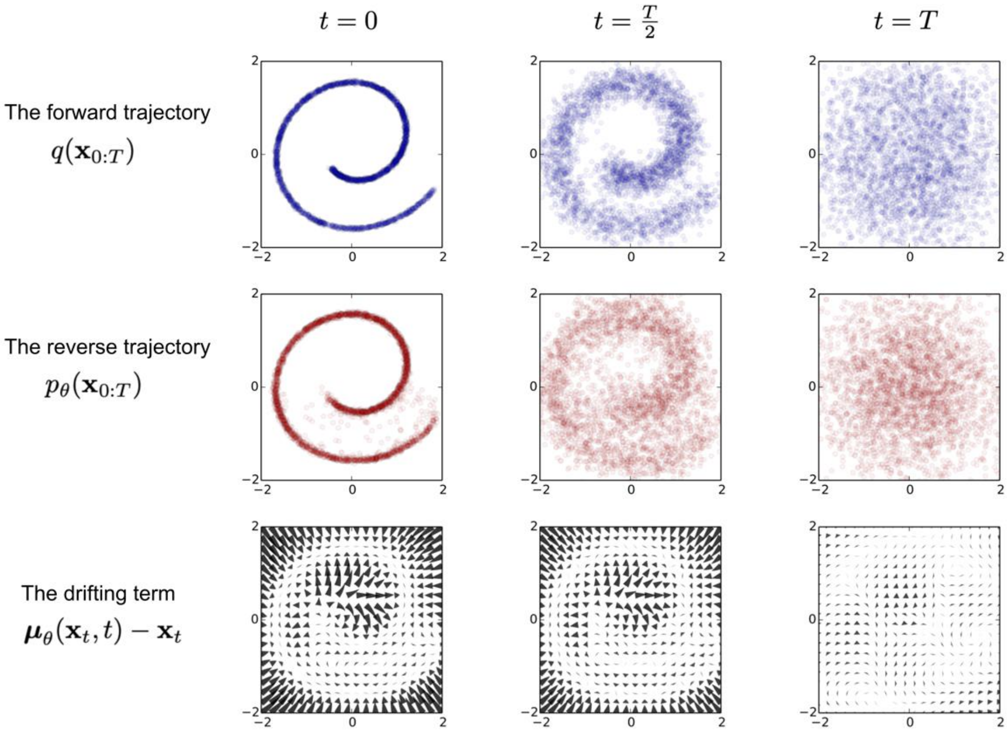
$$\sigma_t = \sqrt{\beta}_t$$

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



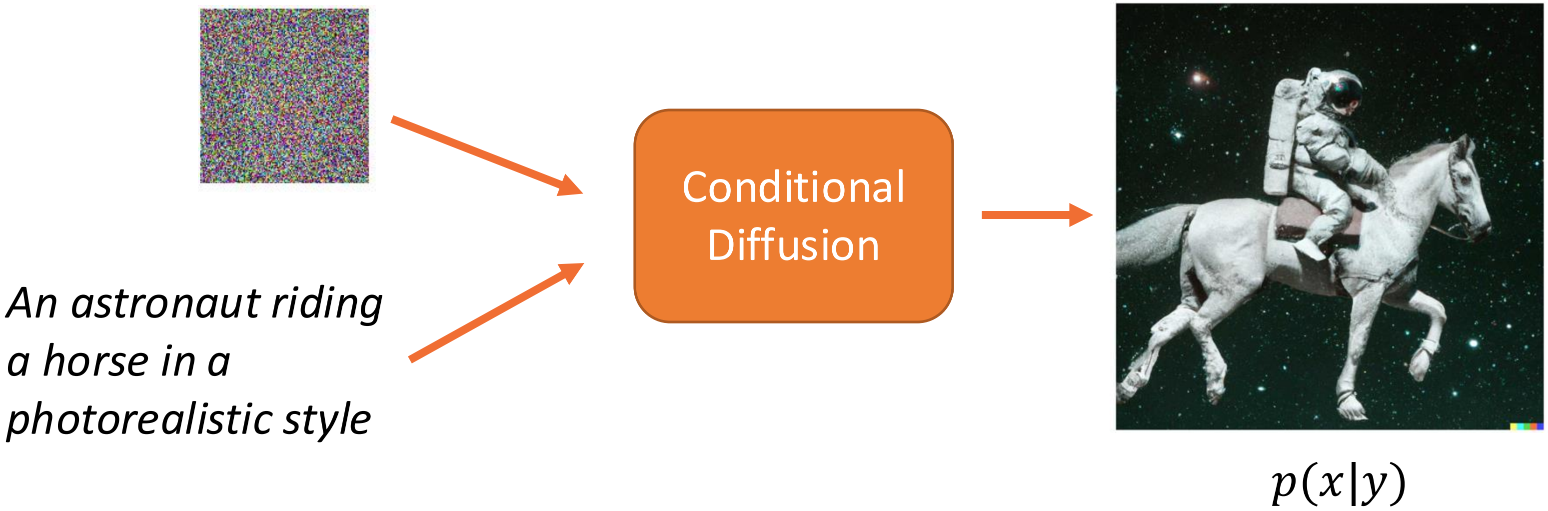
The Denoising Diffusion Probabilistic Models, Ho *et al.*, 2020

Visualizing the Diffusion Process on 2D data

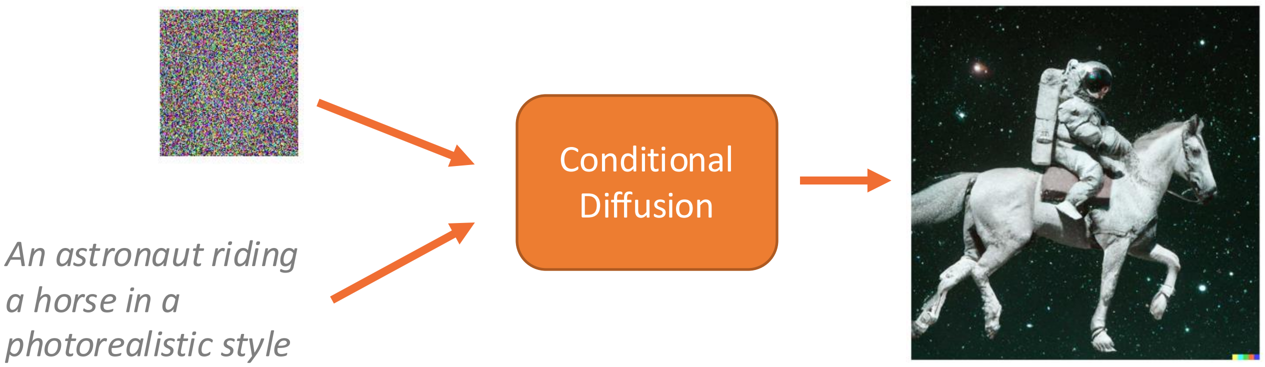


Sohl-Dickstein *et al.*, 2015

Conditional Diffusion Models



Conditional Diffusion Models

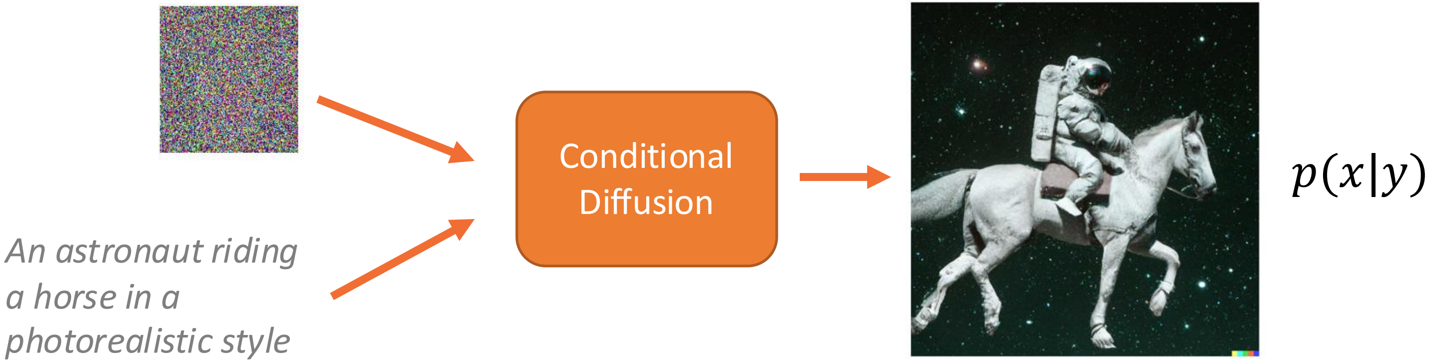


$p(x|y)$

Simple idea: just condition the model on some text labels y!

$$\epsilon_\theta(x_t, y, t)$$

Conditional Diffusion Models

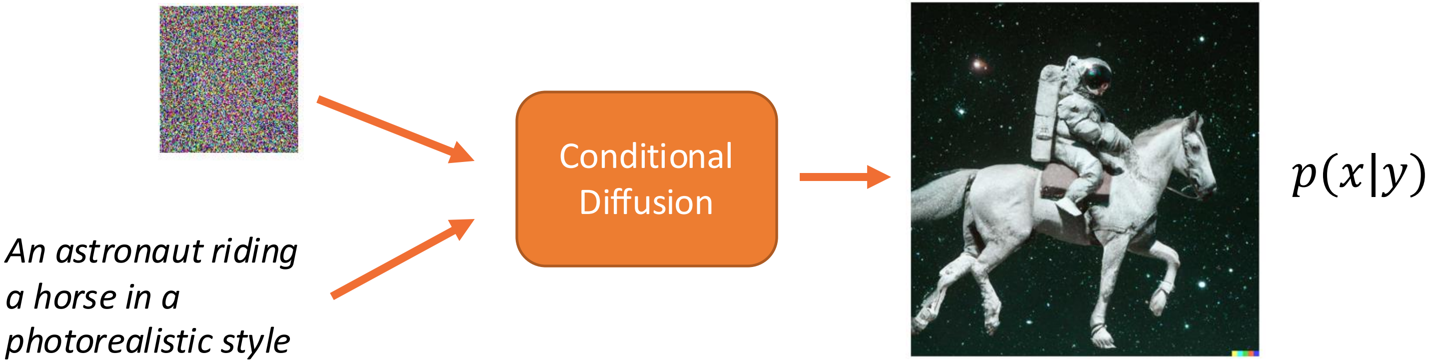


Simple idea: just condition the model on some text labels y!

$$\epsilon_\theta(x_t, y, t)$$

Problem: Very blurry generation

Classifier-guided Diffusion

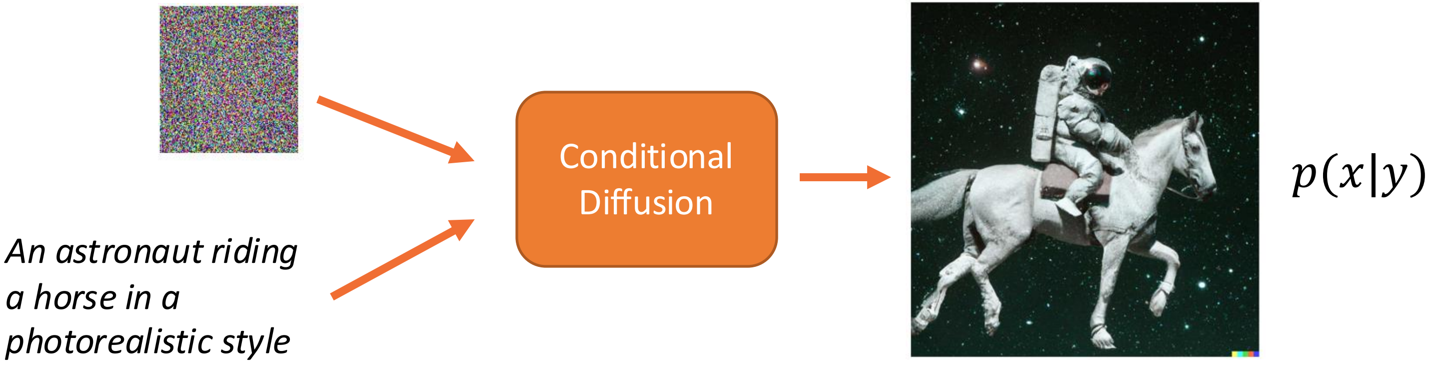


Better idea: use the *gradients* from an image captioning model $f_\varphi(y|x_t)$ to guide the diffusion process!

$$\bar{\epsilon}_\theta(x_t, t) = \epsilon_\theta(x_t, t) - \sqrt{1 - \bar{\alpha}_t}\nabla_{x_t} \log f_\varphi(y|x_t)$$

Dhariwal & Nichol, 2021

Classifier-guided Diffusion



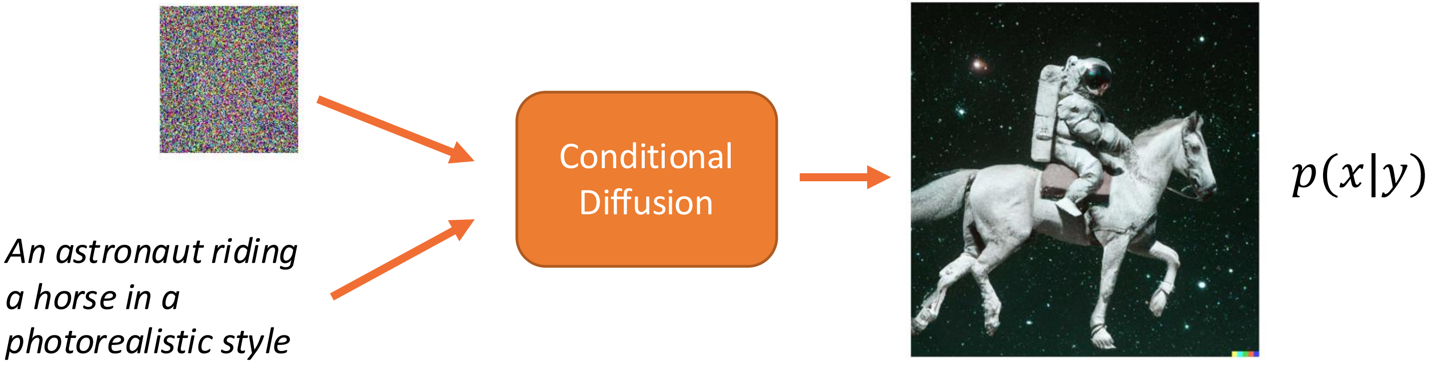
Better idea: use the *gradients* from an image captioning model $f_\varphi(y|x_t)$ to guide the diffusion process!

$$\bar{\epsilon}_\theta(x_t, t) = \epsilon_\theta(x_t, t) - \sqrt{1-\bar{\alpha}_t}\nabla_{x_t}\log f_\varphi(y|x_t)$$

Problem: need a classifier

Dhariwal & Nichol, 2021

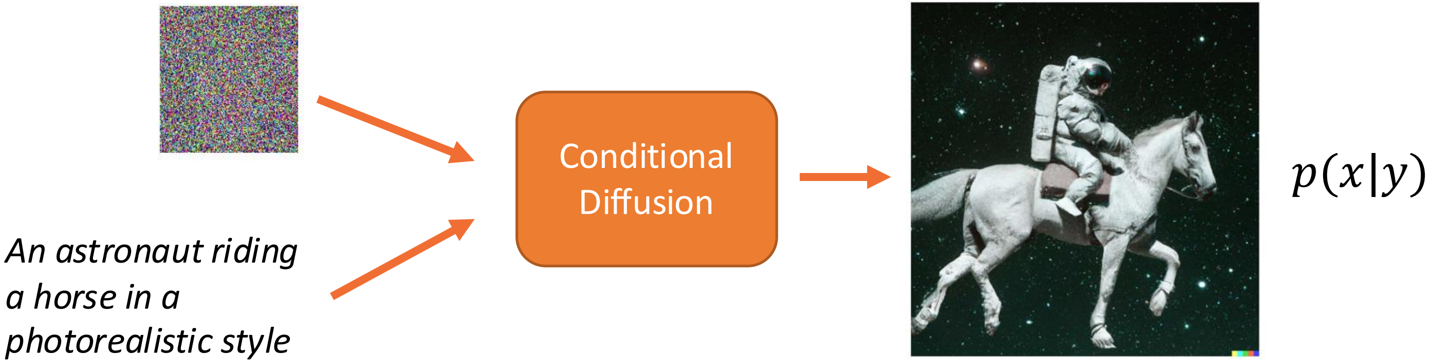
Classifier-free Guided Diffusion



Classifier-free Guided Diffusion: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_\varphi(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\left(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t)\right)$$

Classifier-free Guided Diffusion



Classifier-free Guided Diffusion: estimate the gradient of the classifier model with conditional diffusion models!

$$\nabla_{x_t} \log f_\varphi(y|x_t) = -\frac{1}{\sqrt{1-\bar{\alpha}_t}}\left(\epsilon_\theta(x_t, t, y) - \epsilon_\theta(x_t, t)\right)$$

$$\bar{\epsilon}_\theta(x_t, t, y) = (w+1)\epsilon_\theta(x_t, t, y) - w\epsilon_\theta(x_t, t)$$

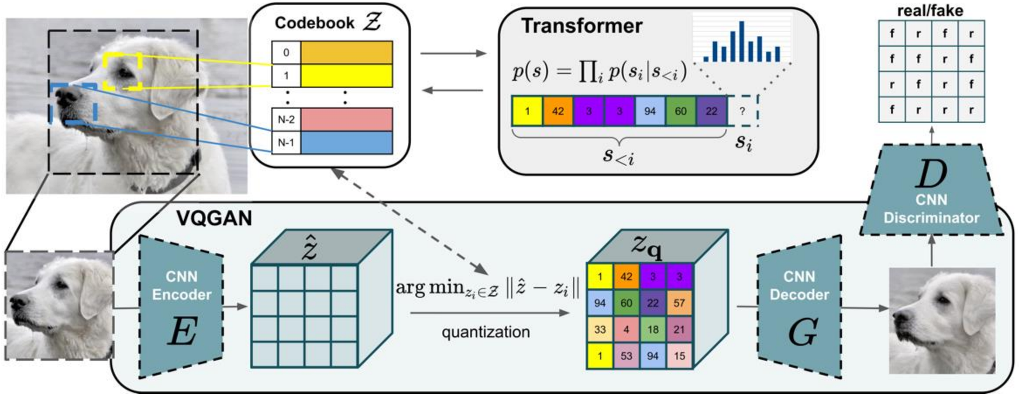
Linearly combine denoisers from an unconditional distribution and a conditional distribution

Ho and Salimans, 2022

Latent-space Diffusion

Problem: Hard to learn diffusion process on high-resolution images

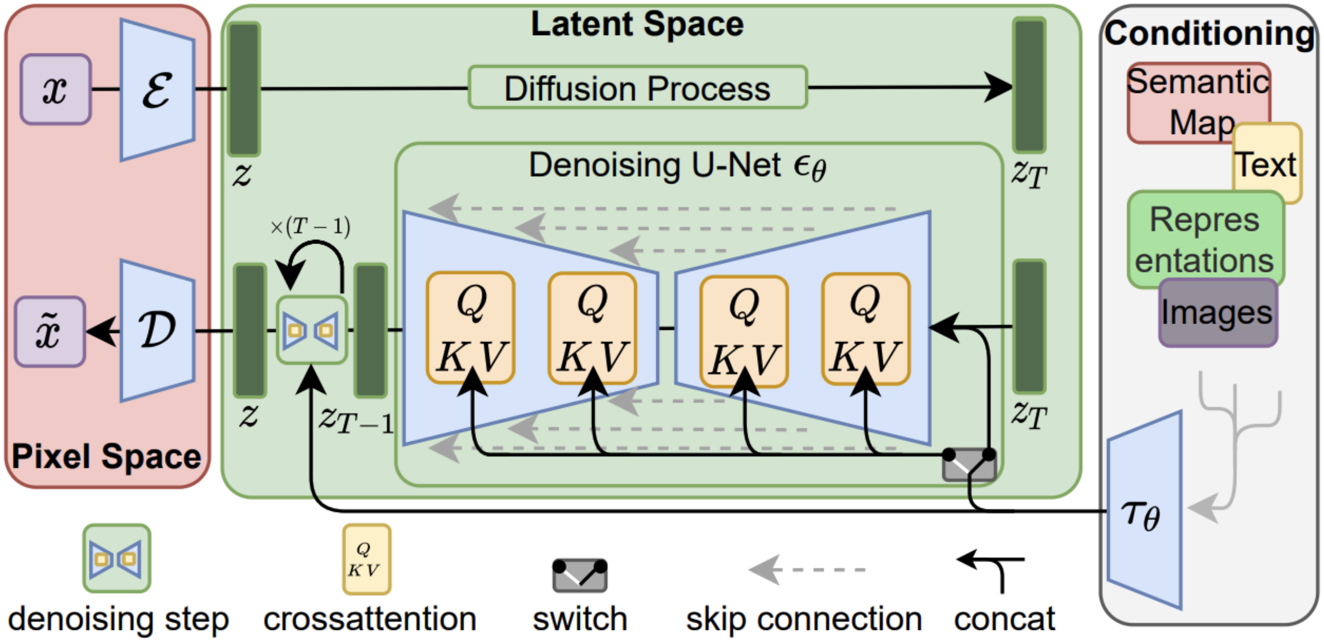
Solution: learn a low-dimensional latent space using a ViT-based autoencoder and *do diffusion on the latent space*!



The latent space autoencoder

Esser and Rombach *et al.*, 2021

“StableDiffusion”



Rombach and Blattmann *et al.*, 2022

“StableDiffusion”

Layout-Conditional Generation

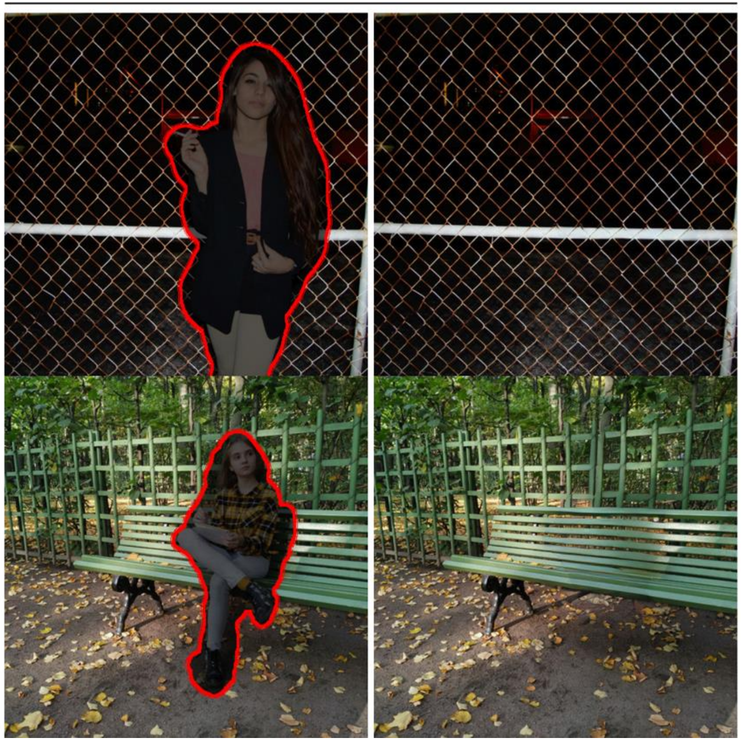
Rombach and Blattmann *et al.*, 2022

“StableDiffusion”

Segmentation-Conditional Generation

Rombach and Blattmann *et al.*, 2022

"StableDiffusion"



Inpainting

Rombach and Blattmann *et al.*, 2022

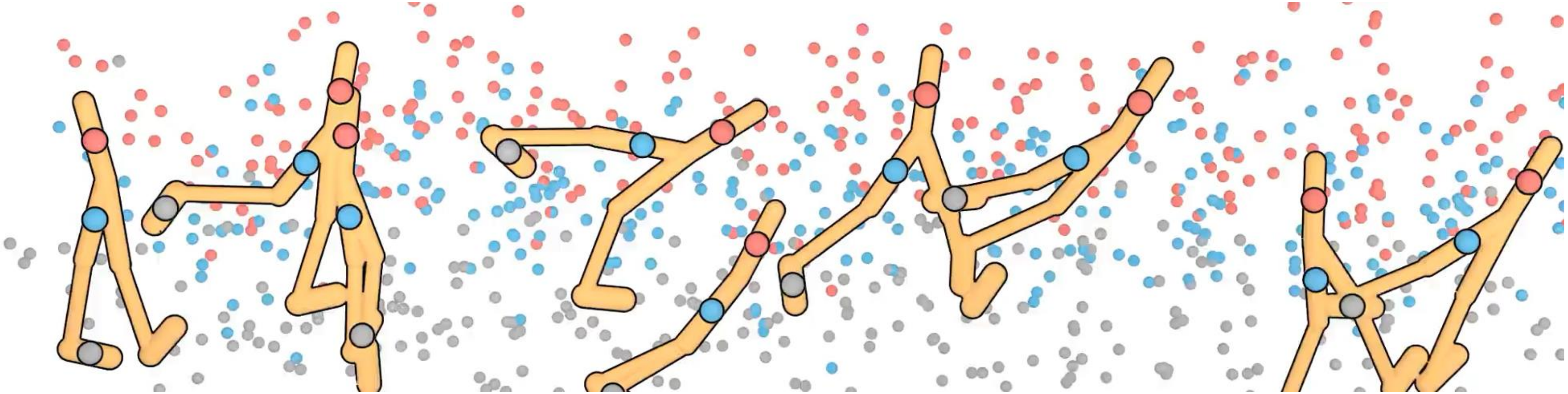
Beyond Image Generation

https://dreamfusion3d.github.io/

Beyond Image Generation

https://ai.facebook.com/blog/generative-ai-text-to-video/

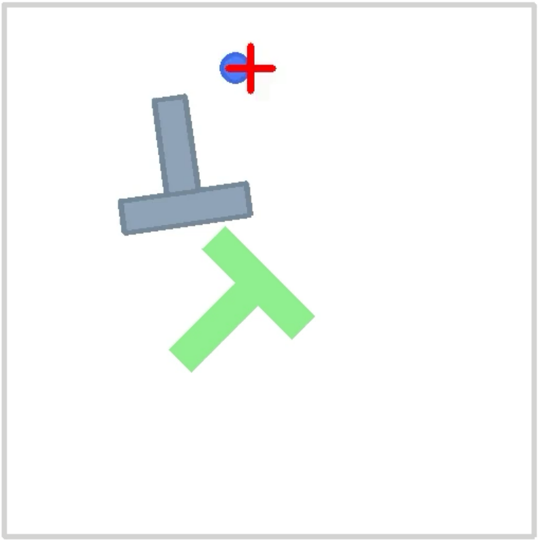
Beyond Image Generation

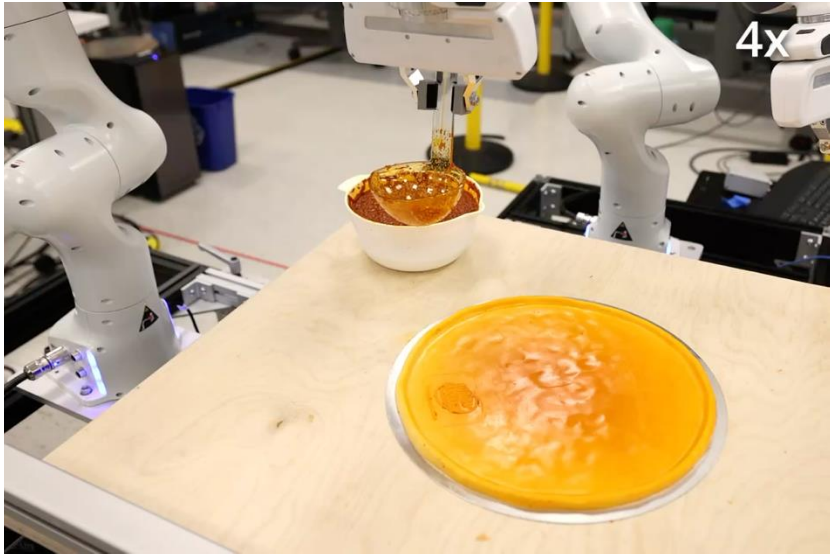


DecisionDiffuser (Ajay, Gupta, Du et al., 2023)
Model future state and reward distributions
$p(r_{t:t+H}, s_{t:t+H} | s_t)$

https://ai.facebook.com/blog/generative-ai-text-to-video/

Beyond Image Generation





Diffusion Policy (Chi et al., 2023)

Model multimodal action distributions (implement this in your HW4!)

$$p(a_{t:t+H}|s_t)$$

https://diffusion-policy.cs.columbia.edu/

Beyond Image Generation

Generative Skill Chaining (Mishra et al., 2023)

https://diffusion-policy.cs.columbia.edu/

Additional resources / tutorials

- Overview of the research landscape: What are Diffusion Models?
- More math! Understanding Diffusion Models: A Unified Perspective
- Tutorial with hands-on example: The Annotated Diffusion Model
- Nice introduction video: What are Diffusion Models?
- CVPR Tutorial: Denoising Diffusion-based Generative Modeling: Foundations and Applications

Summary

- Denoising Diffusion model is a type of generative model that learns the process of “denoising” a known noise source (Gaussian).
- We can construct a learning problem by deriving the evidence lower bound (ELBO) of the denoising process.
- The learning objective is to minimize the KL divergence between the “ground truth” and the learned denoising distribution.
- A simplified learning objective is to estimate the noise of the forward diffusion process.
- The diffusion process can be guided to generate targeted samples.
- Can be applied to many different domains. Same underlying principle.
- Very hot topic!