

Lecture 18: Generative AI Part 2 GANs & Diffusion

Administrative

- Milestone was due last week
- **Quiz 5** (last quiz) will take place last 30 minutes of next lecture
- **Assignment 5** due Friday

Final project details:

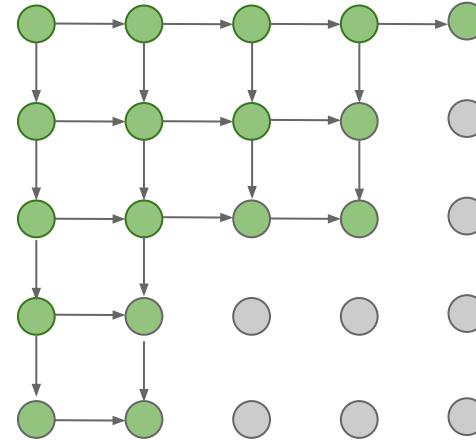
- Submit your **posters** for printing before Friday, March 8th, at 10 a.m.
- **Poster session:** March 11th (Monday), from 10:30AM-12:20PM at HUB 145
- **Final reports** due Mon, Mar 11

Generative AI so far: Autoregressive models

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Very slow during both training and testing; $N \times N$ image requires $2N-1$ sequential steps!



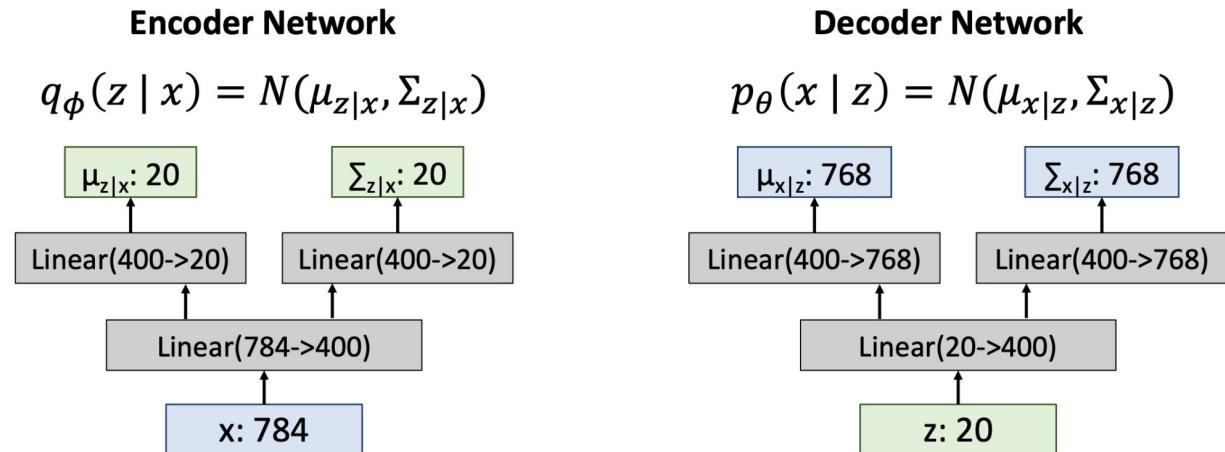
[van der Oord et al. 2016]

Variational Autoencoders: Intractability

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

Another idea: $p_\theta(x) = \frac{p_\theta(x | z)p_\theta(z)}{p_\theta(z | x)}$

x : 28x28 image = 784-dim vector
 z : 20-dim vector



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

Variational Autoencoders

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

We want to
maximize the
data
likelihood

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

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

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

$$= \mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z)) + D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))$$

Decoder network gives $p_\theta(x|z)$, can
compute estimate of this term through
sampling.

This KL term (between
Gaussians for encoder and z
prior) has nice closed-form
solution!

$p_\theta(z|x)$ intractable (saw
earlier), can't compute this KL
term :(But we know KL
divergence always ≥ 0 .

Variational Autoencoders

We want to
maximize the
data
likelihood

$$\begin{aligned}\log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} [\log p_\theta(x^{(i)})] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \frac{q_\phi(z | x^{(i)})}{q_\phi(z | x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z)} \right] + \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z | x^{(i)})} \right] \quad (\text{Logarithms}) \\ &= \underbrace{\mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))}_{\geq 0}\end{aligned}$$

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

Variational Autoencoders

Decoder:
reconstruct
the input data

$$\begin{aligned} \log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} [\log p_\theta(x^{(i)})] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \frac{q_\phi(z | x^{(i)})}{q_\phi(z | x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z)} \right] + \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z | x^{(i)})} \right] \quad (\text{Logarithms}) \\ &= \underbrace{\mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))}_{\geq 0} \end{aligned}$$

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

Encoder:
make approximate posterior distribution close to prior

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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Let's look at computing the KL divergence between the estimated posterior and the prior given some data

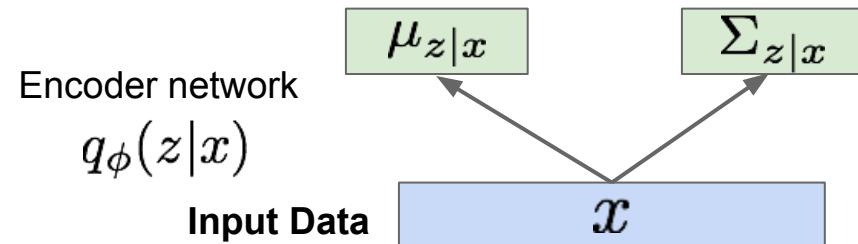
Input Data

x

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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



Variational Autoencoders

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

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

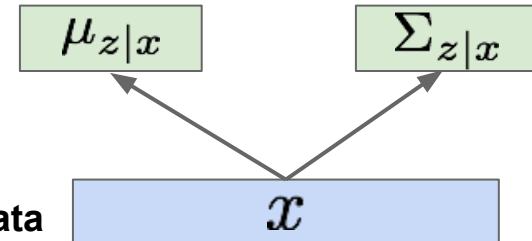
This equation has an analytical solution

Make approximate posterior distribution close to prior

Encoder network

$$q_\phi(z|x)$$

Input Data



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

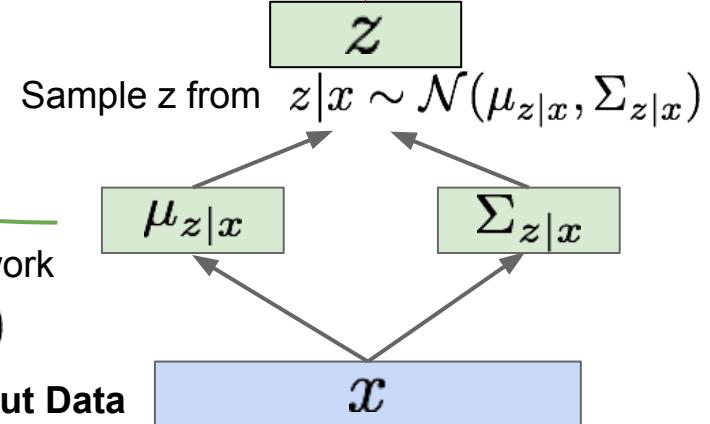
Make approximate posterior distribution close to prior

Encoder network

$$q_\phi(z|x)$$

Input Data

Not part of the computation graph!



Variational Autoencoders

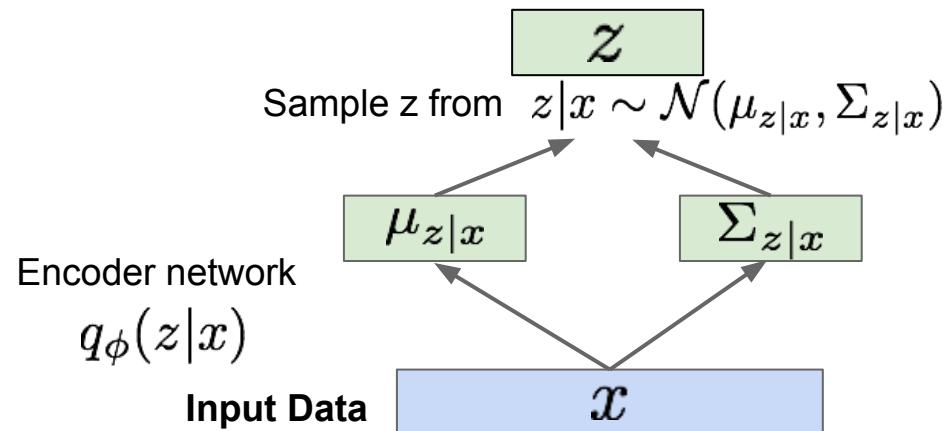
Putting it all together: maximizing the likelihood lower bound

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

Reparameterization trick to make sampling differentiable:

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

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



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

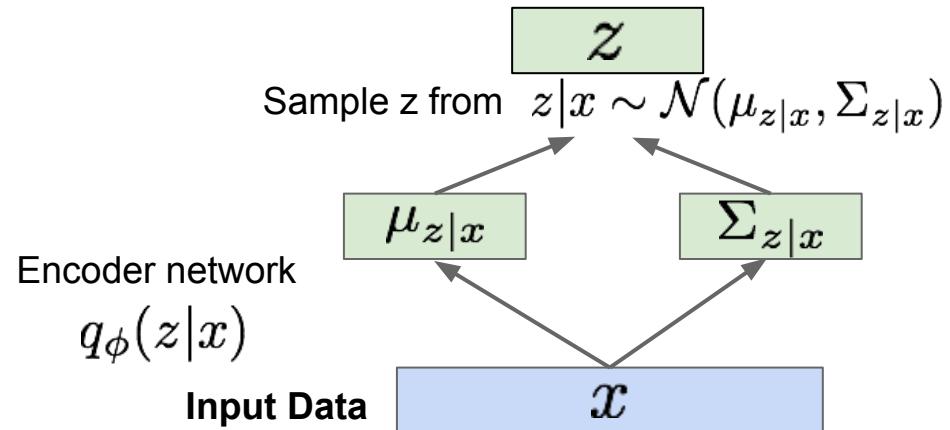
$$\underbrace{\mathbf{E}_z \left[\log p_\theta(x^{(i)} | z) \right] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Reparameterization trick to make sampling differentiable:

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

Sample $\epsilon \sim \mathcal{N}(0, I)$ Input to the graph

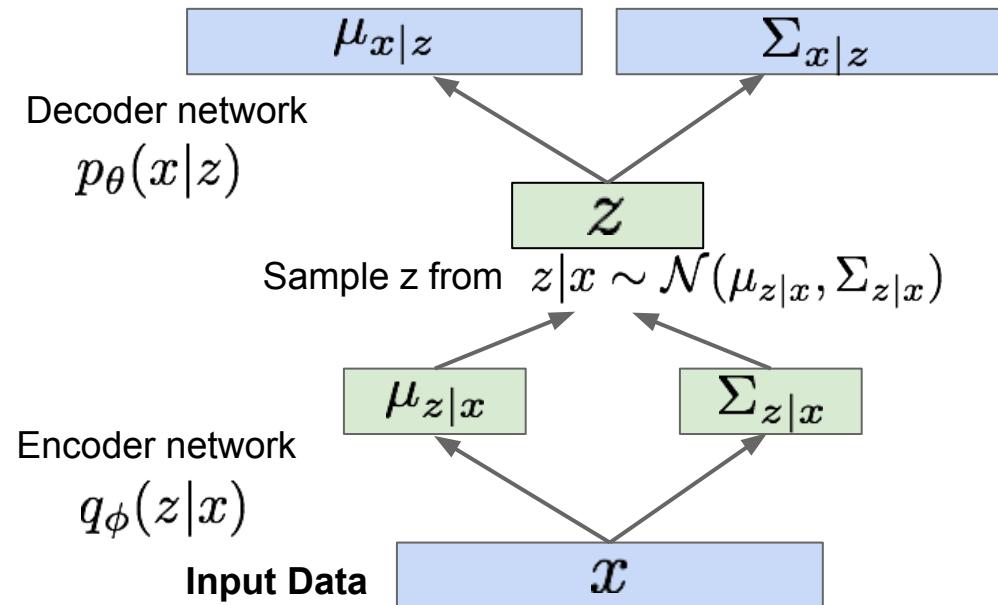
Part of computation graph



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

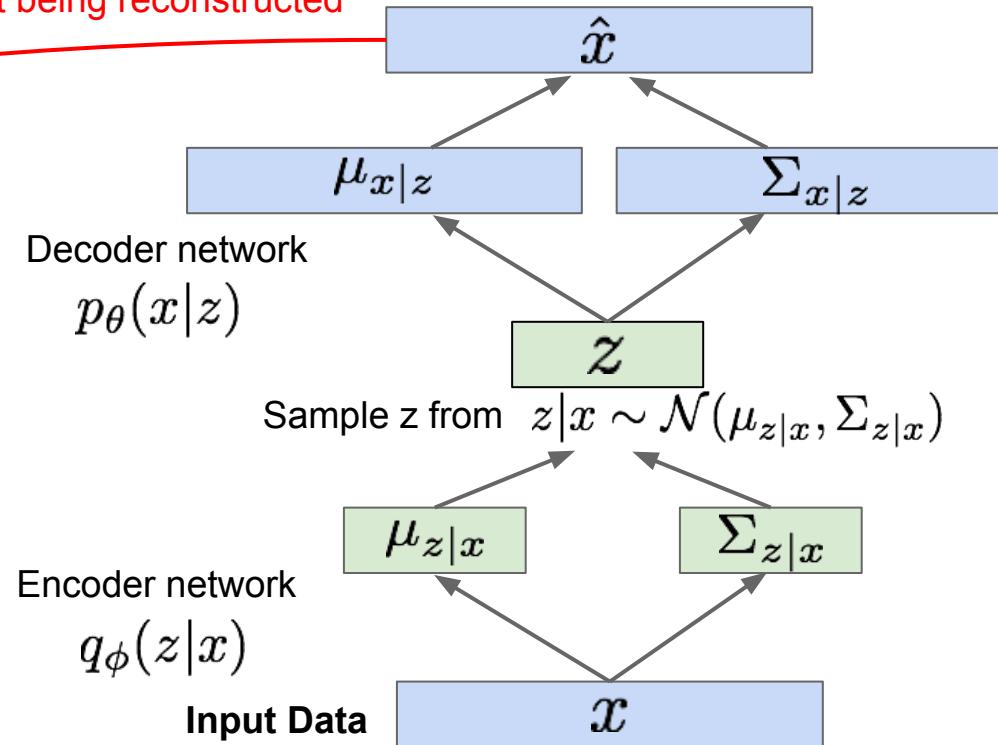


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Maximize likelihood of original input being reconstructed

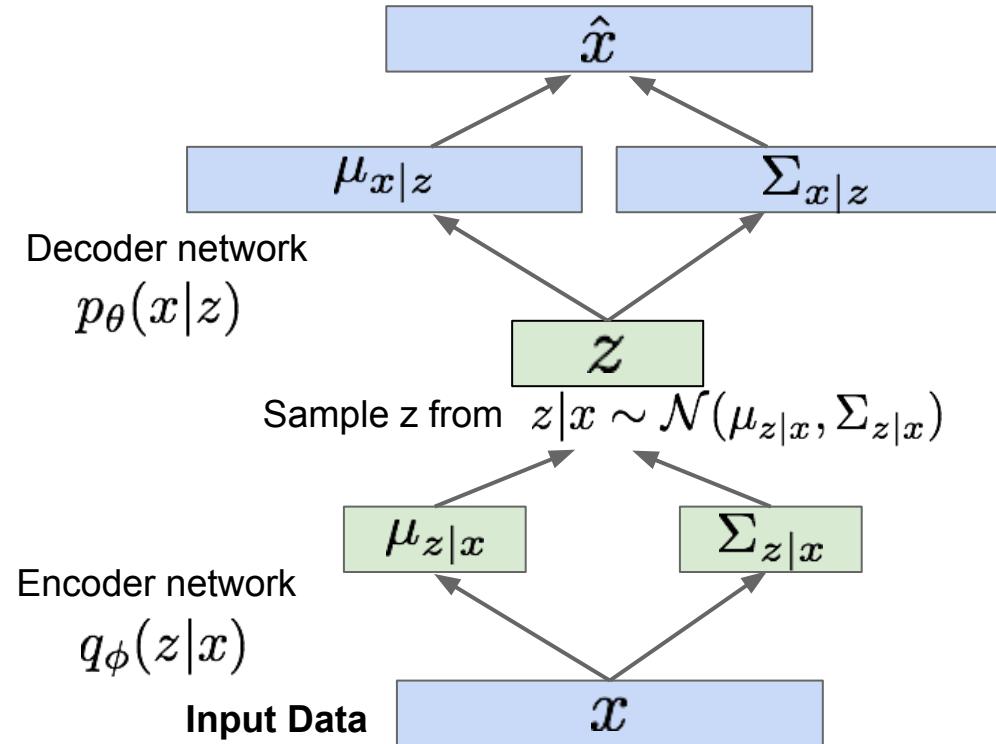


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

For every minibatch of input data: compute this forward pass, and then backprop!



Variational Autoencoders: Generating Data!

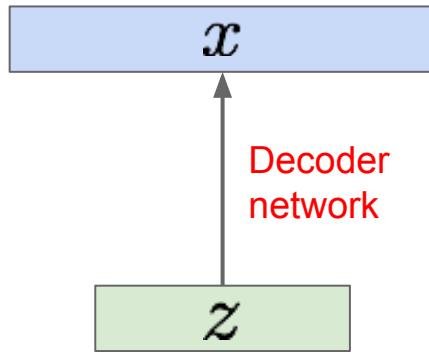
Our assumption about data generation process

Sample from true conditional

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

Sample from true prior

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



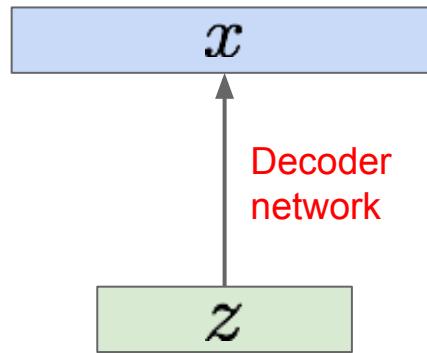
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

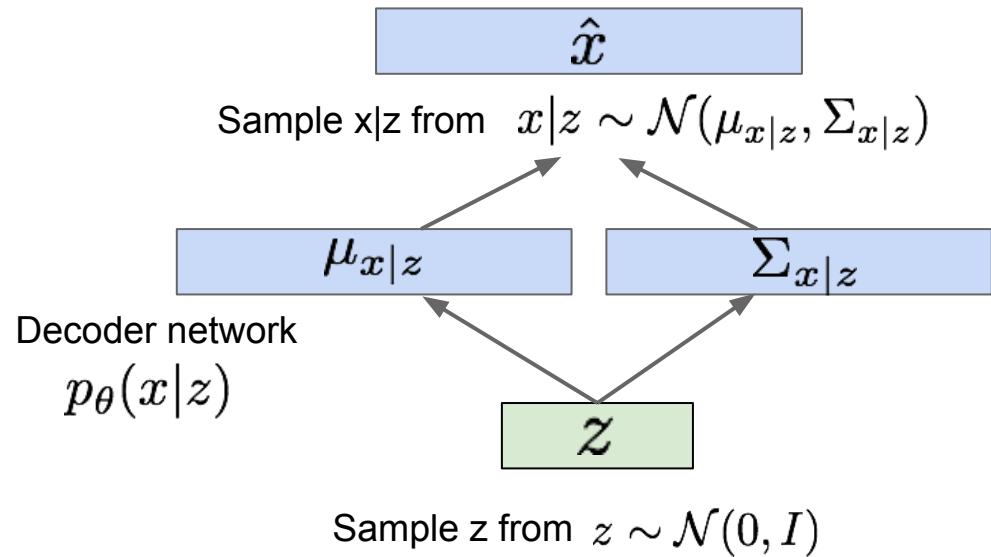
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 $p_{\theta^*}(x | z^{(i)})$

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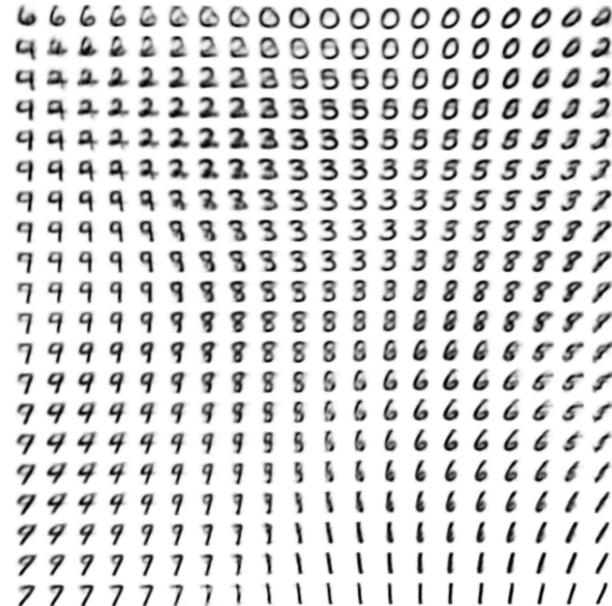
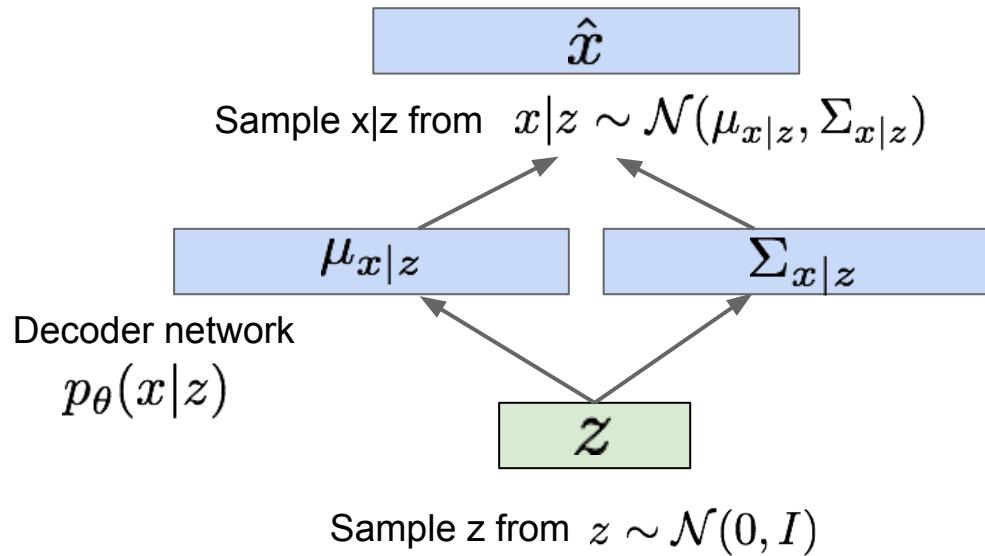
Now given a trained VAE:
use decoder network & sample z from prior!



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

Variational Autoencoders: Generating Data!

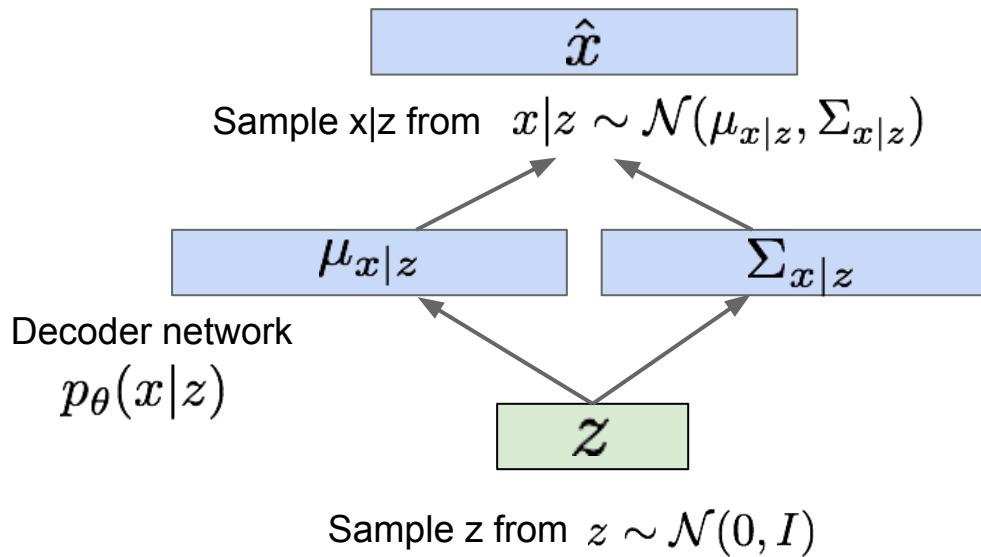
Use decoder network. Now sample z from prior!



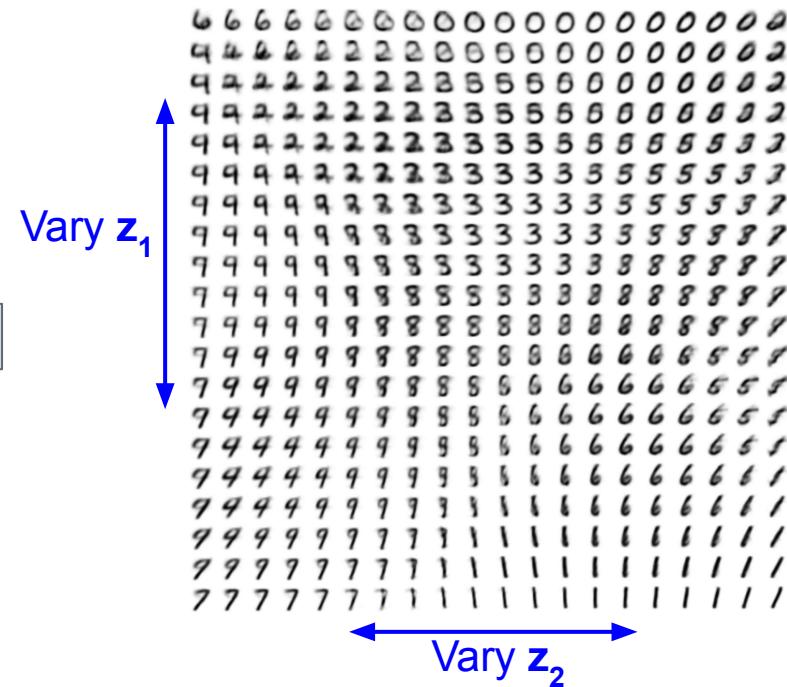
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Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Data manifold for 2-d z

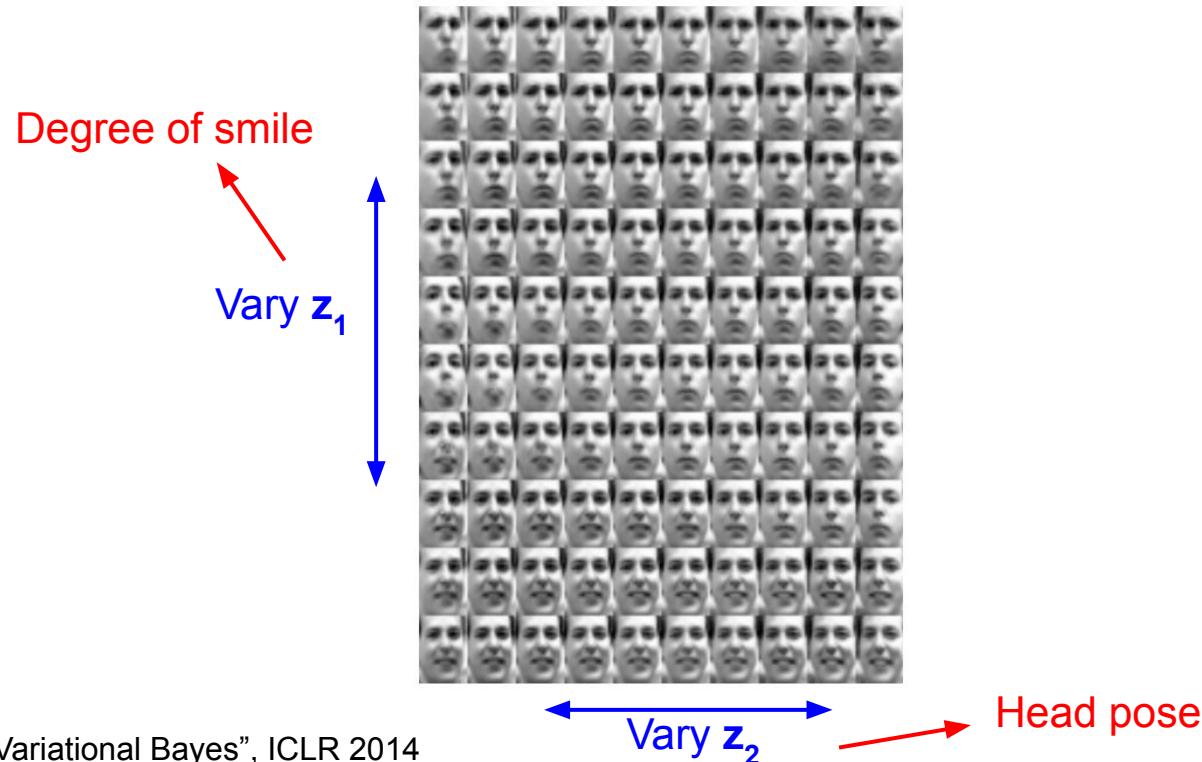


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

Diagonal prior on z
=> independent
latent variables

Different
dimensions of z
encode
interpretable factors
of variation



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

Variational Autoencoders: Generating Data!

Diagonal prior on z
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of variation

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

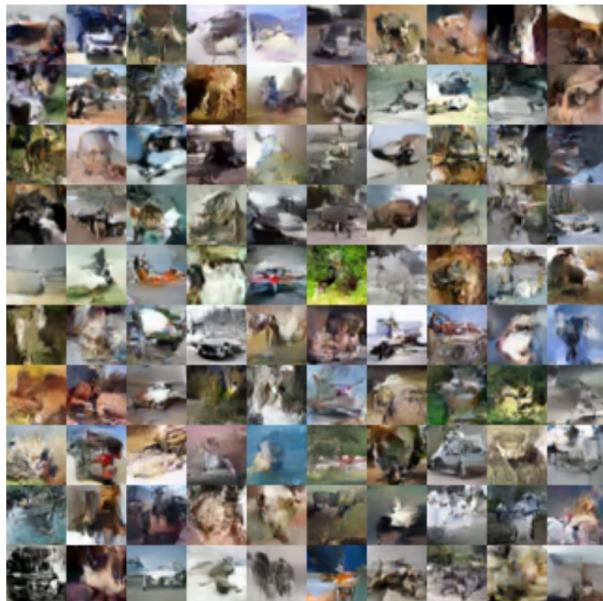
Degree of smile
Vary z_1



Vary z_2 Head pose

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

Variational Autoencoders: Generating Data!



32x32 CIFAR-10

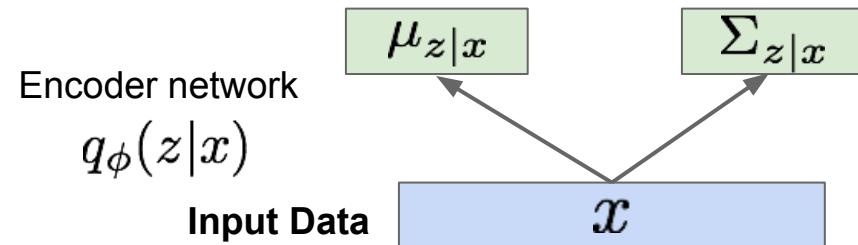


Labeled Faces in the Wild

Figures copyright (L) Dirk Kingma et al. 2016; (R) Anders Larsen et al. 2017. Reproduced with permission.

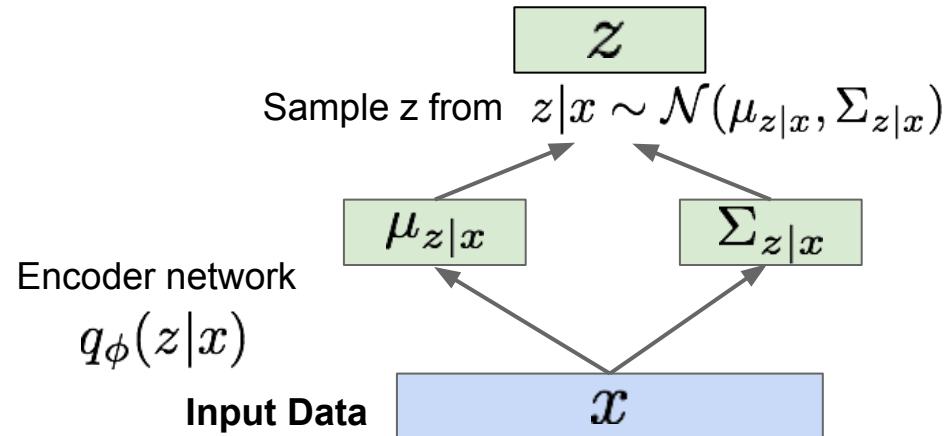
Editing images with VAEs

1. Run input data through encoder to get a distribution over latent codes



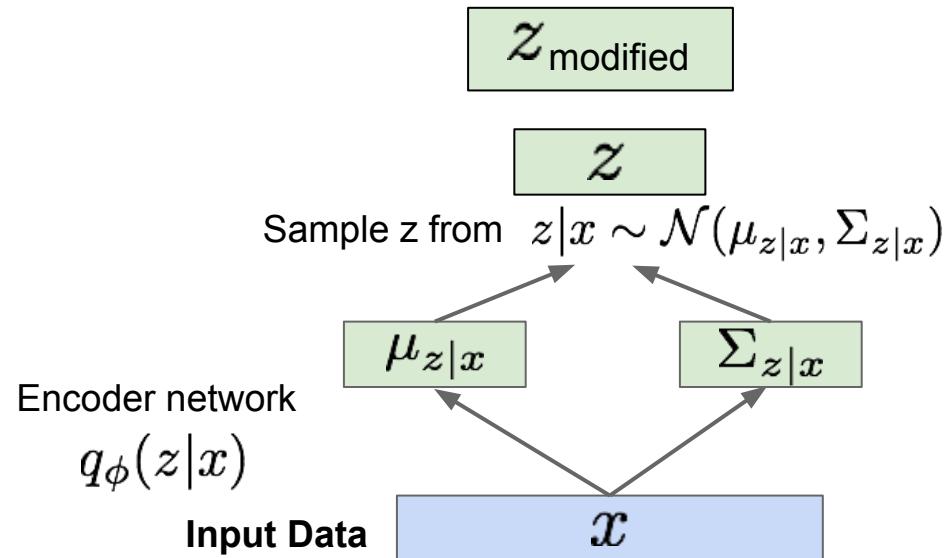
Editing images with VAEs

1. Run input data through encoder to get a distribution over latent codes
2. Sample code z from encoder output



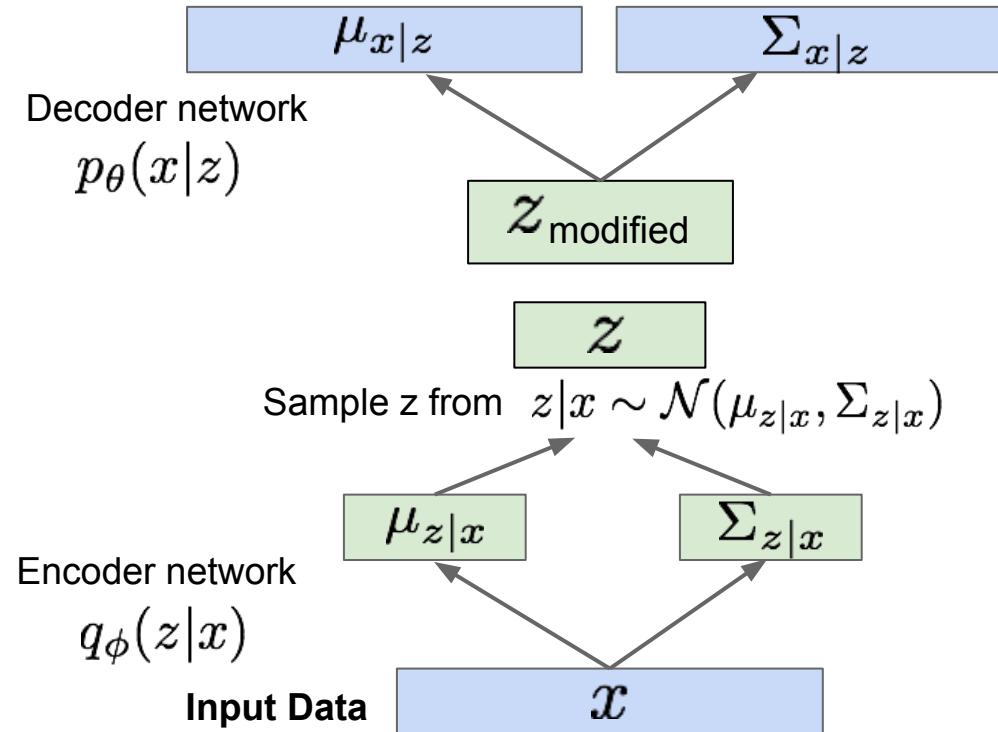
Editing images with VAEs

1. Run input data through encoder to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code



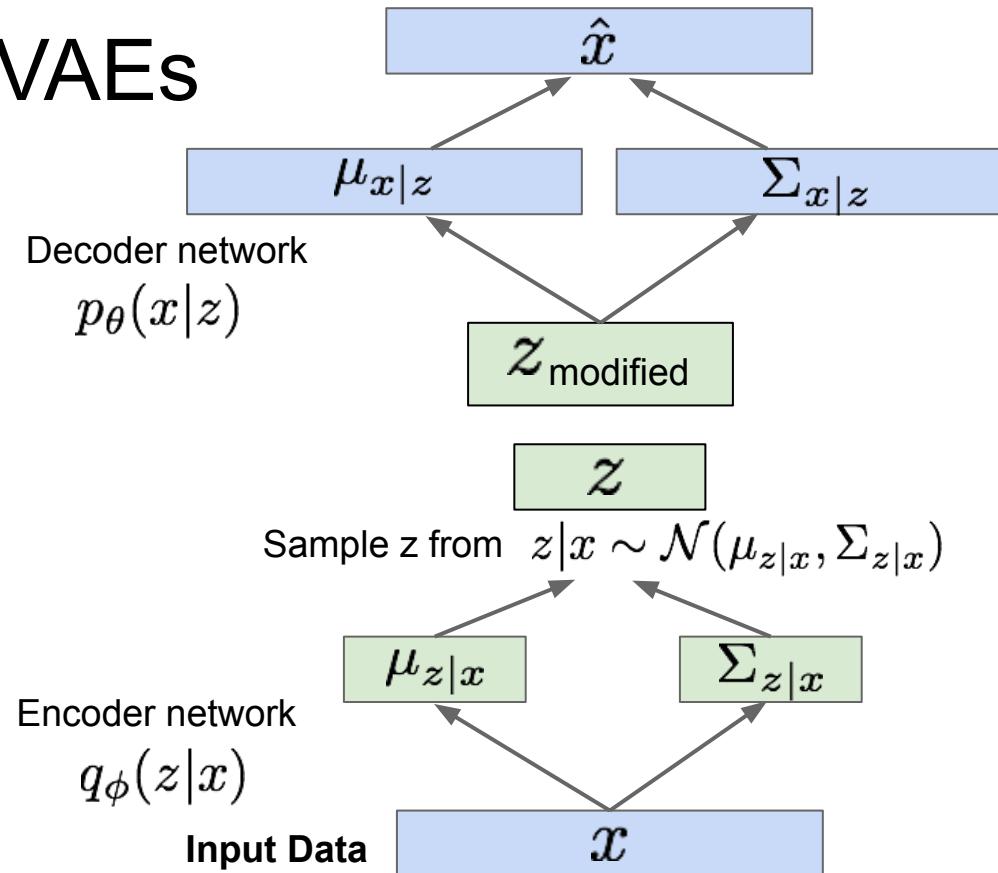
Editing images with VAEs

1. Run input data through encoder to get a distribution over latent codes
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3. Modify some dimensions of sampled code
4. Run modified z through decoder to get a distribution over data sample

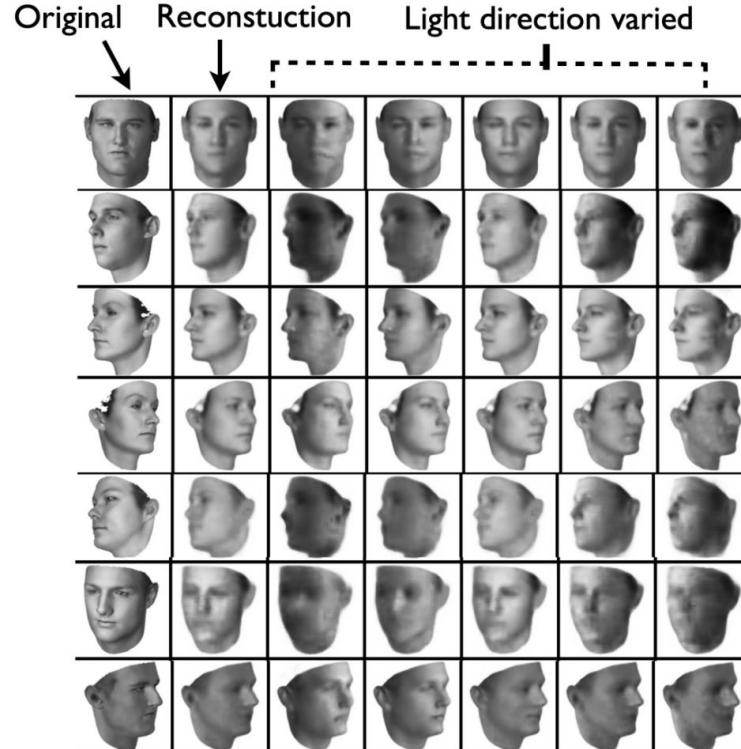
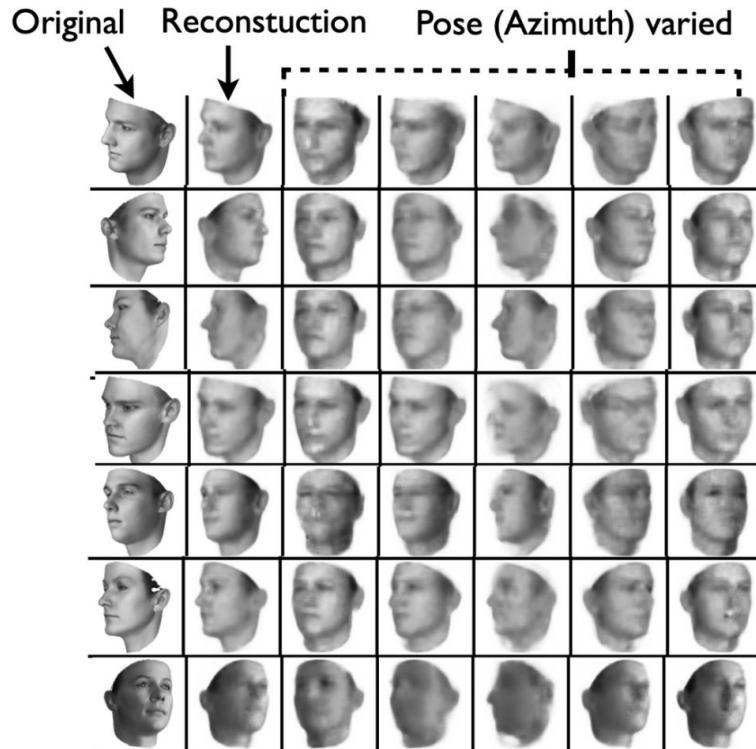


Editing images with VAEs

1. Run input data through encoder to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code
4. Run modified z through decoder to get a distribution over data sample
5. Sample new data from (4)



Editing images with VAEs



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
- Interpretable latent space.
- Allows inference of $q(z|x)$, can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs), Categorical Distributions.
- Learning disentangled representations.

Comparing the two methods so far

Autoregressive model

- Directly maximize $p(\text{data})$
- High-quality generated images
- Slow to generate images
- No explicit latent codes

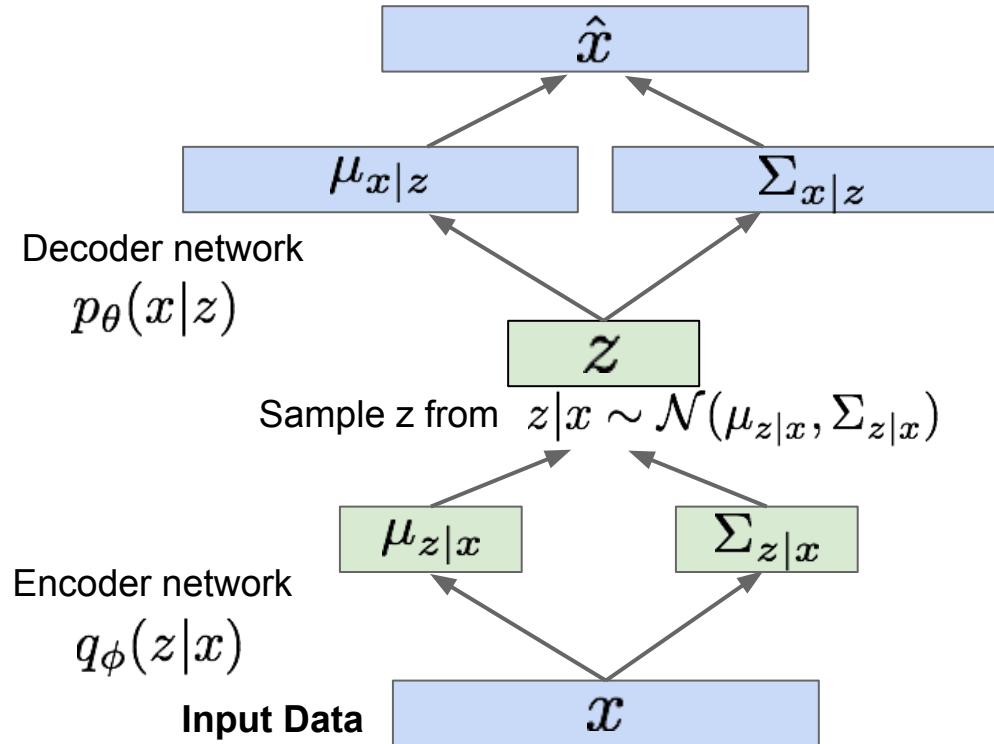
Variational model

- Maximize lower bound on $p(\text{data})$
- Generated images often blurry
- Very fast to generate images
- Learn rich latent codes

Generative AI so far: Variational Autoencoders

Maximizing the likelihood lower bound

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



Taxonomy of Generative Models

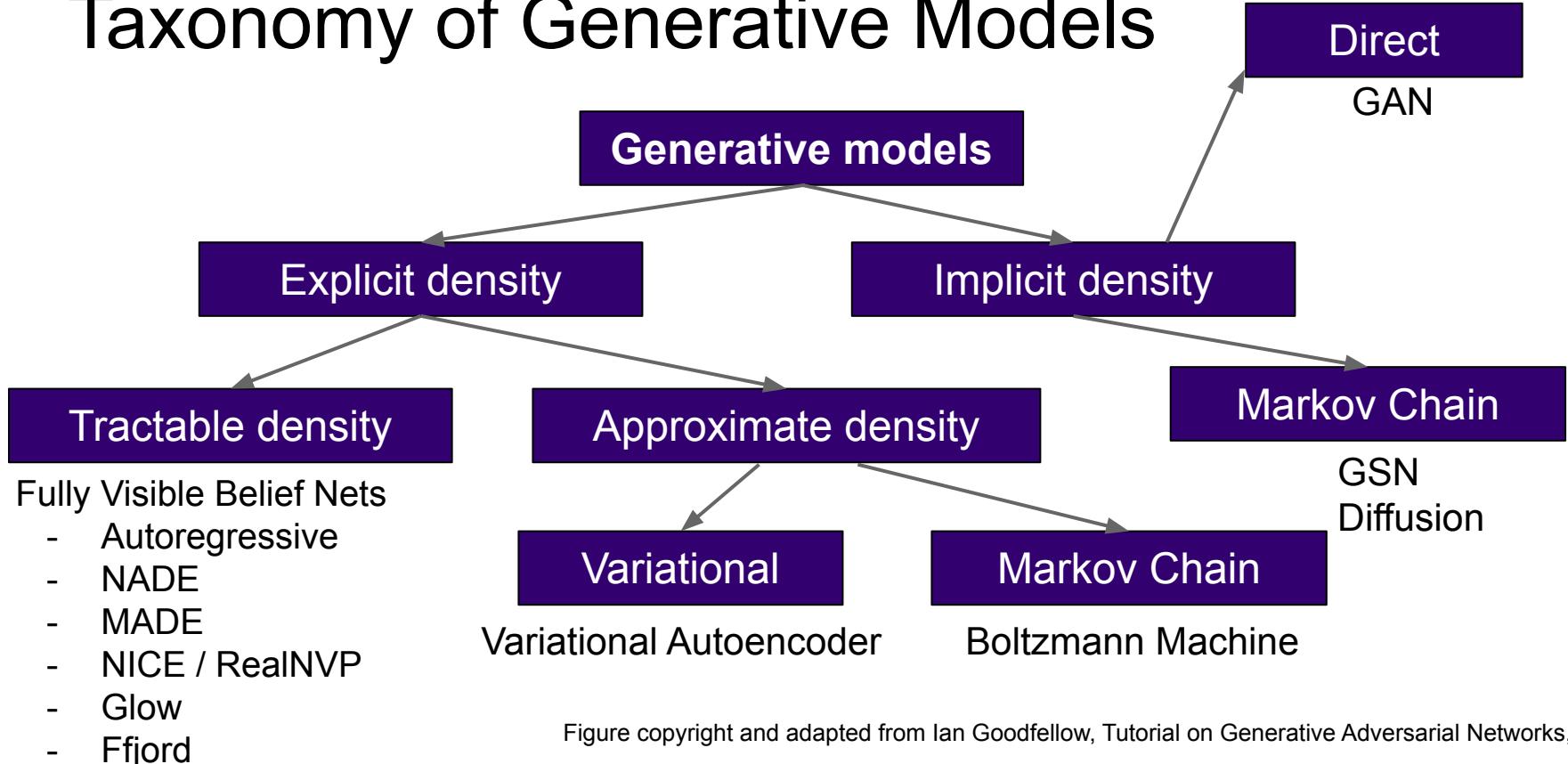


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Today: implicit density models

Generative Adversarial Networks (GANs)

All the models together

Autoregressive models define tractable density function, optimize likelihood of training data:

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

VAEs define intractable density function with latent \mathbf{z} :

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

So far...

Autoregressive define tractable density function, optimize likelihood of training data:

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What if we give up on explicitly modeling density, and just want ability to sample?

So far...

Autoregressive define tractable density function, optimize likelihood of training data:

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Cannot optimize directly, derive and optimize lower bound on likelihood instead

What if we give up on explicitly modeling density, and just want ability to sample?
GANs: not modeling any explicit density function!

Taxonomy of Generative Models

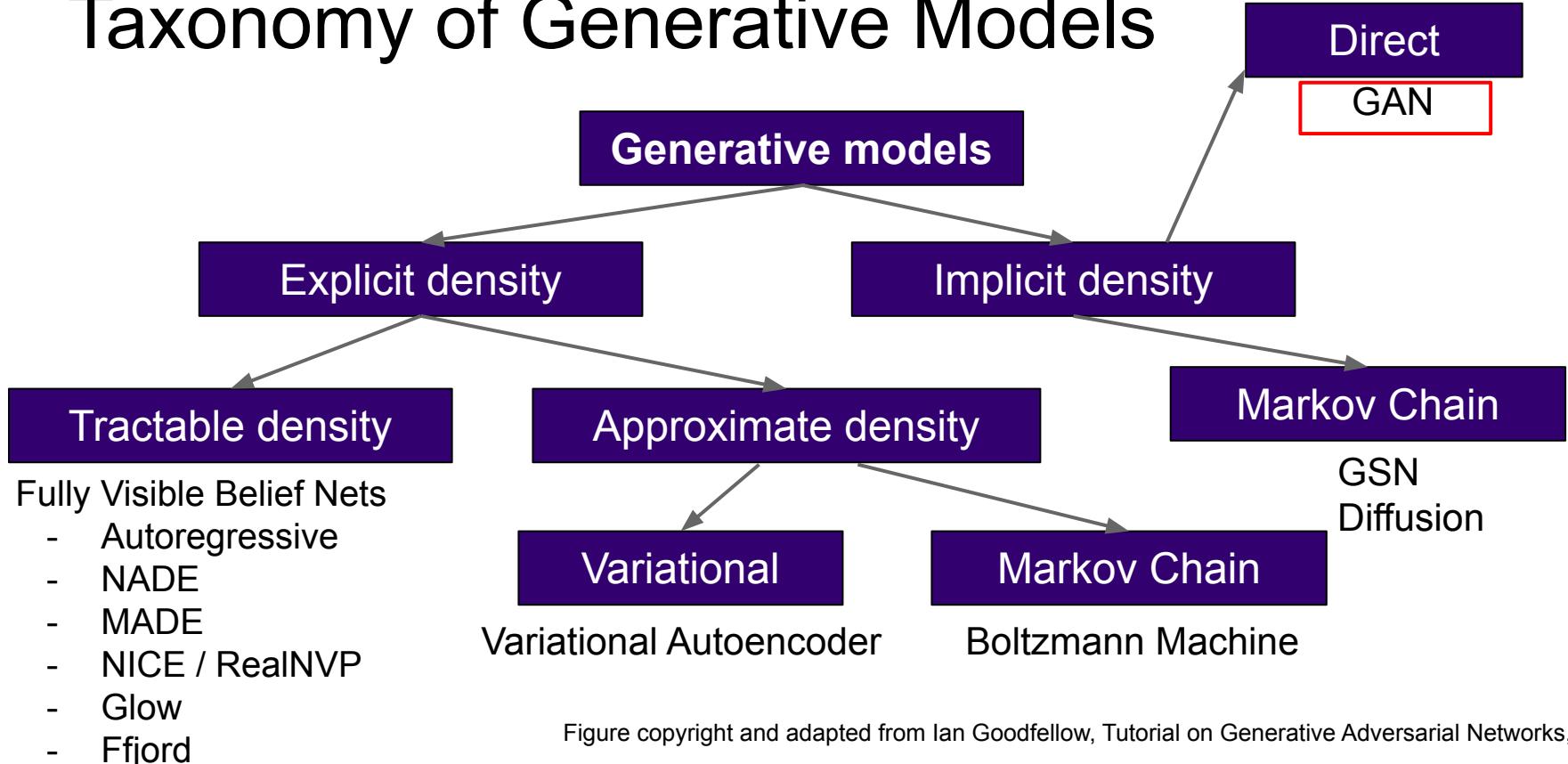


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Generative Adversarial Networks

Setup: Assume we have data x_i drawn from distribution $p_{\text{data}}(x)$. Want to sample from p_{data} .

Generative Adversarial Networks

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Idea: Introduce a latent variable z with simple prior $p(z)$ (e.g. assume z is a multivariate gaussian). Sample $z \sim p(z)$ and pass to a Generator Network $x = G(z)$

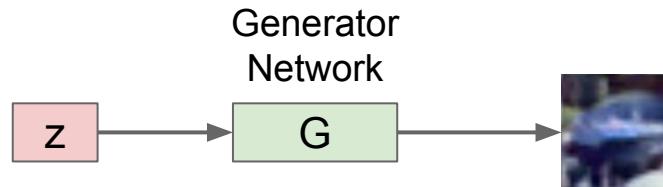
Then x is a sample from the Generator distribution p_G . **We just need to make sure $p_G = p_{\text{data}}$!**

Generative Adversarial Networks

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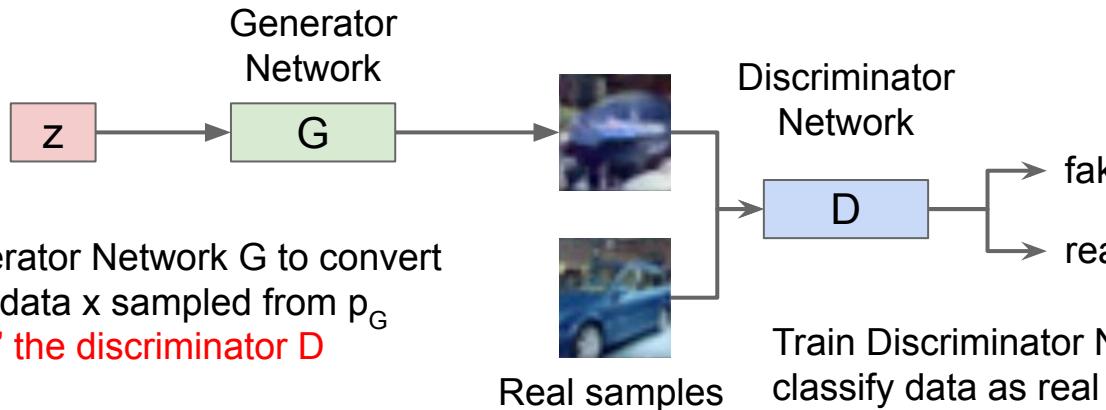
Train Generator Network G to convert z into fake data x sampled from p_G

Generative Adversarial Networks

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Then x is a sample from the Generator distribution p_G . **We just need to make sure $p_G = p_{\text{data}}$!**



Train Generator Network G to convert
 z into fake data x sampled from p_G
by "fooling" the discriminator D

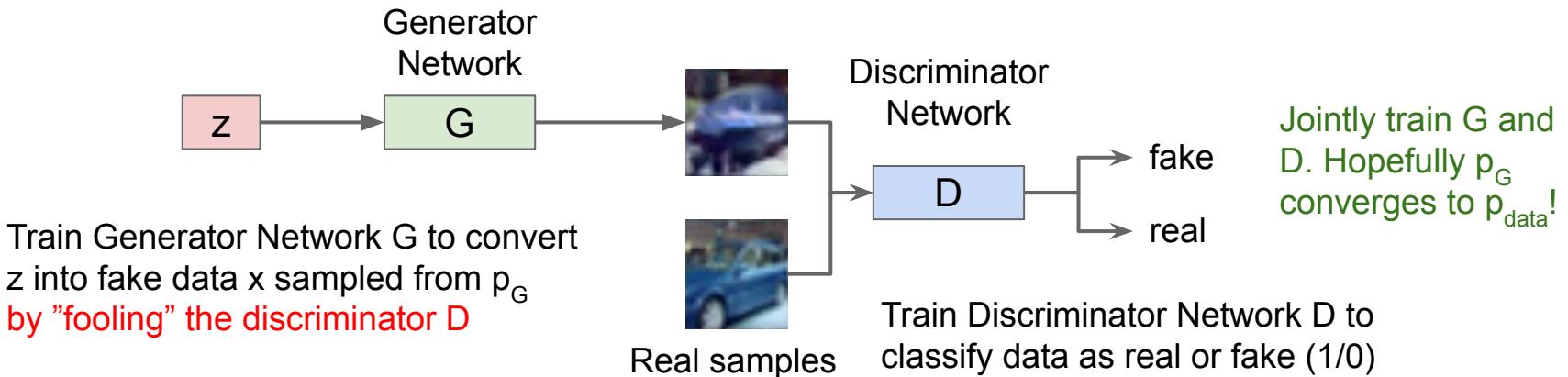
Train Discriminator Network D to
classify data as real or fake (1/0)

Generative Adversarial Networks

Setup: Assume we have data x_i drawn from distribution $p_{\text{data}}(x)$. Want to sample from p_{data} .

Idea: Introduce a latent variable z with simple prior $p(z)$ (e.g. assume z is a multivariate gaussian). Sample $z \sim p(z)$ and pass to a Generator Network $x = G(z)$

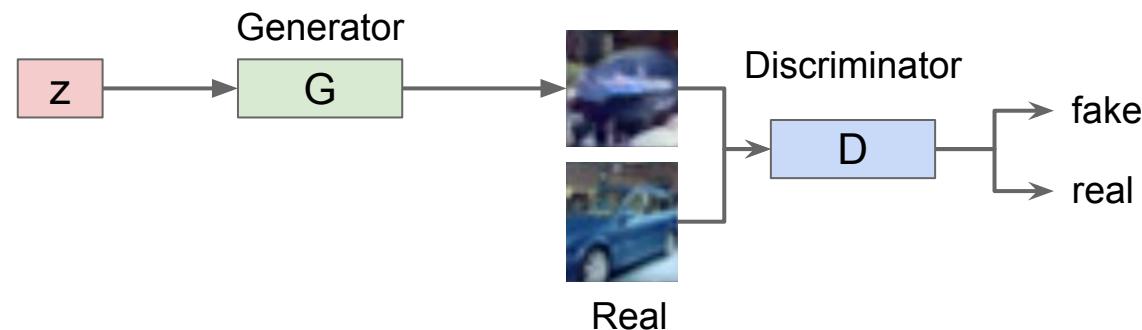
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Generative Adversarial Networks

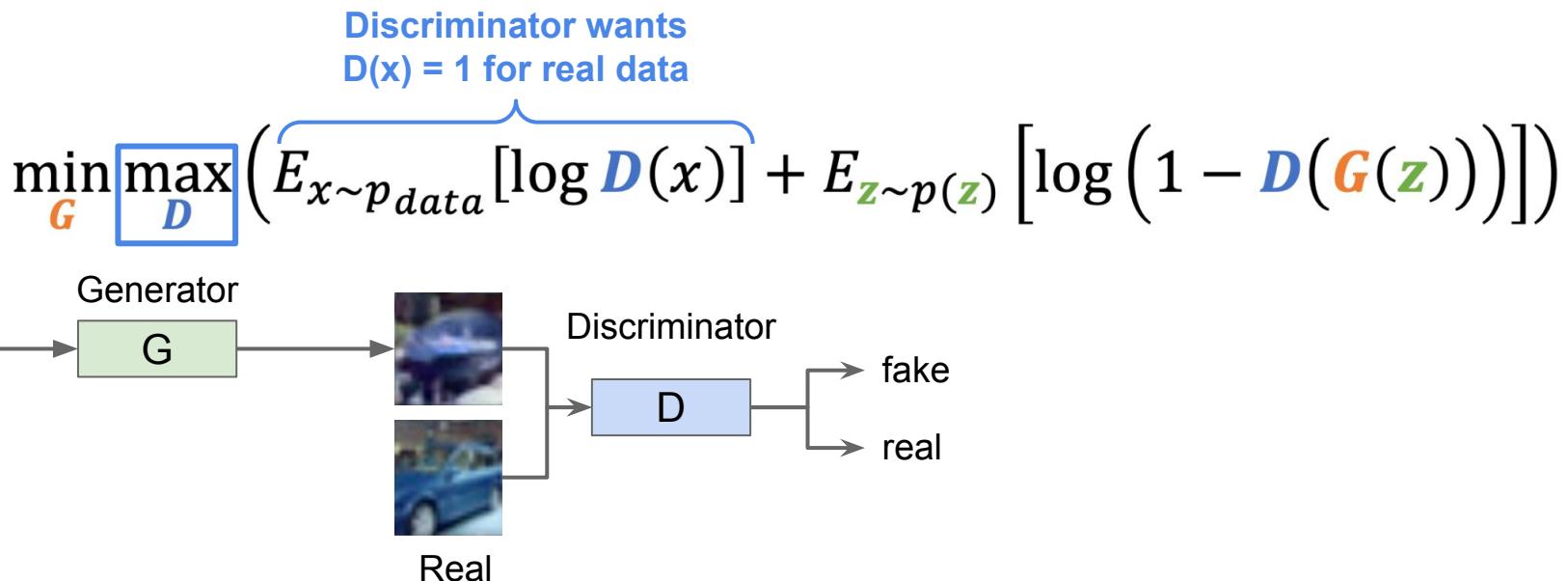
Jointly train generator G and discriminator D with a minimax game

$$\min_{\mathbf{G}} \max_{\mathbf{D}} \left(E_{x \sim p_{data}} [\log \mathbf{D}(x)] + E_{\mathbf{z} \sim p(\mathbf{z})} [\log (1 - \mathbf{D}(\mathbf{G}(\mathbf{z})))] \right)$$



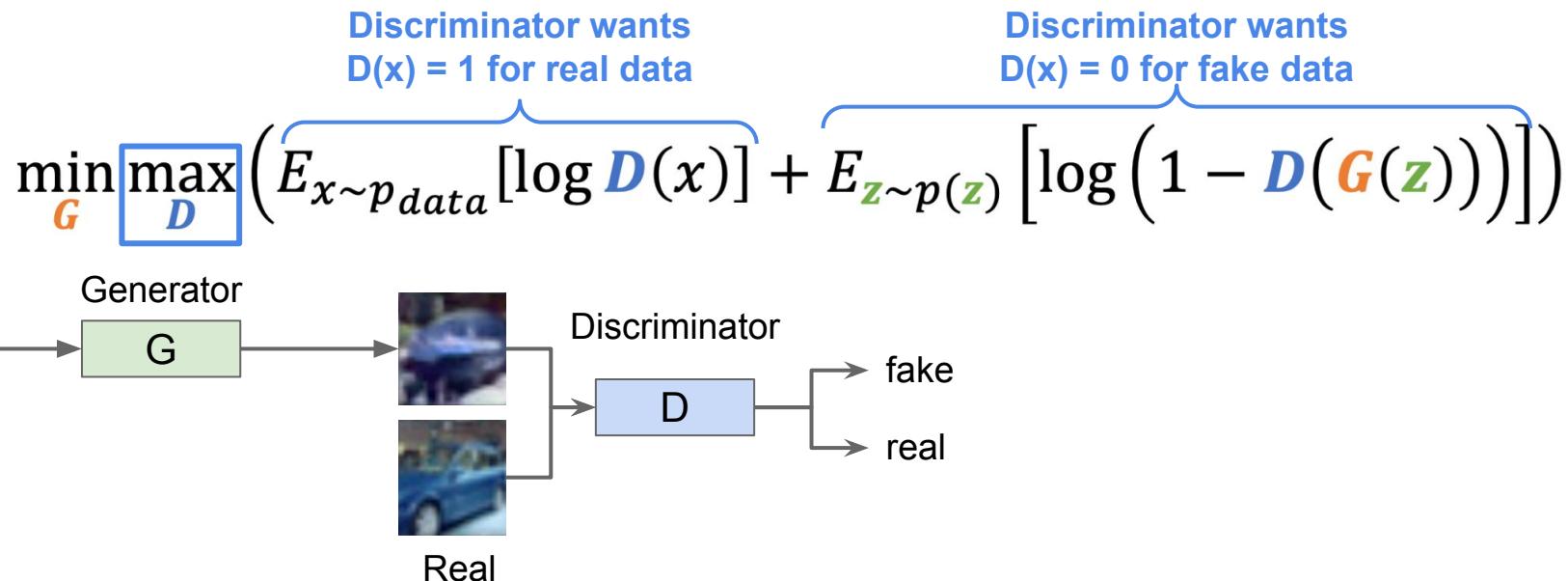
Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game



Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

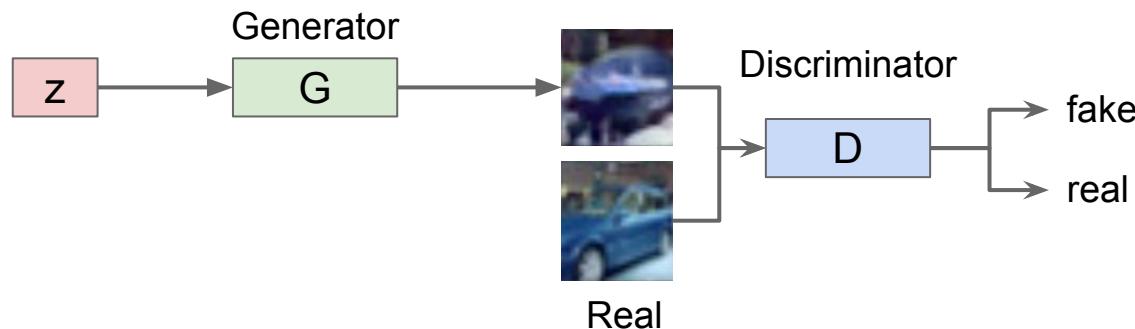


Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

$$\min_G \max_D \left(E_{x \sim p_{data}} [\log D(x)] + E_{z \sim p(z)} [\log (1 - D(G(z)))] \right)$$

Generator wants
 $D(x) = 1$ for fake data



Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

Train G and D using alternating gradient updates

$$\min_{\textcolor{brown}{G}} \max_{\textcolor{blue}{D}} \left(E_{x \sim p_{data}} [\log \textcolor{blue}{D}(x)] + E_{\textcolor{green}{z} \sim p(\textcolor{green}{z})} [\log (1 - \textcolor{blue}{D}(\textcolor{brown}{G}(\textcolor{green}{z})))] \right)$$

Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

Train G and D using alternating gradient updates

$$\begin{aligned} & \min_{\mathbf{G}} \max_{\mathbf{D}} \left(E_{x \sim p_{data}} [\log \mathbf{D}(x)] + E_{\mathbf{z} \sim p(\mathbf{z})} [\log (1 - \mathbf{D}(\mathbf{G}(\mathbf{z})))] \right) \\ &= \min_{\mathbf{G}} \max_{\mathbf{D}} \mathbf{V}(\mathbf{G}, \mathbf{D}) \end{aligned}$$

Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

Train G and D using alternating gradient updates

$$\begin{aligned} & \min_{\mathbf{G}} \max_{\mathbf{D}} \left(E_{x \sim p_{data}} [\log \mathbf{D}(x)] + E_{\mathbf{z} \sim p(\mathbf{z})} [\log (1 - \mathbf{D}(\mathbf{G}(\mathbf{z})))] \right) \\ &= \min_{\mathbf{G}} \max_{\mathbf{D}} \mathbf{V}(\mathbf{G}, \mathbf{D}) \quad \text{For t in 1, ... T:} \end{aligned}$$

1. (Update \mathbf{D}) $\mathbf{D} = \mathbf{D} + \alpha_{\mathbf{D}} \frac{\partial \mathbf{V}}{\partial \mathbf{D}}$
2. (Update \mathbf{G}) $\mathbf{G} = \mathbf{G} - \alpha_{\mathbf{G}} \frac{\partial \mathbf{V}}{\partial \mathbf{G}}$

Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

Train G and D using alternating gradient updates

$$\begin{aligned} & \min_{\mathbf{G}} \max_{\mathbf{D}} \left(E_{x \sim p_{data}} [\log \mathbf{D}(x)] + E_{\mathbf{z} \sim p(\mathbf{z})} [\log (1 - \mathbf{D}(\mathbf{G}(\mathbf{z})))] \right) \\ &= \min_{\mathbf{G}} \max_{\mathbf{D}} \mathbf{V}(\mathbf{G}, \mathbf{D}) \end{aligned}$$

We are not minimizing any overall loss! No training curves to look at!

For t in 1, ... T:

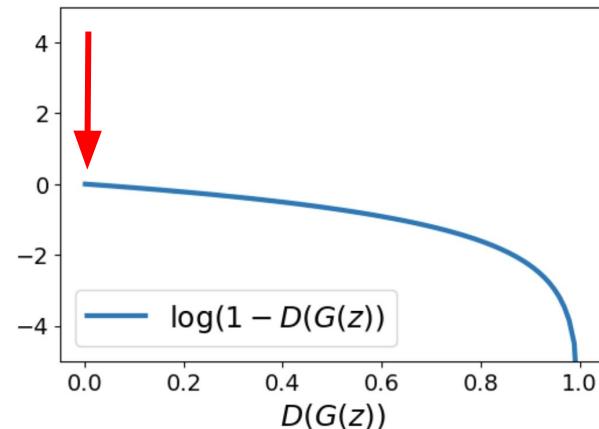
1. (Update D) $\mathbf{D} = \mathbf{D} + \alpha_{\mathbf{D}} \frac{\partial \mathbf{V}}{\partial \mathbf{D}}$
2. (Update G) $\mathbf{G} = \mathbf{G} - \alpha_{\mathbf{G}} \frac{\partial \mathbf{V}}{\partial \mathbf{G}}$

Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

$$\min_{\textcolor{brown}{G}} \max_{\textcolor{blue}{D}} \left(E_{x \sim p_{data}} [\log \textcolor{blue}{D}(x)] + E_{z \sim p(\textcolor{green}{z})} [\log (1 - \textcolor{blue}{D}(\textcolor{brown}{G}(\textcolor{green}{z})))] \right)$$

At start of training, generator is very bad and discriminator can easily tell apart real/fake, so $D(G(z))$ close to 0



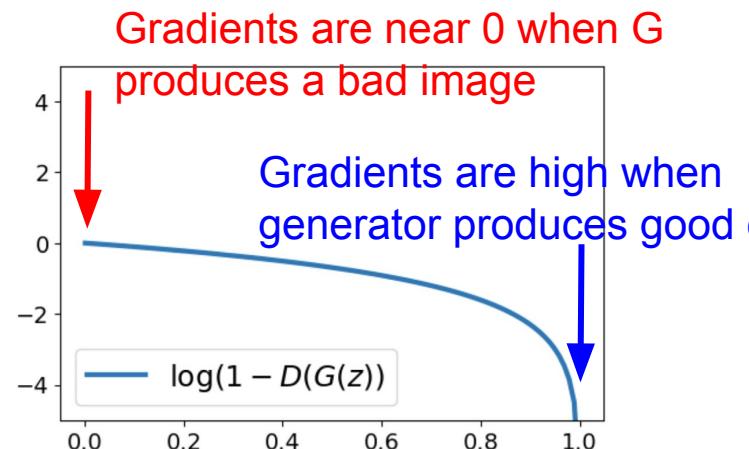
Generative Adversarial Networks

Jointly train generator G and discriminator D with a minimax game

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At start of training, generator is very bad and discriminator can easily tell apart real/fake, so $D(G(z))$ close to 0

Problem: Why is this a problem?



Generative Adversarial Networks

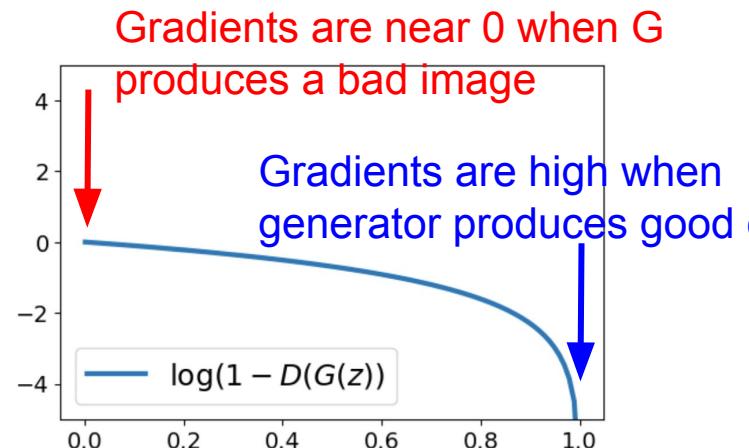
Jointly train generator G and discriminator D with a minimax game

$$\min_{\textcolor{brown}{G}} \max_{\textcolor{blue}{D}} \left(E_{x \sim p_{data}} [\log \textcolor{blue}{D}(x)] + E_{z \sim p(\textcolor{green}{z})} [\log (1 - \textcolor{blue}{D}(\textcolor{brown}{G}(\textcolor{green}{z})))] \right)$$

At start of training, generator is very bad and discriminator can easily tell apart real/fake, so $D(G(z))$ close to 0

Problem: Vanishing gradients for G

How do we fix this?



Generative Adversarial Networks

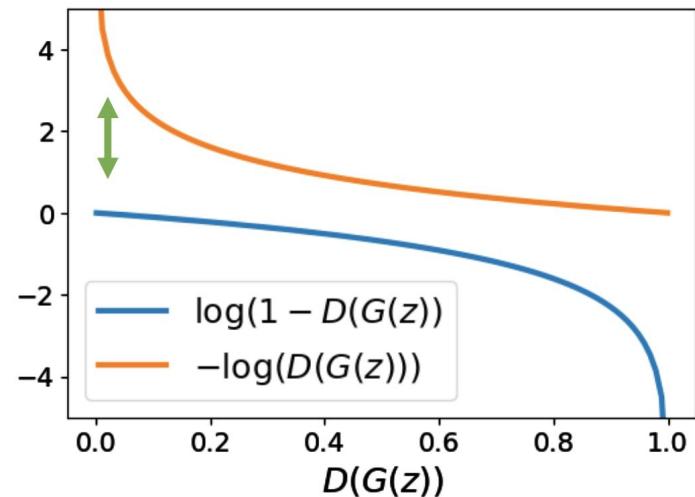
Jointly train generator G and discriminator D with a minimax game

$$\min_{\textcolor{brown}{G}} \max_{\textcolor{blue}{D}} \left(E_{x \sim p_{data}} [\log \textcolor{blue}{D}(x)] + E_{z \sim p(\textcolor{green}{z})} [\log (1 - \textcolor{blue}{D}(\textcolor{brown}{G}(\textcolor{green}{z})))] \right)$$

At start of training, generator is very bad and discriminator can easily tell apart real/fake, so $D(G(z))$ close to 0

Problem: Vanishing gradients for G

Solution: Train G to minimize $-\log(D(G(z)))$, instead of $\log(1-D(G(z)))$. Then G gets strong gradients at start of training!



Generative Adversarial Networks

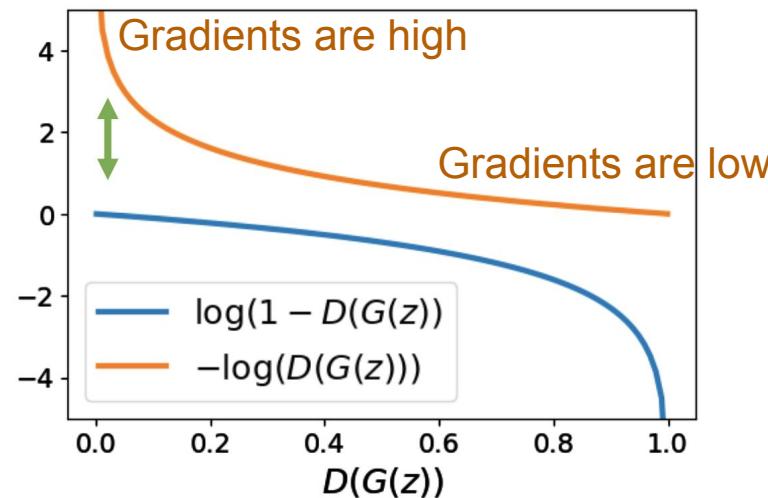
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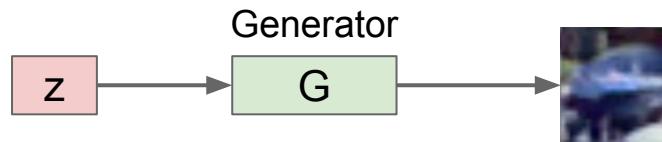
Problem: Vanishing gradients for G

Solution: Train G to minimize $-\log(D(G(z)))$, instead of $\log(1-D(G(z)))$. Then G gets strong gradients at start of training!



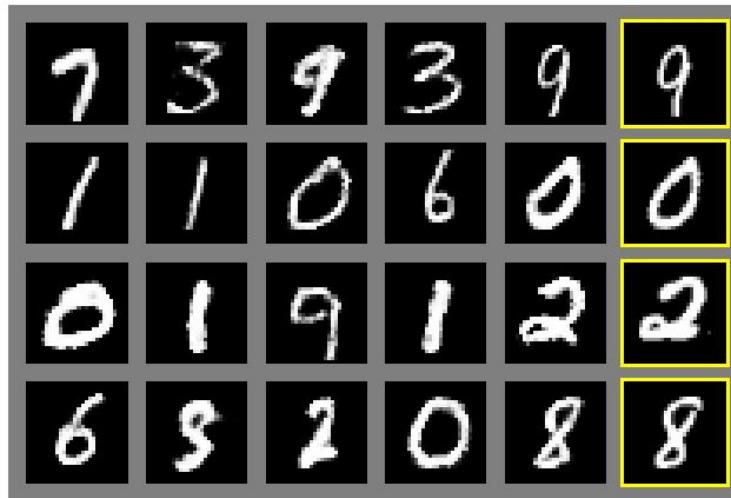
Generative adversarial networks

Once trained, throw away the discriminator and use G to generate new images



Generative Adversarial Nets

Generated samples



Nearest neighbor from training set

Figures copyright Ian Goodfellow et al., 2014. Reproduced with permission.

Generative Adversarial Nets

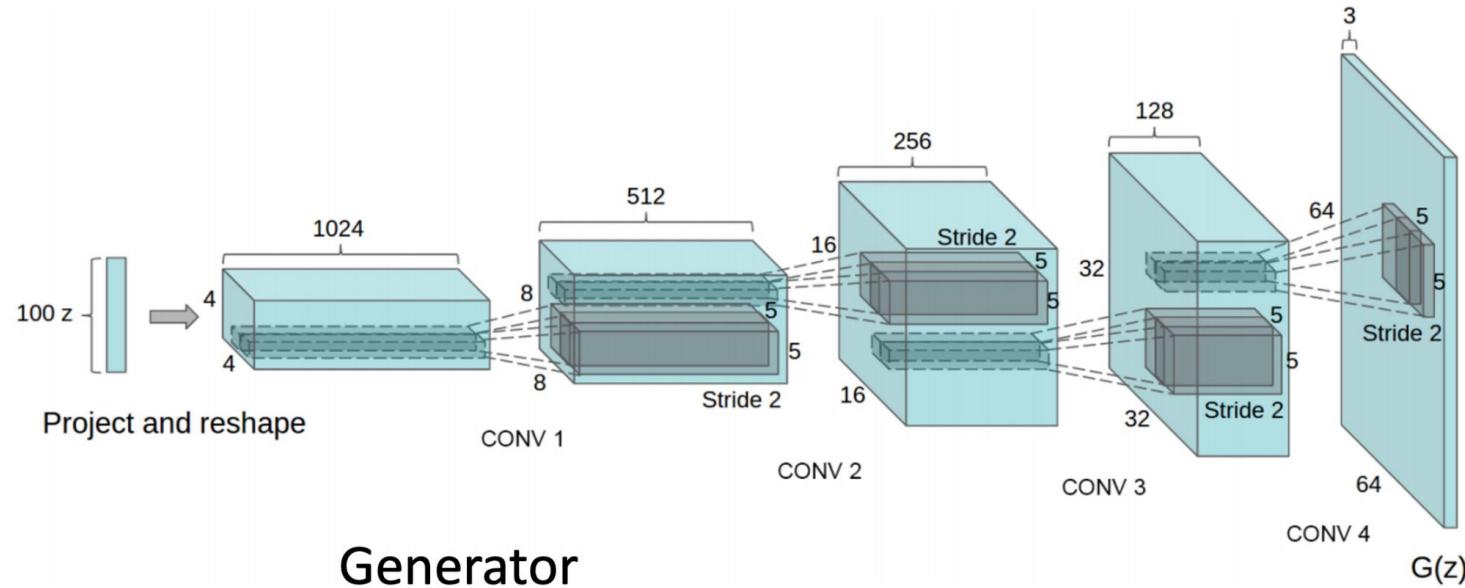
Generated samples (CIFAR-10)



Nearest neighbor from training set

Figures copyright Ian Goodfellow et al., 2014. Reproduced with permission.

Generative Adversarial Nets: Convolutional Architectures



Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Generator is an upsampling network with fractionally-strided convolutions
Discriminator is a convolutional network

Architecture guidelines for stable Deep Convolutional GANs

- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.
- Use LeakyReLU activation in the discriminator for all layers.

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Samples
from the
model look
much
better!



Radford et al,
ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Interpolating
between
random
points in latent
space



Radford et al,
ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

Smiling woman



Neutral woman



Neutral man



Samples
from the
model

Radford et al, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

Smiling woman Neutral woman Neutral man

Samples
from the
model



Average Z
vectors, do
arithmetic



Generative Adversarial Nets: Interpretable Vector Math

Smiling woman Neutral woman Neutral man

Samples
from the
model



Neutral woman



Neutral man



Radford et al, ICLR 2016

Smiling Man



Average Z
vectors, do
arithmetic



Generative Adversarial Nets: Interpretable Vector Math

Glasses man



No glasses man



No glasses woman



Radford et al,
ICLR 2016

Woman with glasses



Since then: Explosion of GANs

“The GAN Zoo”

See also: <https://github.com/soumith/ganhacks> for tips and tricks for trainings GANs

- GAN - Generative Adversarial Networks
- 3D-GAN - Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling
- acGAN - Face Aging With Conditional Generative Adversarial Networks
- AC-GAN - Conditional Image Synthesis With Auxiliary Classifier GANs
- AdAGAN - AdaGAN: Boosting Generative Models
- AEGAN - Learning Inverse Mapping by Autoencoder based Generative Adversarial Nets
- AffGAN - Amortised MAP Inference for Image Super-resolution
- AL-CGAN - Learning to Generate Images of Outdoor Scenes from Attributes and Semantic Layouts
- ALI - Adversarially Learned Inference
- AM-GAN - Generative Adversarial Nets with Labeled Data by Activation Maximization
- AnoGAN - Unsupervised Anomaly Detection with Generative Adversarial Networks to Guide Marker Discovery
- ArtGAN - ArtGAN: Artwork Synthesis with Conditional Categorical GANs
- b-GAN - b-GAN: Unified Framework of Generative Adversarial Networks
- Bayesian GAN - Deep and Hierarchical Implicit Models
- BEGAN - BEGAN: Boundary Equilibrium Generative Adversarial Networks
- BiGAN - Adversarial Feature Learning
- BS-GAN - Boundary-Seeking Generative Adversarial Networks
- CGAN - Conditional Generative Adversarial Nets
- CaloGAN - CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks
- CCGAN - Semi-Supervised Learning with Context-Conditional Generative Adversarial Networks
- CatGAN - Unsupervised and Semi-supervised Learning with Categorical Generative Adversarial Networks
- CoGAN - Coupled Generative Adversarial Networks

- Context-RNN-GAN - Contextual RNN-GANs for Abstract Reasoning Diagram Generation
- C-RNN-GAN - C-RNN-GAN: Continuous recurrent neural networks with adversarial training
- CS-GAN - Improving Neural Machine Translation with Conditional Sequence Generative Adversarial Nets
- CVAE-GAN - CVAE-GAN: Fine-Grained Image Generation through Asymmetric Training
- CycleGAN - Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
- DTN - Unsupervised Cross-Domain Image Generation
- DCGAN - Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks
- DiscoGAN - Learning to Discover Cross-Domain Relations with Generative Adversarial Networks
- DR-GAN - Disentangled Representation Learning GAN for Pose-Invariant Face Recognition
- DualGAN - DualGAN: Unsupervised Dual Learning for Image-to-Image Translation
- EBGAN - Energy-based Generative Adversarial Network
- f-GAN - f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization
- FF-GAN - Towards Large-Pose Face Frontalization in the Wild
- GAWWN - Learning What and Where to Draw
- GeneGAN - GeneGAN: Learning Object Transfiguration and Attribute Subspace from Unpaired Data
- Geometric GAN - Geometric GAN
- GoGAN - Gang of GANs: Generative Adversarial Networks with Maximum Margin Ranking
- GP-GAN - GP-GAN: Towards Realistic High-Resolution Image Blending
- IAN - Neural Photo Editing with Introspective Adversarial Networks
- iGAN - Generative Visual Manipulation on the Natural Image Manifold
- IcGAN - Invertible Conditional GANs for image editing
- ID-CGAN - Image De-raining Using a Conditional Generative Adversarial Network
- Improved GAN - Improved Techniques for Training GANs
- InfoGAN - InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets
- LAGAN - Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics Synthesis
- LAPGAN - Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

<https://github.com/hindupuravinash/the-gan-zoo>

GAN improvements: better loss functions



LSGAN, Zhu 2017.
Wasserstein GAN, Arjovsky 2017.



Improved Wasserstein GAN, Gulrajani 2017.

GAN improvements: higher resolution

256 x 256 bedrooms



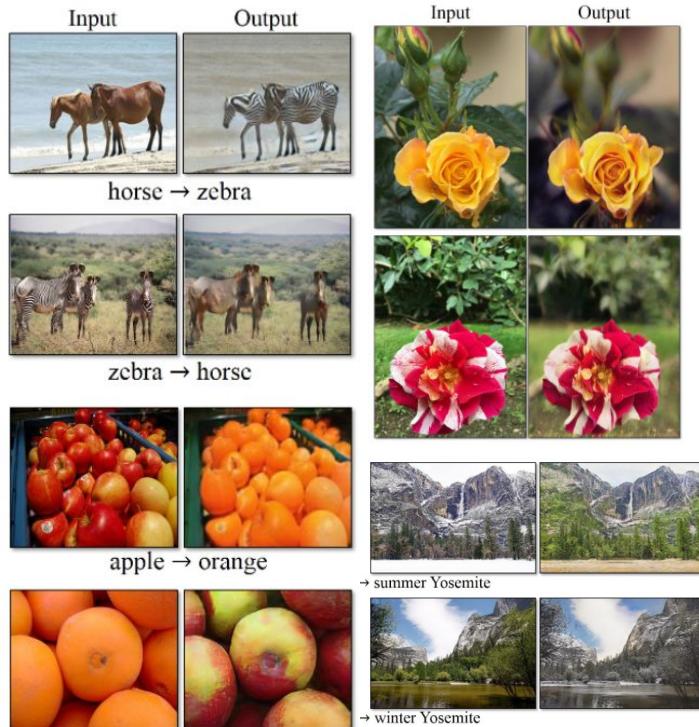
1024 x 1024 faces



Progressive GAN, Karras 2018.

GAN transformations

Source->Target domain transfer



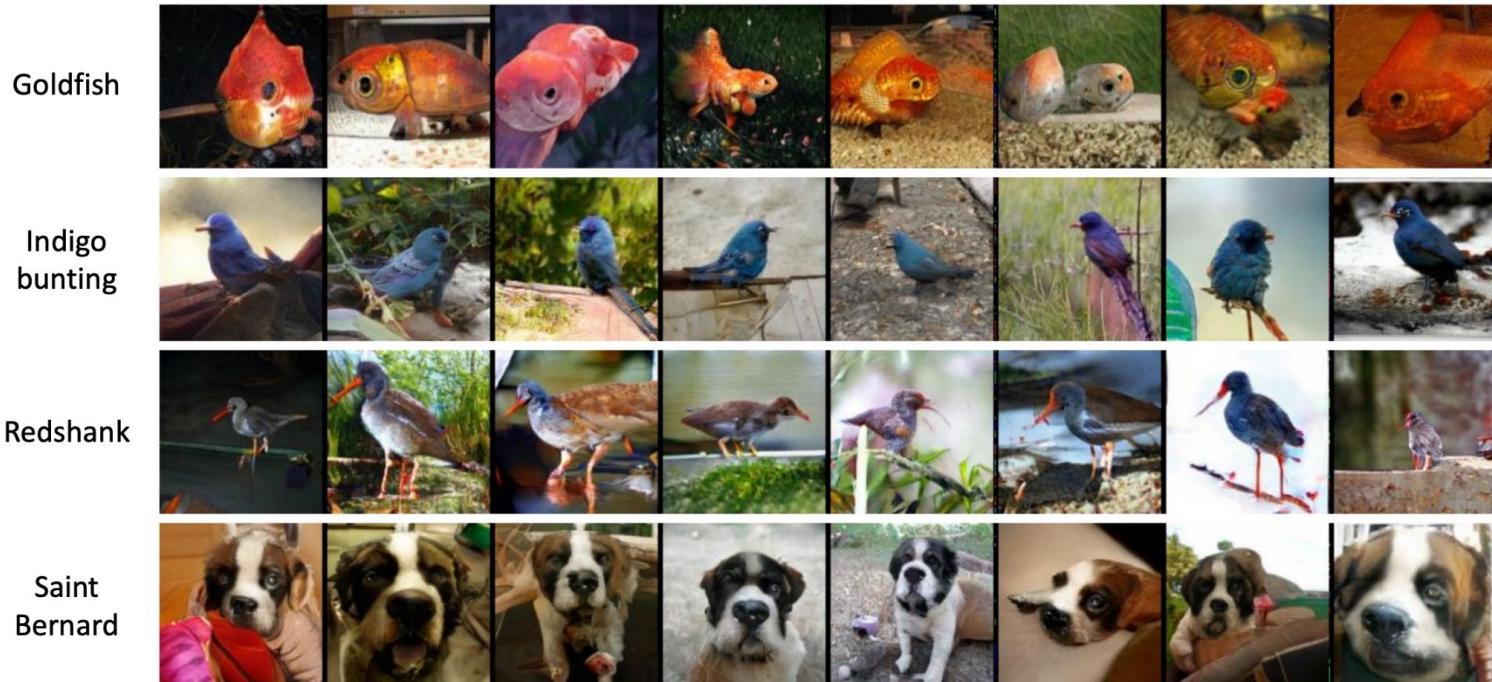
Pix2pix. Isola 2017. Many examples at
<https://phillipi.github.io/pix2pix/>

BigGAN: 512x512 images



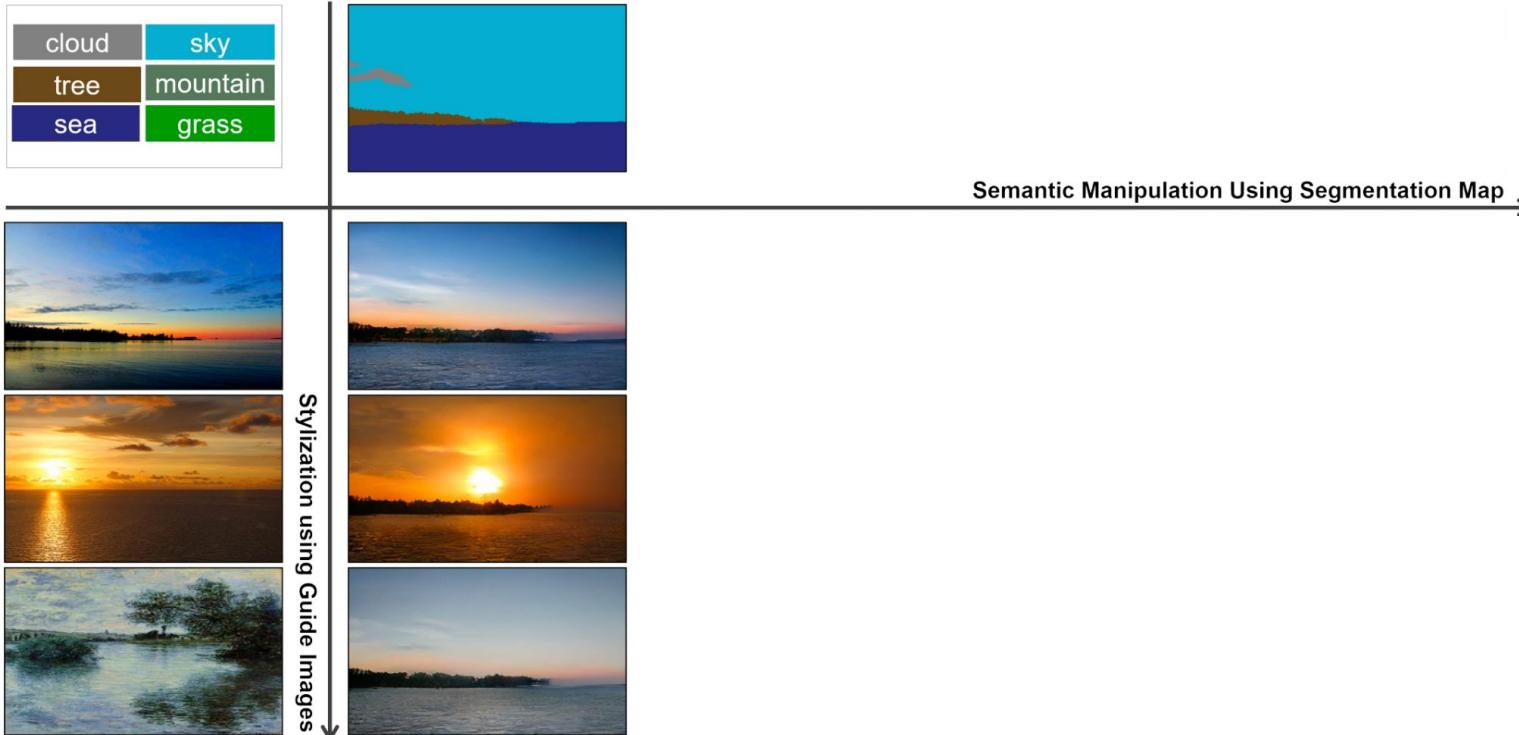
Brock et al., 2019

GANs with self-attention mechanism

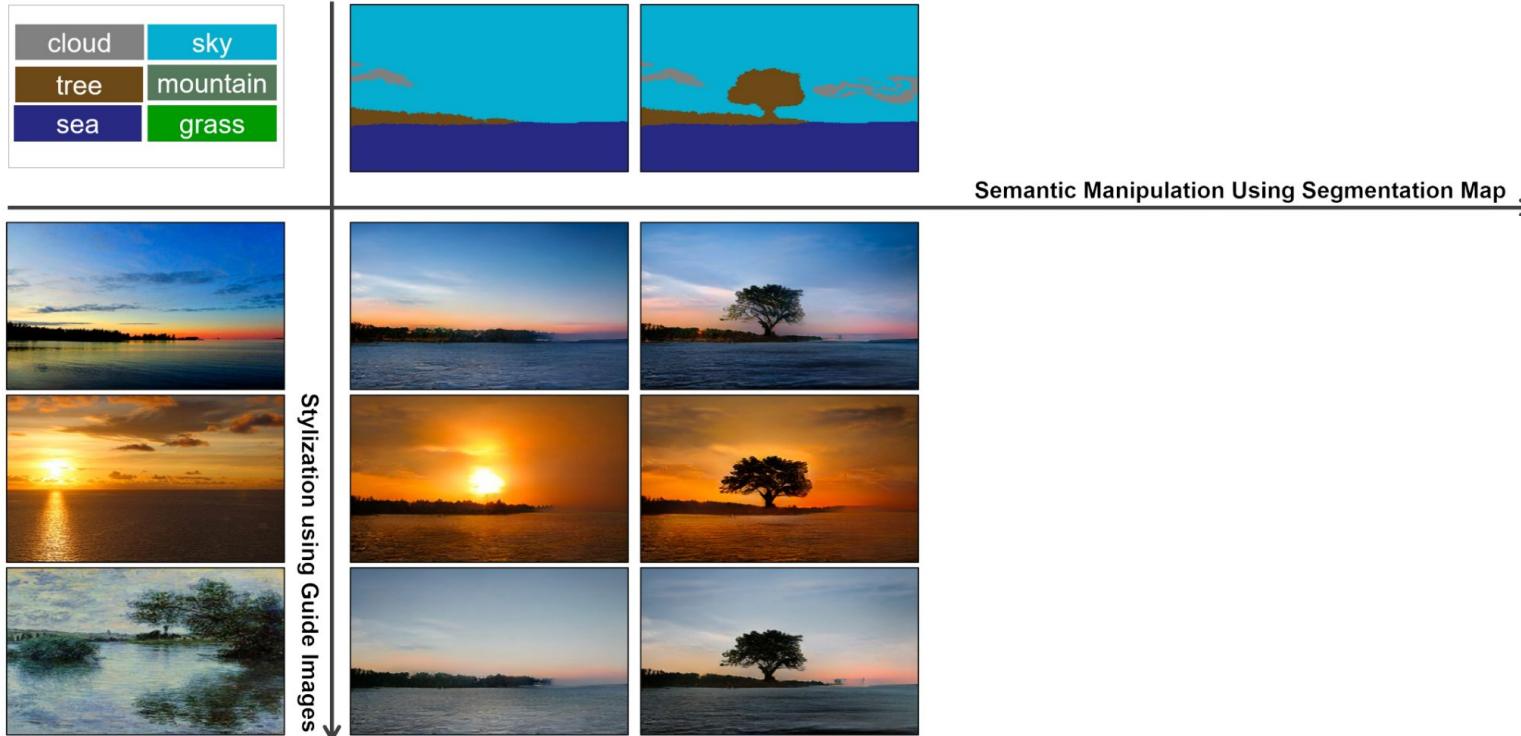


Zhang et al, "Self-Attention Generative Adversarial Networks", ICML 2019

Controlled generation with GANs

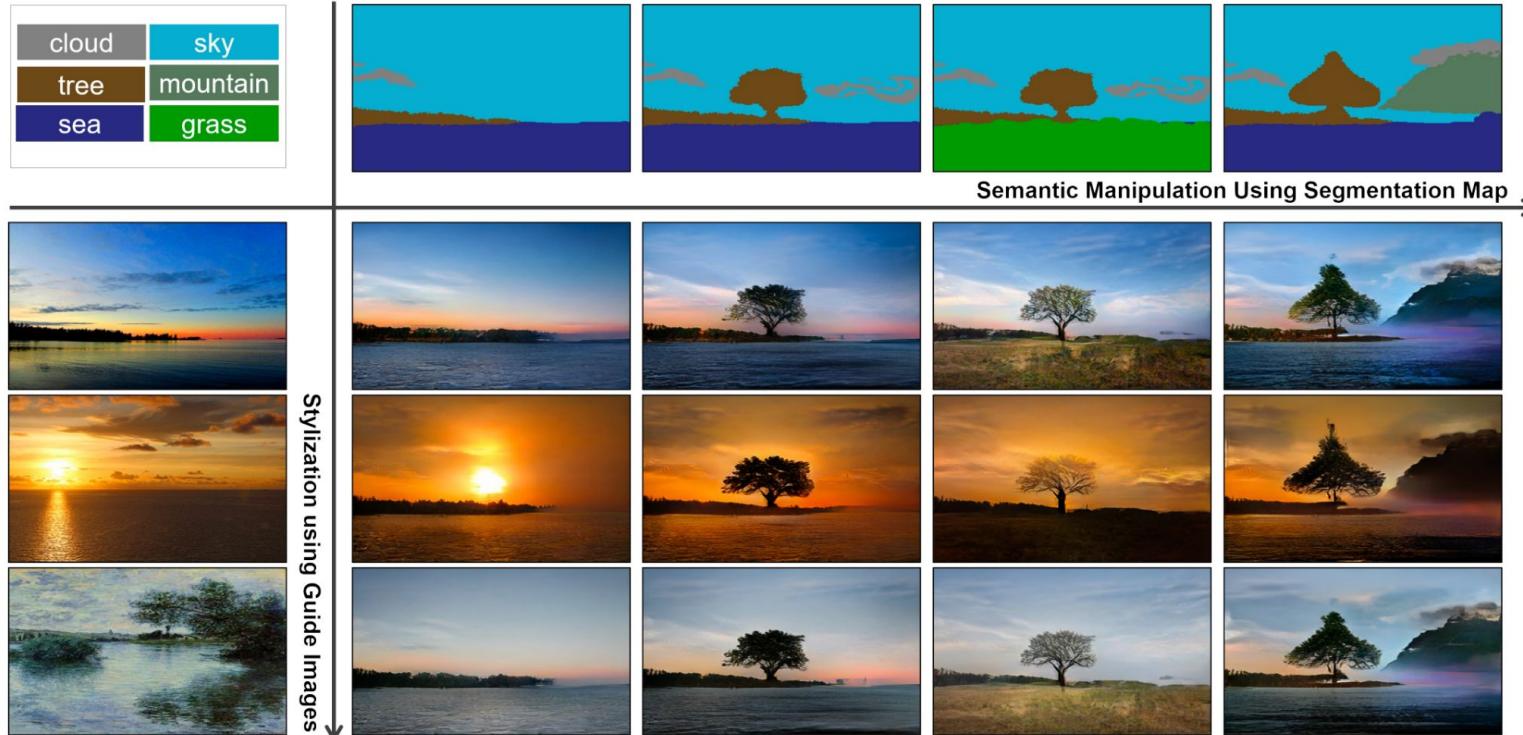


Controlled generation with GANs



Park et al, "Semantic Image Synthesis with Spatially-Adaptive Normalization", CVPR 2019

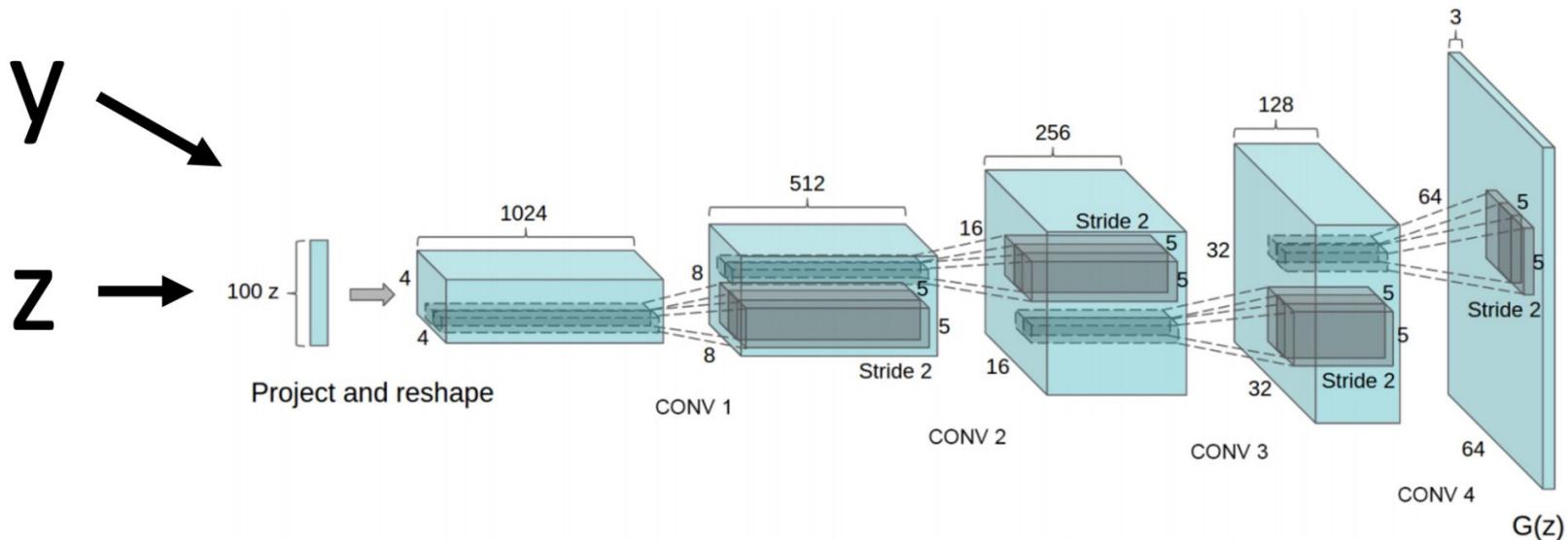
Controlled generation with GANs



Park et al, "Semantic Image Synthesis with Spatially-Adaptive Normalization", CVPR 2019

Conditional GANs: StyleGAN

Y is text that describes the image you want to generate



Karras et al, "Analyzing and Improving the Image Quality of StyleGAN", CVPR 2020

Conditional GANs: StyleGAN

Batch Normalization

$$\mu_j = \frac{1}{N} \sum_{i=1}^N x_{i,j}$$

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{i,j} - \mu_j)^2$$

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}}$$

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Learn a separate scale and shift for each different label y

Conditional Batch Normalization

$$\mu_j = \frac{1}{N} \sum_{i=1}^N x_{i,j}$$

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^N (x_{i,j} - \mu_j)^2$$

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \epsilon}}$$

$$y_{i,j} = \gamma_j^y \hat{x}_{i,j} + \beta_j^y$$

Karras et al, "Analyzing and Improving the Image Quality of StyleGAN", CVPR 2020

Conditional GANs: StyleGAN

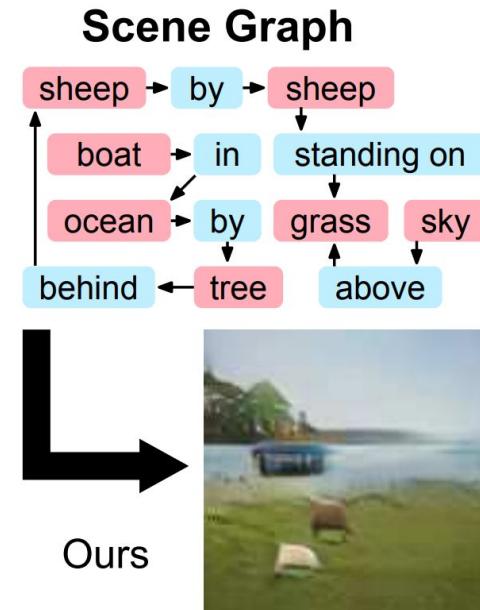


Karras et al, "Analyzing and Improving the Image Quality of StyleGAN", CVPR 2020

Scene graphs to GANs

Specifying exactly what kind of image you want to generate.

The explicit structure in scene graphs provides better image generation for complex scenes.

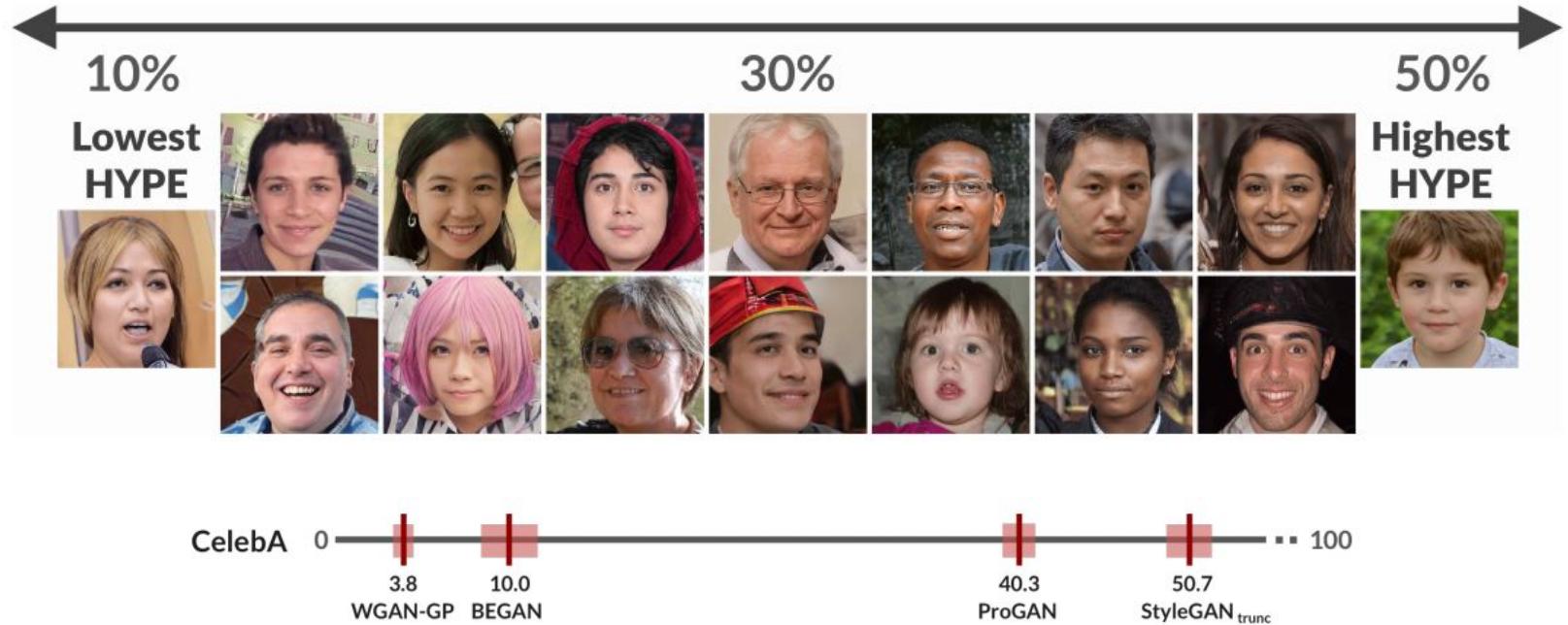


Johnson et al. Image Generation from Scene Graphs, CVPR 2019

Figures copyright 2019. Reproduced with permission.

HYPE: Human eYe Perceptual Evaluations

hype.stanford.edu



Zhou, Gordon, Krishna et al. HYPE: Human eYe Perceptual Evaluations, NeurIPS 2019

Figures copyright 2019. Reproduced with permission.

Summary: GANs

Don't work with an explicit density function

Take game-theoretic approach: learn to generate from training distribution through 2-player game

Pros:

- Beautiful, state-of-the-art samples!

Cons:

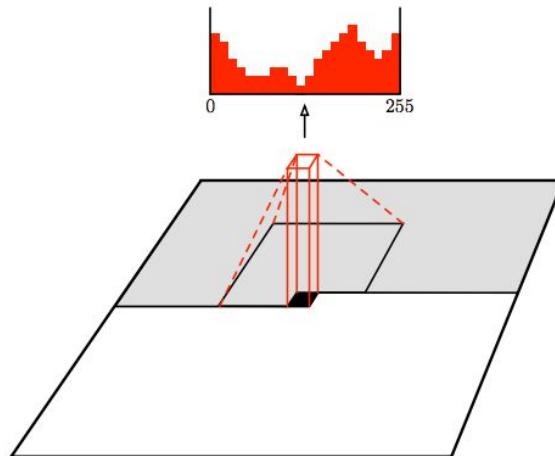
- Trickier / more unstable to train
- Can't solve inference queries such as $p(x)$, $p(z|x)$

Active areas of research:

- Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)
- Conditional GANs, GANs for all kinds of applications

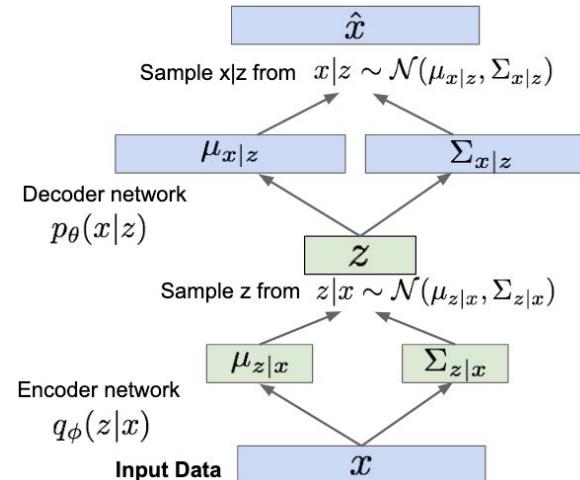
Summary

Autoregressive models: PixelRNN, PixelCNN



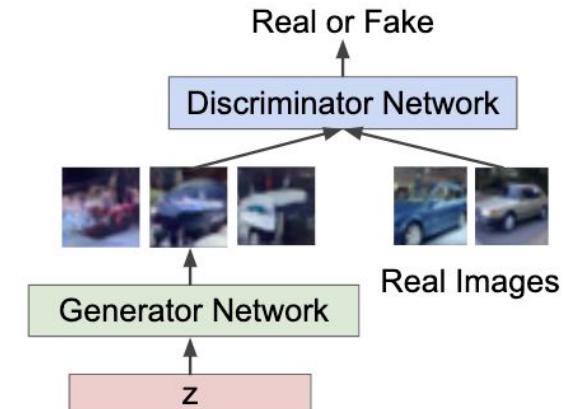
Van der Oord et al, "Conditional image generation with pixelCNN decoders", NIPS 2016

Variational Autoencoders



Kingma and Welling, "Auto-encoding variational bayes", ICLR 2013

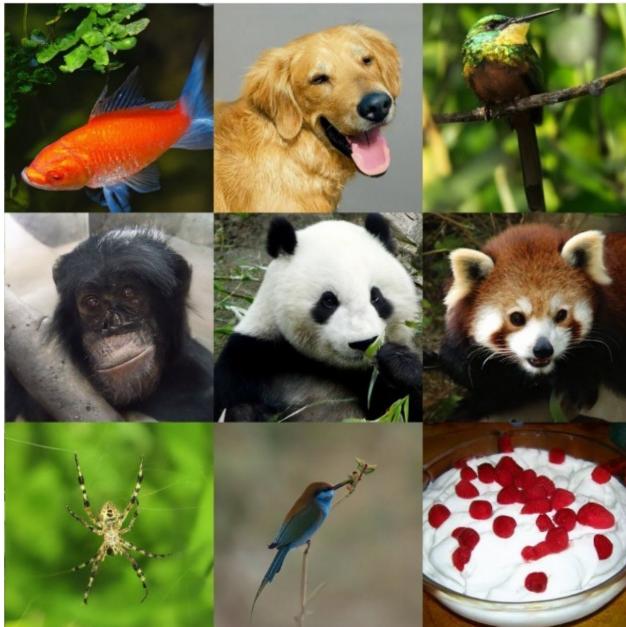
Generative Adversarial Networks (GANs)



Goodfellow et al, "Generative Adversarial Nets", NIPS 2014

Diffusion models

Diffusion Models are outperforming GANs



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



Ho et al. "Cascaded Diffusion Models for High Fidelity Image Generation", Google 2021

Text-to-Image (T2I) Generation

Dall-E2

“a teddy bear on a skateboard in times square”



Ramesh et al. “Hierarchical Text-Conditional Image Generation with CLIP Latents” 2022

Imagen

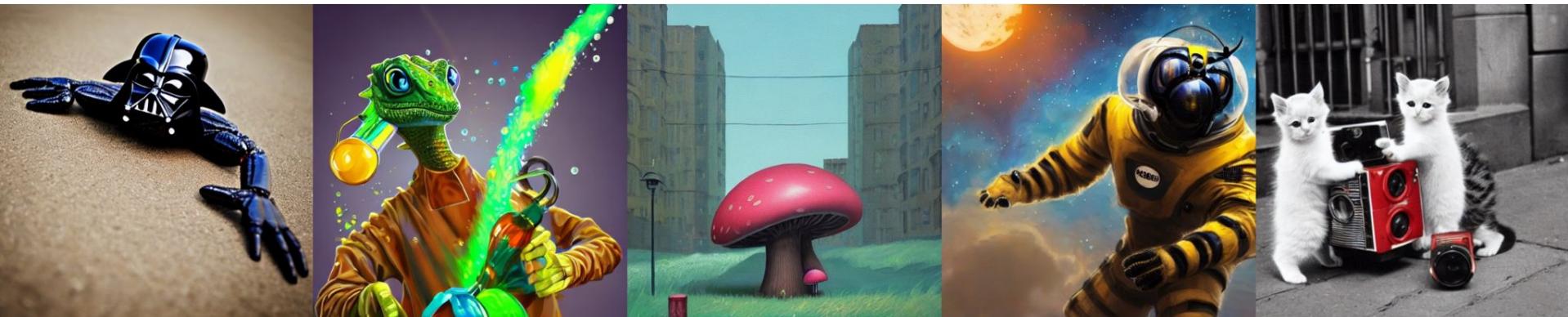
“A group of teddy bears in suit in a corporate office celebrating the birthday of their friend. There is a pizza cake on the desk.”



Saharia et al. “Photorealistic Text-to-Image Diffusion Models with Deep Language Understanding” 2022

Text-to-Image (T2I) Generation

Stable Diffusion



[Mega thread on Twitter/X about Stable Diffusion](#)

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

Application of diffusion: Image Super-resolution

Irish Setter

Saharia et al., Image Super-Resolution via Iterative Refinement, ICCV 2021

Gif on this slide is not displayed in pdf

But what is a diffusion model?

So far...

Autoregressive define tractable density function, optimize likelihood of training data:

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

VAEs define intractable density function with latent \mathbf{z} :

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

GANs give up on explicitly modeling density and just learns to sample “real” data

So far...

Autoregressive define tractable density function, optimize likelihood of training data:

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

VAEs define intractable density function with latent \mathbf{z} :

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead

GANs give up on explicitly modeling density and just learns to sample “real” data

All these methods generate data in one forward step! Why this is hard?

Taxonomy of Generative Models

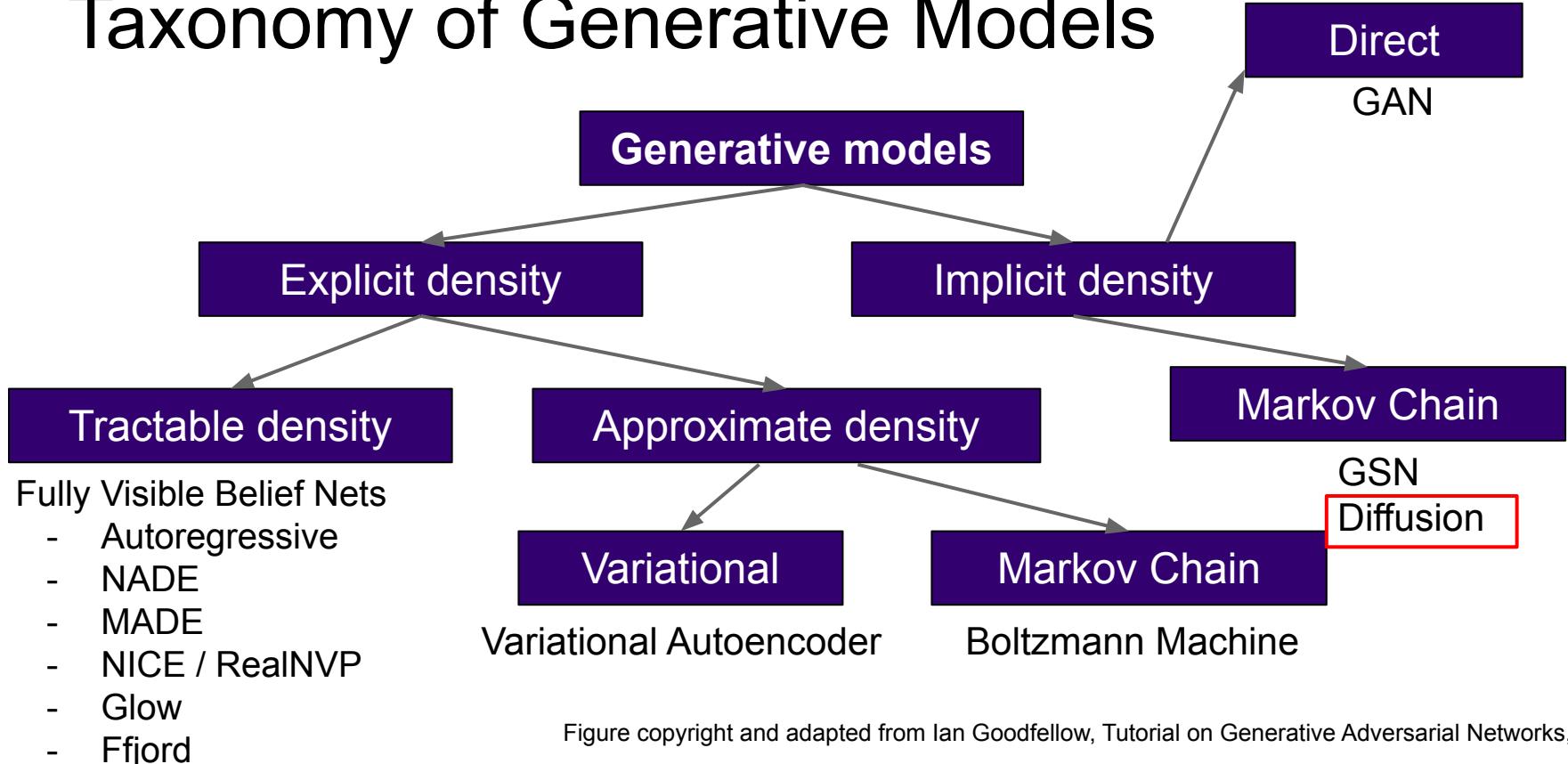


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Recall VAEs

VAEs define intractable density function with latent \mathbf{z} :

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead:

The lower bound we derived last lecture

$$\begin{aligned}\log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} \left[\log p_\theta(x^{(i)}) \right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \frac{q_\phi(z | x^{(i)})}{q_\phi(z | x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_z \left[\log p_\theta(x^{(i)} | z) \right] - \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z)} \right] + \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z | x^{(i)})} \right] \quad (\text{Logarithms}) \\ &= \mathbf{E}_z \left[\log p_\theta(x^{(i)} | z) \right] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z)) + D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))\end{aligned}$$



Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling (need some trick to differentiate through sampling).



This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!



$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always ≥ 0 .

Two loss objectives for VAEs

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

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

Decoder:
reconstruct
the input data

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

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

$$= \underbrace{\mathbf{E}_z [\log p_\theta(x^{(i)} | z)]}_{\mathcal{L}(x^{(i)}, \theta, \phi)} - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z)) + \underbrace{D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))}_{\geq 0}$$

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

Encoder:
make approximate posterior distribution close to prior

First loss for the encoder

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

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

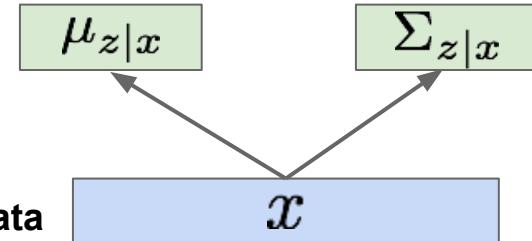
This equation has an analytical solution

Make the latent variable distribution as similar to a unit normal distribution

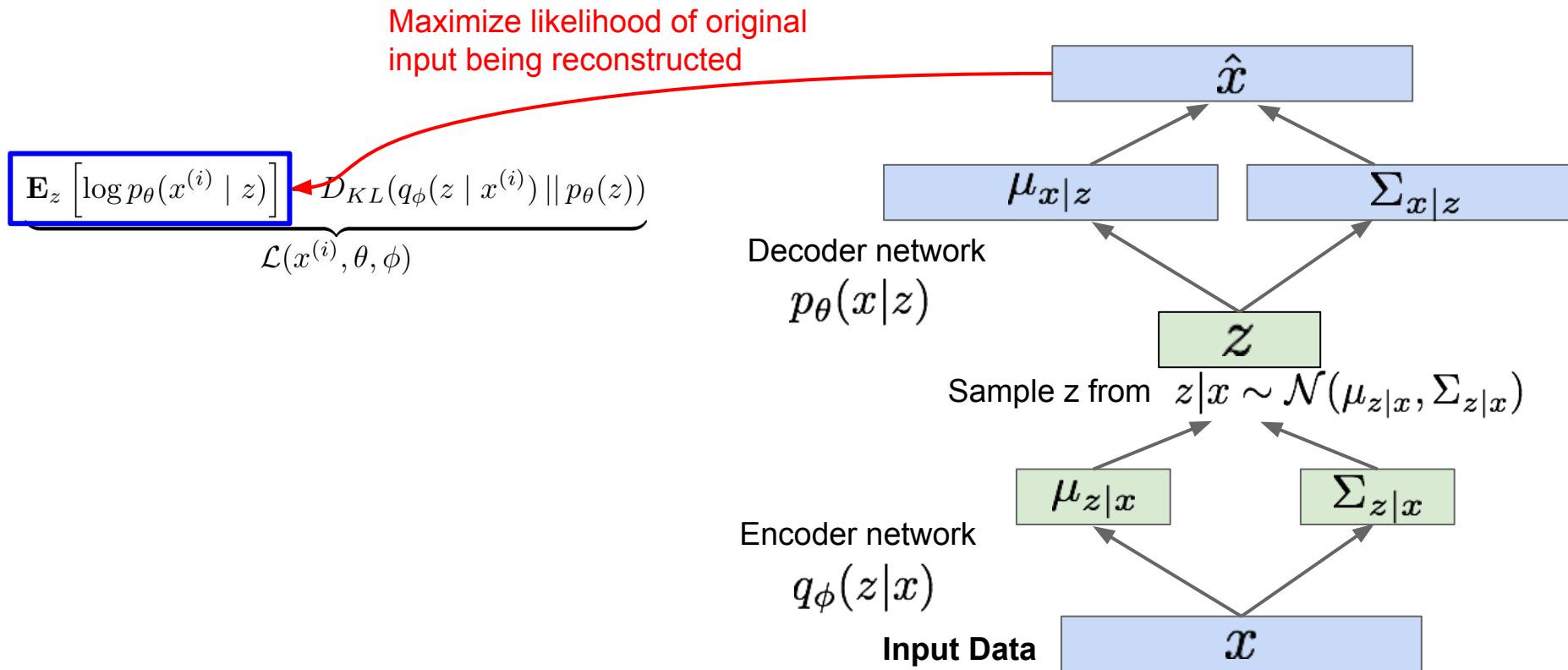
Encoder network

$$q_\phi(z|x)$$

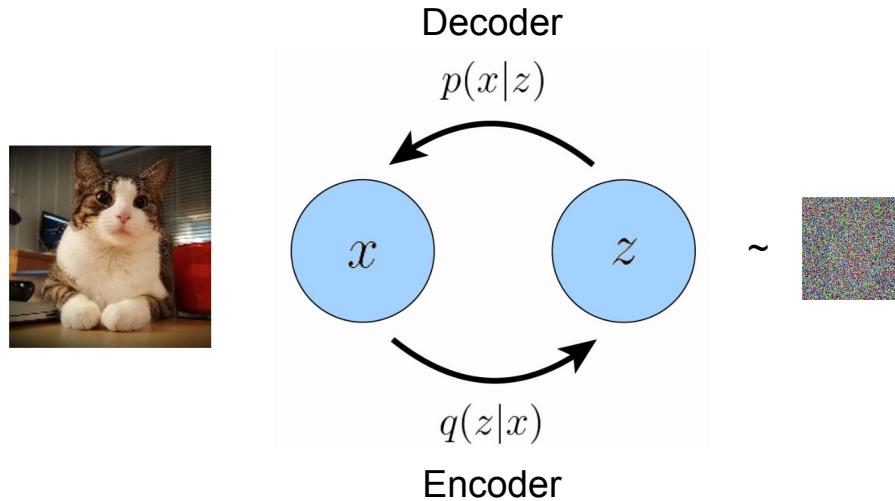
Input Data



Second loss for both decoder and encoder

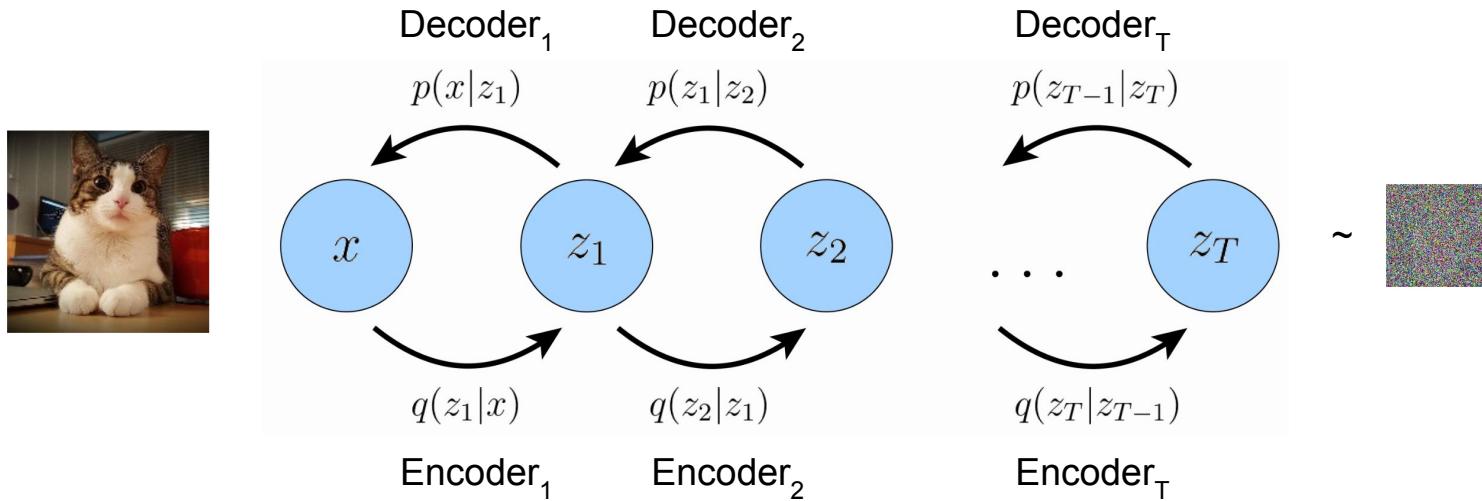


VAEs for images look like this



- We learn **2 networks**, one to encode and one to decode
- We ensure that **z** is similar to a unit normal noise
- To sample new images, we can sample from the unit normal and **decode in 1 step**

Markovian Hierarchical VAEs



- We learn **2T networks**, one to encode and one to decode
- We ensure that z_T is similar to a unit normal noise
- To sample new images, we can sample from the unit normal and **decode in T step**

Markovian Hierarchical VAEs - same derivation

$$\begin{aligned}\log p(x) &= \mathbb{E}_{z_{1:T} \sim q_\phi(z_{1:T}|x)} [\log p_\theta(x^{(i)})] && p_\theta(x) \text{ is independent of } z_{1:T} \\ &= \mathbb{E}_{z_{1:T}} [\log \frac{p_\theta(x|z_{1:T})p_\theta(z_{1:T})}{p_\theta(z_{1:T}|x)}] && \text{Bayes rule}\end{aligned}$$

Markovian Hierarchical VAEs - same derivation

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$$\begin{aligned}\log p(x) &= \mathbb{E}_{z_{1:T} \sim q_\phi(z_{1:T}|x)} [\log p_\theta(x^{(i)})] && p_\theta(x) \text{ is independent of } z_{1:T} \\ &= \mathbb{E}_{z_{1:T}} [\log \frac{p_\theta(x|z_{1:T})p_\theta(z_{1:T})}{p_\theta(z_{1:T}|x)}] && \text{Bayes rule} \\ &= \mathbb{E}_{z_{1:T}} [\log \frac{p_\theta(x|z_{1:T})p_\theta(z_{1:T})}{p_\theta(z_{1:T}|x)} \frac{q_\phi(z_{1:T}|x)}{q_\phi(z_{1:T}|x)}] && \text{Multiplying by a constant} \\ &= \mathbb{E}_{z_{1:T}} [\log p_\theta(x|z_{1:T})] - \mathbb{E}_{z_{1:T}} [\log \frac{q_\phi(z_{1:T}|x)}{p_\theta(z_{1:T})}] + \mathbb{E}_{z_{1:T}} [\log \frac{q_\phi(z_{1:T})}{p(z_{1:T}|x)}]\end{aligned}$$

↑
Reconstruction objective maximizes the likelihood of data $p_\theta(x|z)$

↑
This KL term (between Gaussians for encoder and z prior)

$p_\theta(z|x)$ intractable but we know KL divergence always ≥ 0 .

Markovian Hierarchical VAEs

Keeping just the first two terms:

$$\log p(x) \geq \mathbb{E}_{z_{1:T}} [\log p_\theta(x|z_{1:T})] - \mathbb{E}_{z_{1:T}} [\log \frac{q_\phi(z_{1:T}|x)}{p_\theta(z_{1:T})}]$$

Markovian Hierarchical VAEs

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where the joint probability distribution is: $p(\mathbf{x}, \mathbf{z}_{1:T}) = p(\mathbf{z}_T)p_\theta(\mathbf{x} | \mathbf{z}_1) \prod_{t=2}^T p_\theta(\mathbf{z}_{t-1} | \mathbf{z}_t)$

This is very similar to the autoregressive model formula

Markovian Hierarchical VAEs

Keeping just the first two terms:

$$\begin{aligned}\log p(x) &\geq \mathbb{E}_{z_{1:T}} [\log p_\theta(x|z_{1:T})] - \mathbb{E}_{z_{1:T}} [\log \frac{q_\phi(z_{1:T}|x)}{p_\theta(z_{1:T})}] \\&= \mathbb{E}_{z_{1:T}} [\log \frac{p_\theta(x|z_{1:T})p_\theta(z_{1:T})}{q_\phi(z_{1:T}|x)}] \\&= \mathbb{E}_{z_{1:T}} [\log \frac{p_\theta(x, z_{1:T})}{q_\phi(z_{1:T}|x)}]\end{aligned}$$

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And the encoder posterior is: $q_\phi(\mathbf{z}_{1:T} | \mathbf{x}) = q_\phi(\mathbf{z}_1 | \mathbf{x}) \prod_{t=2}^T q_\phi(\mathbf{z}_t | \mathbf{z}_{t-1})$

Markovian Hierarchical VAEs

Keeping just the first two terms:

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where the joint probability distribution is: $p(\mathbf{x}, \mathbf{z}_{1:T}) = p(\mathbf{z}_T)p_\theta(\mathbf{x} | \mathbf{z}_1) \prod_{t=2}^T p_\theta(\mathbf{z}_{t-1} | \mathbf{z}_t)$

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Markovian Hierarchical VAEs

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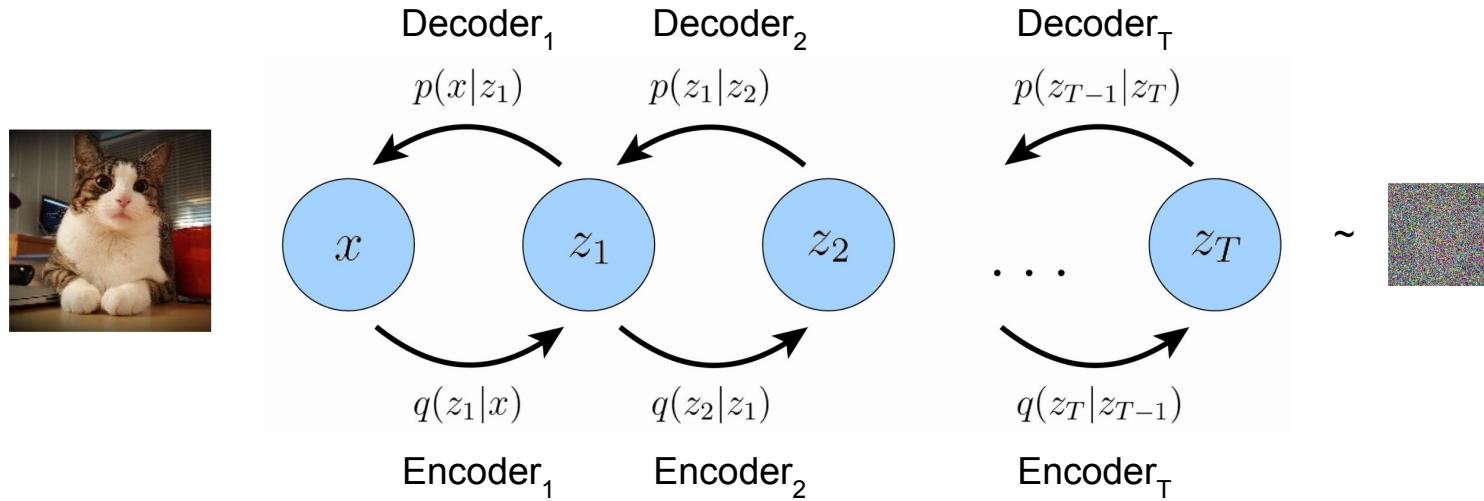
Why is this a hard objective to train?

1. There are too many networks to learn
2. The objective function is expensive!
3. It collapses easily!

where the joint probability distribution is: $p(\mathbf{x}, \mathbf{z}_{1:T}) = p(\mathbf{z}_T)p_\theta(\mathbf{x} | \mathbf{z}_1) \prod_{t=2}^T p_\theta(\mathbf{z}_{t-1} | \mathbf{z}_t)$

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Markovian Hierarchical VAEs



Diffusion models are a special case
With a more interpretable, simpler objective.

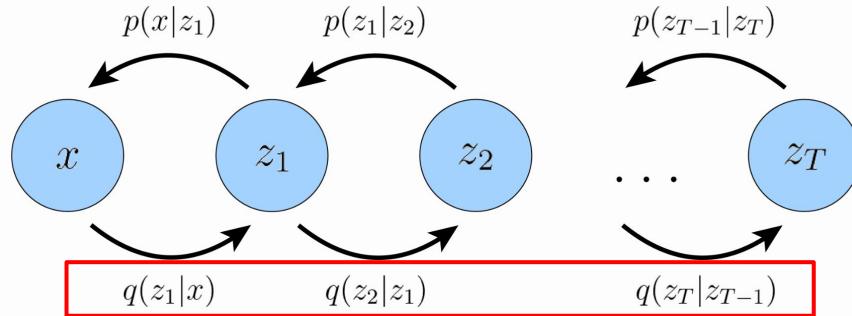
How are diffusion models different?

1. The latent dimension size is exactly equal to the data dimension



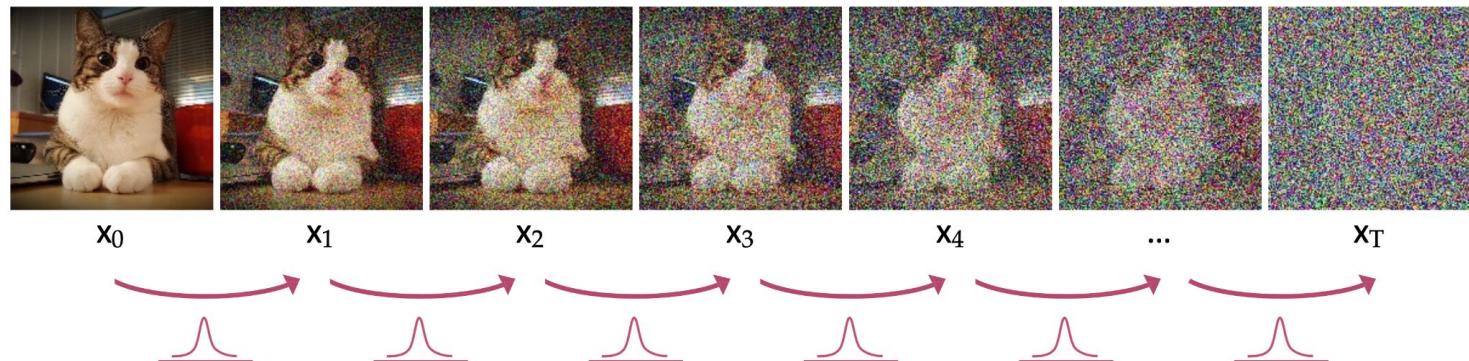
How are diffusion models different?

1. The latent dimension size is exactly equal to the data dimension
2. The encoders are **pre-defined** and **not learned**.



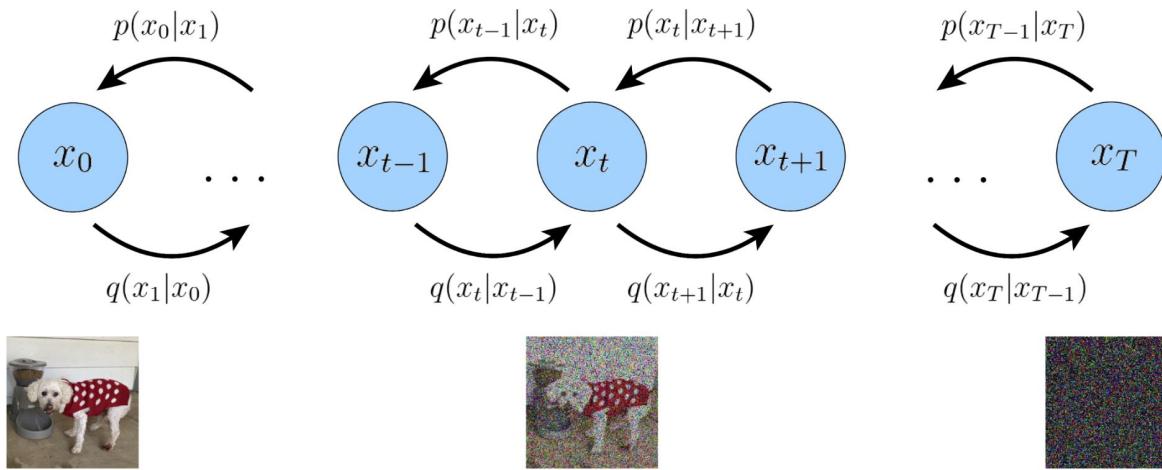
How are diffusion models different?

1. The latent dimension size is exactly equal to the data dimension
2. The encoders are pre-defined and not learned.
3. Encoders are designed as a **linear Gaussian model** conditioned on the time step: Add noise at every time step

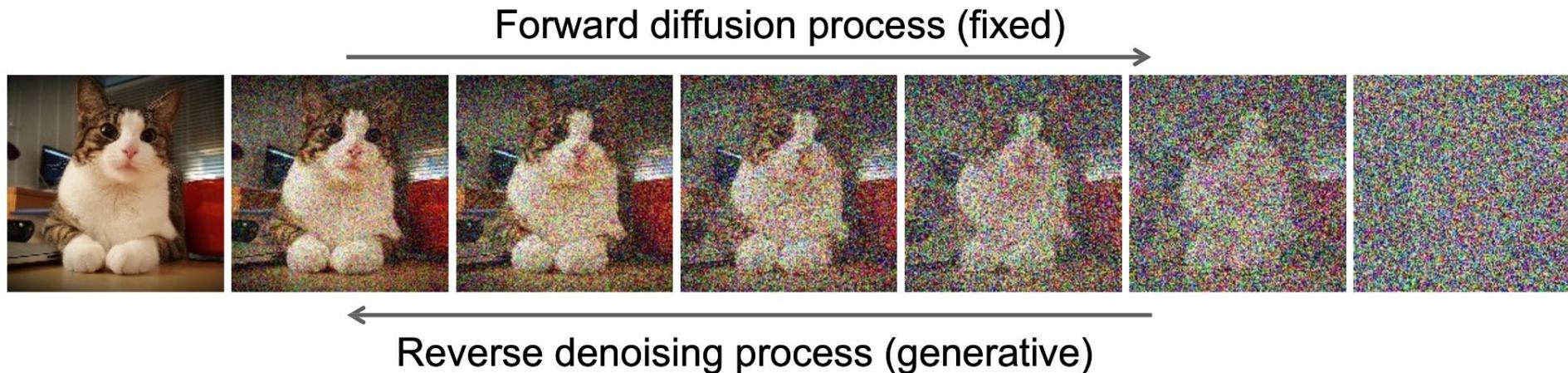


How are diffusion models different?

4. The Gaussian parameters vary over time in such a way that the distribution of the **latent at final step T** is a **standard Gaussian**



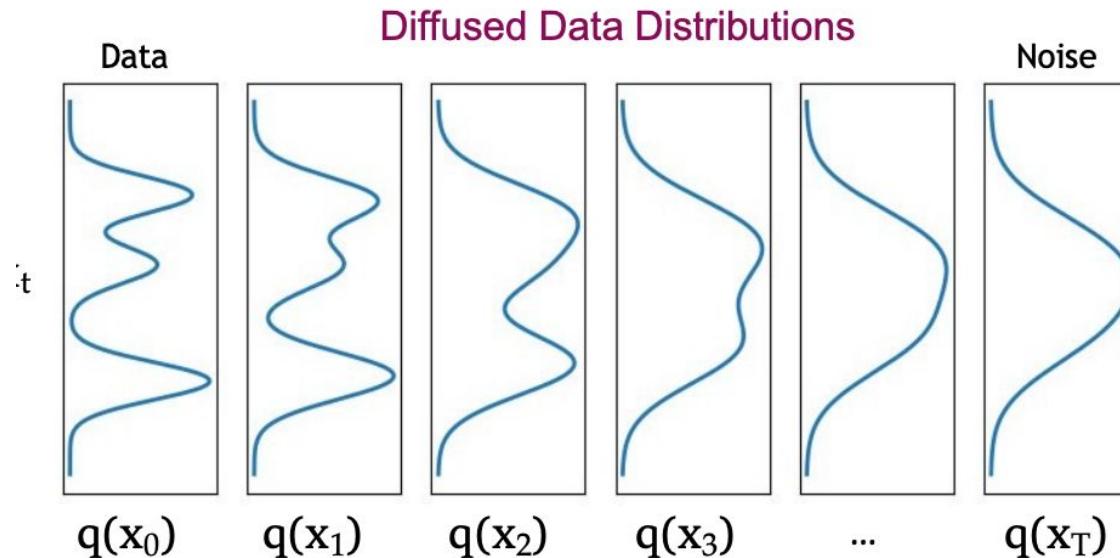
Terminology: Forward and backward process



Note: reverse or backward here doesn't mean the same thing as backpropagation

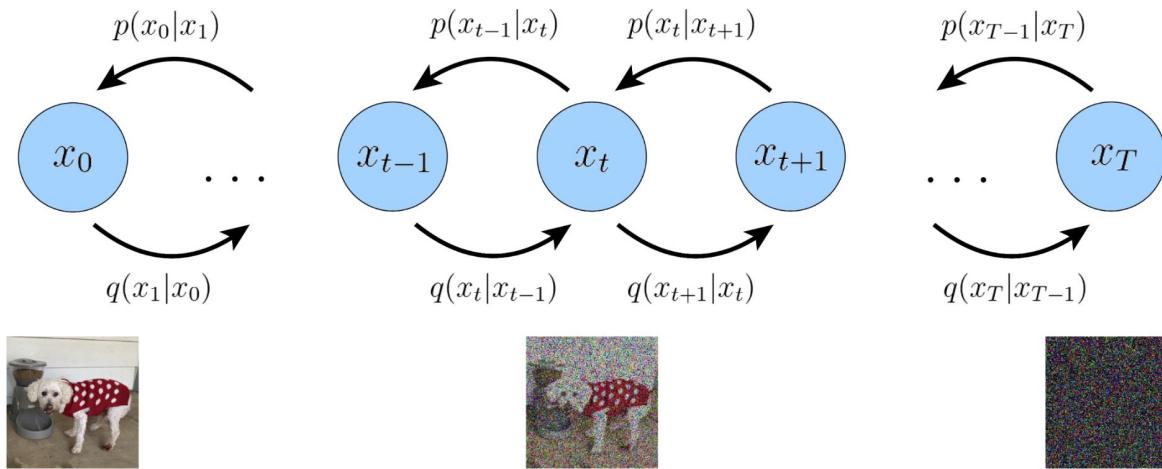
The distribution perspective

Over time, as we add more noise sampled from a Gaussian distribution, it begins to look more like a unit normal



How do we define a loss objective?

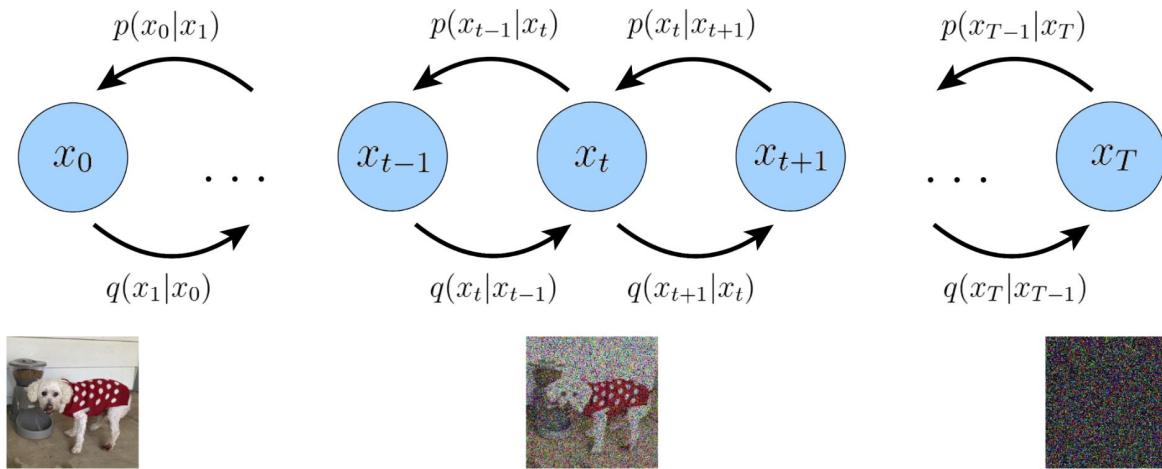
Q. What do we have to learn to generate new samples from noise?



How do we define a loss objective?

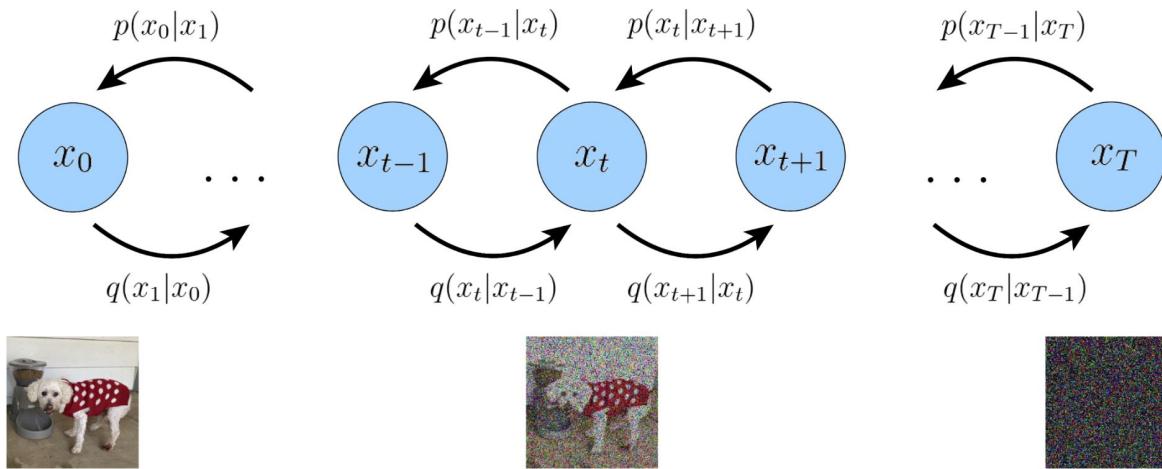
Q. What do we have to learn to generate new samples from noise?

A. We want to define a neural network to predict $p_{\theta}(x_{t-1} | x_t)$



How do we define a loss objective?

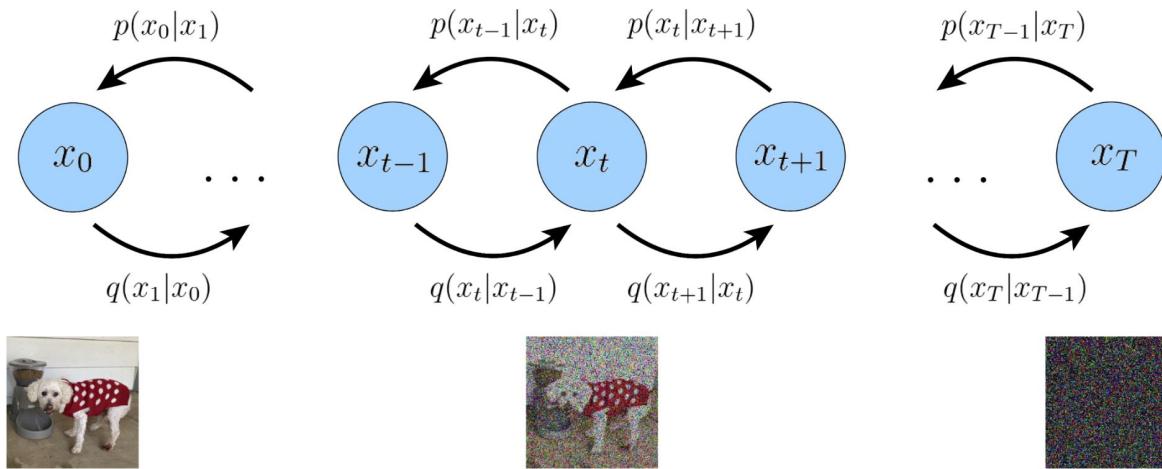
Q. How should we train $p_{\theta}(x_{t-1} | x_t)$?



How do we define a loss objective?

Q. How should we train $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$?

A. We can get it to match $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$!

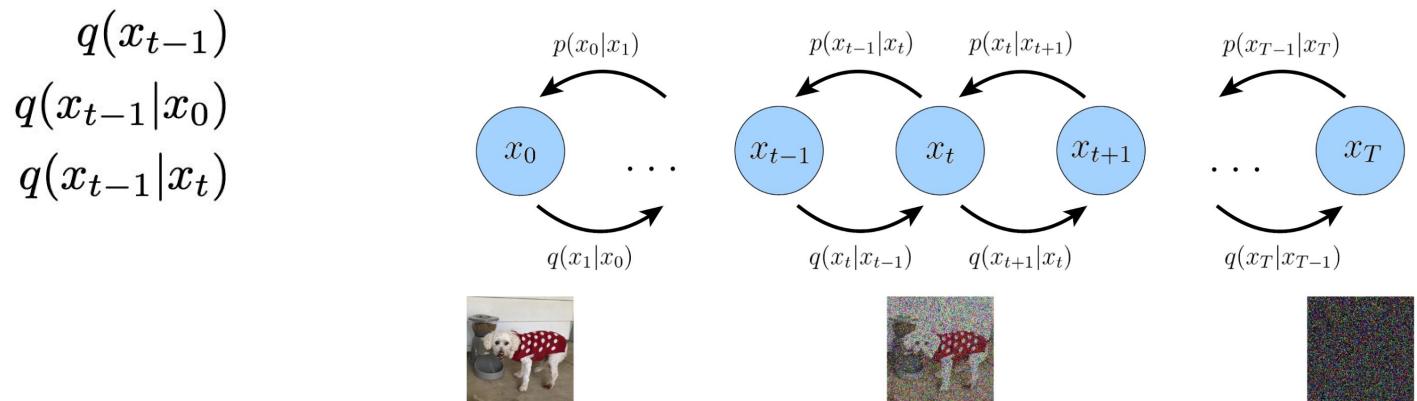


How do we define a loss objective?

Q. How should we train $p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$?

A. We can get it to match $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$!

Q. But why $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$ and not:



Ok so our loss function is:

Q. How should we train $p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$?

A. We can get it to match $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$!

Minimize the distance between the two distributions:

$$\arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t))$$

Ok so our loss function is:

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Problem: How do we estimate $q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$?

The forward diffusion step

The distribution at step t is a Gaussian

$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t} \mathbf{x}_{t-1}, (1 - \alpha_t) \mathbf{I})$$

The forward diffusion step

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The **mean** defined by \mathbf{x}_{t-1} : $\mu_t(\mathbf{x}_t) = \sqrt{\alpha_t} \mathbf{x}_{t-1}$

α_t is a **predefined** value for each step t

The forward diffusion step

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The **mean** defined by \mathbf{x}_{t-1} : $\mu_t(\mathbf{x}_t) = \sqrt{\alpha_t} \mathbf{x}_{t-1}$

α_t is a **predefined** value for each step t

The **covariance** is **independent** of \mathbf{x}_{t-1} (an assumption)

$$\Sigma_t(\mathbf{x}_t) = (1 - \alpha_t) \mathbf{I}$$

How the forward step was designed:

The distribution at step t is a Gaussian

$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t} \mathbf{x}_{t-1}, (1 - \alpha_t) \mathbf{I})$$

$$\boldsymbol{\mu}_t(\mathbf{x}_t) = \sqrt{\alpha_t} \mathbf{x}_{t-1}$$

$$\boldsymbol{\Sigma}_t(\mathbf{x}_t) = (1 - \alpha_t) \mathbf{I}$$

So, given \mathbf{x}_{t-1} we can sample \mathbf{x}_t using:

$$\mathbf{x}_t \sim \sqrt{\alpha_t} \mathbf{x}_{t-1} + (1 - \alpha_t) \boldsymbol{\epsilon}$$

where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{x}; \mathbf{0}, \mathbf{I})$

Why was it designed like this?

$$\boldsymbol{x}_t = \sqrt{\alpha_t} \boldsymbol{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^*$$

Why was it designed like this?

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\ &= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \leftarrow \text{Substituting } \mathbf{x}_{t-1}\end{aligned}$$

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We can interpret this $\sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^*$ as a sample from $\mathcal{N}(\mathbf{0}, (1 - \alpha_t)\mathbf{I})$

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Notice that $\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^*$ is the sum of two Gaussian samples

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Notice that $\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^*$ is the sum of two Gaussian samples

Using the property: $\mathcal{N}(x; 0, \sigma_1^2 I) + \mathcal{N}(x; 0, \sigma_2^2 I) = \mathcal{N}(x; 0, \sqrt{\sigma_1^2 + \sigma_2^2} I)$

Why was it designed like this?

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \epsilon_{t-1}^* \\&= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \epsilon_{t-2}^* \right) + \sqrt{1 - \alpha_t} \epsilon_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \boxed{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \epsilon_{t-2}^* + \sqrt{1 - \alpha_t} \epsilon_{t-1}^*} \quad \text{Opening the parentheses}\end{aligned}$$

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We can interpret this $\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \epsilon_{t-2}^*$ as a sample from $\mathcal{N}(\mathbf{0}, (\alpha_t - \alpha_t \alpha_{t-1})\mathbf{I})$

Notice that $\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \epsilon_{t-2}^* + \sqrt{1 - \alpha_t} \epsilon_{t-1}^*$ is the sum of two Gaussian samples

Using the property: $\mathcal{N}(x; 0, \sigma_1^2 I) + \mathcal{N}(x; 0, \sigma_2^2 I) = \mathcal{N}(x; 0, \sqrt{\sigma_1^2 + \sigma_2^2} I)$

We can rewrite $\sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \epsilon_{t-2}^* + \sqrt{1 - \alpha_t} \epsilon_{t-1}^*$ as $\sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \epsilon_{t-2}$

Why was it designed like this?

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\&= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Opening the parentheses} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \boldsymbol{\epsilon}_{t-2} \quad \text{Sum of two Gaussians}\end{aligned}$$

Why was it designed like this?

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\&= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Opening the parentheses} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \boldsymbol{\epsilon}_{t-2} \quad \text{Sum of two Gaussians} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t} \boldsymbol{\epsilon}_{t-2} \quad \text{Squaring the terms}\end{aligned}$$

Why was it designed like this?

$$\begin{aligned} \mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\ &= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Opening the parentheses} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \boldsymbol{\epsilon}_{t-2} \quad \text{Sum of two Gaussians} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t} \boldsymbol{\epsilon}_{t-2} \quad \text{Squaring the terms} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2} \quad \text{Simplifying} \end{aligned}$$

Why was it designed like this?

$$\begin{aligned} \mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\ &= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* && \text{Substituting } \mathbf{x}_{t-1} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* && \text{Opening the parentheses} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \boldsymbol{\epsilon}_{t-2} && \text{Sum of two Gaussians} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t} \boldsymbol{\epsilon}_{t-2} && \text{Squaring the terms} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2} && \text{Simplifying} \\ &= \dots \\ &= \sqrt{\prod_{i=1}^t \alpha_i} \mathbf{x}_0 + \sqrt{1 - \prod_{i=1}^t \alpha_i} \boldsymbol{\epsilon}_0 && \text{Substituting till } \mathbf{x}_0 \end{aligned}$$

Why was it designed like this?

$$\begin{aligned} \mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \epsilon_{t-1}^* \\ &= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \epsilon_{t-2}^* \right) + \sqrt{1 - \alpha_t} \epsilon_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \epsilon_{t-2}^* + \sqrt{1 - \alpha_t} \epsilon_{t-1}^* \quad \text{Opening the parentheses} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \epsilon_{t-2} \quad \text{Sum of two Gaussians} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t} \epsilon_{t-2} \quad \text{Squaring the terms} \\ &= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \epsilon_{t-2} \quad \text{Simplifying} \\ &= \dots \\ &= \sqrt{\prod_{i=1}^t \alpha_i} \mathbf{x}_0 + \sqrt{1 - \prod_{i=1}^t \alpha_i} \epsilon_0 \quad \text{Substituting till } \mathbf{x}_0 \\ &= \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \epsilon_0 \quad \text{Let } \bar{\alpha}_t = \prod_{i=1}^t \alpha_i \end{aligned}$$

Why was it designed like this?

$$\begin{aligned}\mathbf{x}_t &= \sqrt{\alpha_t} \mathbf{x}_{t-1} + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \\&= \sqrt{\alpha_t} \left(\sqrt{\alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* \right) + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Substituting } \mathbf{x}_{t-1} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2}^* + \sqrt{1 - \alpha_t} \boldsymbol{\epsilon}_{t-1}^* \quad \text{Opening the parentheses} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\sqrt{\alpha_t - \alpha_t \alpha_{t-1}}^2 + \sqrt{1 - \alpha_t}^2} \boldsymbol{\epsilon}_{t-2} \quad \text{Sum of two Gaussians} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{\alpha_t - \alpha_t \alpha_{t-1} + 1 - \alpha_t} \boldsymbol{\epsilon}_{t-2} \quad \text{Squaring the terms} \\&= \sqrt{\alpha_t \alpha_{t-1}} \mathbf{x}_{t-2} + \sqrt{1 - \alpha_t \alpha_{t-1}} \boldsymbol{\epsilon}_{t-2} \quad \text{Simplifying} \\&= \dots \\&= \sqrt{\prod_{i=1}^t \alpha_i} \mathbf{x}_0 + \sqrt{1 - \prod_{i=1}^t \alpha_i} \boldsymbol{\epsilon}_0 \quad \text{Substituting till } \mathbf{x}_0 \\&= \sqrt{\bar{\alpha}_t} \mathbf{x}_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}_0 \quad \text{Let } \bar{\alpha}_t = \prod_{i=1}^t \alpha_i \\&\sim \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I}) \quad \text{x}_t \text{ is now a Gaussian characterized by } \mathbf{x}_0\end{aligned}$$

Takeaway from the previous slides:

$$\boldsymbol{x}_t \sim \mathcal{N}(\boldsymbol{x}_t; \sqrt{\bar{\alpha}_t} \boldsymbol{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})$$

We can instantly sample \boldsymbol{x}_t given any input data \boldsymbol{x}_0

What about the reverse?

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0)$$

What about the reverse?

$$q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) = \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)}$$

Applying Bayes rule

What about the reverse?

$$\begin{aligned} q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)} \\ &= \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1 - \alpha_t)\mathbf{I}) \end{aligned}$$

The first term is just a single forward diffusion process:

$$q(\mathbf{x}_t \mid \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1 - \alpha_t)\mathbf{I})$$

What about the reverse?

$$\begin{aligned} q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0) q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)} \\ &= \frac{\mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t} \mathbf{x}_{t-1}, (1 - \alpha_t) \mathbf{I}) \mathcal{N}(\mathbf{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0, (1 - \bar{\alpha}_{t-1}) \mathbf{I})}{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})} \end{aligned}$$

The second term is also a Gaussian using the formula we just derived:

$$\mathbf{x}_t \sim \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t} \mathbf{x}_0, (1 - \bar{\alpha}_t) \mathbf{I})$$

What about the reverse?

$$\begin{aligned} q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)} \\ &= \frac{\mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1 - \alpha_t)\mathbf{I})\mathcal{N}(\mathbf{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0, (1 - \bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I})} \end{aligned}$$

The third term is also a Gaussian using the same formula:

$$\mathbf{x}_t \sim \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I})$$

What about the reverse?

$$\begin{aligned} q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)} \\ &= \frac{\mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1 - \alpha_t)\mathbf{I})\mathcal{N}(\mathbf{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0, (1 - \bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I})} \\ &\propto \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)\mathbf{x}_0}{1 - \bar{\alpha}_t}}_{\mu_q(\mathbf{x}_t, \mathbf{x}_0)}, \underbrace{\frac{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}\mathbf{I}}_{\Sigma_q(t)}) \end{aligned}$$

The product of these 3 Gaussian distributions simplify to a Gaussian as well!

Let's call its mean $\mu_q(\mathbf{x}_t, \mathbf{x}_0)$ and variance $\Sigma_q(t)$

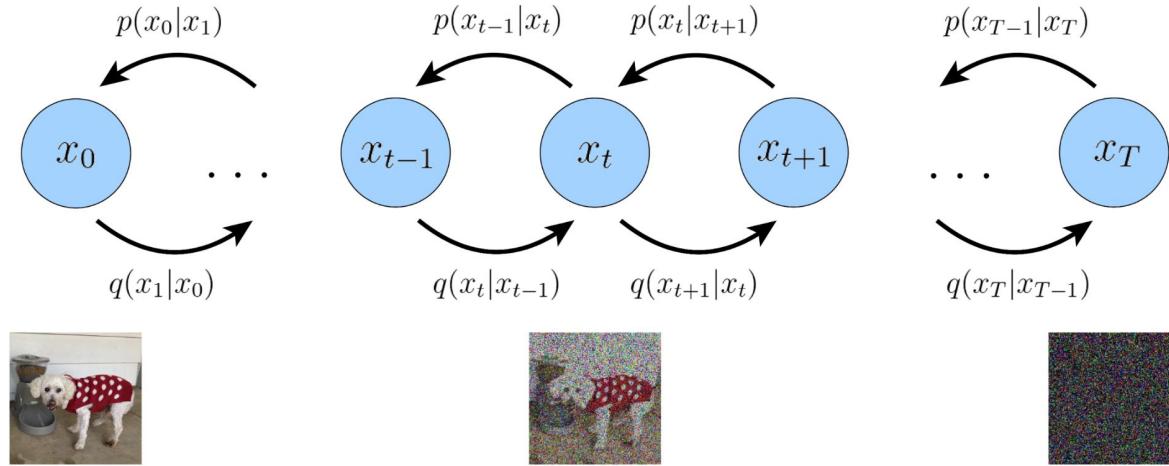
Proof (out of scope for the class)

$$\begin{aligned}
q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) &= \frac{q(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \mathbf{x}_0)q(\mathbf{x}_{t-1} \mid \mathbf{x}_0)}{q(\mathbf{x}_t \mid \mathbf{x}_0)} \\
&= \frac{\mathcal{N}(\mathbf{x}_t; \sqrt{\alpha_t}\mathbf{x}_{t-1}, (1 - \alpha_t)\mathbf{I})\mathcal{N}(\mathbf{x}_{t-1}; \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0, (1 - \bar{\alpha}_{t-1})\mathbf{I})}{\mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1 - \bar{\alpha}_t)\mathbf{I})} \\
&\propto \exp \left\{ - \left[\frac{(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{2(1 - \alpha_t)} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{2(1 - \bar{\alpha}_{t-1})} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{2(1 - \bar{\alpha}_t)} \right] \right\} \\
&= \exp \left\{ - \frac{1}{2} \left[\frac{(\mathbf{x}_t - \sqrt{\alpha_t}\mathbf{x}_{t-1})^2}{1 - \alpha_t} + \frac{(\mathbf{x}_{t-1} - \sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0)^2}{1 - \bar{\alpha}_{t-1}} - \frac{(\mathbf{x}_t - \sqrt{\bar{\alpha}_t}\mathbf{x}_0)^2}{1 - \bar{\alpha}_t} \right] \right\} \\
&= \exp \left\{ - \frac{1}{2} \left[\frac{(-2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1} + \alpha_t\mathbf{x}_{t-1}^2)}{1 - \alpha_t} + \frac{(\mathbf{x}_{t-1}^2 - 2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_{t-1}\mathbf{x}_0)}{1 - \bar{\alpha}_{t-1}} + C(\mathbf{x}_t, \mathbf{x}_0) \right] \right\} \\
&\propto \exp \left\{ - \frac{1}{2} \left[- \frac{2\sqrt{\alpha_t}\mathbf{x}_t\mathbf{x}_{t-1}}{1 - \alpha_t} + \frac{\alpha_t\mathbf{x}_{t-1}^2}{1 - \alpha_t} + \frac{\mathbf{x}_{t-1}^2}{1 - \bar{\alpha}_{t-1}} - \frac{2\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_{t-1}\mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right] \right\} \\
&= \exp \left\{ - \frac{1}{2} \left[\left(\frac{\alpha_t}{1 - \alpha_t} + \frac{1}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1}^2 - 2 \left(\frac{\sqrt{\alpha_t}\mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1} \right] \right\} \\
&= \exp \left\{ - \frac{1}{2} \left[\frac{\alpha_t(1 - \bar{\alpha}_{t-1}) + 1 - \alpha_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})} \mathbf{x}_{t-1}^2 - 2 \left(\frac{\sqrt{\alpha_t}\mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}}\mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1} \right] \right\}
\end{aligned}$$

Proof (out of scope for the class)

$$\begin{aligned}
&= \exp \left\{ -\frac{1}{2} \left[\frac{\alpha_t - \bar{\alpha}_t + 1 - \alpha_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})} \mathbf{x}_{t-1}^2 - 2 \left(\frac{\sqrt{\alpha_t} \mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1} \right] \right\} \\
&= \exp \left\{ -\frac{1}{2} \left[\frac{1 - \bar{\alpha}_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})} \mathbf{x}_{t-1}^2 - 2 \left(\frac{\sqrt{\alpha_t} \mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right) \mathbf{x}_{t-1} \right] \right\} \\
&= \exp \left\{ -\frac{1}{2} \left(\frac{1 - \bar{\alpha}_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})} \right) \left[\mathbf{x}_{t-1}^2 - 2 \frac{\left(\frac{\sqrt{\alpha_t} \mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right)}{\frac{1 - \bar{\alpha}_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}} \mathbf{x}_{t-1} \right] \right\} \\
&= \exp \left\{ -\frac{1}{2} \left(\frac{1 - \bar{\alpha}_t}{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})} \right) \left[\mathbf{x}_{t-1}^2 - 2 \frac{\left(\frac{\sqrt{\alpha_t} \mathbf{x}_t}{1 - \alpha_t} + \frac{\sqrt{\bar{\alpha}_{t-1}} \mathbf{x}_0}{1 - \bar{\alpha}_{t-1}} \right) (1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{x}_{t-1} \right] \right\} \\
&= \exp \left\{ -\frac{1}{2} \left(\frac{1}{\frac{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t}} \right) \left[\mathbf{x}_{t-1}^2 - 2 \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1}) \mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t) \mathbf{x}_0}{1 - \bar{\alpha}_t} \mathbf{x}_{t-1} \right] \right\} \\
&\propto \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1}) \mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t) \mathbf{x}_0}{1 - \bar{\alpha}_t}}_{\mu_q(\mathbf{x}_t, \mathbf{x}_0)}, \underbrace{\frac{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{I}}_{\Sigma_q(t)})
\end{aligned}$$

Let's go back to the Markovian VAE

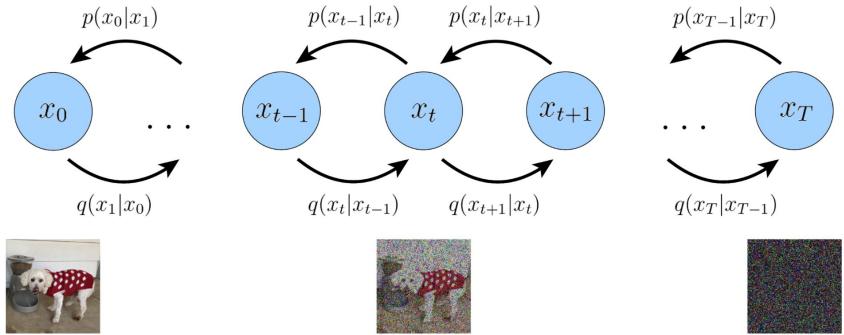


We are ready to set up a simple intuitive loss function to train the decoder!

Given an image x_0 :

We want to generate $p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t)$ to match the Gaussian we just derived: $q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0)$

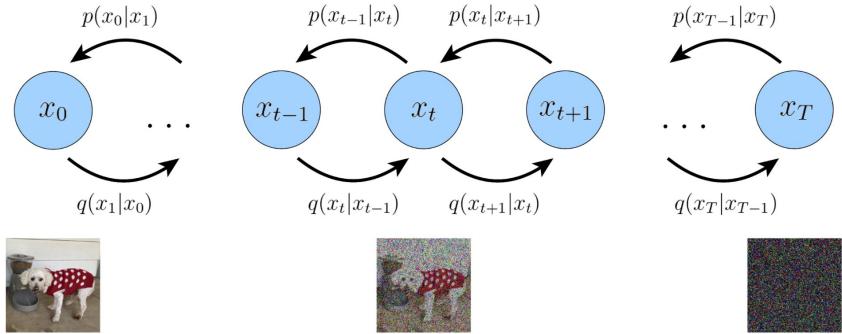
The loss function tries to match distributions



The loss function

$$\arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t))$$

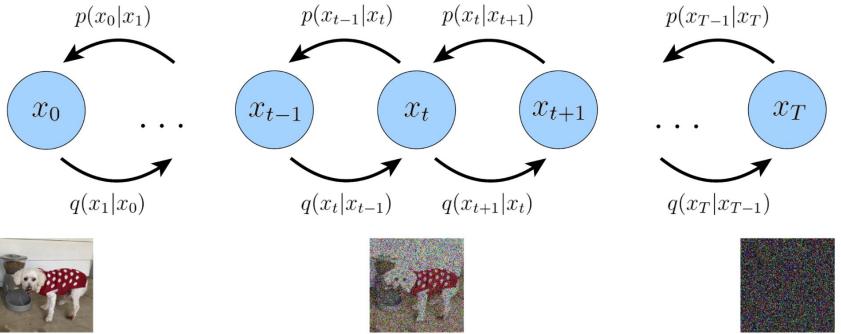
We can model $p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ as a Gaussian



The loss function

$$\begin{aligned} & \arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)) \\ &= \arg \min_{\theta} \mathcal{D}_{\text{KL}} (\mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) \parallel \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_q(t))) \end{aligned}$$

We can model $p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)$ as a Gaussian



The loss function

$$\begin{aligned} & \arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)) \\ &= \arg \min_{\theta} \mathcal{D}_{\text{KL}} (\mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) \parallel \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_q(t))) \\ &= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\|\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q\|_2^2 \right] \end{aligned}$$

Proof (out of scope for class)

$$\arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} | \mathbf{x}_t, \mathbf{x}_0) || p_{\theta}(\mathbf{x}_{t-1} | \mathbf{x}_t))$$

$$= \arg \min_{\theta} \mathcal{D}_{\text{KL}}(\mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) || \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_q(t)))$$

$$= \arg \min_{\theta} \frac{1}{2} \left[\log \frac{|\boldsymbol{\Sigma}_q(t)|}{|\boldsymbol{\Sigma}_q(t)|} - d + \text{tr}(\boldsymbol{\Sigma}_q(t)^{-1} \boldsymbol{\Sigma}_q(t)) + (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q)^T \boldsymbol{\Sigma}_q(t)^{-1} (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q) \right]$$

$$= \arg \min_{\theta} \frac{1}{2} \left[\log 1 - d + d + (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q)^T \boldsymbol{\Sigma}_q(t)^{-1} (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q) \right]$$

$$= \arg \min_{\theta} \frac{1}{2} [(\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q)^T \boldsymbol{\Sigma}_q(t)^{-1} (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q)]$$

$$= \arg \min_{\theta} \frac{1}{2} \left[(\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q)^T (\sigma_q^2(t) \mathbf{I})^{-1} (\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q) \right]$$

$$= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} [\|\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q\|_2^2]$$

Ok we are close to the objective:

The loss we want to minimize is $\arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\|\mu_{\theta} - \mu_q\|_2^2 \right]$

Ok we are close to the objective:

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From the previous slide, we got the mean from this:

$$\mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)\mathbf{x}_0}{1 - \bar{\alpha}_t}, \underbrace{\frac{(1 - \alpha_t)(1 - \bar{\alpha}_{t-1})}{1 - \bar{\alpha}_t} \mathbf{I}}_{\Sigma_q(t)}}_{\mu_q(\mathbf{x}_t, \mathbf{x}_0)})$$

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So, we can write the mean to be: $\boldsymbol{\mu}_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{\sqrt{\alpha_t}(1 - \bar{\alpha}_{t-1})\mathbf{x}_t + \sqrt{\bar{\alpha}_{t-1}}(1 - \alpha_t)\mathbf{x}_0}{1 - \bar{\alpha}_t}$

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Our neural network can predict **noise** instead!

$$\mu_q(\mathbf{x}_t, \mathbf{x}_0) = \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \epsilon_0$$

We can also set our predicted mean to be:

$$\mu_{\theta}(\mathbf{x}_t, t) = \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \hat{\epsilon}_{\theta}(\mathbf{x}_t, t)$$

Why is this helpful?

Our neural network can predict **noise** instead!

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Why is this helpful? Because now our model needs to predict the noise that was injected, which turns out to be empirically more stable of an objective than predicting the image mean.

The two loss objectives are equivalent

The loss function

$$\arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t))$$

$$= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\|\boldsymbol{\mu}_{\theta} - \boldsymbol{\mu}_q\|_2^2 \right]$$

Instead of predicting the mean image values

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Instead of predicting the mean image values

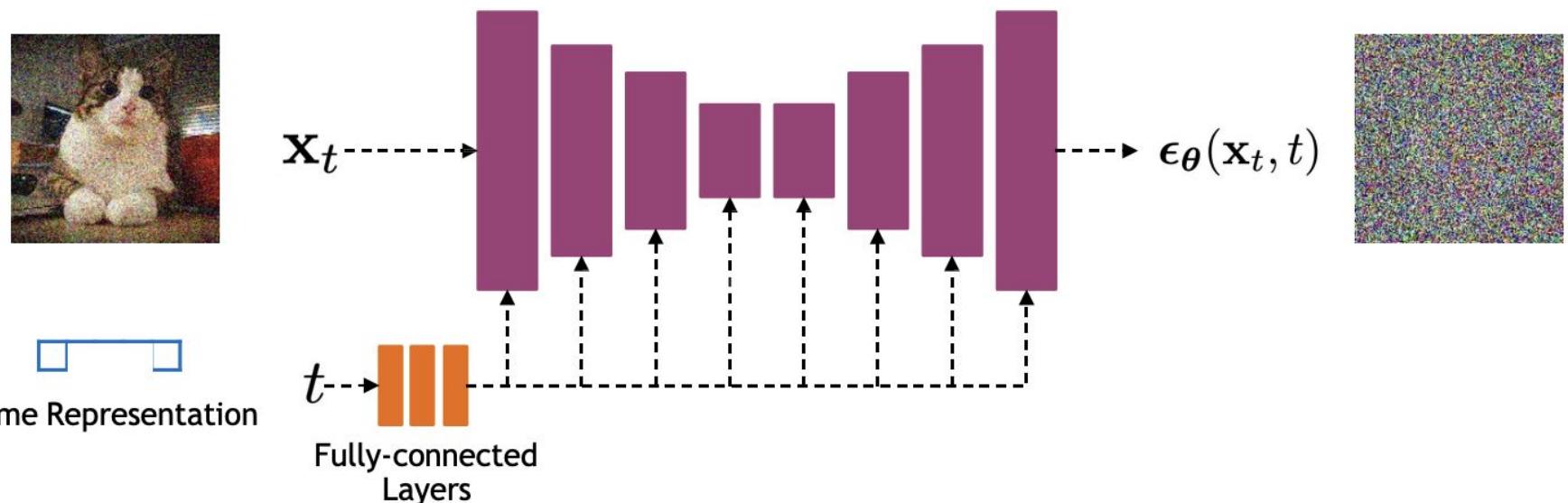
$$= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \frac{(1 - \alpha_t)^2}{(1 - \bar{\alpha}_t)\alpha_t} \left[\|\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_t, t)\|_2^2 \right]$$

The neural network can predict the added noise

Proof: (out of scope)

$$\begin{aligned} & \arg \min_{\theta} \mathcal{D}_{\text{KL}}(q(\mathbf{x}_{t-1} \mid \mathbf{x}_t, \mathbf{x}_0) \parallel p_{\theta}(\mathbf{x}_{t-1} \mid \mathbf{x}_t)) \\ &= \arg \min_{\theta} \mathcal{D}_{\text{KL}}(\mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q(t)) \parallel \mathcal{N}(\mathbf{x}_{t-1}; \boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_q(t))) \\ &= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\left\| \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_t, t) - \frac{1}{\sqrt{\alpha_t}} \mathbf{x}_t + \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \boldsymbol{\epsilon}_0 \right\|_2^2 \right] \\ &= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\left\| \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \boldsymbol{\epsilon}_0 - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_t, t) \right\|_2^2 \right] \\ &= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\left\| \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} (\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_t, t)) \right\|_2^2 \right] \\ &= \arg \min_{\theta} \frac{1}{2\sigma_q^2(t)} \left[\frac{(1 - \alpha_t)^2}{(1 - \bar{\alpha}_t)\alpha_t} \left[\|\boldsymbol{\epsilon}_0 - \hat{\boldsymbol{\epsilon}}_{\theta}(\mathbf{x}_t, t)\|_2^2 \right] \right] \end{aligned}$$

The denoising architecture



Time representation: sinusoidal positional embeddings.

How do we sample a new image?

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

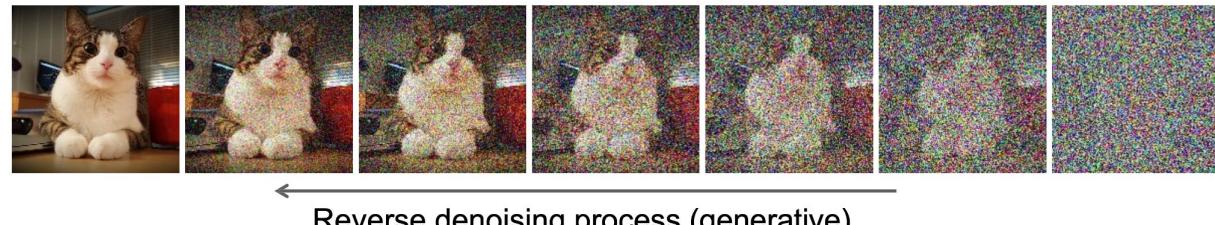
For $t = T \dots 1$ do

Predict $\hat{\epsilon}_t = p_\theta(x_t)$

$$\mu_{t-1} = \frac{1}{\sqrt{\alpha_t}} x_t - \frac{1 - \alpha_t}{\sqrt{1 - \bar{\alpha}_t} \sqrt{\alpha_t}} \sqrt{1 - \bar{\alpha}_{t-1}} \hat{\epsilon}_t$$

Sample $x_{t-1} \sim \mathcal{N}(\mu_{t-1}, \Sigma_{t-1})$

Return x_0

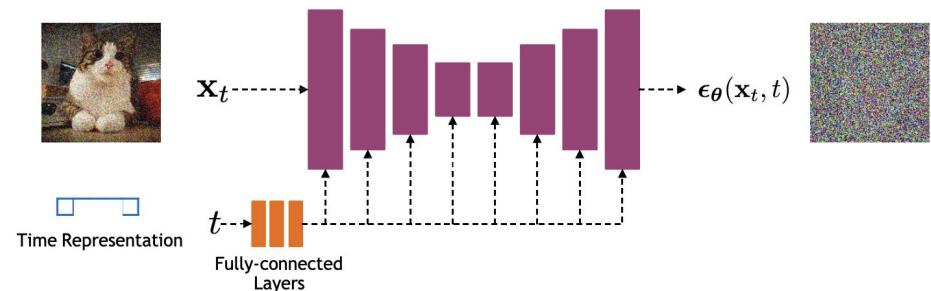


How is the time step inputted:

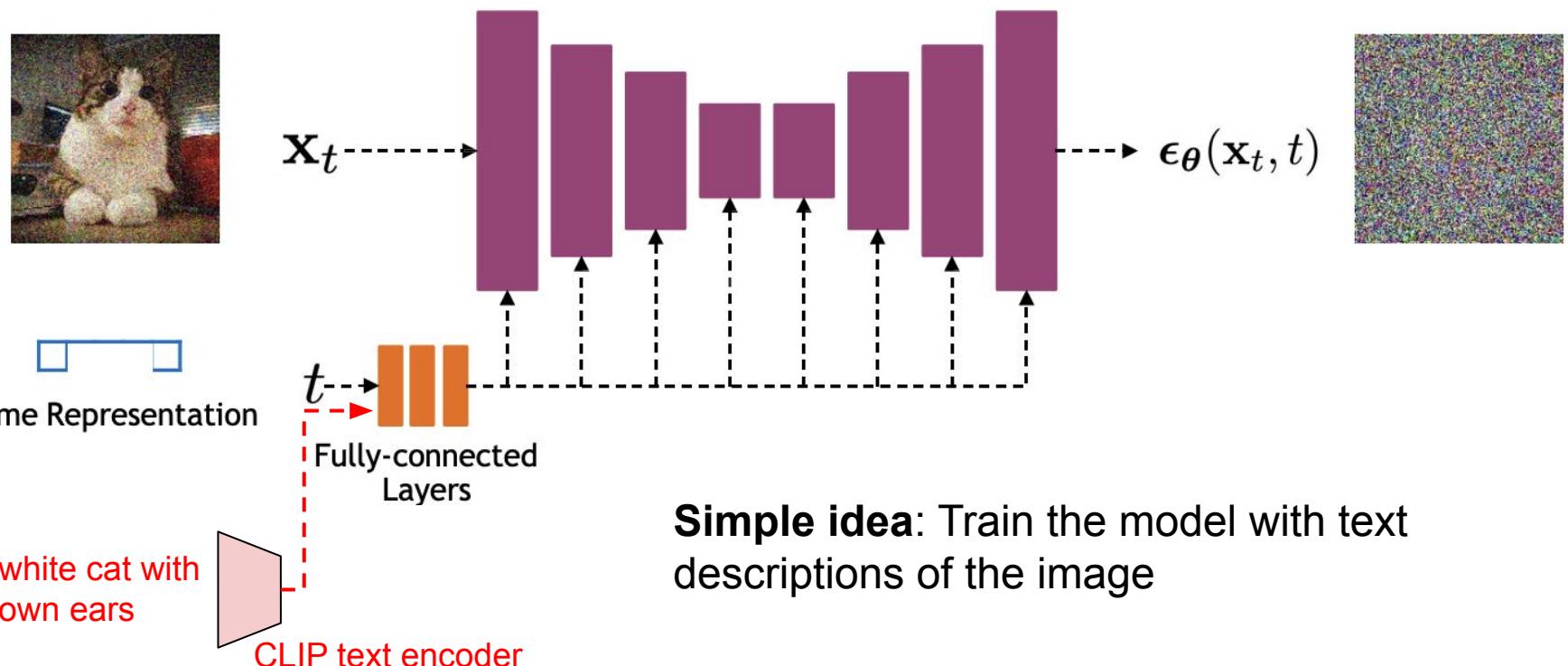
Time representation: sinusoidal positional embeddings.

Added in using: $\text{AdaGN}(h, y) = y_s \text{ GroupNorm}(h) + y_b$

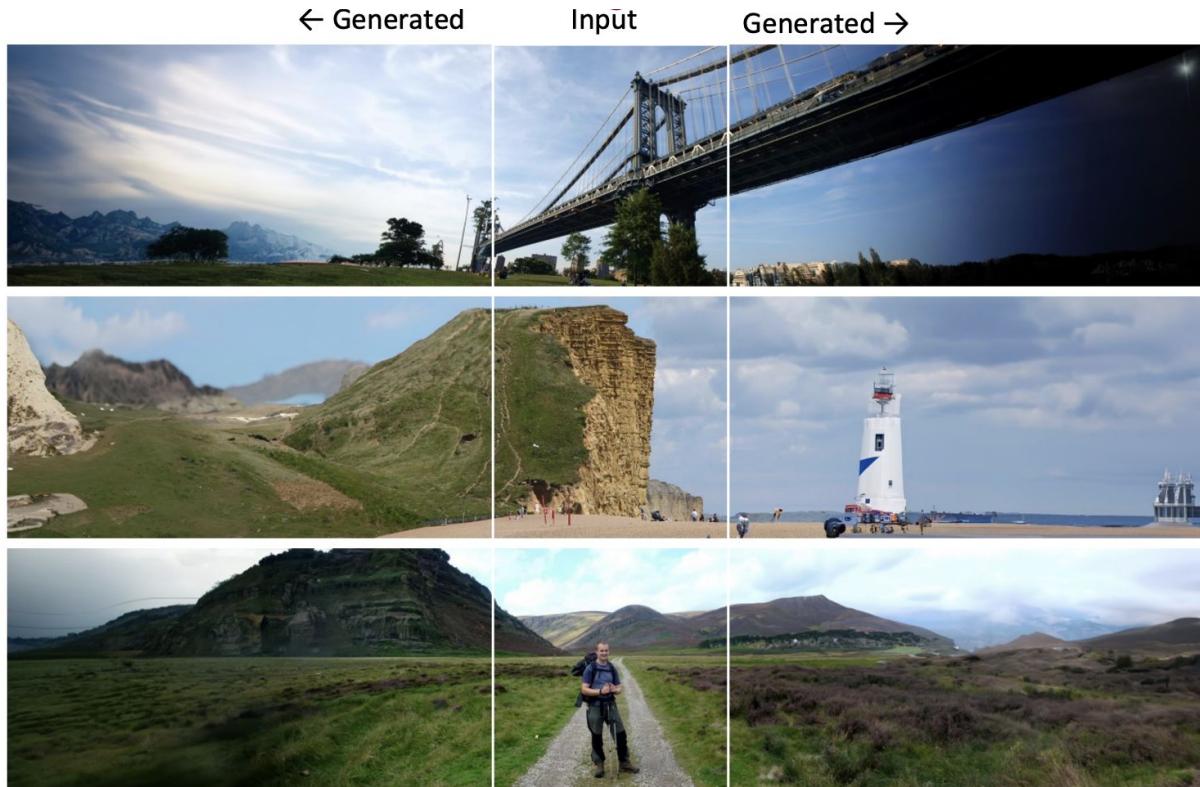
- h is the intermediate activations of the residual block following the first convolution in each layer,
- $y = [y_s, y_b]$ is obtained from a linear projection of the timestep



Text-conditioned generation



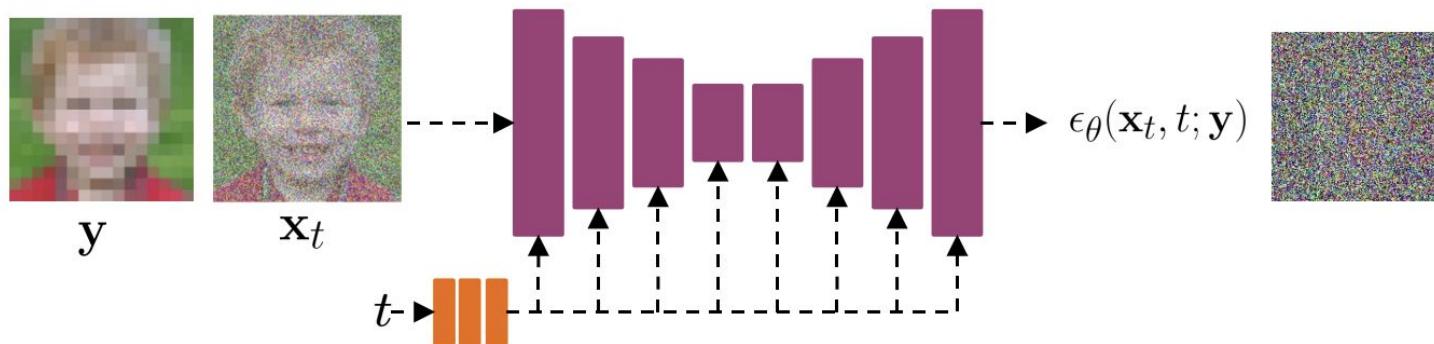
Application: panorama generation



Application: super-resolution

Learn a superresolution diffusion model conditioned on a low resolution image.
 y is a low resolution input image, x is a high resolution output image

$$\mathbb{E}_{\mathbf{x}, \mathbf{y}} \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \mathbb{E}_t \|\epsilon_\theta(\mathbf{x}_t, t; \mathbf{y}) - \epsilon\|_p^p$$



Saharia et al., Image Super-Resolution via Iterative Refinement, 2021

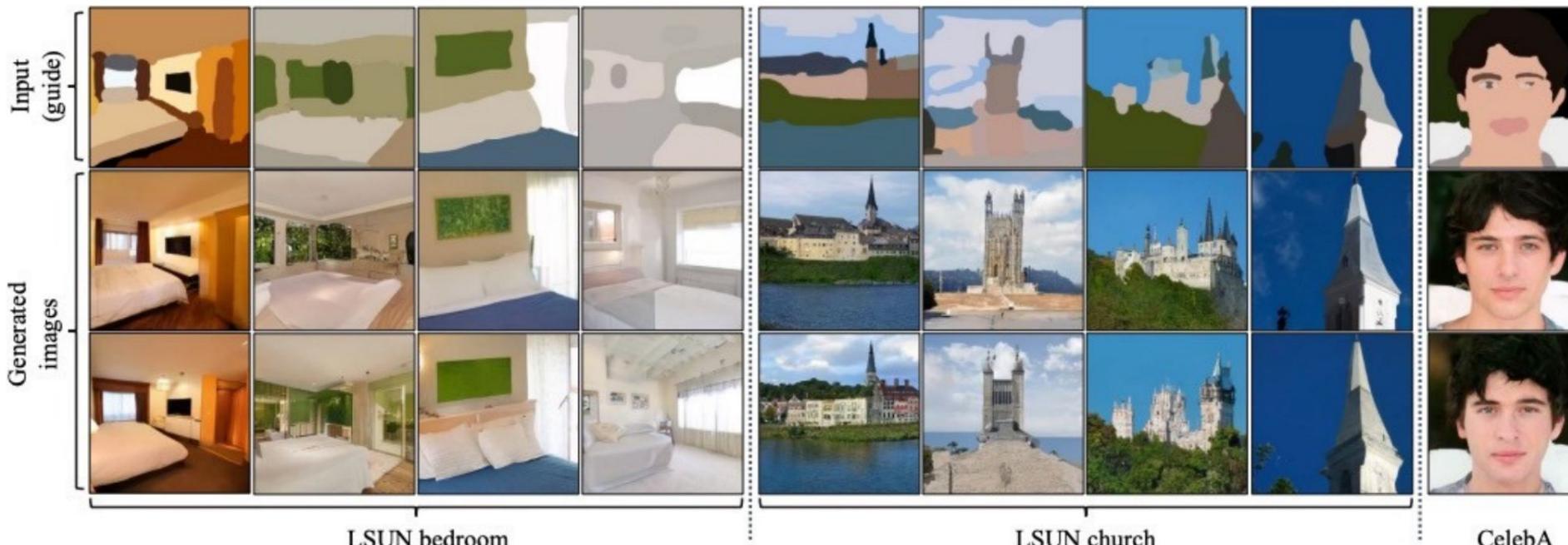
Application: super resolution

Natural Image Super-Resolution $64 \times 64 \rightarrow 256 \times 256$



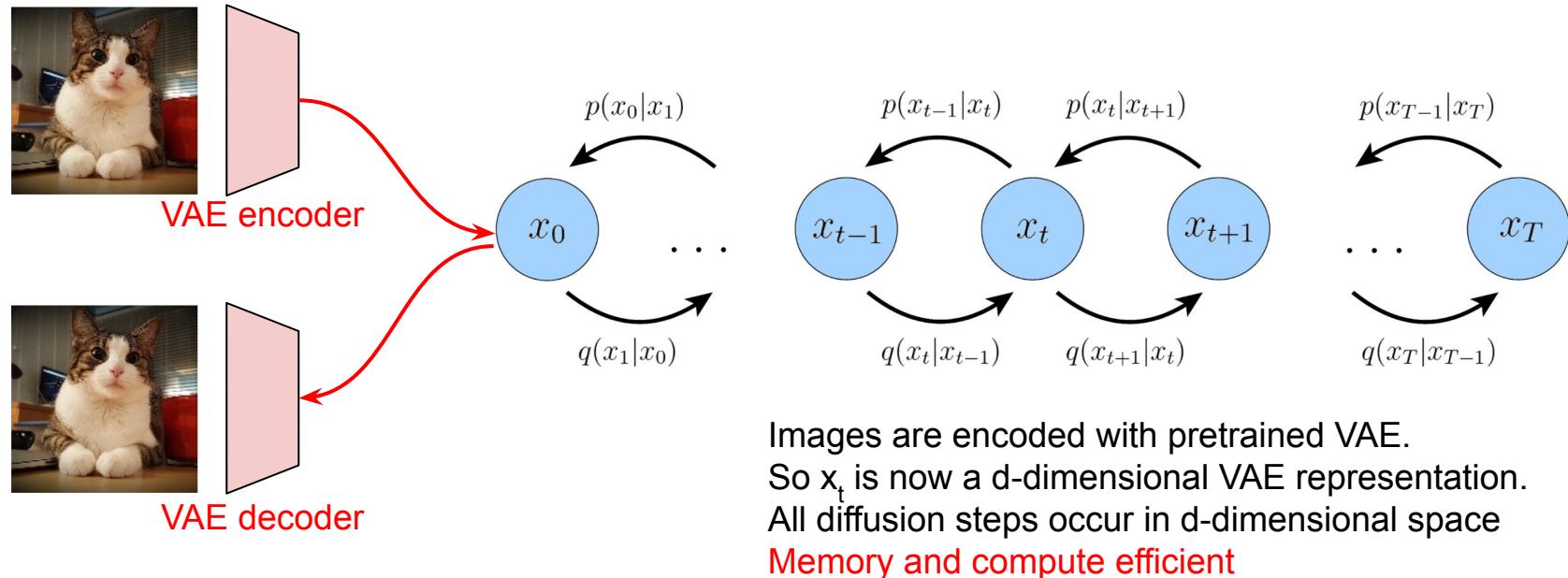
Saharia et al., Image Super-Resolution via Iterative Refinement, 2021

Application: image editing



Meng et al., SDEdit: Guided Image Synthesis and Editing with Stochastic Differential Equations, ICLR 2022

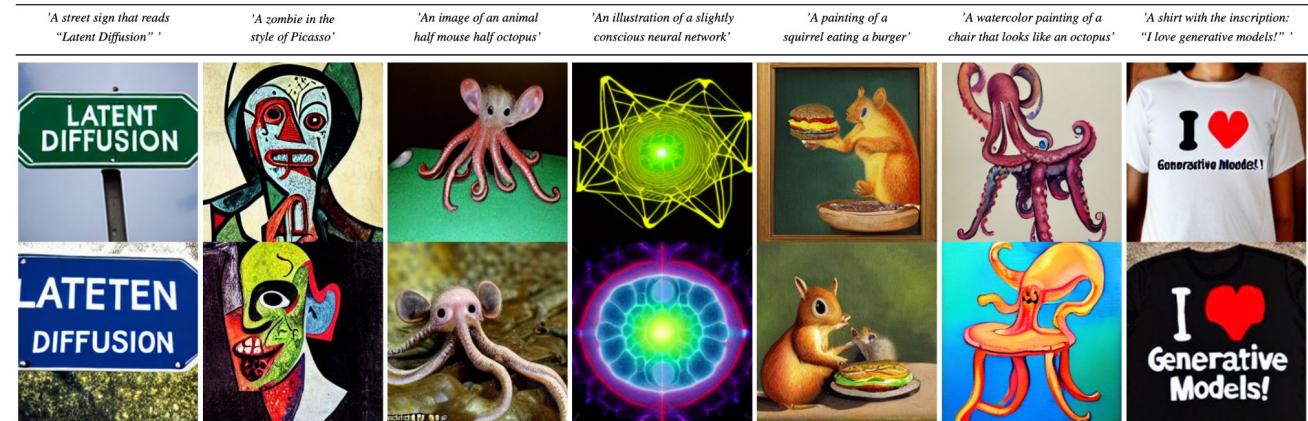
Latent diffusion models: perform diffusion over latent VAE encodings



Rombach et al. High-Resolution Image Synthesis with Latent Diffusion Models ArXiv 2022

Stable diffusion - from Stability AI

- Open sourced diffusion model - main model used for research
- Produces 512x512 images
- UNet with 860M params
- ViT-L text encoder with 123M params
- Fits in 10GB VRAM - fits on most GPUs



Rombach et al. High-Resolution Image Synthesis with Latent Diffusion Models ArXiv 2022

Imagen - Google

Combines:

- Latent diffusion model
- text conditioning
- 2 super-resolution models

To produce high quality 1024x1024 images

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

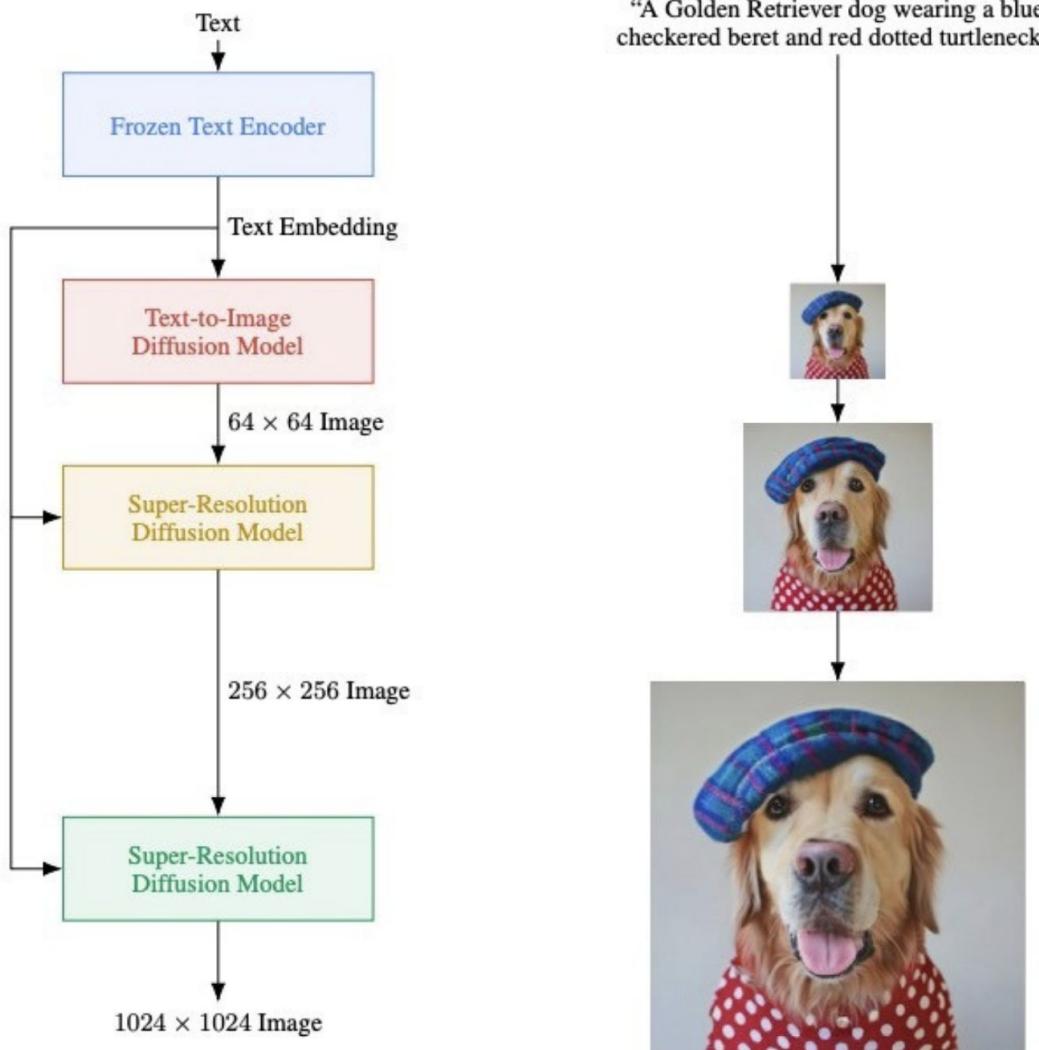


Imagen examples



A dragon fruit wearing karate belt in the snow.



A relaxed garlic with a blindfold reading a newspaper while floating in a pool of tomato soup.



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

Last week: Sora video diffusion model

<https://openai.com/sora>

How did they do it?

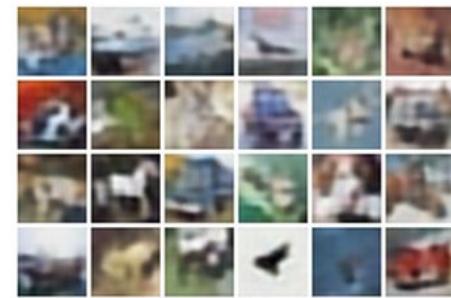
- More data (unknown data source)
- Replaced U-Net architecture with transformers

Comparing the different generative models

Q. Which ones are VAEs good at?

	Autoregressive (VAEs)	GANs	Diffusion
Mode coverage / diversity of generations			
Fast sampling			
High quality samples			

Comparing the different generative



VAEs are bad at generating high quality samples

	Autoregressive (VAEs)	GANs	Diffusion
Mode coverage / diversity of generations	✓		
Fast sampling	✓		
High quality samples	✗		

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Q. Which ones are GANs good at?

	Autoregressive (VAEs)	GANs	Diffusion
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Comparing the different generative models

GANs suffer from mode collapse

	Autoregressive (VAEs)	GANs	Diffusion
Mode coverage / diversity of generations	✓	✗	
Fast sampling	✓	✓	
High quality samples	✗	✓	

Comparing the different generative models

Q. Which ones are Diffusion models good at?

	Autoregressive (VAEs)	GANs	Diffusion
Mode coverage / diversity of generations	✓	✗	
Fast sampling	✓	✓	
High quality samples	✗	✓	

Comparing the different generative models

Diffusion models are bad at sampling fast.

	Autoregressive (VAEs)	GANs	Diffusion
Mode coverage / diversity of generations	✓	✗	✓
Fast sampling	✓	✓	✗
High quality samples	✗	✓	✓

Next: Deep Reinforcement Learning