Lecture 15: Generative Models

Administrative

- A3 is out. Due May 23.
- Milestone was due May 19th
  - Read website page for milestone requirements.
  - Need to Finish data preprocessing and initial results by then.

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Supervised vs Unsupervised Learning

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Cat

Classification

Supervised vs Unsupervised Learning

Supervised Learning

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A cat sitting on a suitcase on the floor

Image captioning

Supervised vs Unsupervised Learning

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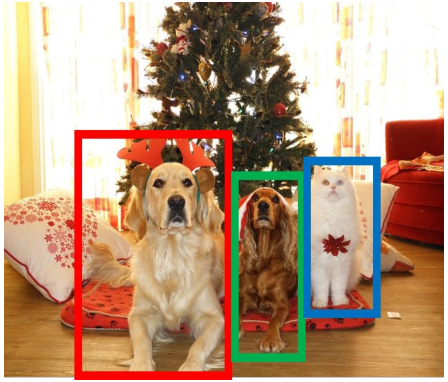

DOG, DOG, CAT

Object Detection

Supervised vs Unsupervised Learning

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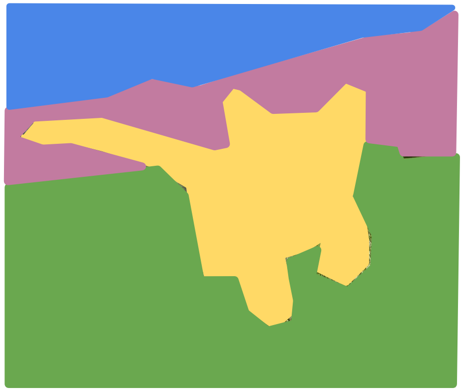
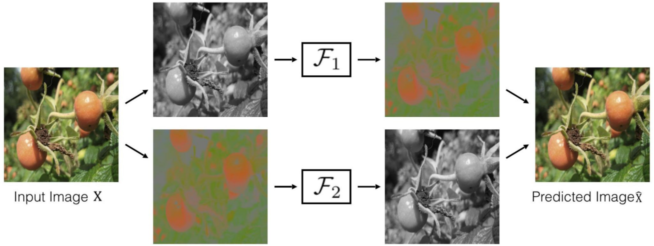


GRASS, CAT, TREE, SKY

Semantic Segmentation

Supervised vs Unsupervised Learning

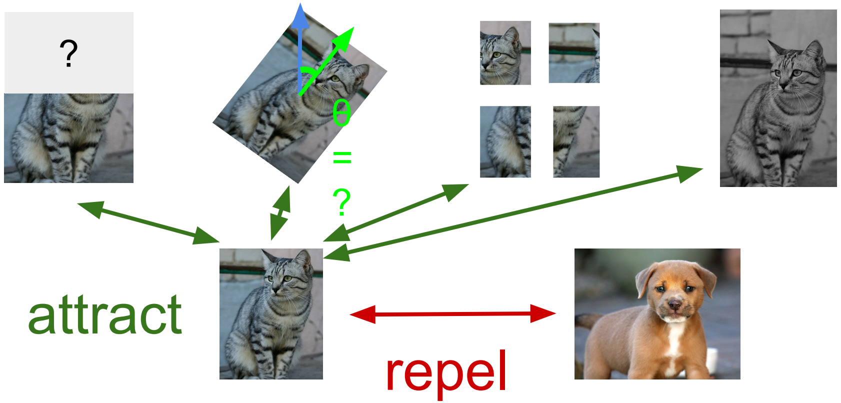
Self-Supervised Learning



Data: (x, y)
x is data, y is a proxy label

Goal: Learn a *function* to map x -> y

Examples: Inpainting, colorization, contrastive learning.



Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, **no labels!**

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
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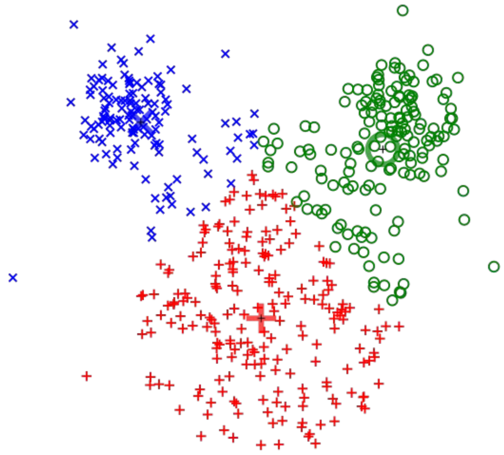
Examples: Clustering, dimensionality reduction, density estimation, etc.



K-means clustering

Supervised vs Unsupervised Learning

Unsupervised Learning

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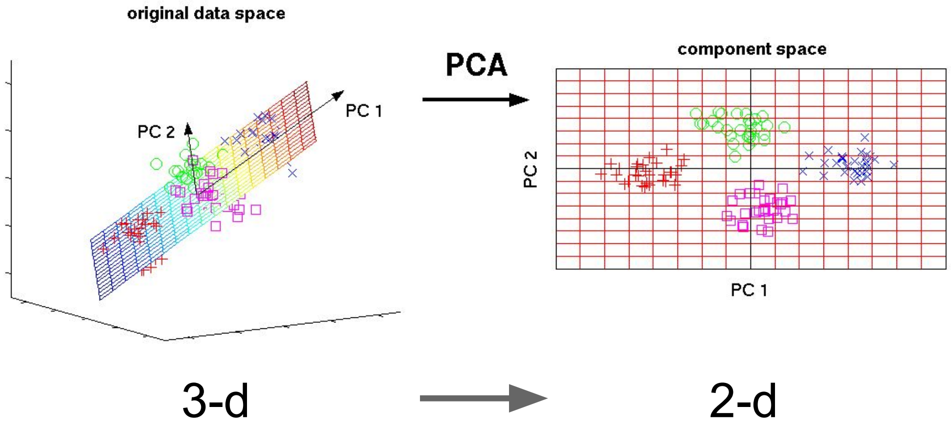
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.



Principal Component Analysis
(Dimensionality reduction)

Supervised vs Unsupervised Learning

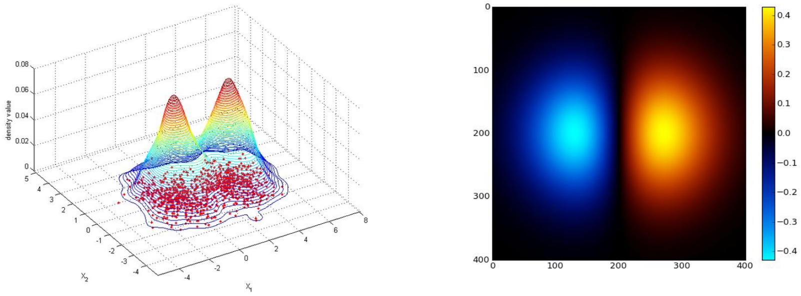
Unsupervised Learning

Data: x
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

1-d density estimation



2-d density estimation

Modeling p(x)

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Unsupervised Learning

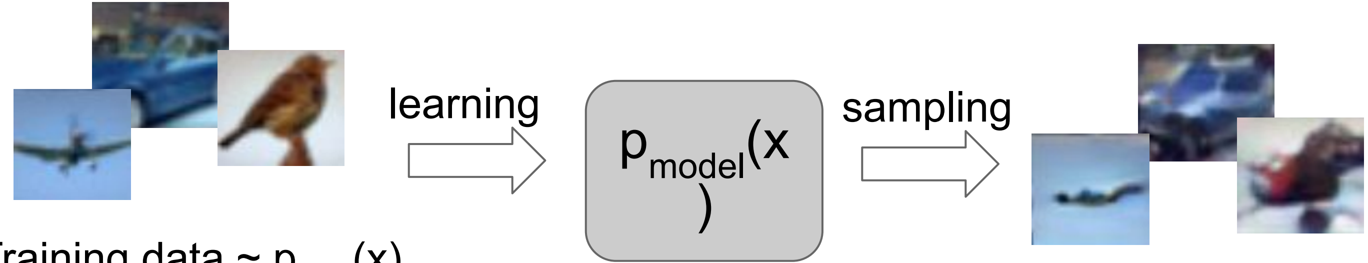
Data: x
Just data, no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, density estimation, etc.

Generative Modeling

Given training data, generate new samples from same distribution



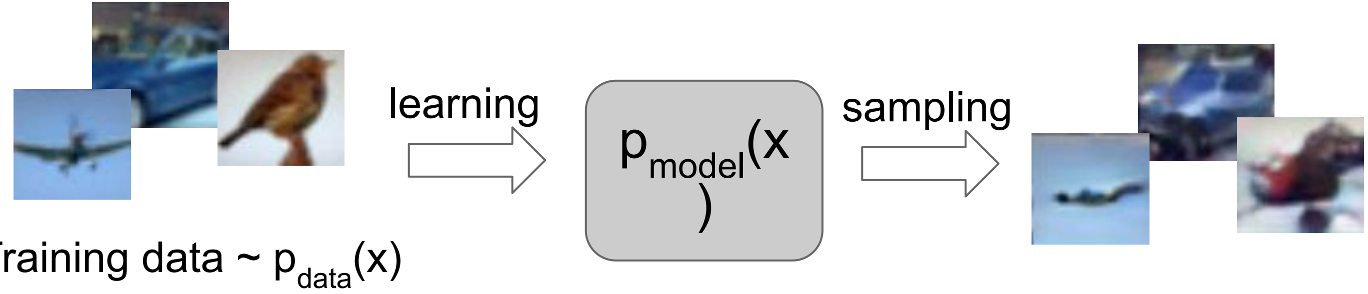
Training data ~ $p_{data}(x)$

Objectives:

1. Learn $p_{model}(x)$ that approximates $p_{data}(x)$
2. **Sampling new x from $p_{model}(x)$**

Generative Modeling

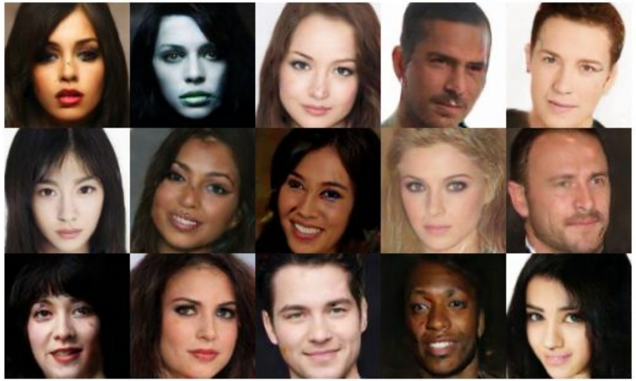
Given training data, generate new samples from same distribution



Formulate as density estimation problems:

- **Explicit density estimation**: explicitly define and solve for $p_{model}(x)$
- **Implicit density estimation**: learn model that can sample from $p_{model}(x)$ **without explicitly defining it.**

Why Generative Models?



- Realistic samples for artwork, super-resolution, colorization, etc.
- Learn useful features for downstream tasks such as classification.
- Getting insights from high-dimensional data (physics, medical imaging, etc.)
- Modeling physical world for simulation and planning (robotics and reinforcement learning applications)
- Many more ...

Taxonomy of Generative Models

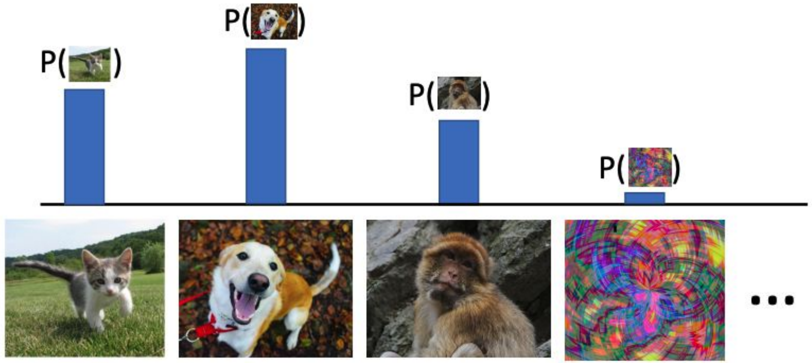
Generative models

Model can compute p(x)

Explicit density

Model does not compute p(x)
But can sample from p(x)

Implicit density



p(x) measures the likelihood of an image

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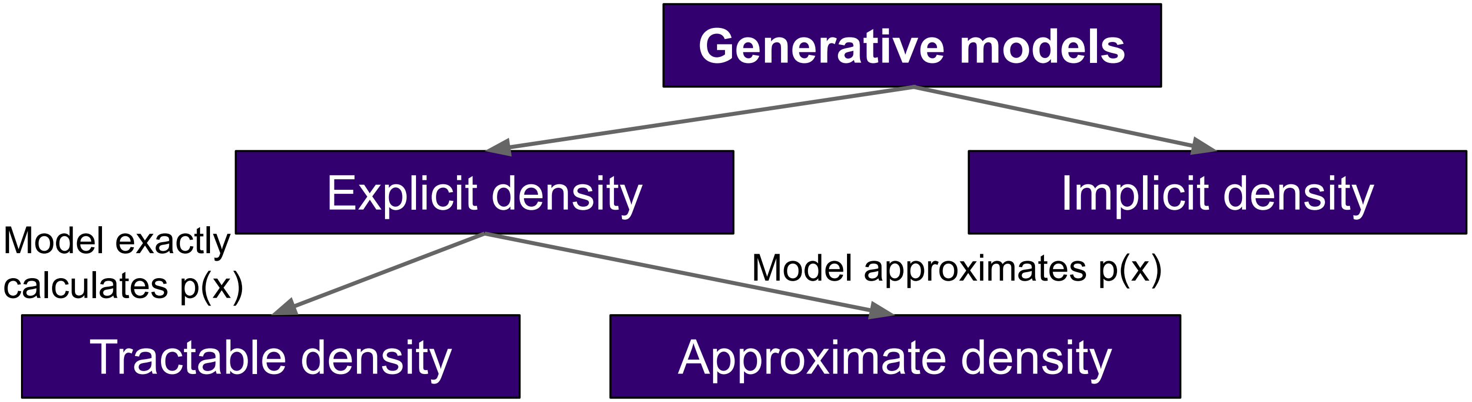
Taxonomy of Generative Models



Fully Visible Belief Nets
- Autoregressive
- NADE
- MADE
- NICE / RealNVP
- Glow
- Ffjord

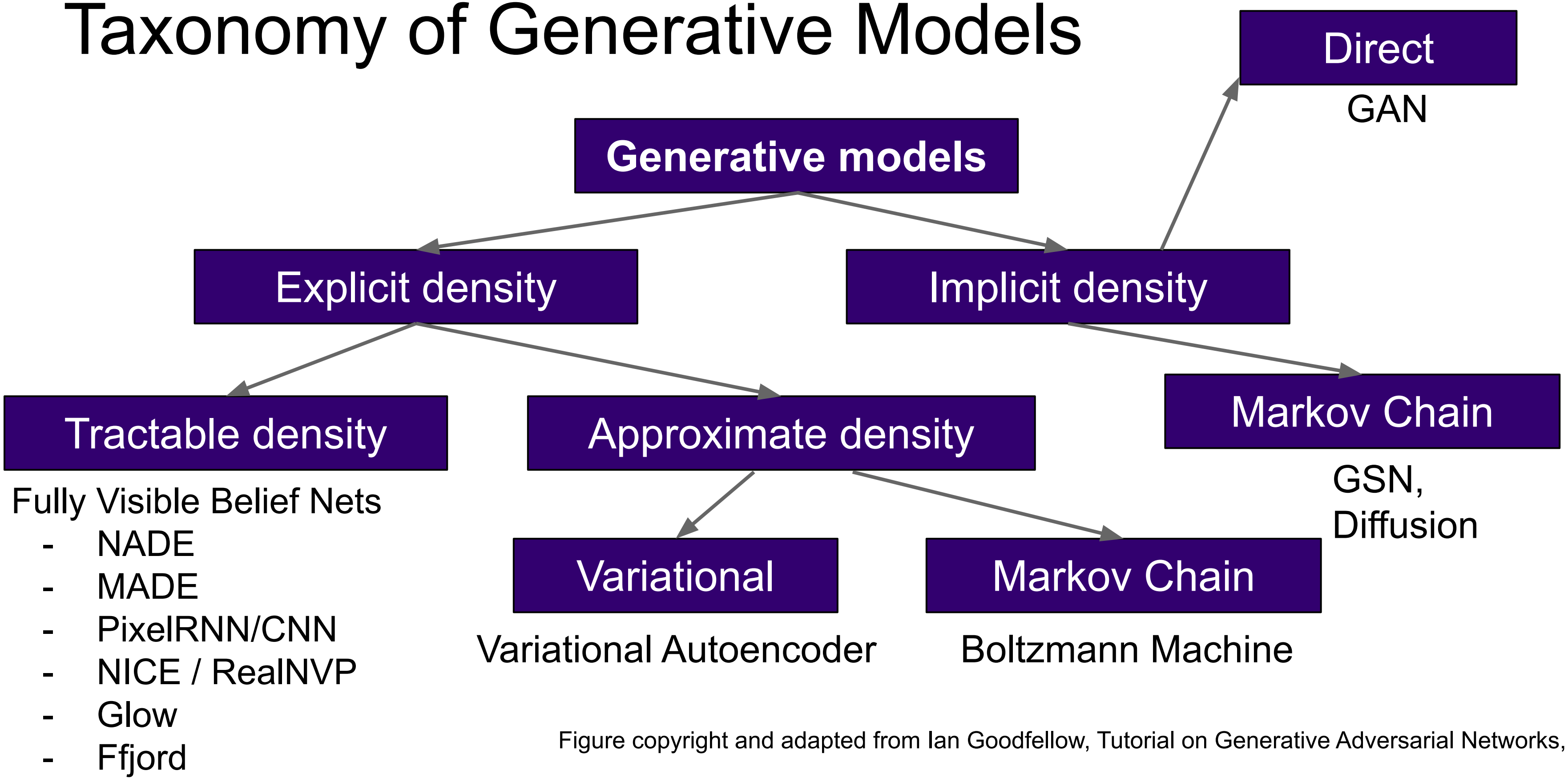
Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Taxonomy of Generative Models

- **Generative models**
  - Explicit density
    - Tractable density
      - Fully Visible Belief Nets
        - Autoregressive
        - NADE
        - MADE
        - NICE / RealNVP
        - Glow
        - Ffjord
    - Approximate density
      - Variational
        - Variational Autoencoder
      - Markov Chain
        - Boltzmann Machine
  - Implicit density

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

Taxonomy of Generative Models



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Taxonomy of Generative Models

Today: discuss 3 types of generative models today

- **Generative models**
  - Explicit density
    - Tractable density
      - Fully Visible Belief Nets
        - Autoregressive
        - NADE
        - MADE
        - NICE / RealNVP
        - Glow
        - Ffjord
    - Approximate density
      - Variational
        - Variational Autoencoder
      - Markov Chain
        - Boltzmann Machine
  - Implicit density
    - Direct
      - GAN
    - Markov Chain
      - GSN, Diffusion

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

Autorgressive models

(PixelRNN and PixelCNN)

Fully visible belief network (FVBN)

Explicit density model

$$p(x) = p(x_1, x_2, \ldots, x_n)$$

Likelihood of image x

Joint likelihood of each pixel in the image

Fully visible belief network (FVBN)

Explicit density model

Remember the probability chain rule:

$$p(x) = p(x_n | x_1, x_2, \ldots, x_{n-1}) p(x_1, x_2, \ldots, x_{n-1})$$

Fully visible belief network (FVBN)

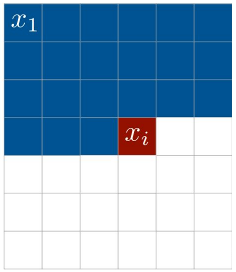
Explicit density model

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

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

Likelihood of image x

Probability of i'th pixel value given all previous pixels



Then maximize likelihood of training data

Fully visible belief network (FVBN)

Explicit density model

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

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Likelihood of image x

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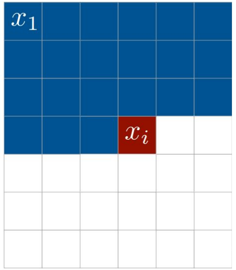
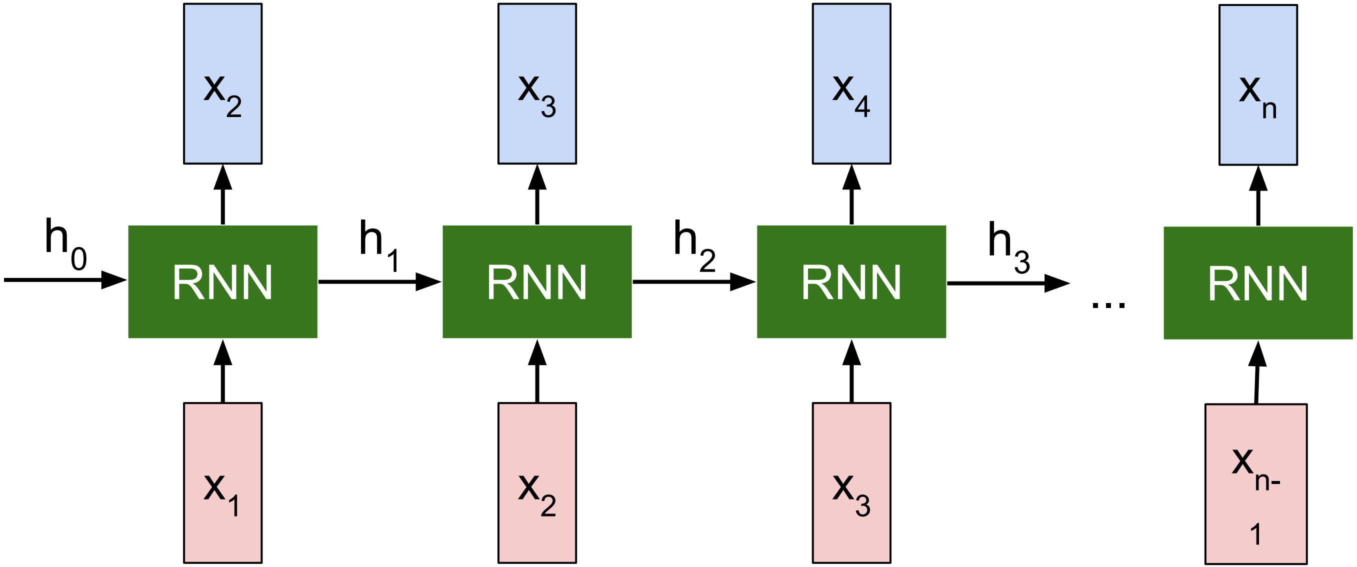


Complex distribution over pixel values => Express using a neural network!

Then maximize likelihood of training data

Recurrent Neural Network

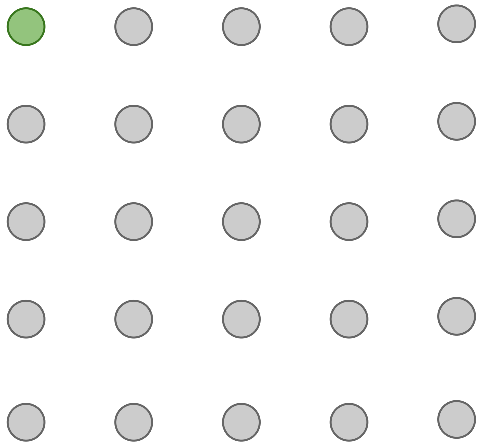


$$p(x_i|x_1, ..., x_{i-1})$$

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

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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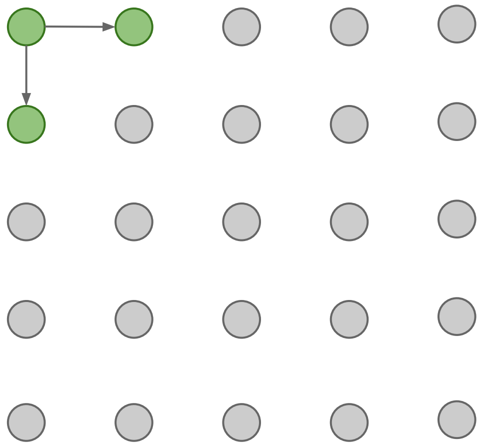

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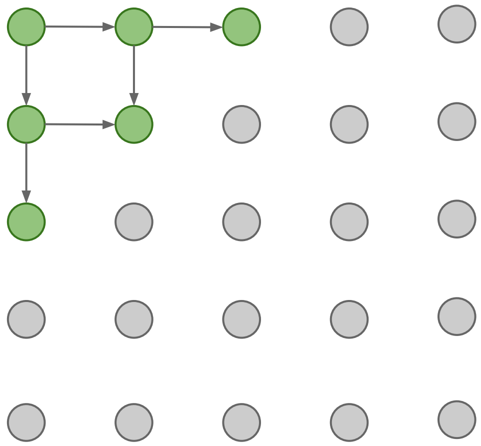

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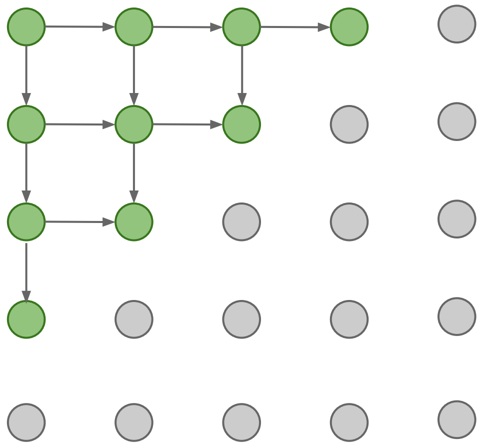
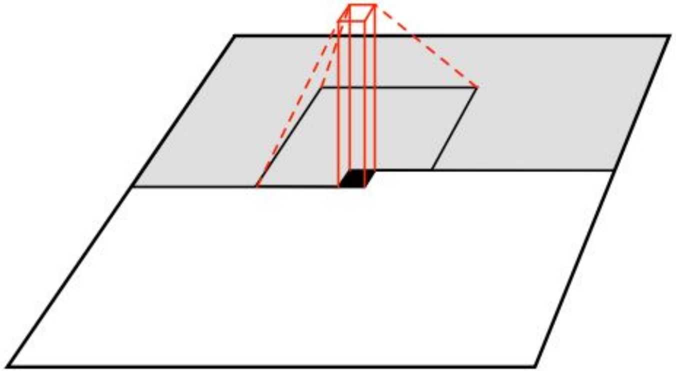


Drawback: sequential generation is slow in both training and inference!

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

Still generate image pixels starting from corner

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



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

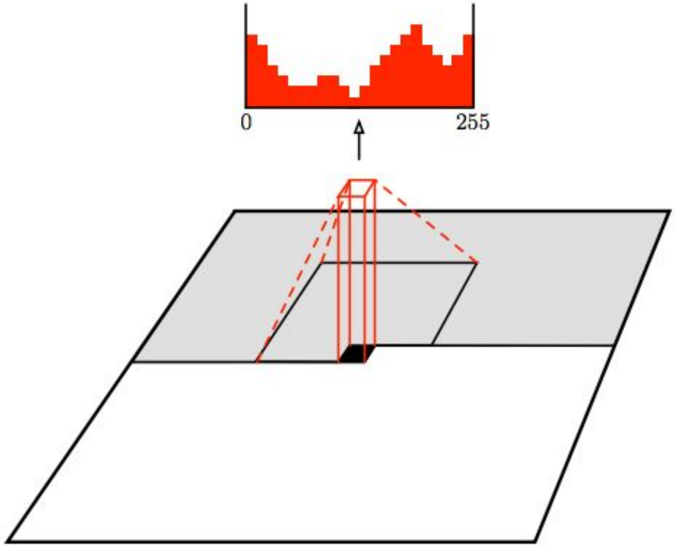
Still generate image pixels starting from corner

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

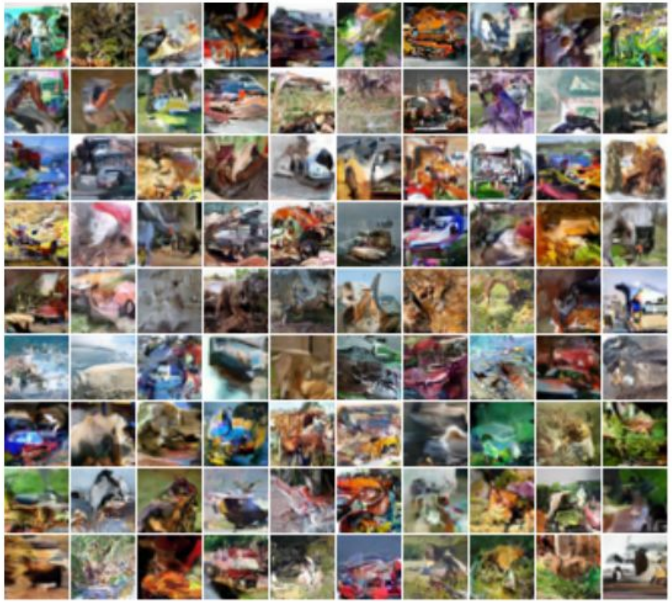
Training is faster than PixelRNN
(can parallelize convolutions since context region values known from training images)

Generation is still slow:
For a 32x32 image, we need to do forward passes of the network 1024 times for a single image

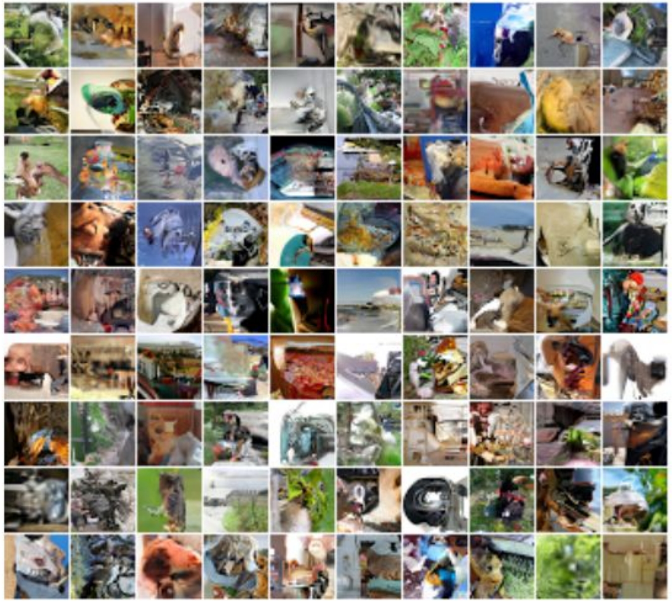
Softmax loss over pixel values at every location



Generation Samples



32x32 CIFAR-10



32x32 ImageNet

PixelRNN and PixelCNN

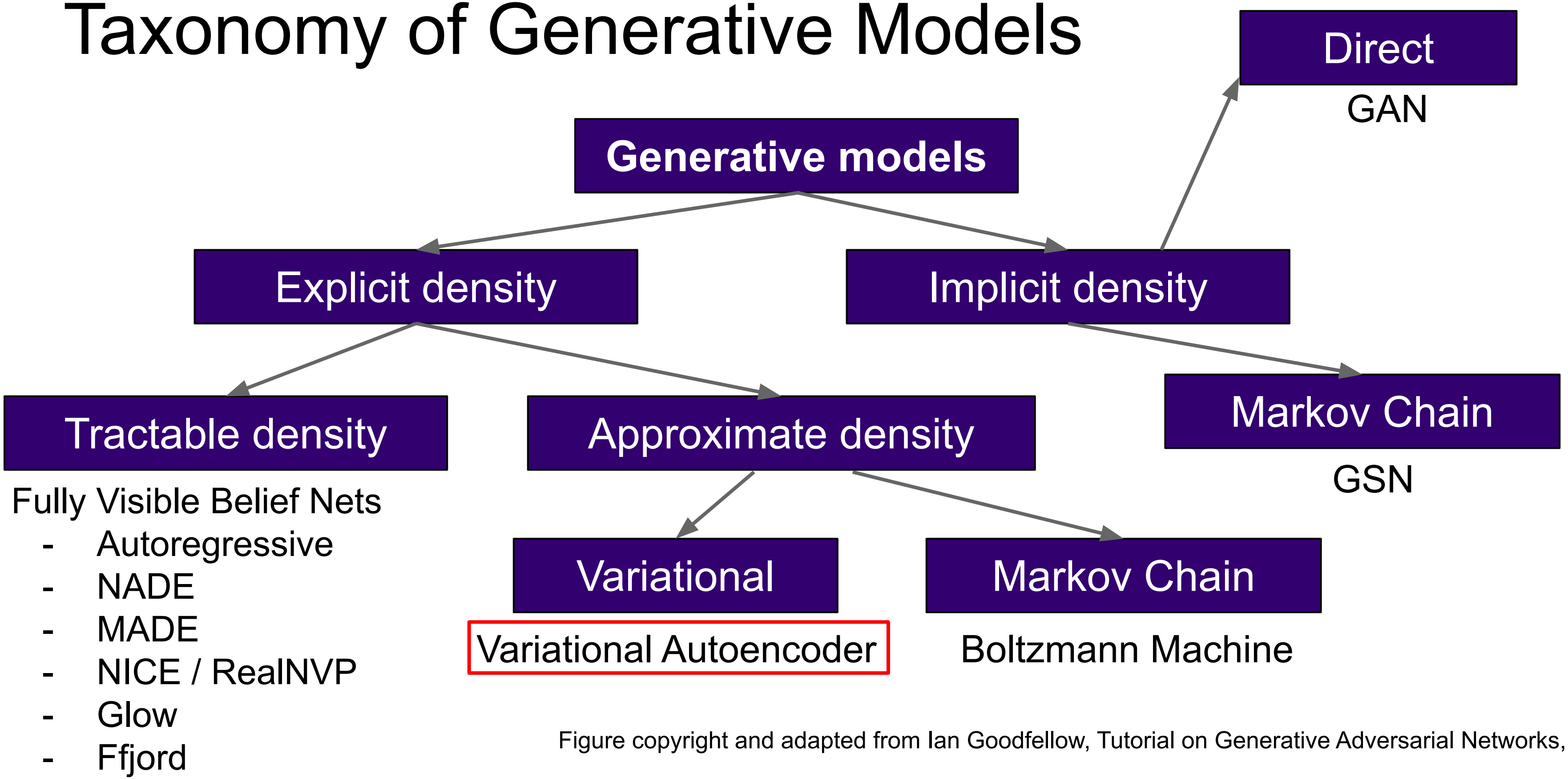
Pros:
- Can explicitly compute likelihood p(x)
- Easy to optimize
- Good samples

Con:
- Sequential generation => slow

Improving PixelCNN performance
- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See
- Van der Oord et al. NIPS 2016
- Salimans et al. 2017 (PixelCNN++)

Taxonomy of Generative Models



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Variational Autoencoders (VAE)

So far...

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

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

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

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

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

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

So far...

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

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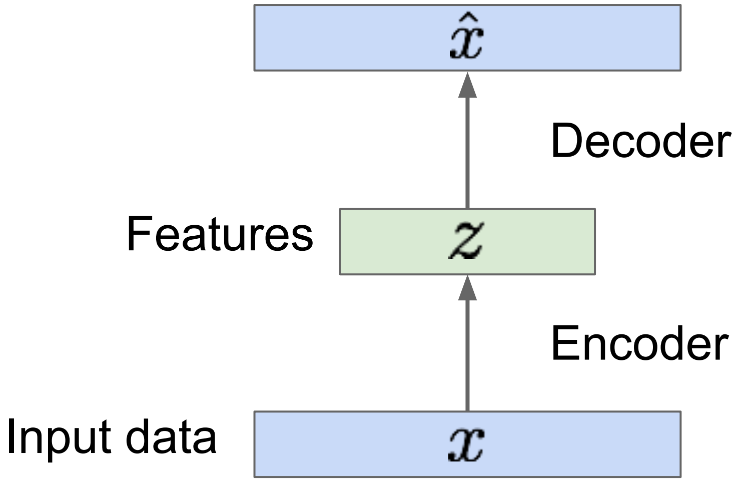
Why latent z?

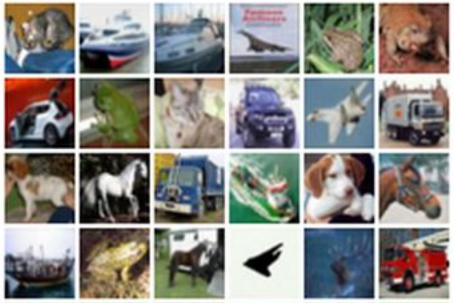
~~Variational~~ Autoencoders

Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data



Z should extract useful information (maybe object identities, properties, scene type, etc) that we can use for downstream tasks

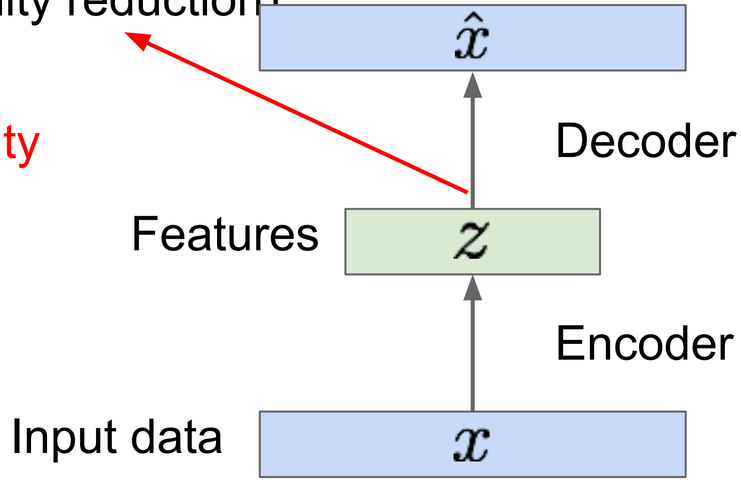


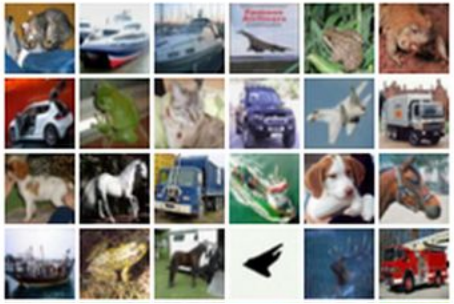
Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x**
(dimensionality reduction)

Q: Why dimensionality reduction?





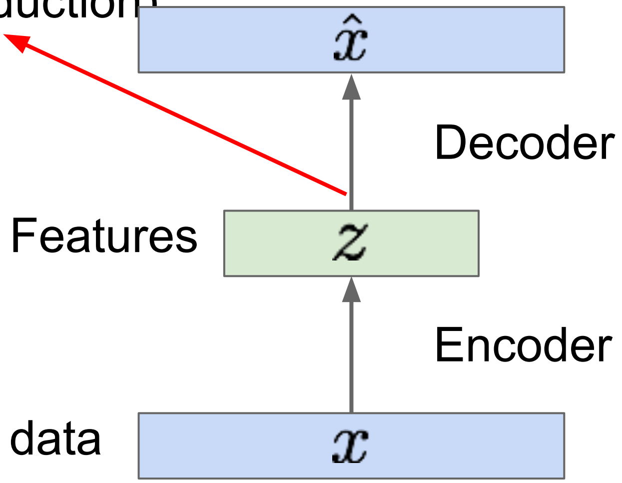
Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

z usually smaller than **x** (dimensionality reduction)

Q: Why dimensionality reduction?

A: Want features to capture meaningful factors of variation in data



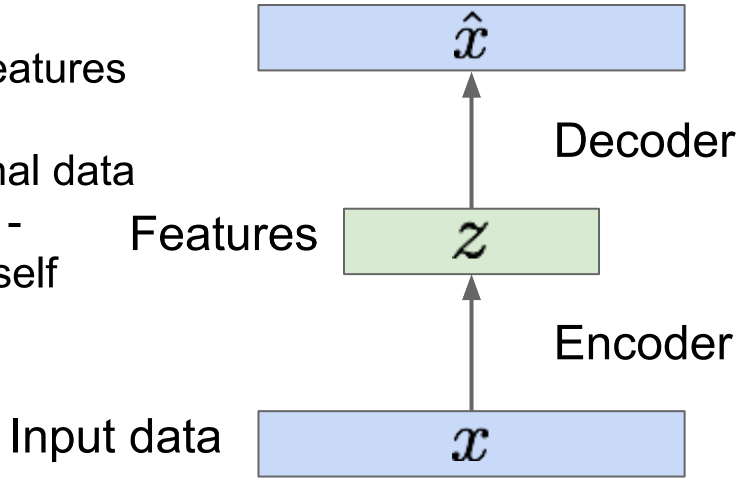
Some background first: Autoencoders

Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

How do we learn this z?

Train such that features can be used to reconstruct original data "**Autoencoding**" - encoding input itself

$$\|\hat{x} - x\|_2^2$$

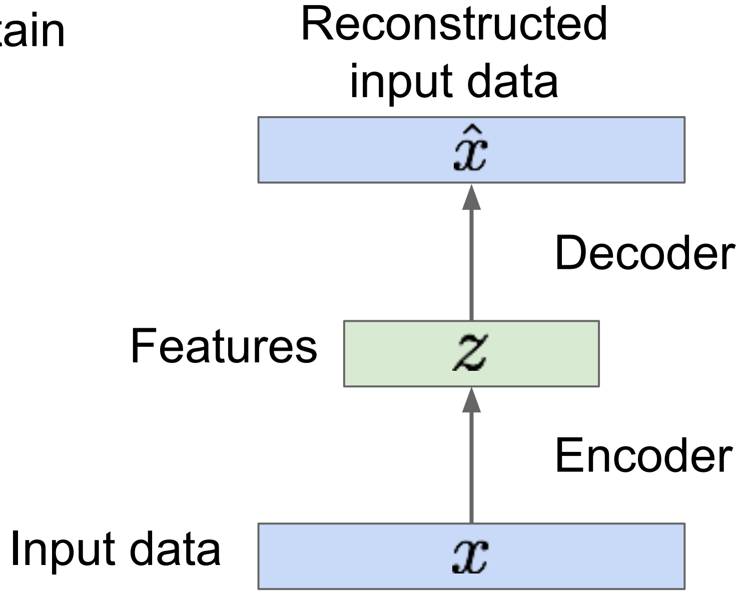


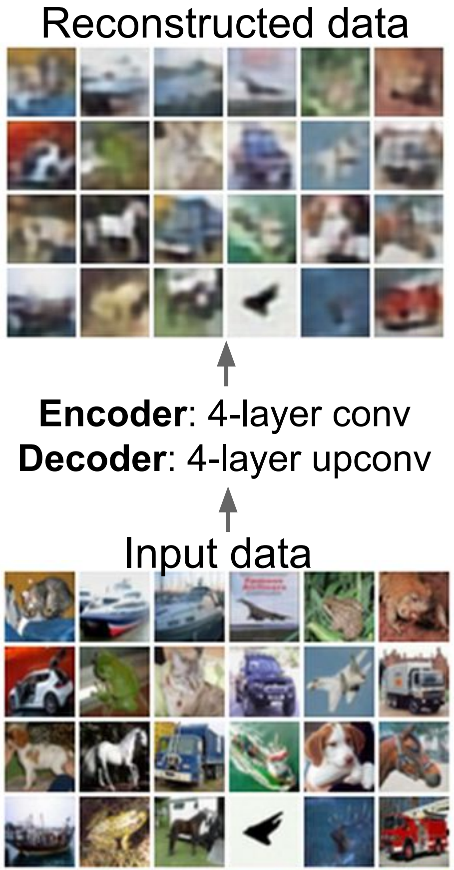
Learning objective: reconstruct the image and use l2 loss.

No labels are necessary!!

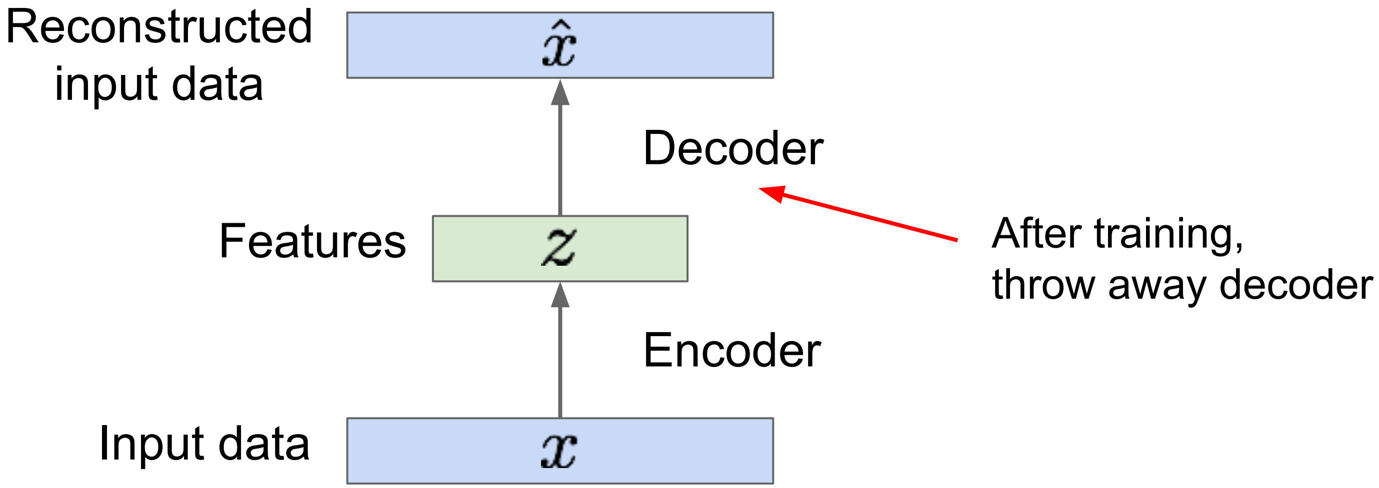
Some background first: Autoencoders

Images reconstructed are blurry because they don't contain pixel-perfect information





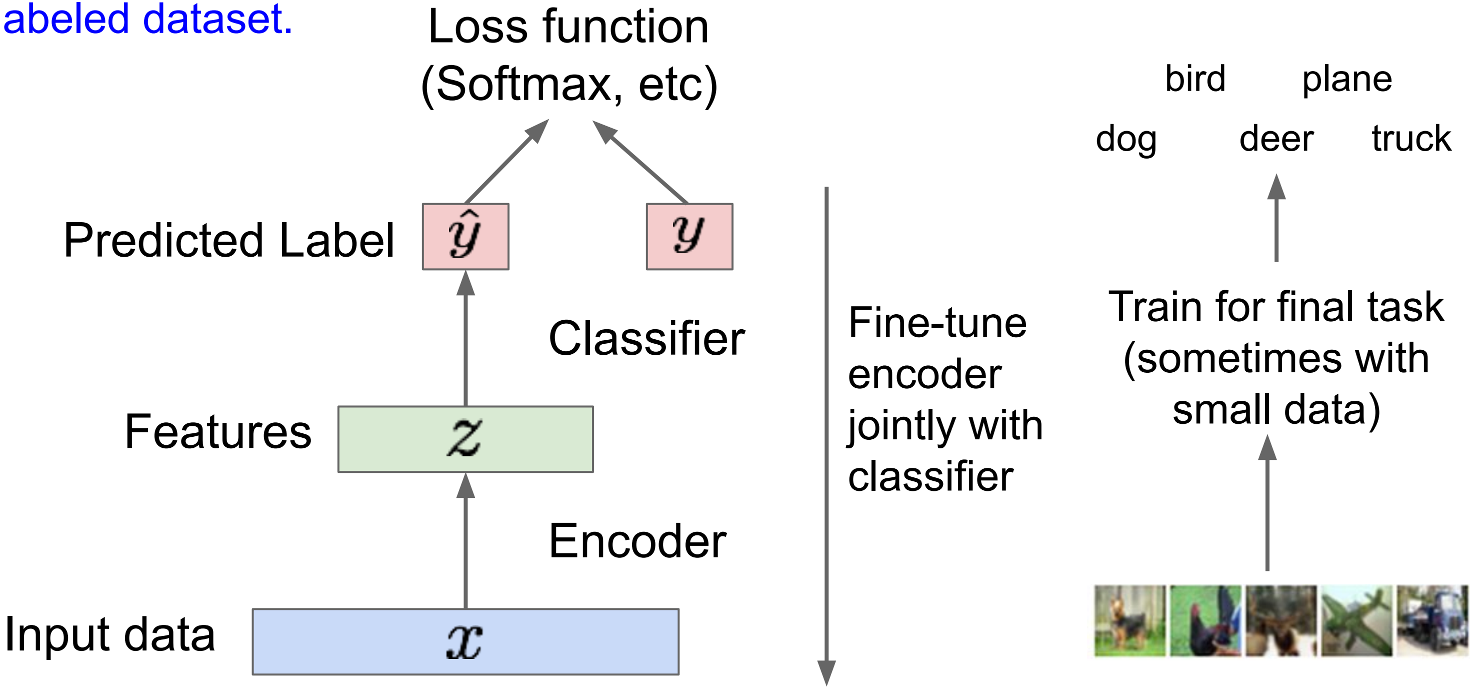
Some background first: Autoencoders



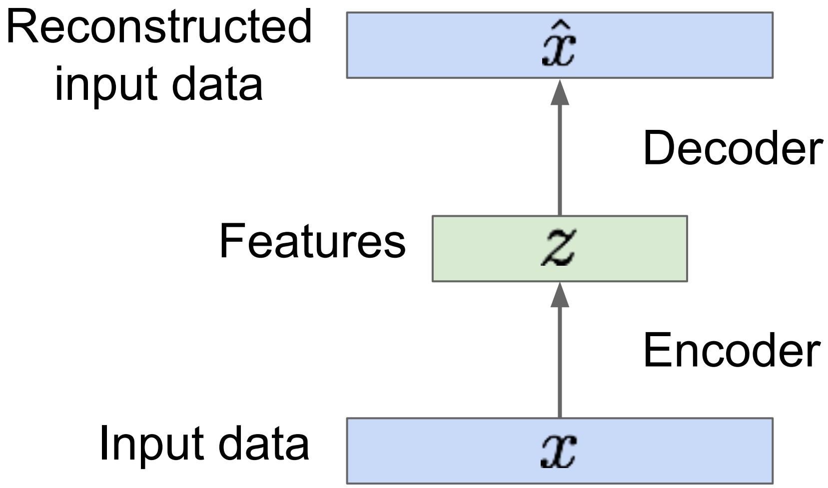
Some background first: Autoencoders

Transfer from large, unlabeled dataset to small, labeled dataset.

Encoder can be used to initialize a **supervised** model



Some background first: Autoencoders



Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

But we can't generate **new images** from an autoencoder because we don't know the space of z.

How do we make autoencoder a **generative model**?

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

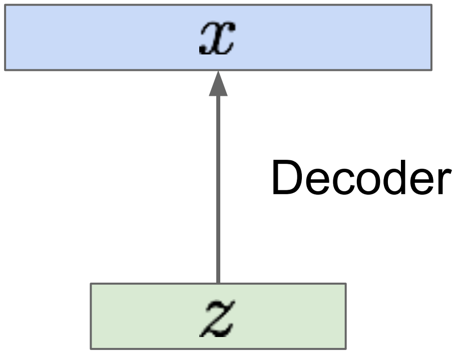
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

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

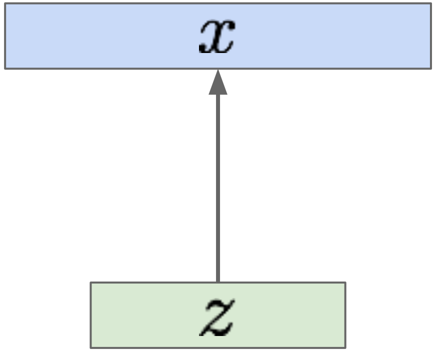
Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from the distribution of unobserved (latent) representation **z**

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

Sample from true conditional

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



Sample from true prior

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

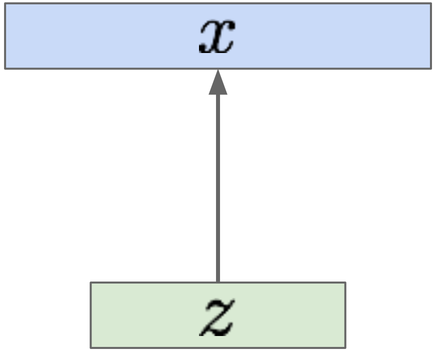
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

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

Sample from true conditional

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



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Variational Autoencoders

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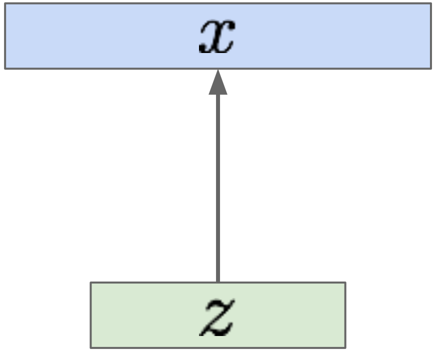
Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior $z^{(i)} \sim p_{\theta^*}(z)$



How should we represent this model?

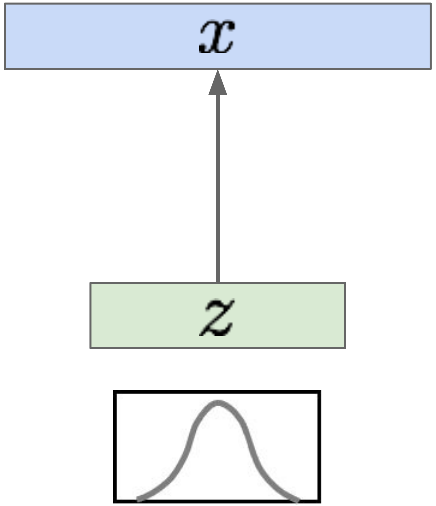
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

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

Sample from true conditional

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



Sample from true prior

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

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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

Variational Autoencoders

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

Sample from true conditional

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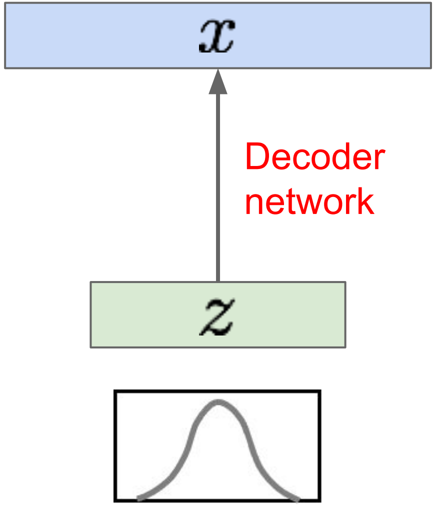


Sample from true prior

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

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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

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

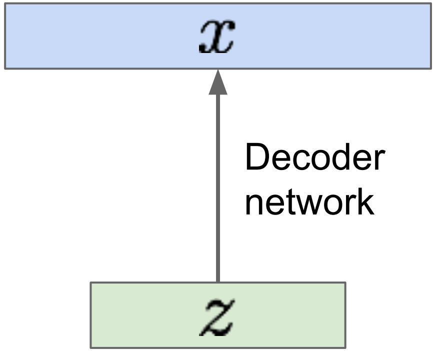
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

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



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How to train the model?

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

Variational Autoencoders

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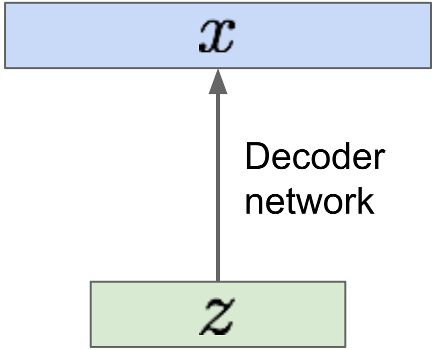

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$z^{(i)} \sim p_{\theta^*}(z)$

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How to train the model?

Learn model parameters to maximize likelihood of training data

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

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

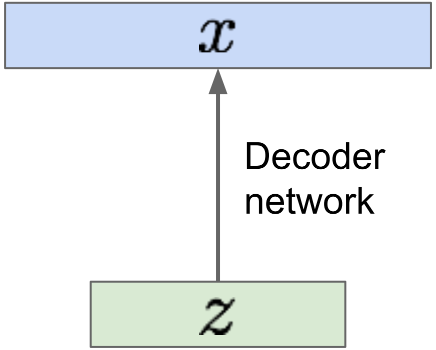
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

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



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Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

Intractable!

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

Variational Autoencoders: Intractability

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

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

Variational Autoencoders: Intractability

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

Simple Gaussian prior

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

Variational Autoencoders: Intractability

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

Decoder neural network

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

Variational Autoencoders: Intractability

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

Intractable to compute p(x|z) for every z!

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

Variational Autoencoders: Intractability

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

Intractable to compute p(x|z) for every z!

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

Monte Carlo estimation is too high variance

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

Variational Autoencoders: Intractability

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

Another idea: $p_\theta(x) = \dfrac{p_\theta(x \mid z) p_\theta(z)}{p_\theta(z \mid x)}$ Use Bayes rule

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

Variational Autoencoders: Intractability

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

Another idea: $p_\theta(x) = \frac{\boxed{p_\theta(x \mid z)p_\theta(z)}}{p_\theta(z \mid x)}$ We know how to calculate these

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

Variational Autoencoders: Intractability

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

Another idea: $p_\theta(x) = \dfrac{p_\theta(x \mid z)p_\theta(z)}{\boxed{p_\theta(z \mid x)}}$

But how do you calculate this?

Solution: In addition to modeling $p_\theta(x|z)$, learn $q_\phi(z|x)$ that approximates the true posterior $p_\theta(z|x)$.

Will see that the approximate posterior allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize.

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

Variational Autoencoders

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

Variational Autoencoders

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Taking expectation wrt. z
(using encoder network) will
come in handy later

Variational Autoencoders

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

Variational Autoencoders

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Variational Autoencoders

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

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The expectation wrt. z (using encoder network) let us write nice KL terms

Variational Autoencoders

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

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

Variational Autoencoders

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

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We want to maximize the data likelihood

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

Variational Autoencoders

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Decoder:
reconstruct
the input data

Encoder:
make approximate
posterior distribution
close to prior

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

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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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

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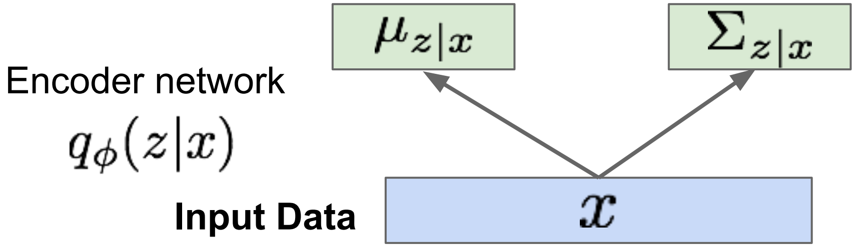


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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

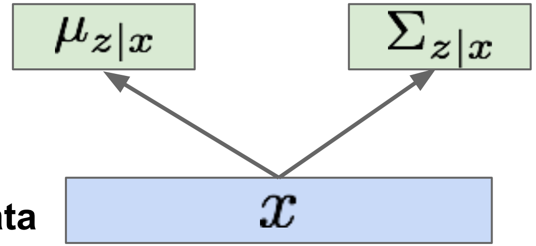
Have analytical solution

Make approximate posterior distribution close to prior

Encoder network

$q_\phi(z|x)$

Input Data



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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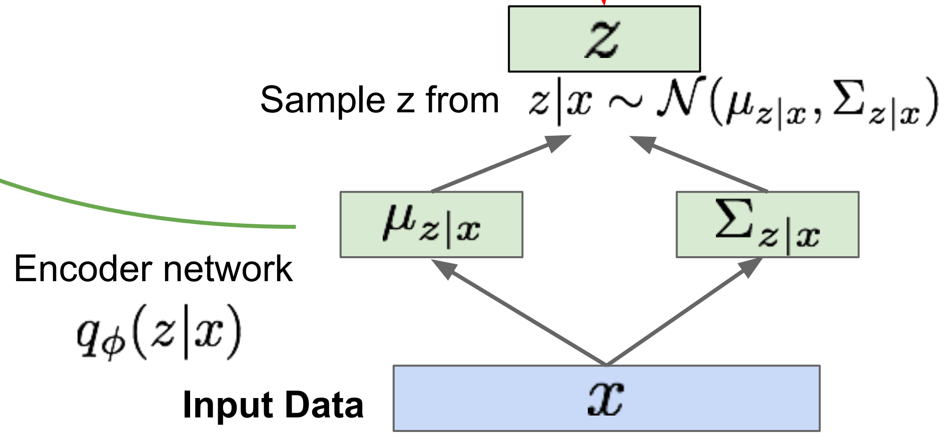
Not part of the computation graph!

Make approximate posterior distribution close to prior



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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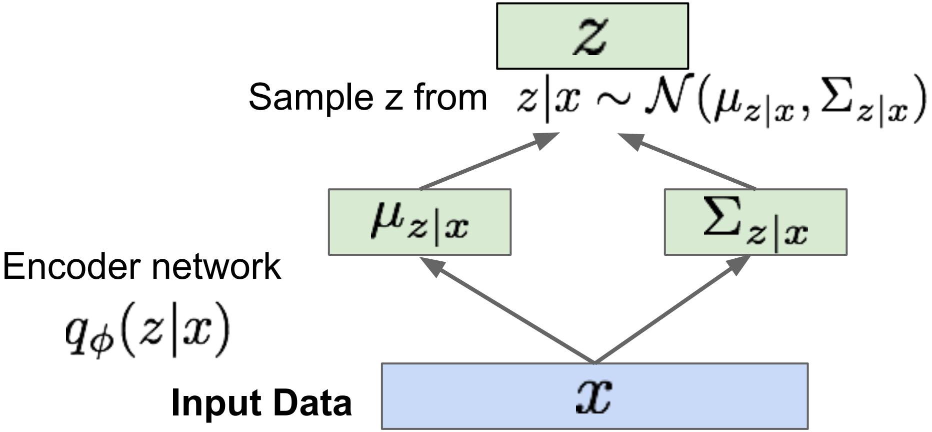
Reparameterization trick to make sampling differentiable:

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

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



Variational Autoencoders

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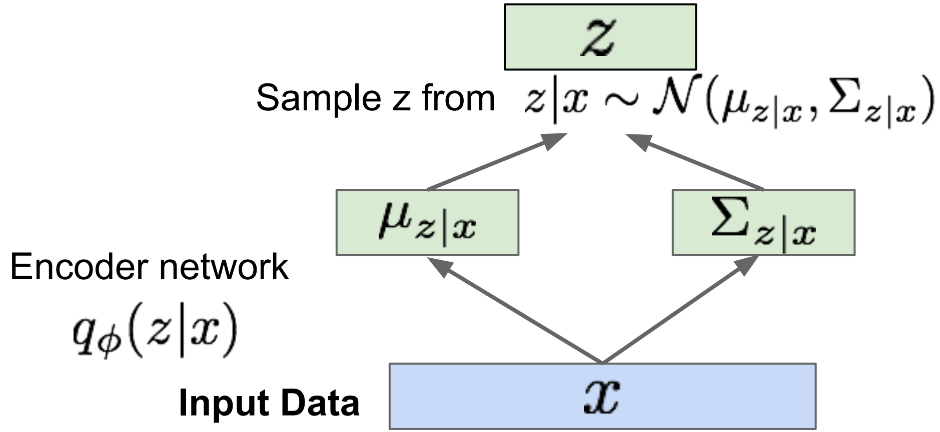
Sample $\epsilon \sim \mathcal{N}(0, I)$

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

Input to the graph

Part of computation graph



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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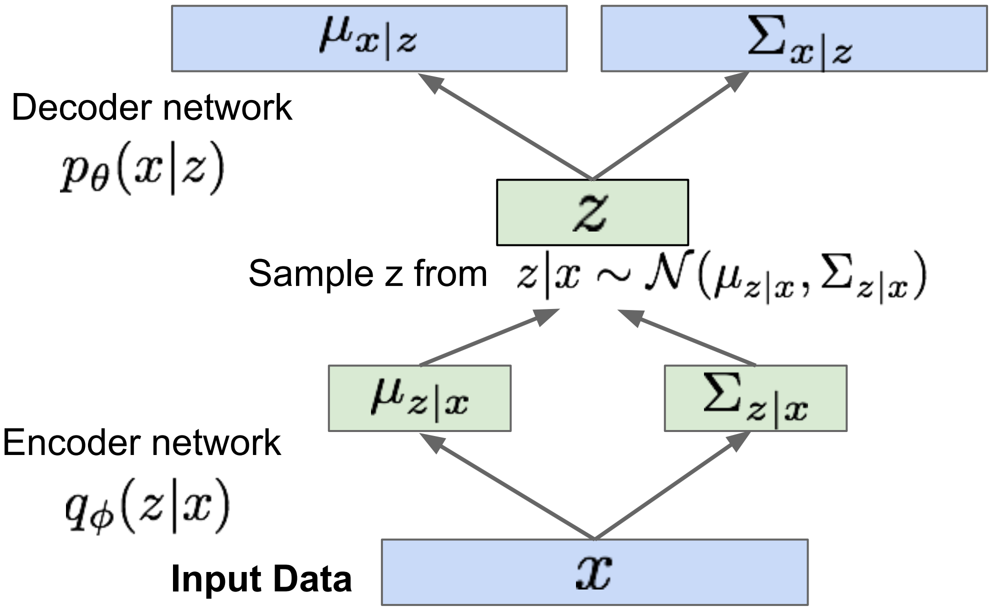
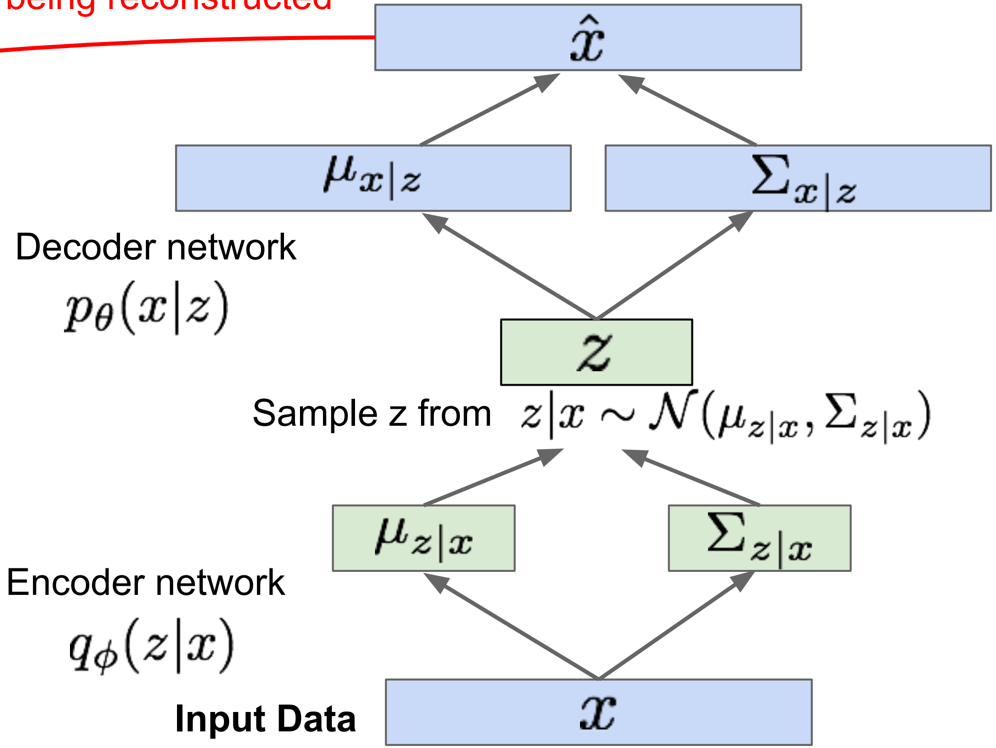


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

Maximize likelihood of original input being reconstructed

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

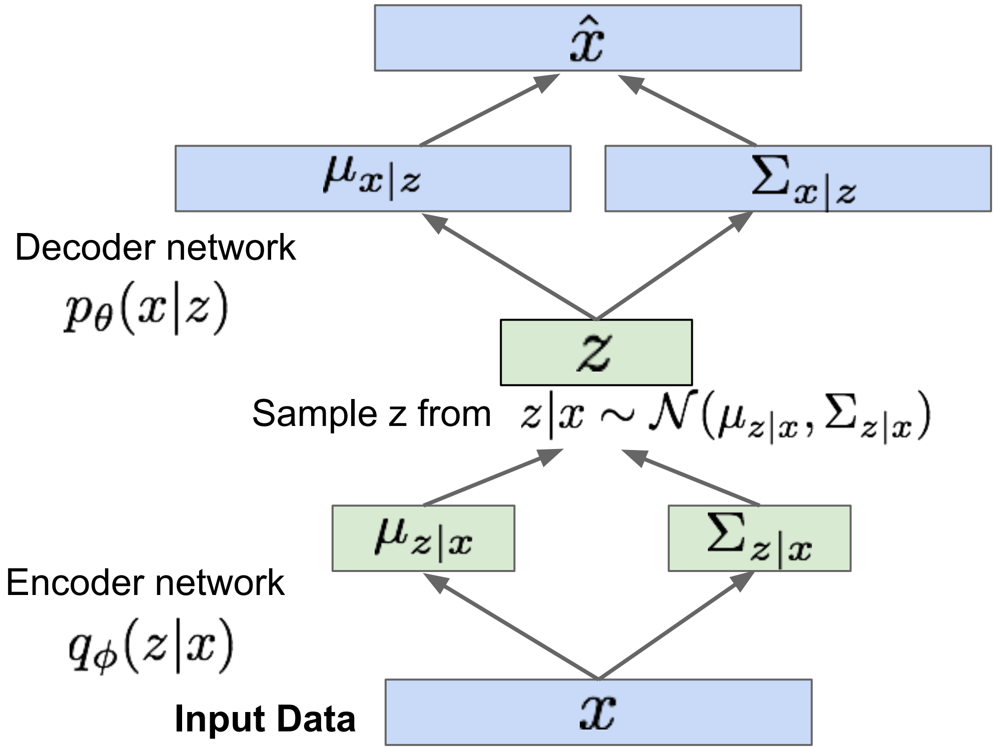


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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



Variational Autoencoders: Generating Data!

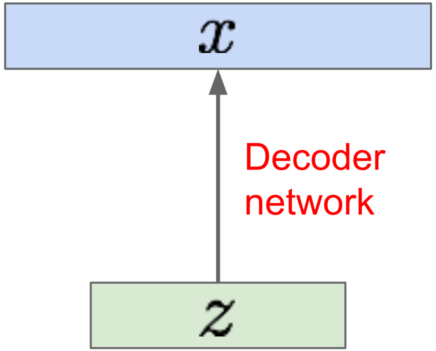
Our assumption about data generation process

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

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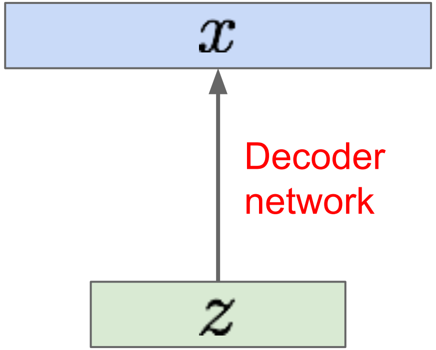
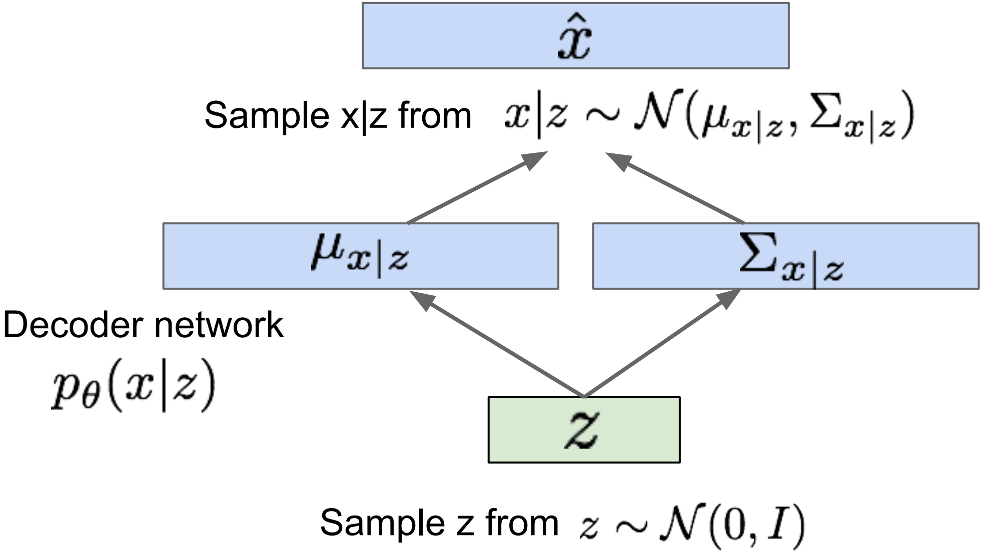


Now given a trained VAE: use decoder network & sample z from prior!



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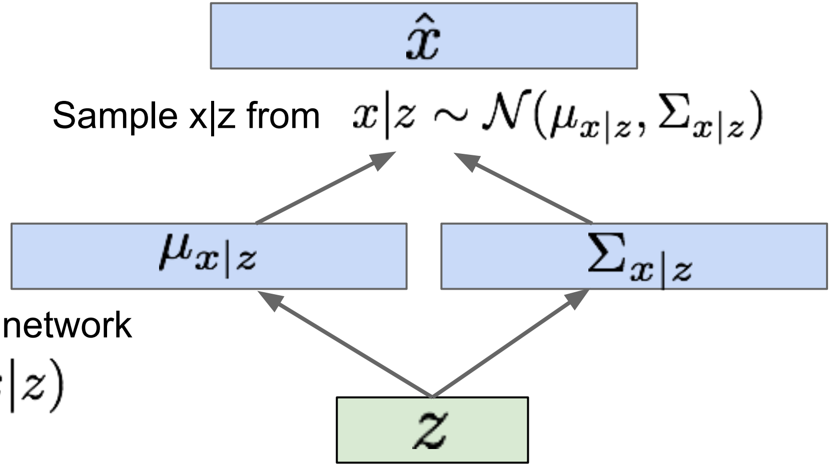
Variational Autoencoders: Generating Data!

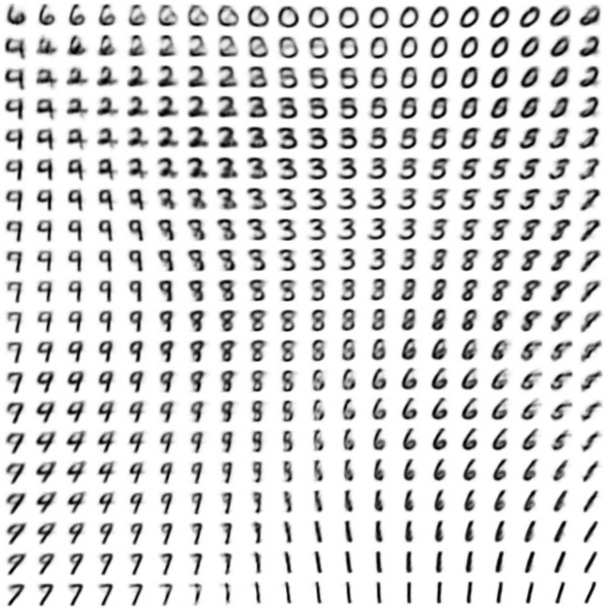
Use decoder network. Now sample z from prior!



Decoder network

$p_\theta(x|z)$

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



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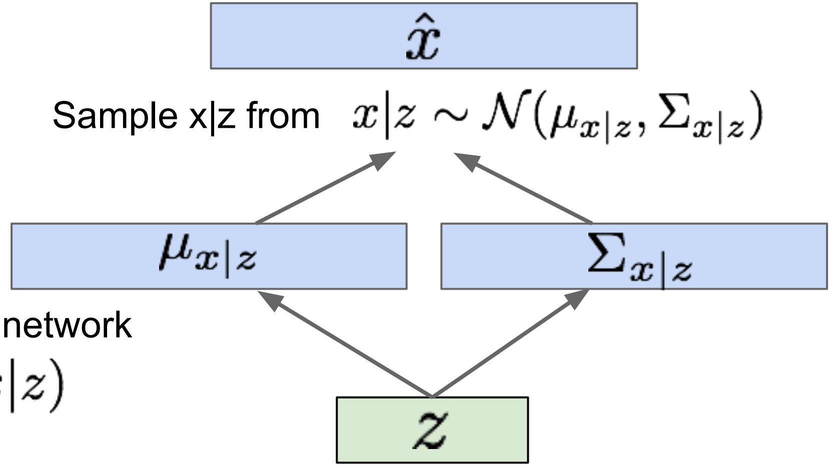

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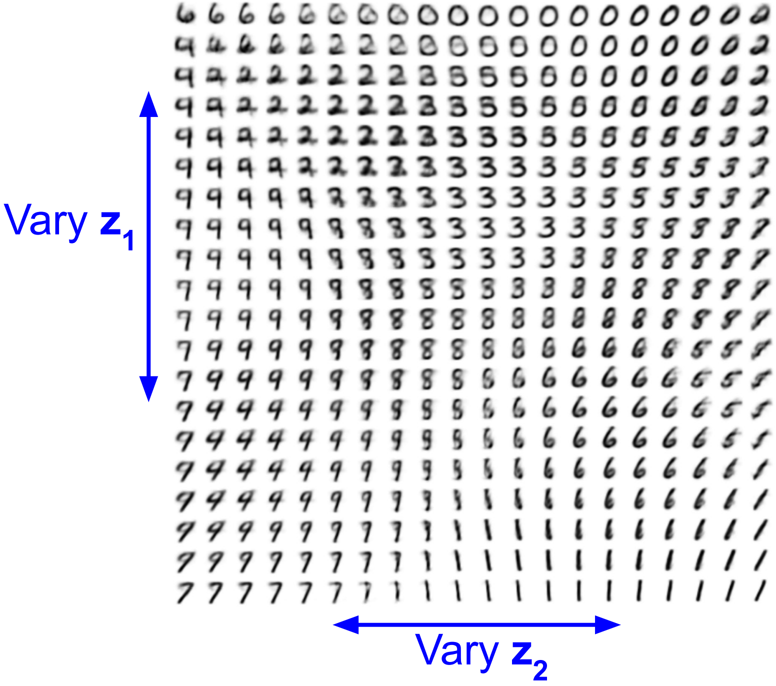
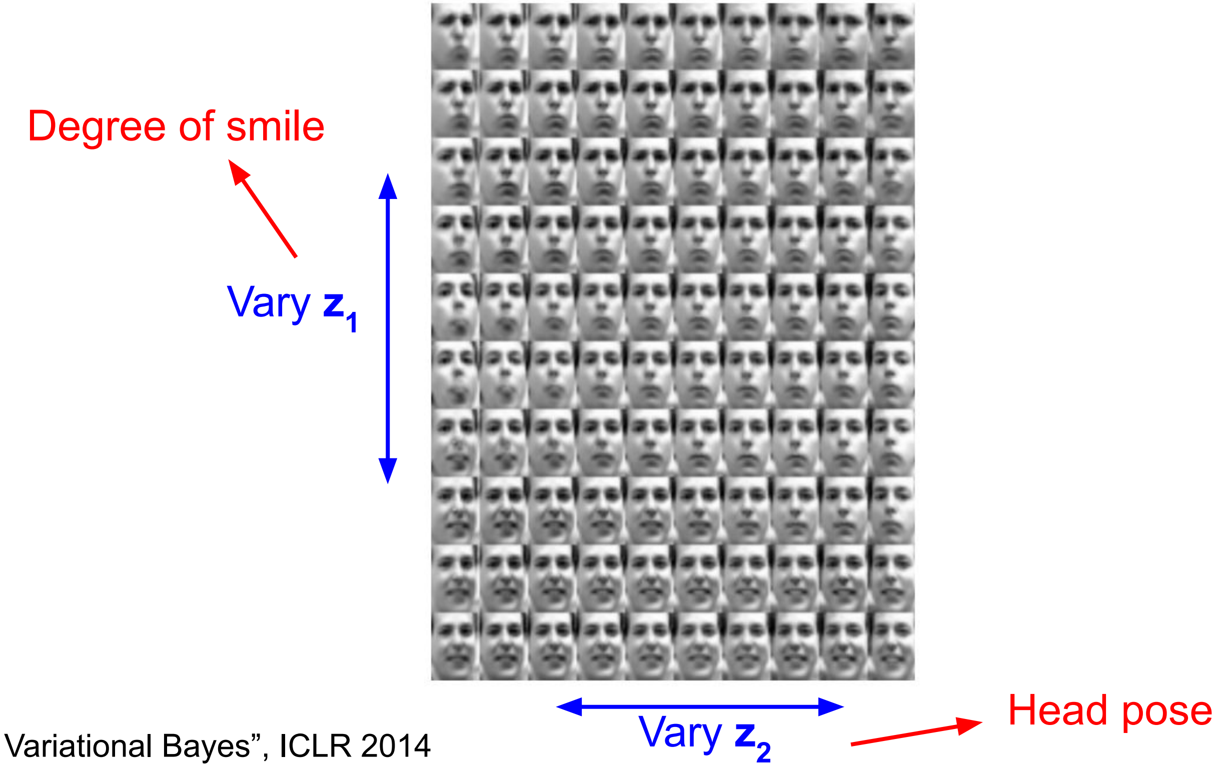
Data manifold for 2-d **z**



Variational Autoencoders: Generating Data!

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

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



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Variational Autoencoders: Generating Data!

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

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

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

Degree of smile

Vary $\mathbf{z}_1$

Vary $\mathbf{z}_2$

Head pose

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

Variational Autoencoders: Generating Data!

32x32 CIFAR-10

Labeled Faces in the Wild

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(data)
- High-quality generated images
- Slow to generate images
- No explicit latent codes

Variational model
- Maximize lower bound on p(data)
- Generated images often blurry
- Very fast to generate images
- Learn rich latent codes

Taxonomy of Generative Models

Direct

GAN

Generative models

Explicit density

Implicit density

Markov Chain

GSN

Tractable density

Approximate density

Fully Visible Belief Nets
- Autoregressive
- NADE
- MADE
- NICE / RealNVP
- Glow
- Ffjord

Variational

Markov Chain

Variational Autoencoder

Boltzmann Machine

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

Generative Adversarial Networks (GANs)

So far...

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

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

VAEs define intractable density function with latent **z**:

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

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

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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!

Generative Adversarial Networks

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

Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

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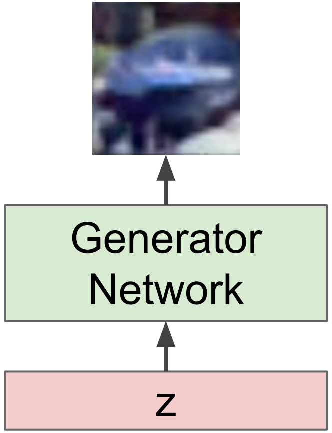
Output: Sample from training distribution

Input: Random noise



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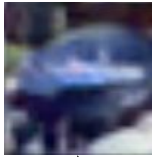

Generator Network

Input: Random noise

z

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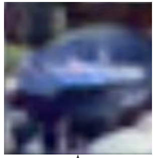

Objective: generated images should look “real”

Generator Network

Input: Random noise

z

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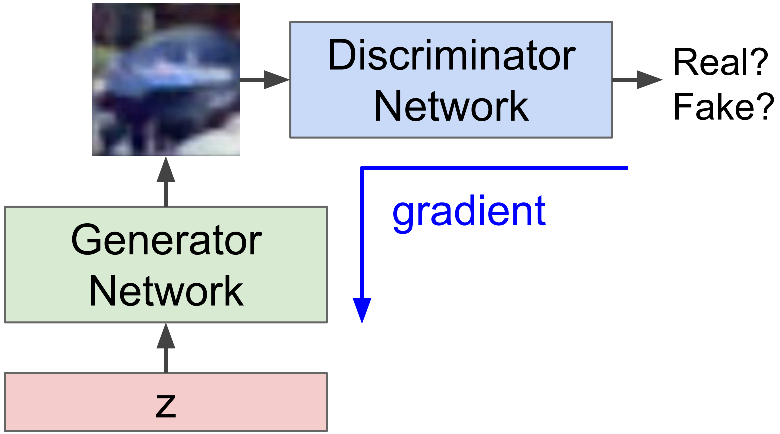
Solution: Sample from a simple distribution we can easily sample from, e.g. random noise. Learn transformation to training distribution.

But we don't know which sample z maps to which training image -> can't learn by reconstructing training images

Solution: Use a discriminator network to tell whether the generate image is within data distribution ("real") or not

Output: Sample from training distribution

Input: Random noise



Training GANs: Two-player game

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

Discriminator network: try to distinguish between real and fake images
Generator network: try to fool the discriminator by generating real-looking images

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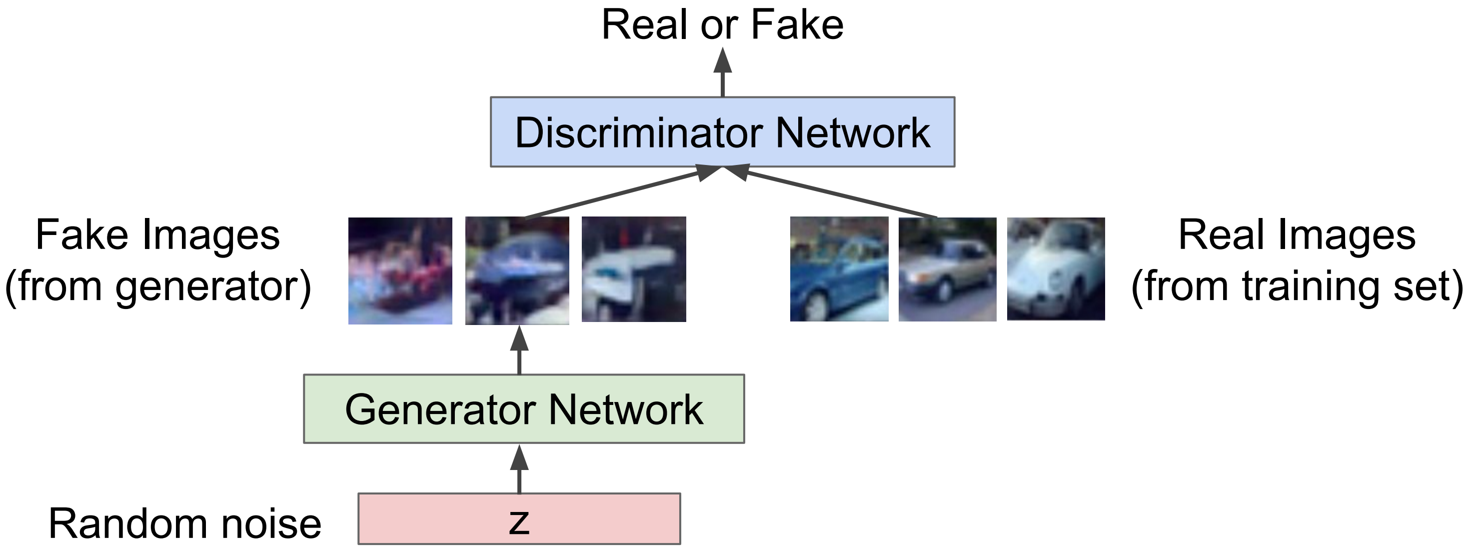

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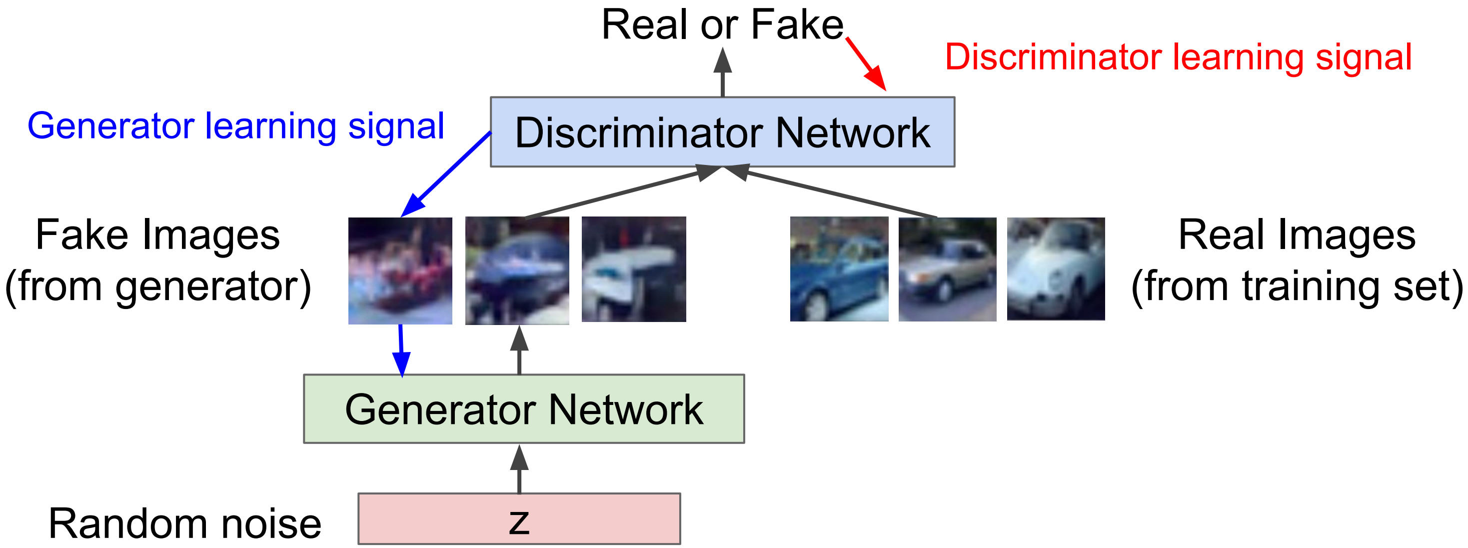

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Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Generator objective

Discriminator objective

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Discriminator outputs likelihood in (0,1) of real image

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- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

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

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Alternate between:

1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

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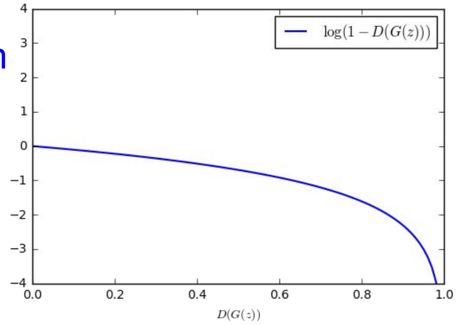
$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).



In practice, optimizing this generator objective does not work well!

Training GANs: Two-player game

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

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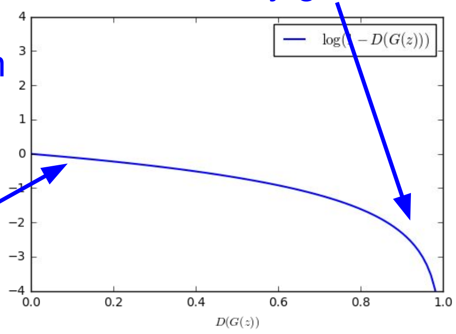
In practice, optimizing this generator objective does not work well!

When sample is likely fake, want to learn from it to improve generator (move to the right on X axis).

But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



Training GANs: Two-player game

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

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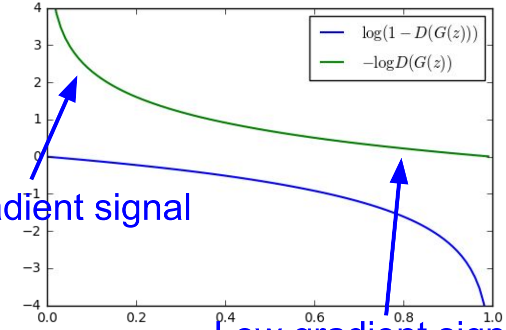
2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.



Training GANs: Two-player game

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

Putting it together: GAN training algorithm

for number of training iterations **do**

  for k steps **do**

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
  - Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

  end for

  - Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
  - Update the generator by ascending its stochastic gradient (improved objective):

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Training GANs: Two-player game

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

Putting it together: GAN training algorithm

Some find k=1 more stable, others use k > 1, no best rule.

Followup work (e.g. Wasserstein GAN, BEGAN) alleviates this problem, better stability!

for number of training iterations **do**
  for $\boxed{k \text{ steps}}$ **do**
- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
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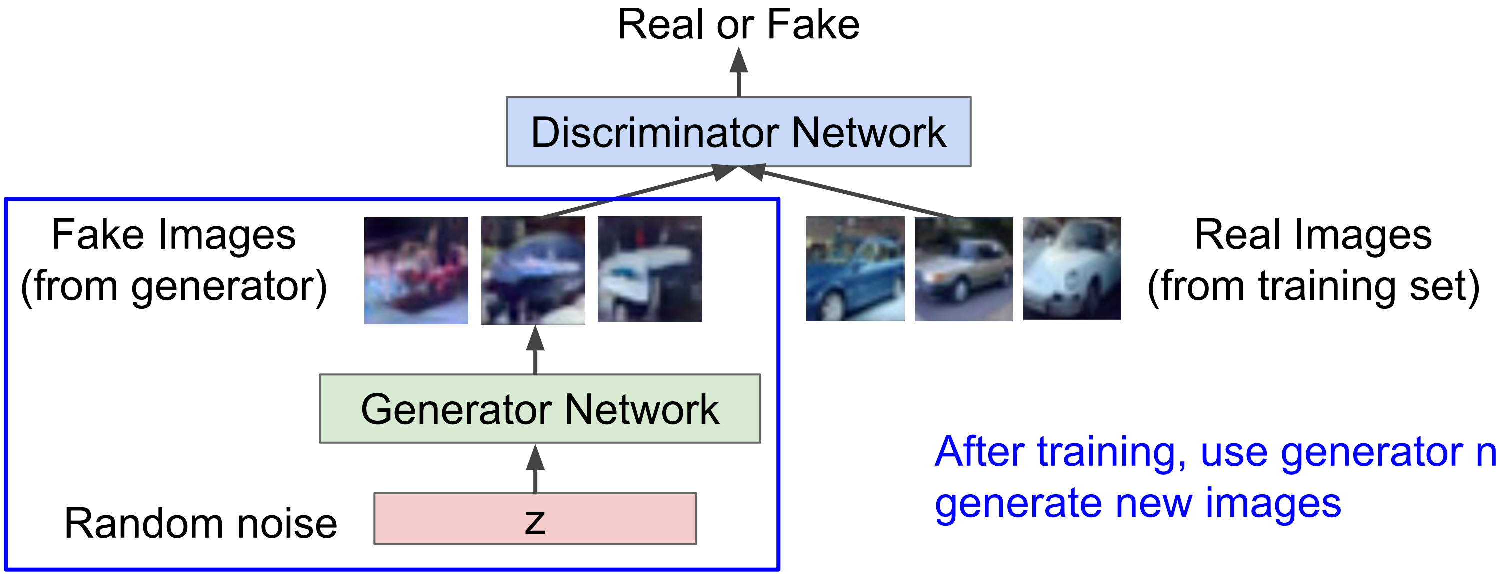
end for

Arjovsky et al. "Wasserstein gan." arXiv preprint arXiv:1701.07875 (2017)
Berthelot, et al. "Began: Boundary equilibrium generative adversarial networks." arXiv preprint arXiv:1703.10717 (2017)

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images

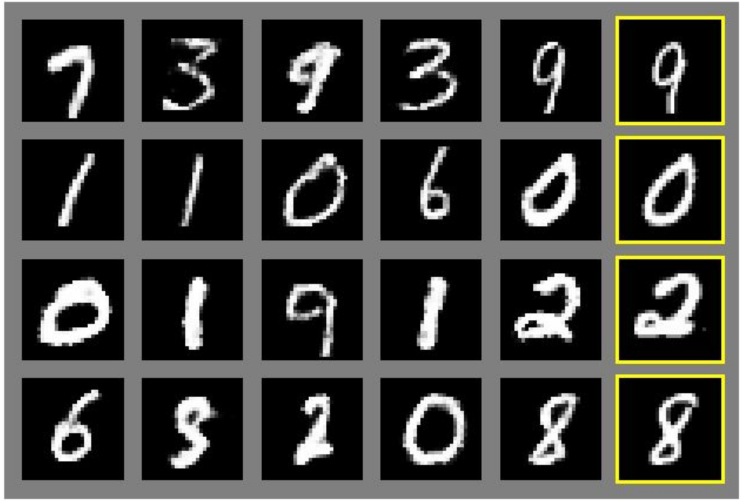


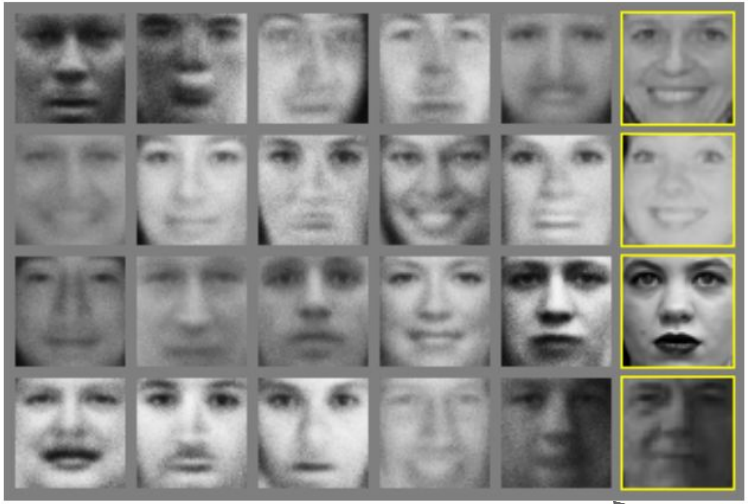
After training, use generator network to generate new images

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples



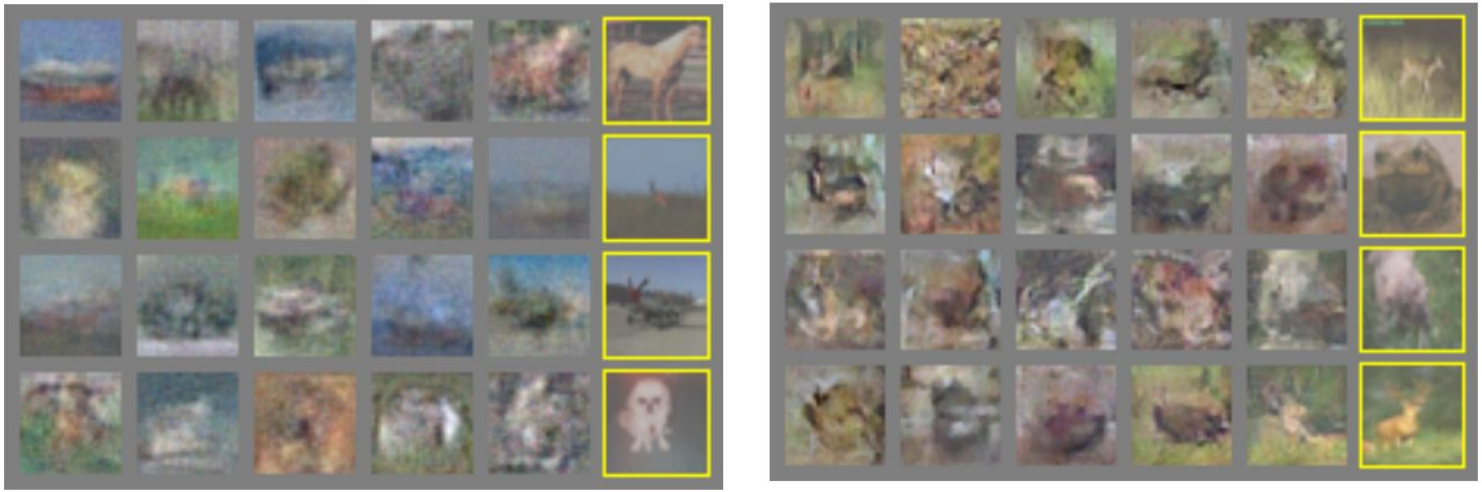


Nearest neighbor from training set

Generative Adversarial Nets

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

Generated samples (CIFAR-10)



Nearest neighbor from training set

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 laten space

Radford et al, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

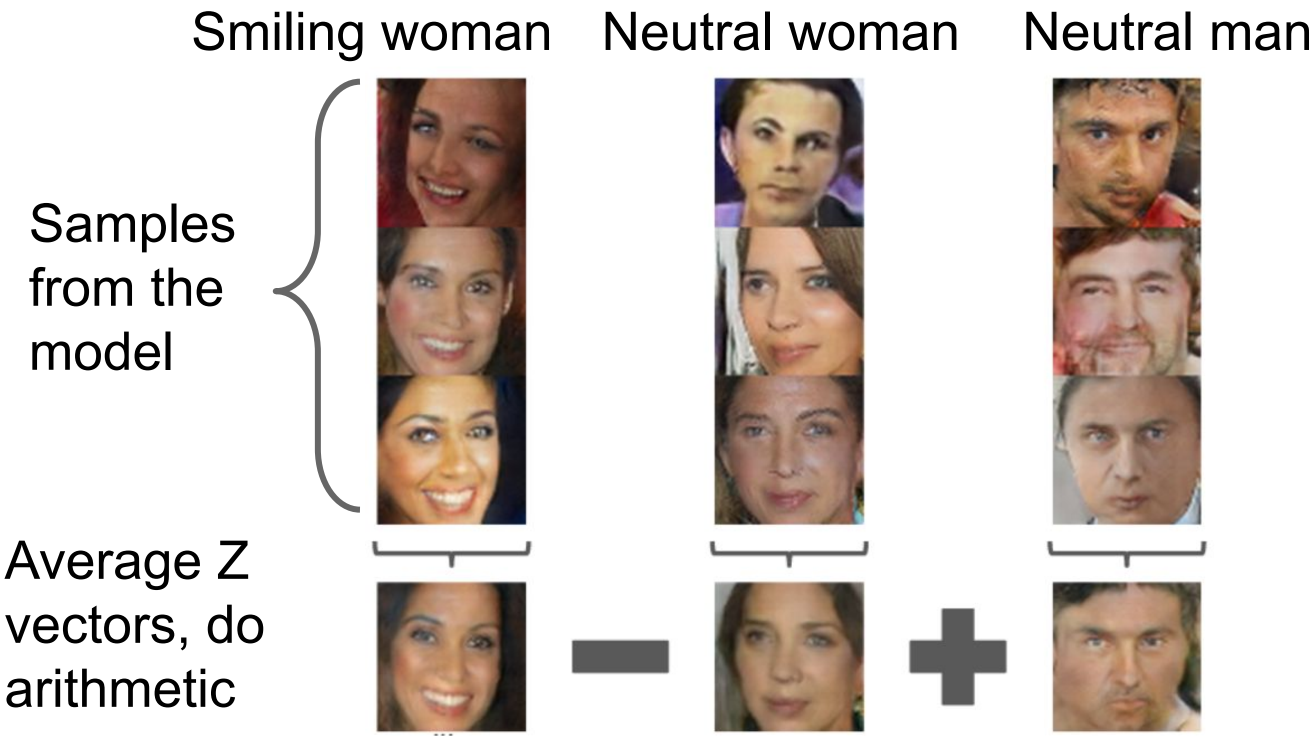
Radford et al, ICLR 2016

Smiling woman Neutral woman Neutral man

Samples from the model

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016



Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

Smiling woman | Neutral woman | Neutral man

Smiling Man

Samples from the model

Average Z vectors, do arithmetic

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

Since then: Explosion of GANs

"The GAN Zoo"

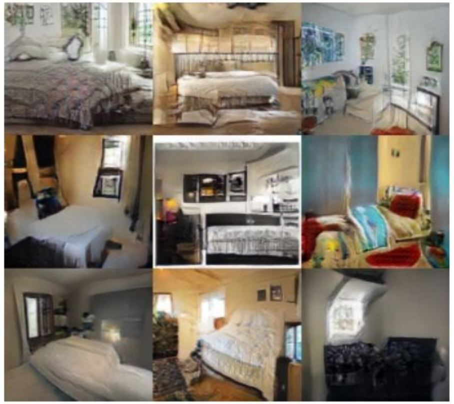
See also: https://github.com/soumith/ganhacks for tips and tricks for trainings GANs

- 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 Categorial 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

2017: Explosion of GANs

Better training and generation



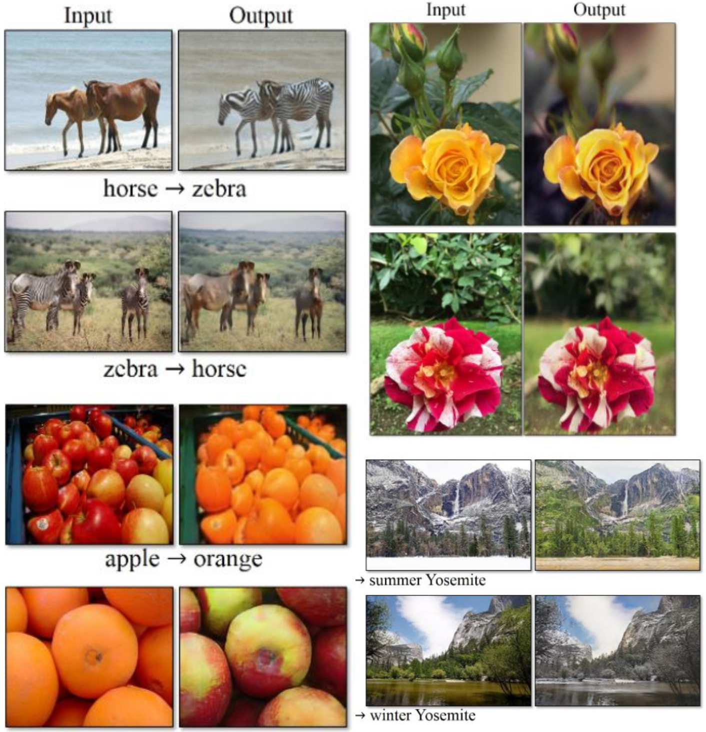
LSGAN, Zhu 2017.

Wasserstein GAN, Arjovsky 2017. Improved Wasserstein GAN, Gulrajani 2017.

Progressive GAN, Karras 2018.

2017: Explosion of GANs

Source->Target domain transfer



CycleGAN. Zhu et al. 2017.

Text -> Image Synthesis

Reed et al. 2017.

Many GAN applications

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

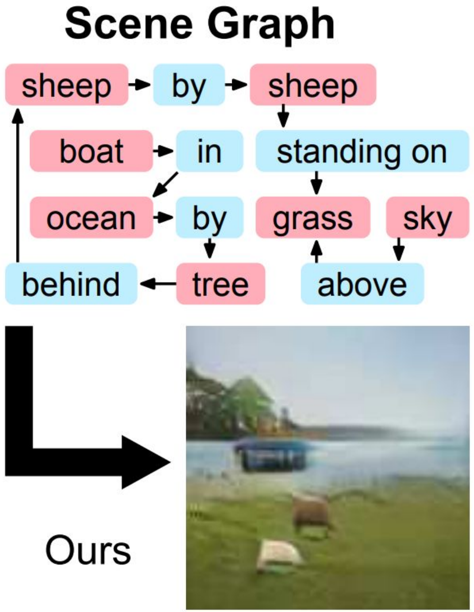
2019: BigGAN

Brock et al., 2019

2019: Scene graphs to GANs

Specifying exactly what kind of image you want to generate.

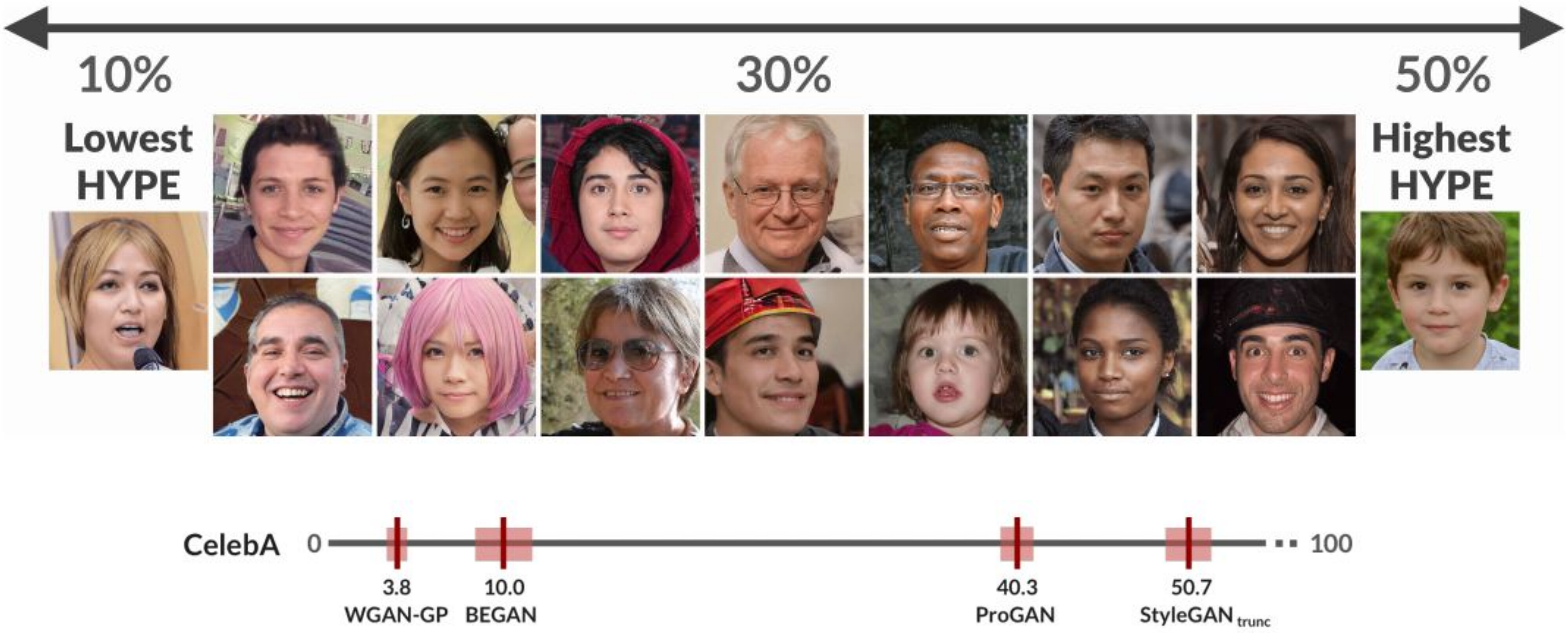
The explicit structure in scene graphs provides better image generation for complex scenes.



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

HYPE: Human eYe Perceptual Evaluations

hype.stanford.edu



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

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:

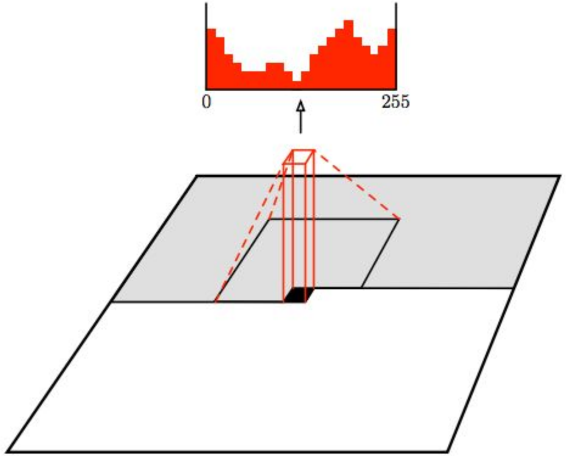
- Trickier / more unstable to train
- Can't solve inference queries such as p(x), p(z|x)

Active areas of research:

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

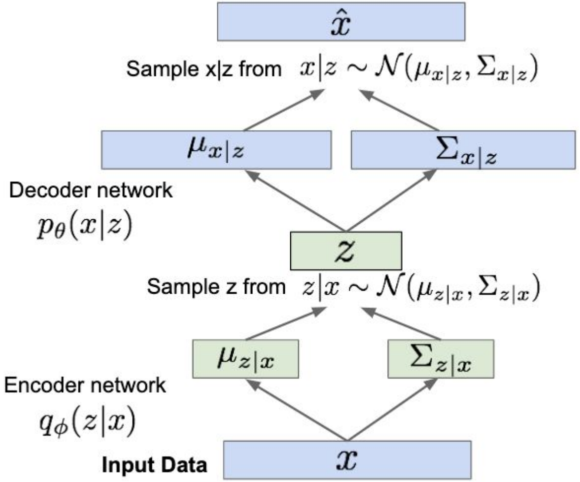
Summary

Autoregressive models:
PixelRNN, PixelCNN



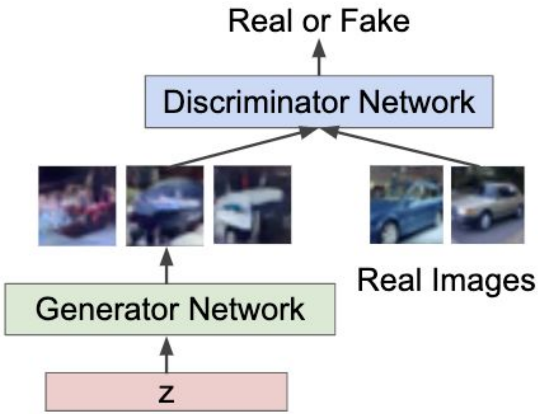
Van der Oord et al, “Conditional image generation with pixelCNN decoders”, NIPS 2016

Variational Autoencoders



Kingma and Welling, “Auto-encoding variational bayes”, ICLR 2013

Generative Adversarial Networks (GANs)



Goodfellow et al, “Generative Adversarial Nets”, NIPS 2014

Next: Reinforcement Learning