

# CS 7643: Deep Learning

## Topics:

- Generative Models (PixelRNNs, VAEs, GANs)
- Key Ideas
  - AE, Reparameterization
  - Variational Inference

Dhruv Batra  
Georgia Tech

# Invited Talk

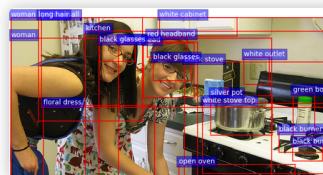
- Peter Anderson, ANU
  - *Visual Understanding in Natural Language*
  - Co-located as ML@GT Seminar, Nov 27 11am, Nano 1117



PhD student in Computer Vision / Deep Learning

- 📍 Sydney / Canberra
- ✉ Email
- 🐦 Twitter
- LinkedIn
- Google Scholar

## Publications



### Bottom-Up and Top-Down Attention for Image Captioning and Visual Question Answering

Peter Anderson, Xiaodong He, Chris Buehler, Damien Teney, Mark Johnson, Stephen Gould, Lei Zhang

preprint arXiv:1707.07998, 2017.

[Project](#) [PDF](#) [Code](#)

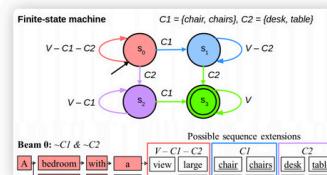


### Tips and Tricks for Visual Question Answering: Learnings from the 2017 Challenge

Damien Teney, Peter Anderson, Xiaodong He, Anton van den Hengel

preprint arXiv:1708.02711, 2017.

[PDF](#) [Slides](#)

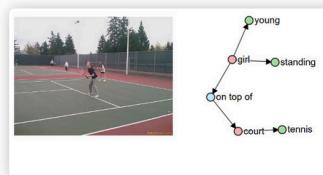


### Guided Open Vocabulary Image Captioning with Constrained Beam Search

Peter Anderson, Basura Fernando, Mark Johnson and Stephen Gould

In Conference on Empirical Methods for Natural Language Processing (EMNLP), 2017.

[PDF](#)



### SPICE: Semantic Propositional Image Caption Evaluation

Peter Anderson, Basura Fernando, Mark Johnson and Stephen Gould

In Proceedings of the European Conference on Computer Vision (ECCV), 2016.

[Project](#) [PDF](#) [Code](#)

# Administrivia

- **Poster Presentation:** **Best Project Award!**
  - Wed 11/29, 2-4pm
    - In two sessions
  - **Klaus Auditorium**
  - Less text, more pictures.

# Overview

- Unsupervised Learning
- Generative Models
  - PixelRNN and PixelCNN
  - Variational Autoencoders (VAE)
  - Generative Adversarial Networks (GAN)

# Supervised vs Unsupervised Learning

## Supervised Learning

**Data:**  $(x, y)$

x is data, y is label

**Goal:** Learn a *function* to map  $x \rightarrow y$

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

# Supervised vs Unsupervised Learning

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→ Cat

Classification

[This image](#) is CC0 public domain

# Supervised vs Unsupervised Learning

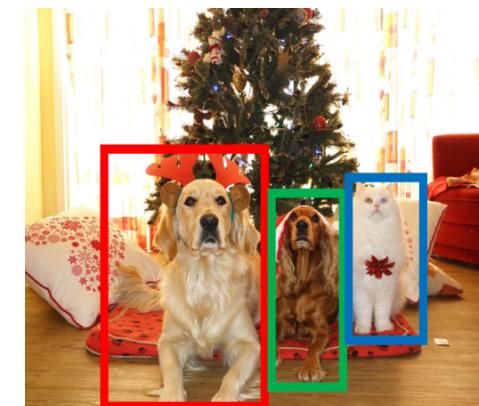
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**DOG, DOG, CAT**

Object Detection

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# Supervised vs Unsupervised Learning

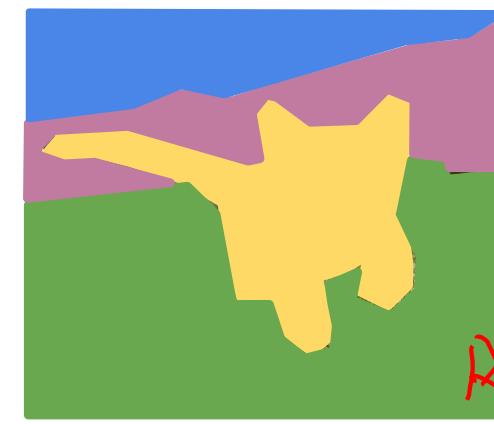
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GRASS, CAT,  
TREE, SKY

Semantic Segmentation

# Supervised vs Unsupervised Learning

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$x$



$y$

A cat sitting on a suitcase on the floor

Image captioning

Caption generated using [neuraltalk2](#)  
[Image](#) is [CC0 Public domain](#)

# 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

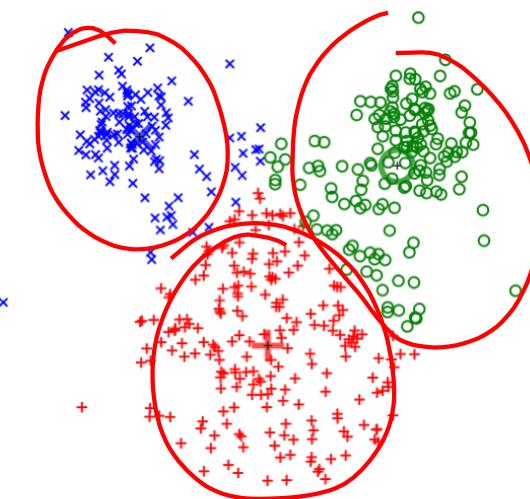
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K-means clustering

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# Supervised vs Unsupervised Learning

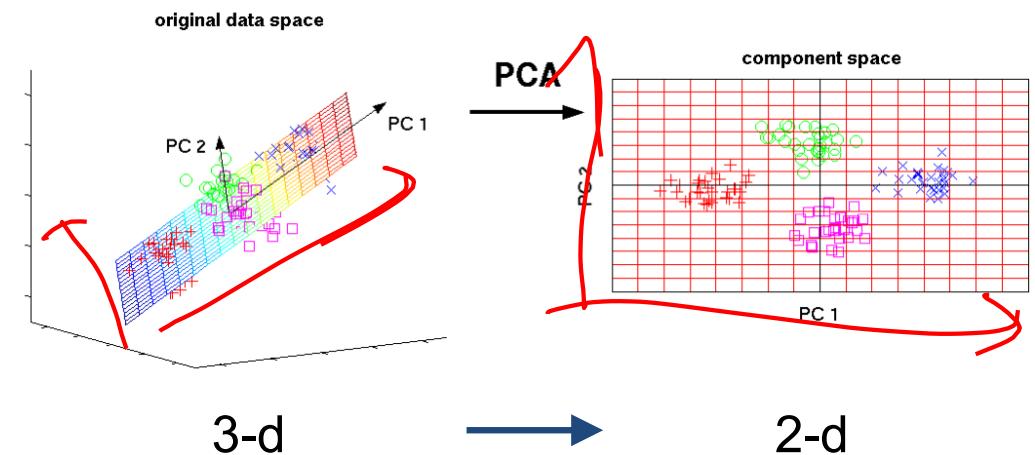
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Principal Component Analysis  
(Dimensionality reduction)

This image from Matthias Scholz  
is CC0 public domain

$P(x)$   
model

# Supervised vs Unsupervised Learning

## Unsupervised Learning

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Just data, no labels!

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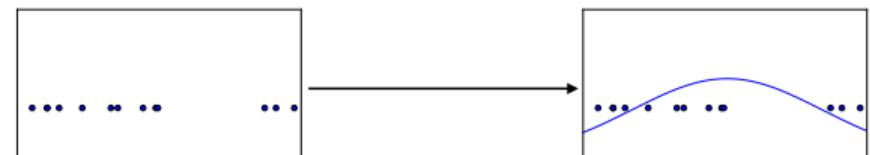
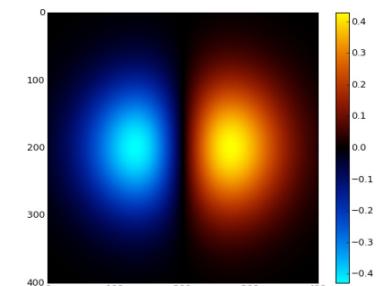
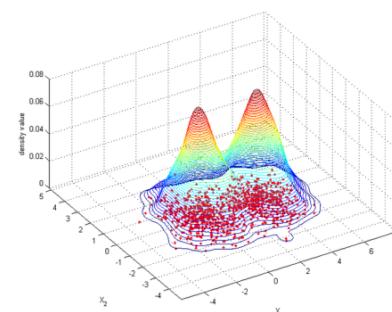


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1-d density estimation



2-d density estimation

2-d density images [left](#) and [right](#) are [CC0 public domain](#)

# Supervised vs Unsupervised Learning

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## Unsupervised Learning

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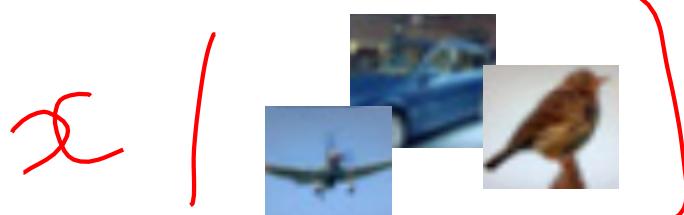
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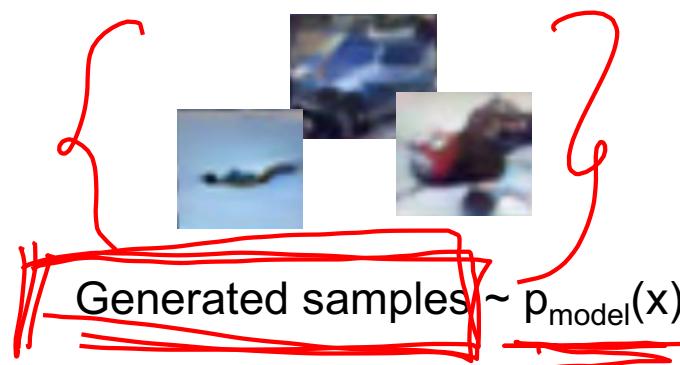
# Generative Models

Given training data, generate new samples from same distribution



Training data  $\sim p_{\text{data}}(x)$

Want to learn  $p_{\text{model}}(x)$  similar to  $p_{\text{data}}(x)$



# Generative Models

Given training data, generate new samples from same distribution



Training data  $\sim p_{\text{data}}(x)$



Generated samples  $\sim p_{\text{model}}(x)$

Want to learn  $p_{\text{model}}(x)$  similar to  $p_{\text{data}}(x)$

Addresses density estimation, a core problem in unsupervised learning

## Several flavors:

- Explicit density estimation: explicitly define and solve for  $p_{\text{model}}(x)$
- Implicit density estimation: learn model that can sample from  $p_{\text{model}}(x)$  w/o explicitly defining it

# Taxonomy of Generative Models

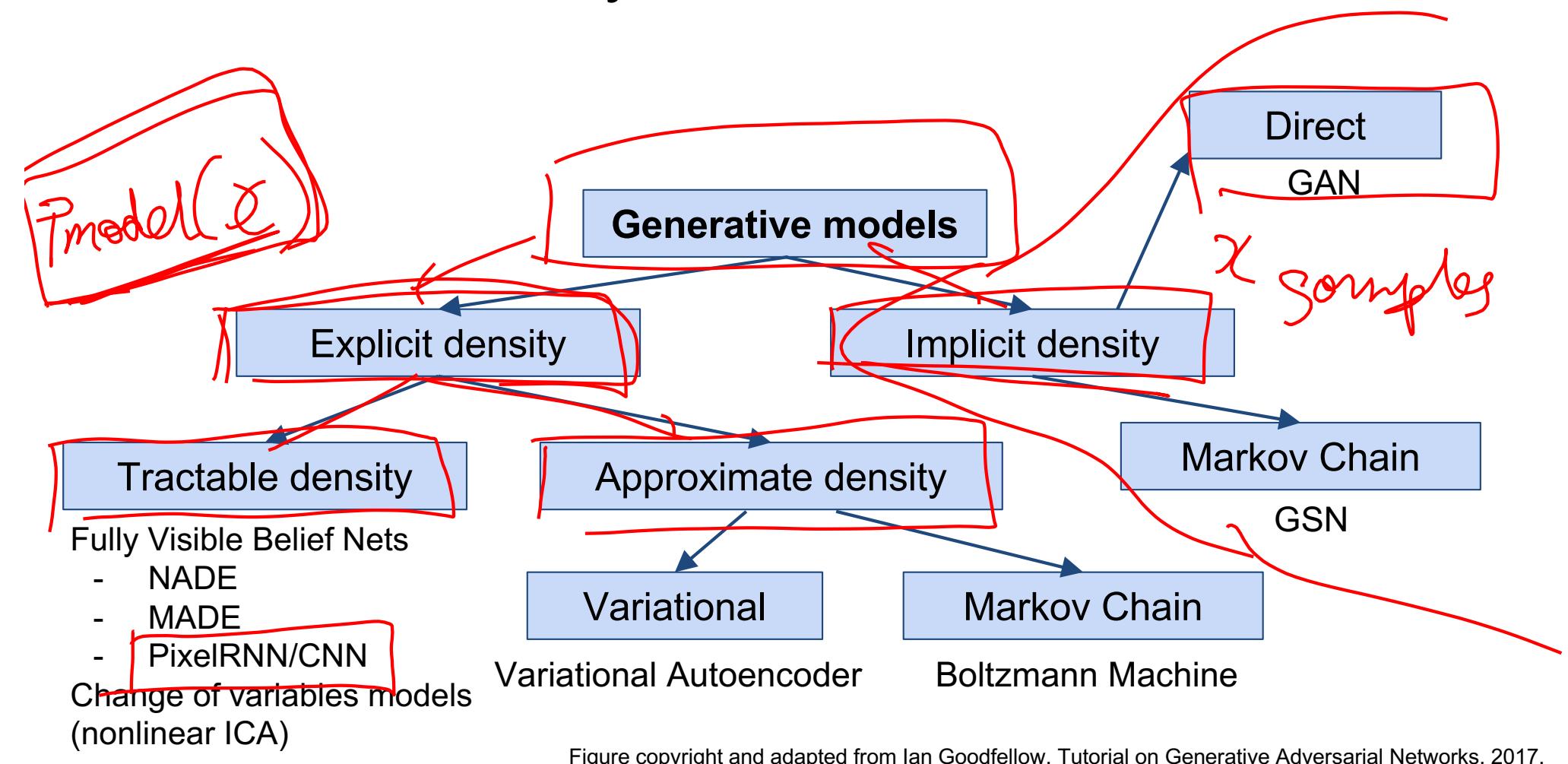


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

# Taxonomy of Generative Models

Today: discuss 3 most popular types of generative models today

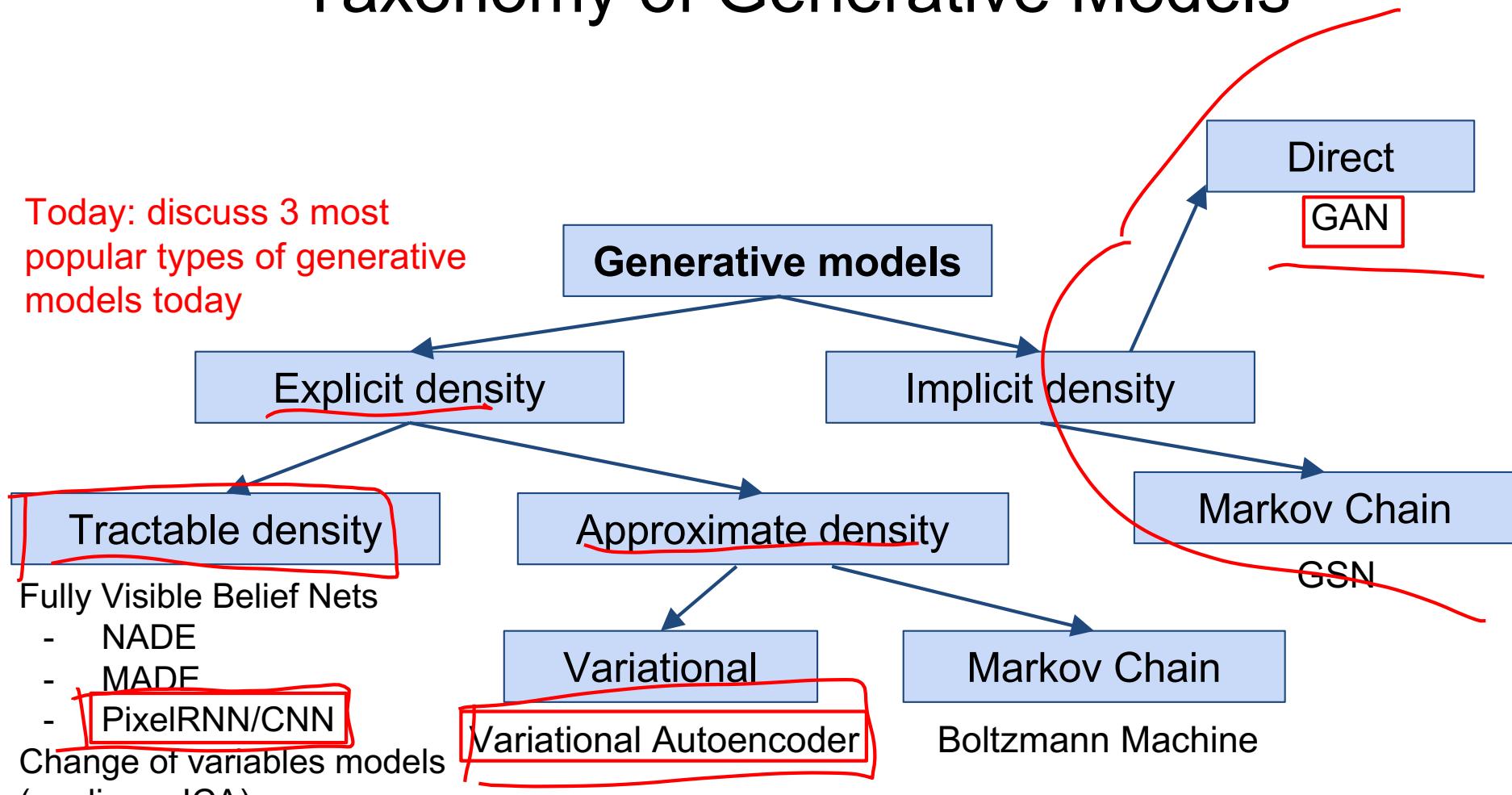
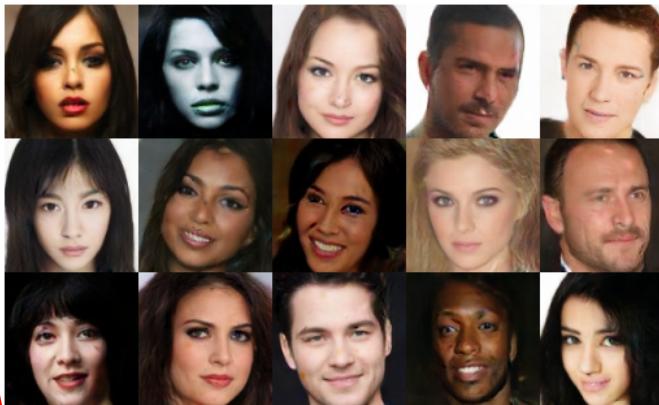


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# Why Generative Models?

- Realistic samples for artwork, super-resolution, colorization, etc.



- Generative models of time-series data can be used for simulation and planning (reinforcement learning applications!)
- Training generative models can also enable inference of latent representations that can be useful as general features

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# PixelRNN and PixelCNN

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# Fully Observable Model

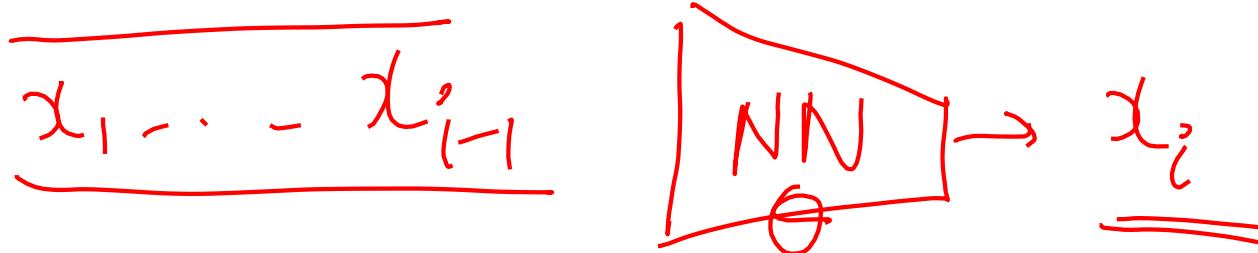
## Explicit density model

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

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

Likelihood of image  $x$                           Probability of  $i$ 'th pixel value given all previous pixels

Then maximize likelihood of training data



# Fully Observable Model

## 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  $x$

↑  
Probability of  $i$ 'th pixel value  
given all previous pixels

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

Then maximize likelihood of training data

# Fully Observable Model

## Explicit density model

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

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

↑                              ↑  
Likelihood of image  $x$       Probability of  $i$ 'th pixel value  
                                  given all previous pixels

Will need to define ordering  
of “previous pixels”

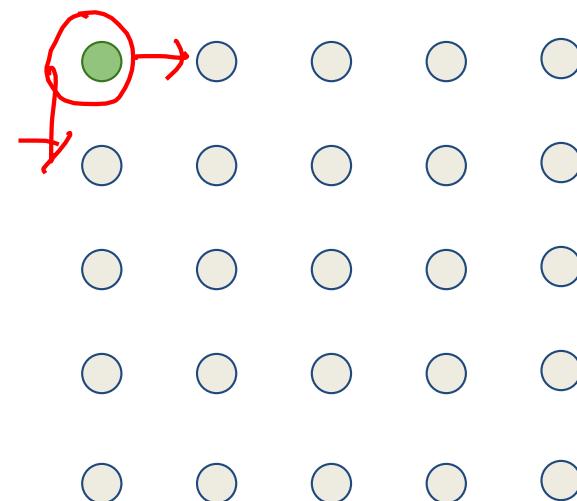
Complex distribution over pixel values  
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Then maximize likelihood of training data

# PixelRNN [van der Oord et al. 2016]

Generate image pixels starting from corner

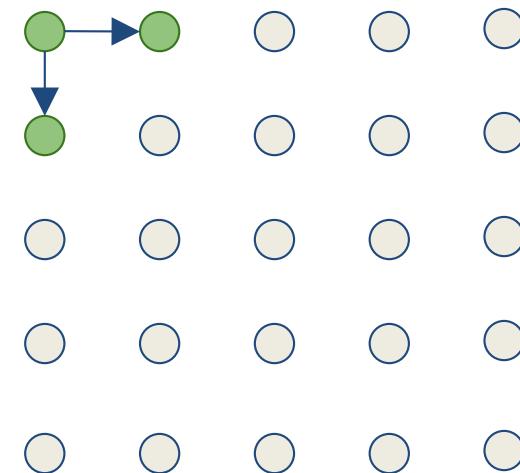
Dependency on previous pixels modeled using an RNN (LSTM)



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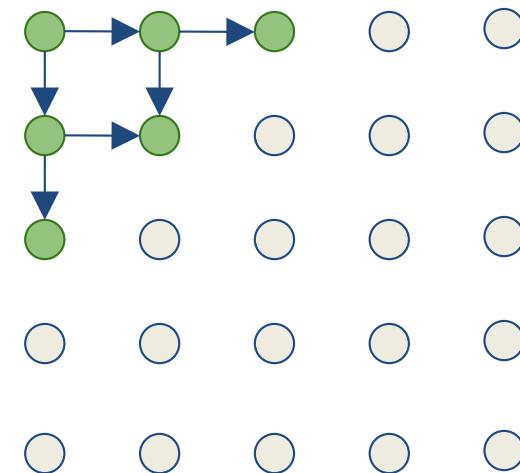
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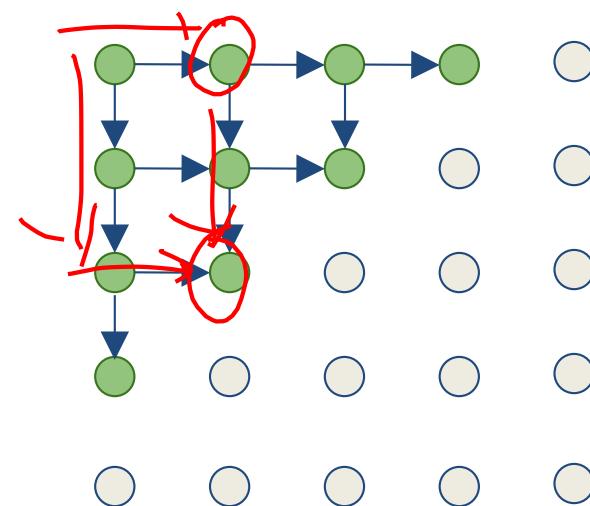


# PixelRNN [van der Oord et al. 2016]

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow!



$$P(x_i | \dots \rightarrow) \sim RNN(\text{Softmax}(\rightarrow | h_i))$$

# 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

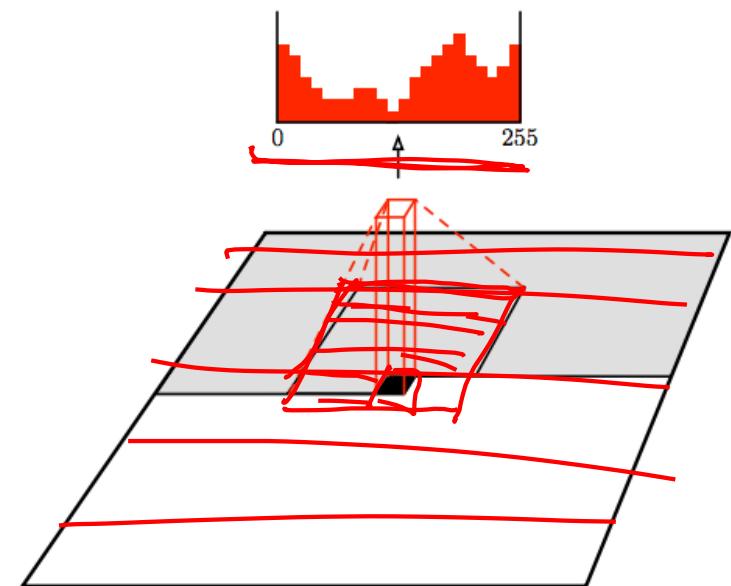


Figure copyright van der Oord et al., 2016. Reproduced with permission.

# PixelCNN

[van der Oord et al. 2016]

$$\mathcal{D} = \{\mathcal{R}_1, \dots, \mathcal{R}_n\}$$

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region

Training: maximize likelihood of training images

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

Softmax loss at each pixel

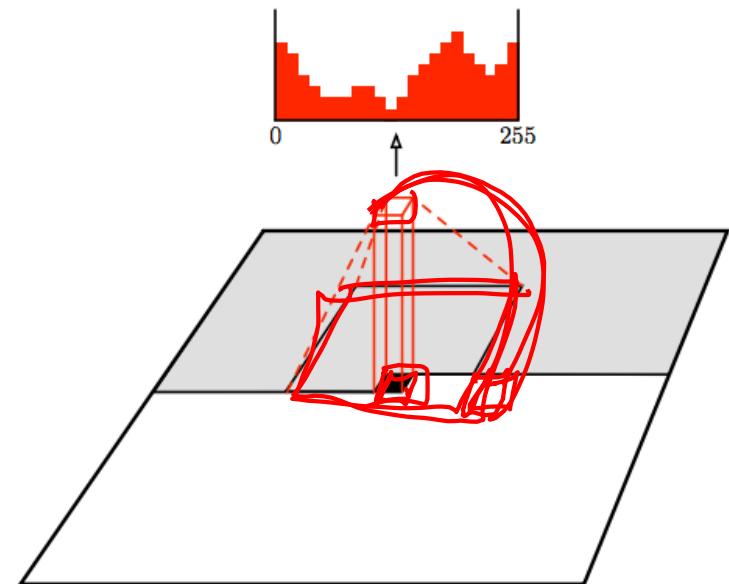


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# PixelCNN [van der Oord et al. 2016]

Still generate image pixels starting from corner

Dependency on previous pixels now modeled using a CNN over context region

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

Generation must still proceed sequentially  
=> still slow

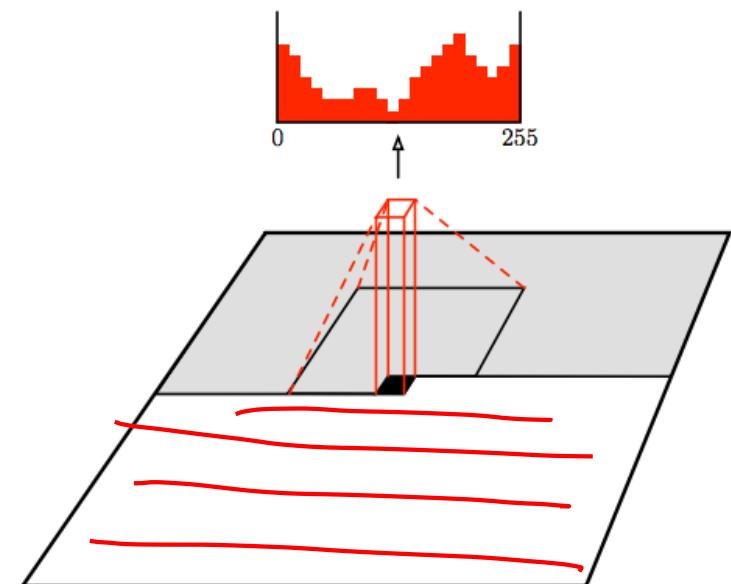
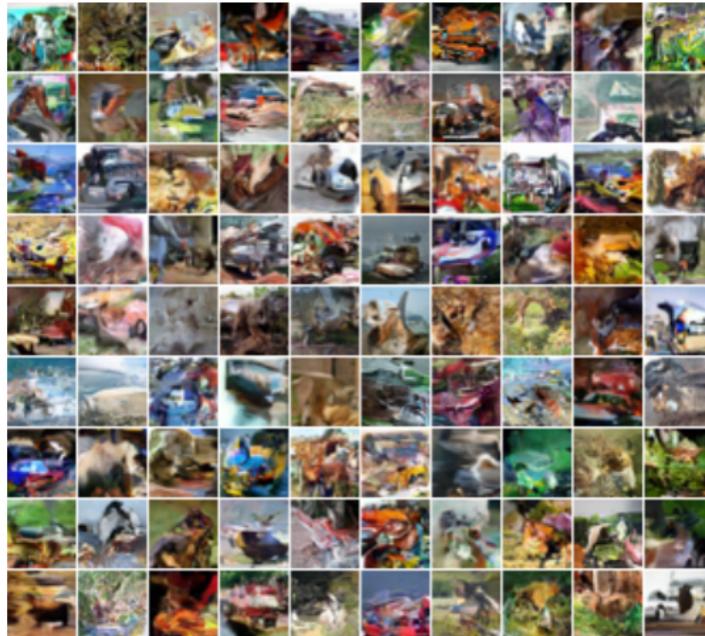
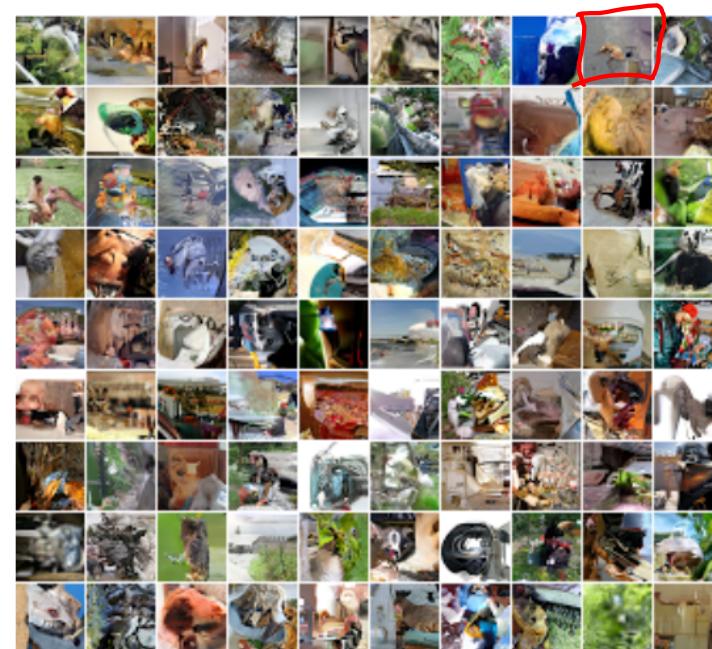


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# Generation Samples



32x32 CIFAR-10



32x32 ImageNet

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# PixelRNN and PixelCNN

Pros:

- Can explicitly compute likelihood  $p(x)$
- Explicit likelihood of training data gives good evaluation metric
- 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++)

# Variational Autoencoders (VAE)

# So far...

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

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

# So far...

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

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

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



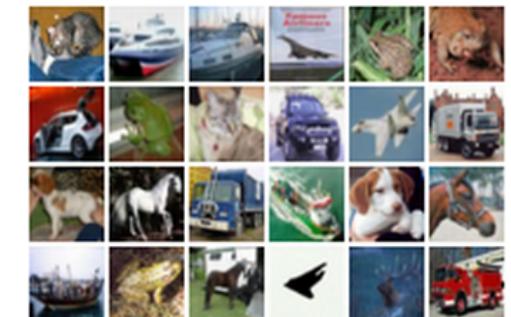
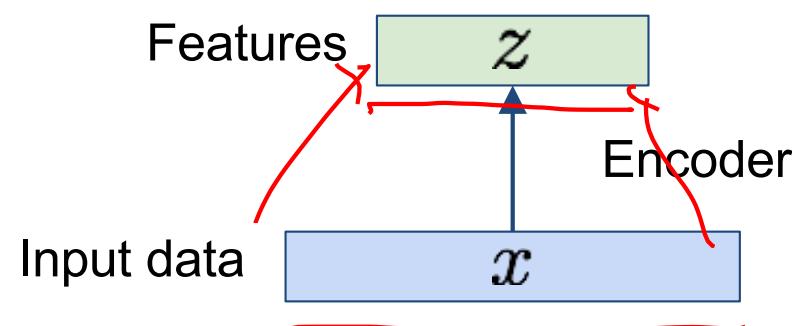
# Variational Auto Encoders

VAEs are a combination of the following ideas:

1. Auto Encoders
2. Variational Approximation
  - Variational Lower Bound / ELBO
3. Amortized Inference Neural Networks
4. “Reparameterization” Trick

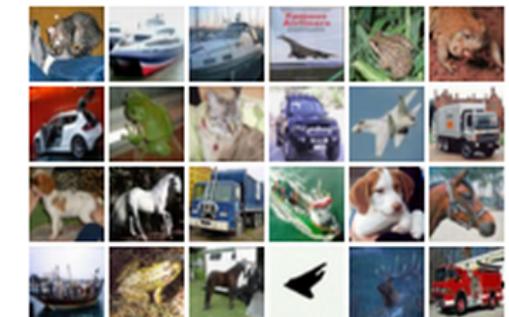
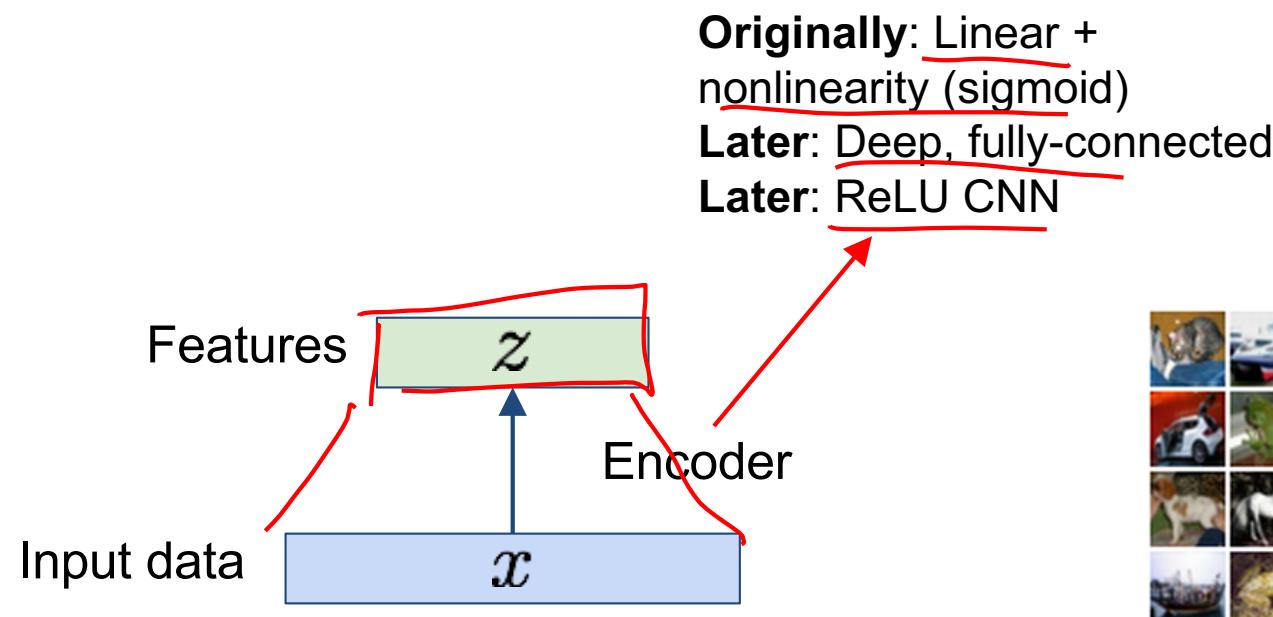
# Autoencoders

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



# Autoencoders

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

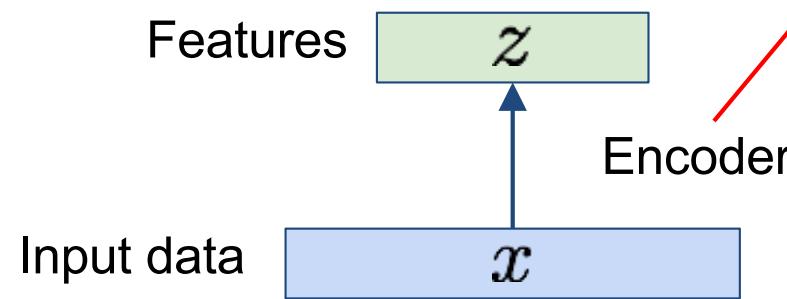


# Autoencoders

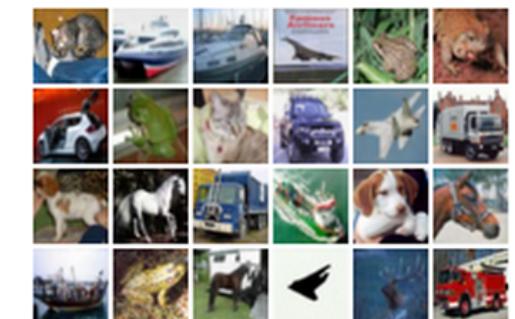
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

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

Q: Why dimensionality reduction?



**Originally:** Linear +  
nonlinearity (sigmoid)  
**Later:** Deep, fully-connected  
**Later:** ReLU CNN



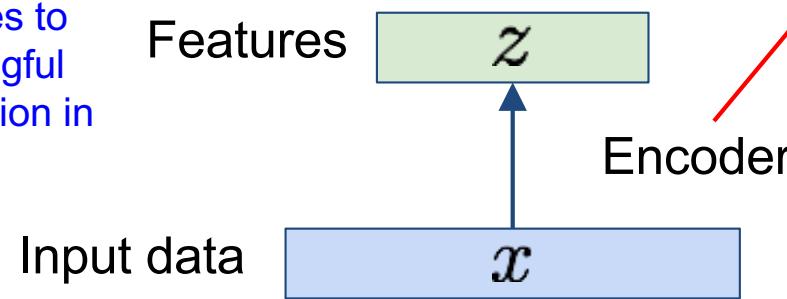
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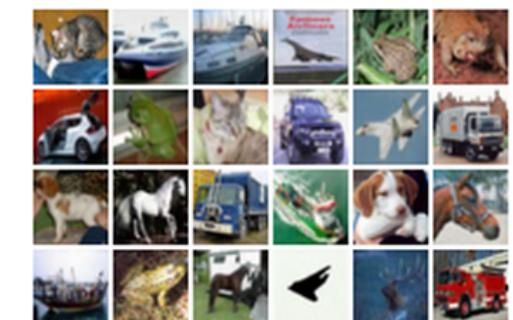
$z$  usually smaller than  $x$   
(dimensionality reduction)

Q: Why dimensionality reduction?

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

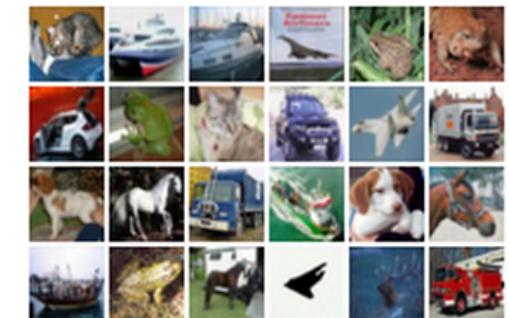
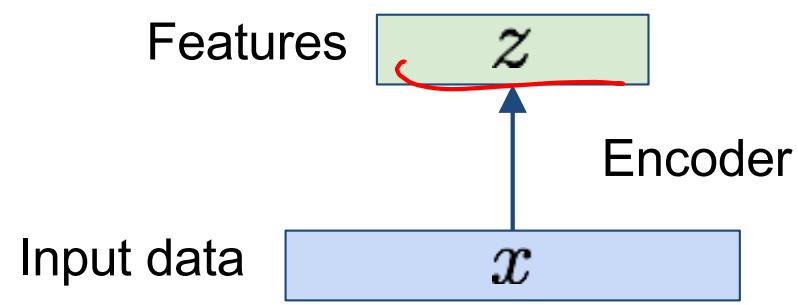


**Originally:** Linear + nonlinearity (sigmoid)  
**Later:** Deep, fully-connected  
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# Autoencoders

How to learn this feature representation?

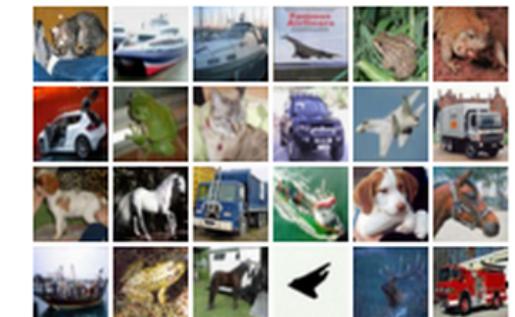
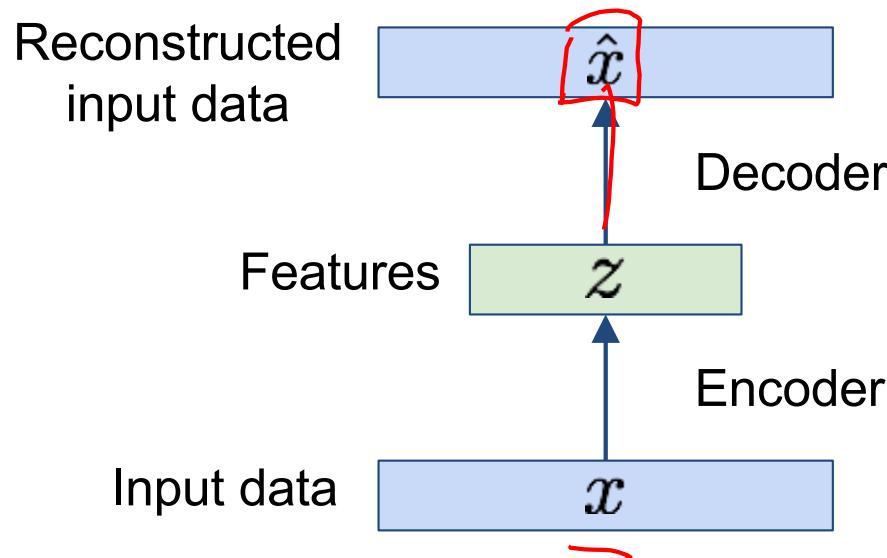


# Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data

“Autoencoding” - encoding itself

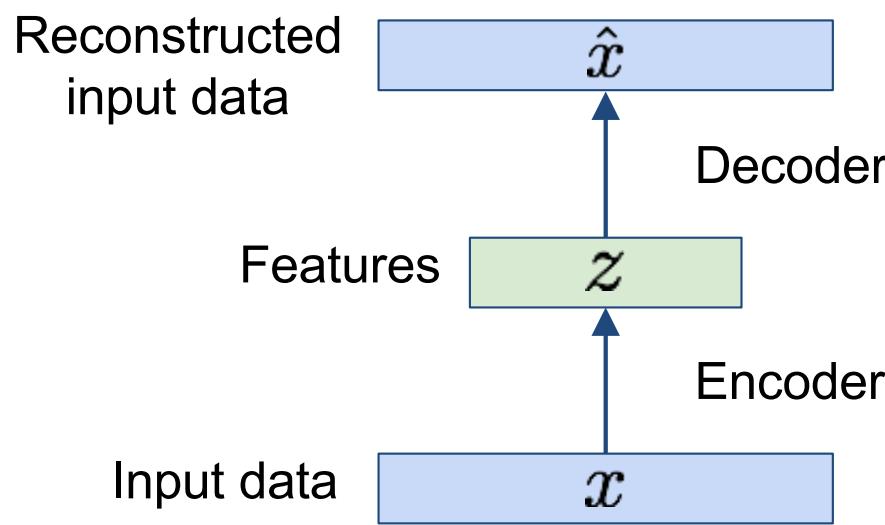


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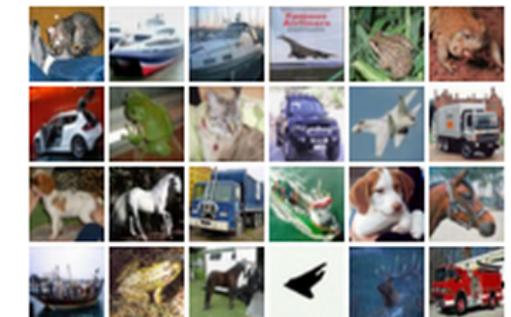
# How to learn this feature representation?

Train such that features can be used to reconstruct original data

## “Autoencoding” - encoding itself



- Originally: Linear + nonlinearity (sigmoid)
- Later: Deep, fully-connected
- Later: ReLU CNN (upconv)

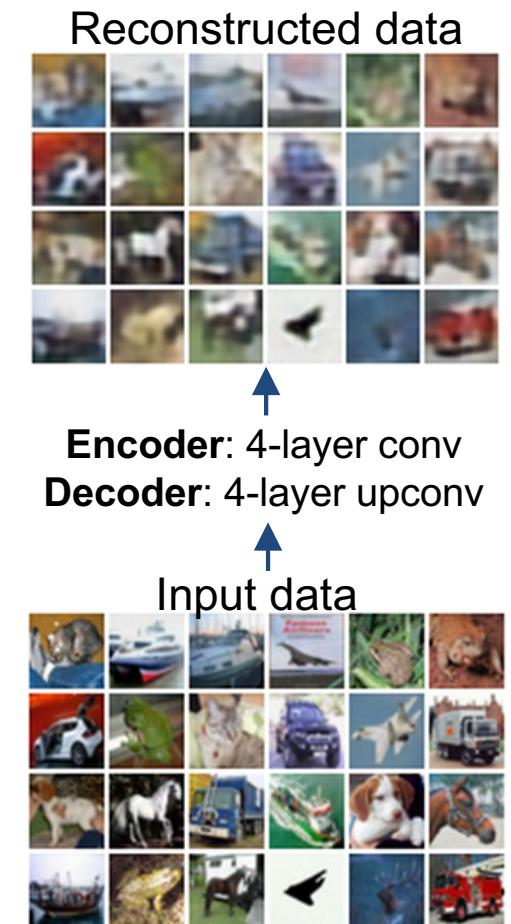
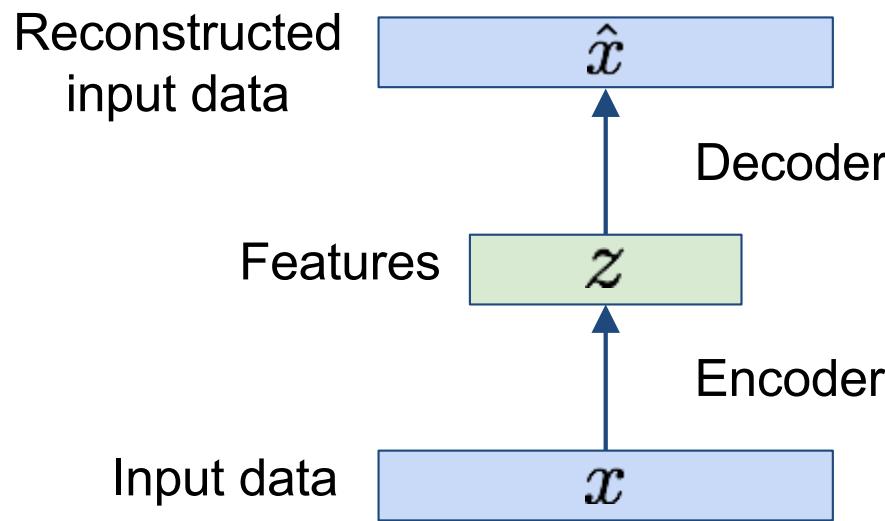


# Autoencoders

How to learn this feature representation?

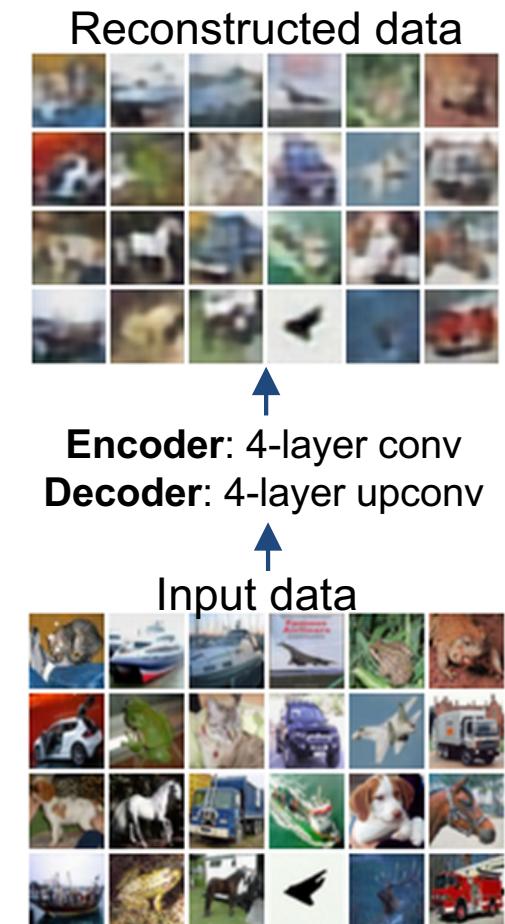
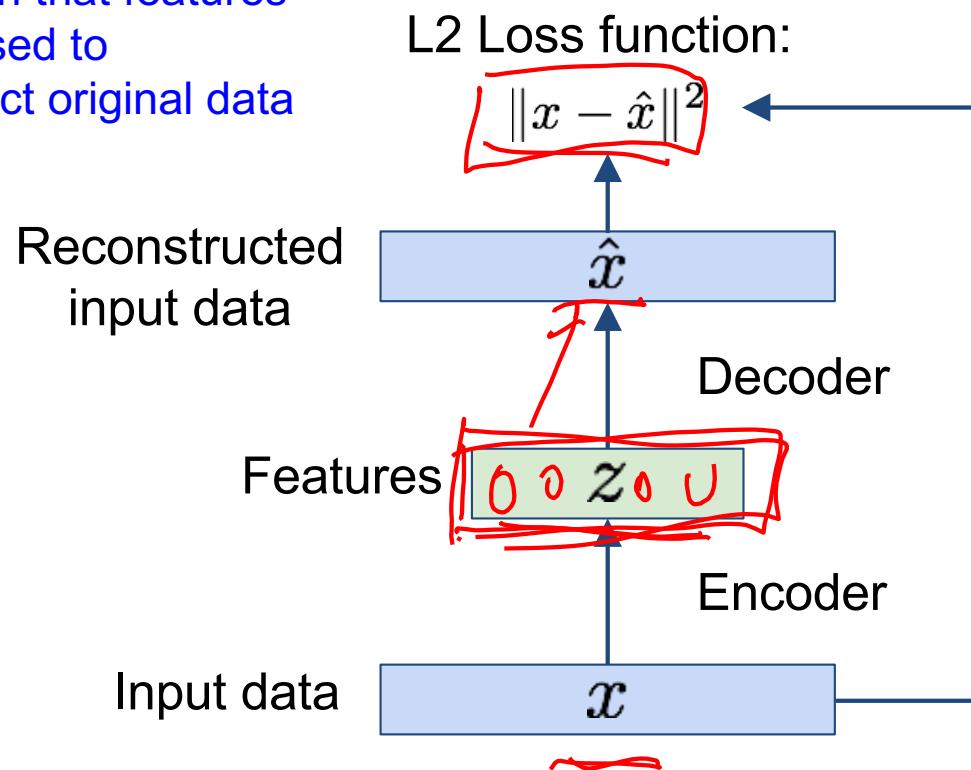
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“Autoencoding” - encoding itself



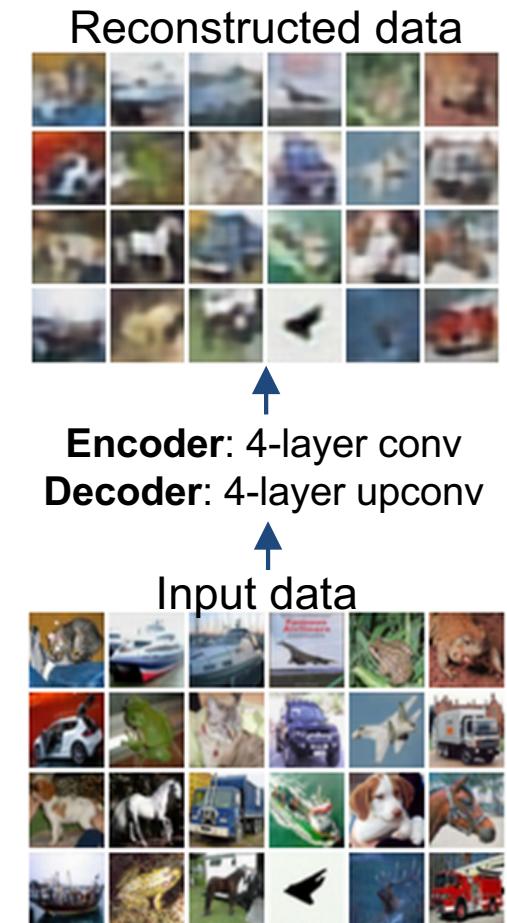
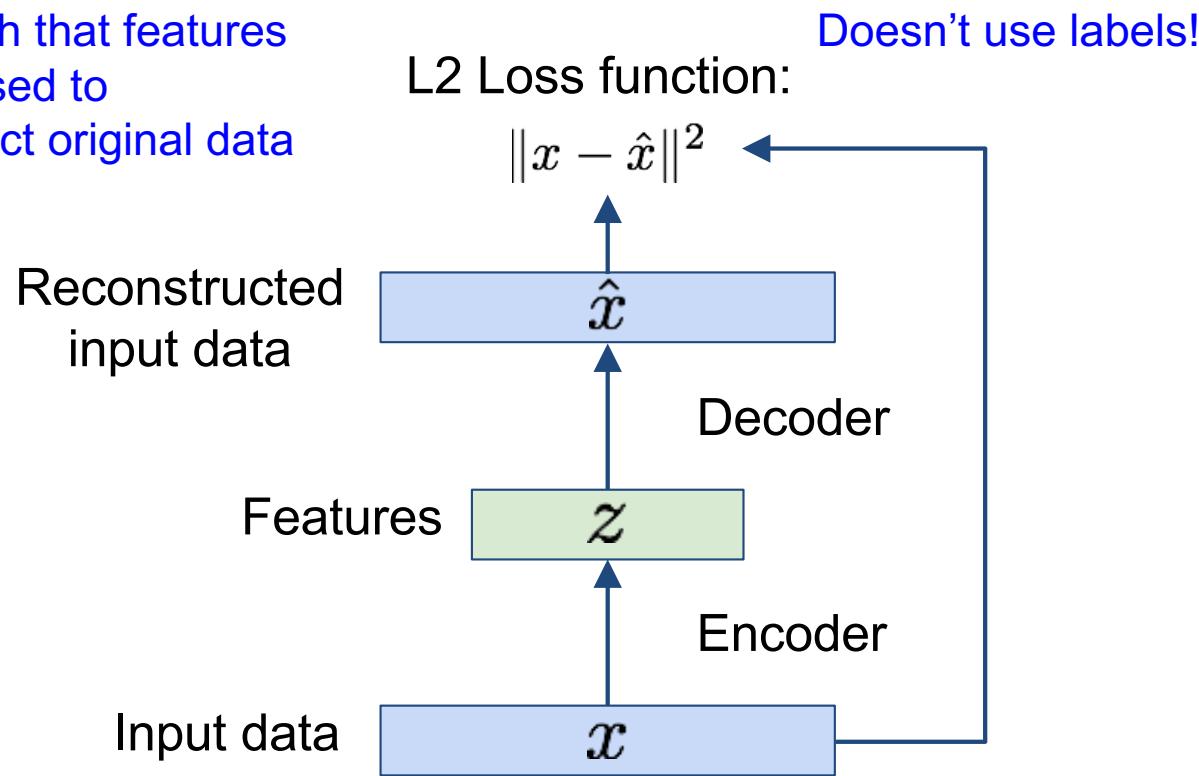
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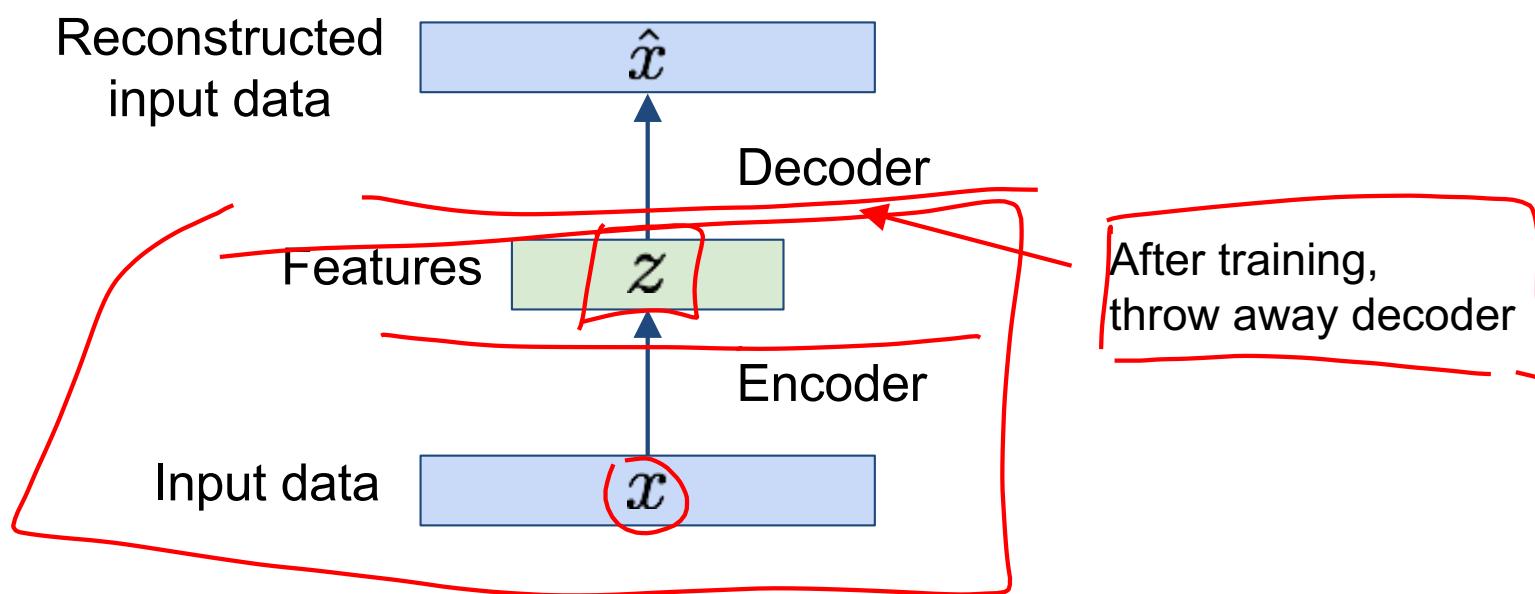


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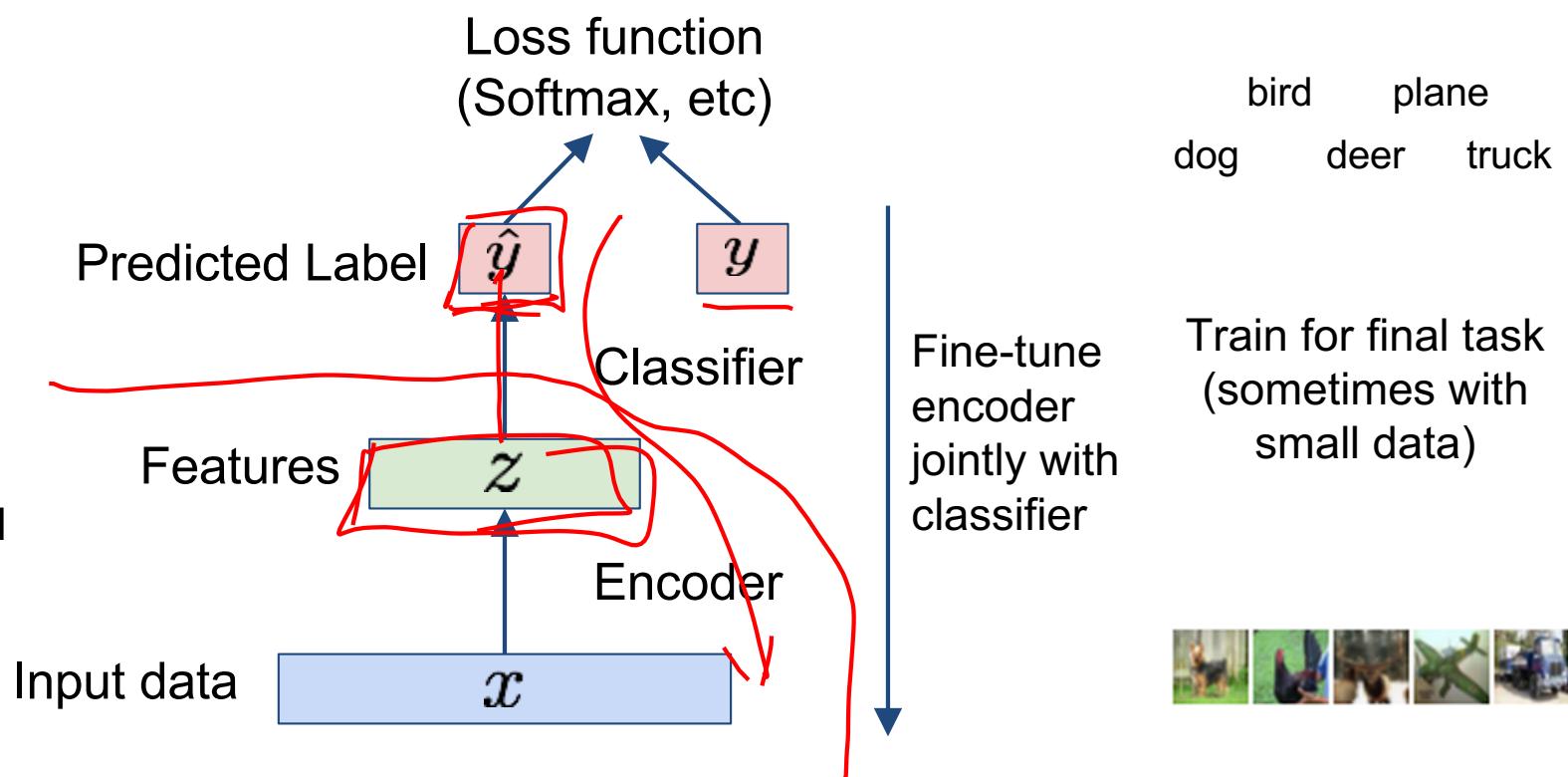


# Autoencoders



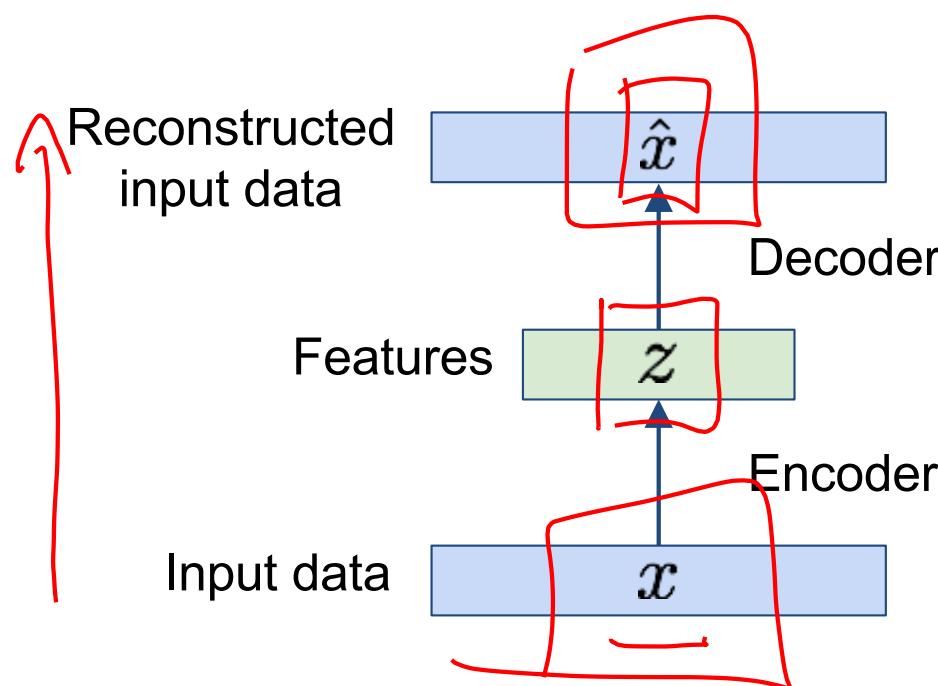
# Autoencoders

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



# Autoencoders

$$g(f(x)) \sim p(z|x)$$



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

Features capture factors of variation in training data. Can we generate new images from an autoencoder?

# Variational Autoencoders

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

# Variational Auto Encoders

VAEs are a combination of the following ideas:

1. Auto Encoders

2. Variational Approximation

- Variational Lower Bound / ELBO

3. Amortized Inference Neural Networks

4. “Reparameterization” Trick

# Basic Problem

- Goal

$$\min_{\theta} \mathbb{E}_{z \sim p_{\theta}(z)} [f(z)]$$

- Need to compute:

$$\nabla_{\theta} \mathbb{E}_{x,y \sim p_{\text{data}}} [l(x,y,\theta)]$$

$$\nabla_{\theta} \mathbb{E}_{z \sim p_{\theta}(z)} [f(z)]$$

$$l(x,y,\theta)$$

$$\approx \frac{1}{N} \sum_i \nabla_{\theta} l(x_i, y_i, \theta)$$

# Example

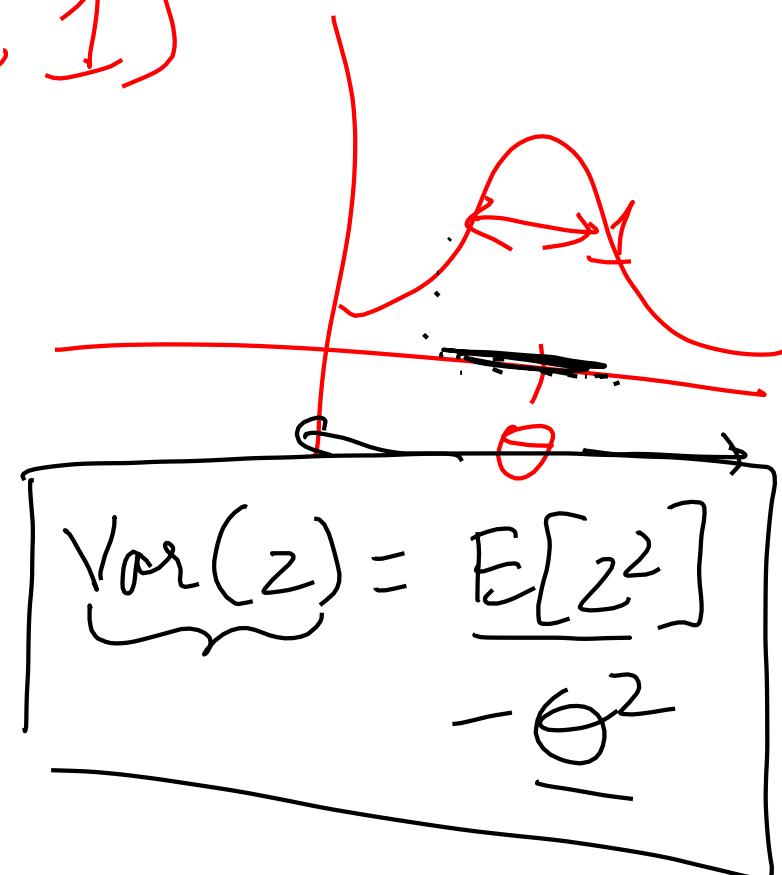
$$z \sim p_{\theta}(z) = N(\theta, 1)$$

$$f(z) = z^2$$

$$\min \mathbb{E}[fz^2]$$

$$\min_{\theta} \left\{ \int p(z) z^2 dz \right\}$$

$\int e^{-\frac{(z-\theta)^2}{2}} z^2 dz$



# Example

# Two Options

- Score Function based Gradient Estimator  
aka REINFORCE (and variants)

$$\underline{\nabla_{\theta} \mathbb{E}_z [f(z)]} = \underline{\mathbb{E}_z [f(z) \nabla_{\theta} \log p_{\theta}(z)]}$$

- Path Derivative Gradient Estimator  
aka “reparameterization trick”

$$\frac{\partial}{\partial \theta} \mathbb{E}_{\underline{z \sim p_{\theta}}} [f(z)] = \frac{\partial}{\partial \theta} \mathbb{E}_{\epsilon} [f(g(\underline{\theta}, \epsilon))] = \mathbb{E}_{\epsilon \sim p_{\epsilon}} \left[ \frac{\partial f}{\partial g} \frac{\partial g}{\partial \theta} \right]$$

# Option 1

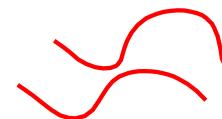
- Score Function based Gradient Estimator  
aka REINFORCE (and variants)

$$\nabla_{\theta} \mathbb{E}_z [f(z)] = \mathbb{E}_z [f(z) \nabla_{\theta} \log p_{\theta}(z)]$$

$$\int f(z) \nabla_{\theta} p_{\theta}(z) dz \cdot \frac{p_{\theta}(z)}{p_{\theta}(z)} = \int [f(z) \nabla_{\theta} \log p(z)] p(z) dz$$

$$\nabla_{\theta} \log p_{\theta}(z) = \mathbb{E} [\underline{f(z) \nabla_{\theta} \log p(z)}]$$

$\frac{1}{N}$



# Example

$$p_0(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(z-\theta)^2}{2}}$$

$$\frac{\partial}{\partial \theta} \log p(z) = -\frac{(z-\theta)^2}{2} - \frac{1}{2} \cancel{\log 2\pi}$$

$$= -\frac{(z-\theta)(-1)}{2}$$

$$\bar{E}[z^2(z-\theta)] \approx \frac{1}{N} \sum z_i^2 (z_i - \theta)$$

# Two Options

- Score Function based Gradient Estimator  
aka REINFORCE (and variants)

$$\nabla_{\theta} \mathbb{E}_z [f(z)] = \mathbb{E}_z [f(z) \nabla_{\theta} \log p_{\theta}(z)]$$

- Path Derivative Gradient Estimator  
aka “reparameterization trick”

$$\frac{\partial}{\partial \theta} \mathbb{E}_{\underline{z \sim p_{\theta}}} [f(z)] = \frac{\partial}{\partial \theta} \mathbb{E}_{\epsilon} [f(g(\theta, \epsilon))] = \mathbb{E}_{\epsilon \sim p_{\epsilon}} \left[ \frac{\partial f}{\partial g} \frac{\partial g}{\partial \theta} \right]$$

# Option 2

- Path Derivative Gradient Estimator  
aka “reparameterization trick”

$$\frac{\partial}{\partial \theta} \mathbb{E}_{z \sim p_\theta} [f(z)] = \frac{\partial}{\partial \theta} \mathbb{E}_\epsilon [f(g(\theta, \epsilon))] = \mathbb{E}_{\epsilon \sim p_\epsilon} \left[ \frac{\partial f}{\partial g} \frac{\partial g}{\partial \theta} \right] \frac{1}{N} \sum$$

$$z \sim p_\theta(z)$$

$$z = g(\underline{\theta}, \underline{\epsilon}) \quad \epsilon \sim N(0, 1)$$

$$\mathbb{E}_{z \sim p(z)} [f(z)] = \mathbb{E}_{\epsilon \sim p(\epsilon)} [f(g(\theta, \epsilon))]$$

# Example

$$z \sim N(0, \sigma^2)$$

$$\varepsilon \sim N(0, 1)$$

$$\underline{z} = \underline{\theta} + \underline{\sigma \varepsilon}$$

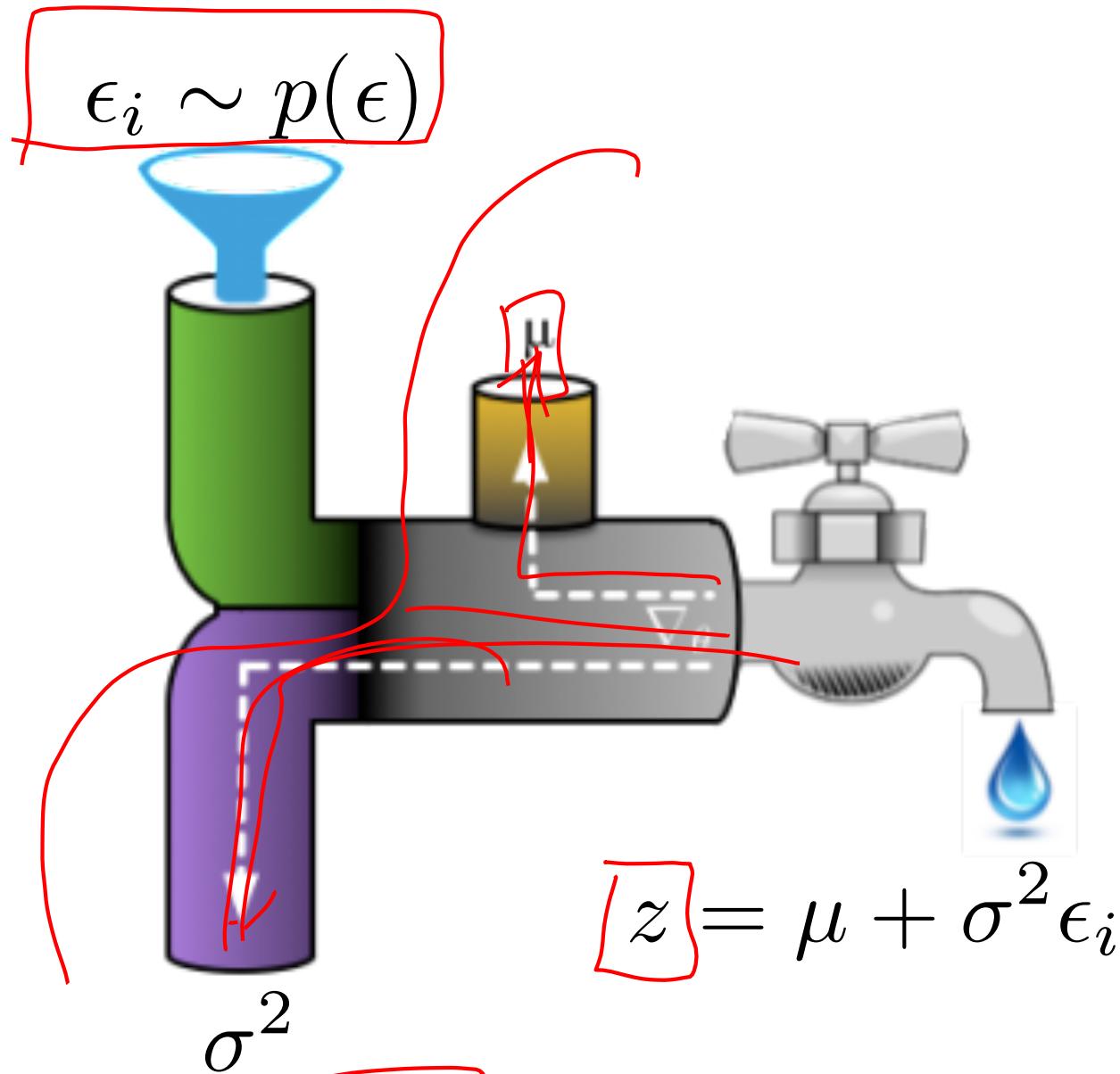
$$\frac{\partial z}{\partial \theta} = 1$$

$$f(z) = z^2$$

$$\frac{\partial f}{\partial \theta} = 2z$$

$$\begin{aligned} E_{\varepsilon \sim p(\varepsilon)}[2z] &= E_{\varepsilon} [2(\underline{\theta} + \underline{\sigma \varepsilon})] \\ &= \frac{1}{N} \sum (\text{---}) \end{aligned}$$

# Reparameterization Intuition



# Two Options

- Score Function based Gradient Estimator  
aka REINFORCE (and variants)

$$\nabla_{\theta} \mathbb{E}_z [f(z)] = \mathbb{E}_z [f(z) \nabla_{\theta} \log p_{\theta}(z)]$$

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$$\frac{\partial}{\partial \theta} \mathbb{E}_{z \sim p_{\theta}} [f(z)] = \frac{\partial}{\partial \theta} \mathbb{E}_{\epsilon} [f(g(\theta, \epsilon))] = \mathbb{E}_{\epsilon \sim p_{\epsilon}} \left[ \frac{\partial f}{\partial g} \frac{\partial g}{\partial \theta} \right]$$

# Example

```
import numpy as np
N = 1000
theta = 2.0
x = np.random.randn(N) + theta
eps = np.random.randn(N)

grad1 = lambda x: np.sum(np.square(x)*(x-theta)) / x.size
grad2 = lambda eps: np.sum(2*(theta + eps)) / x.size

print grad1(x)
print grad2(eps)
```

4.46239612174  
4.1840532024

# Example

```
Ns = [10, 100, 1000, 10000, 100000]
reps = 100

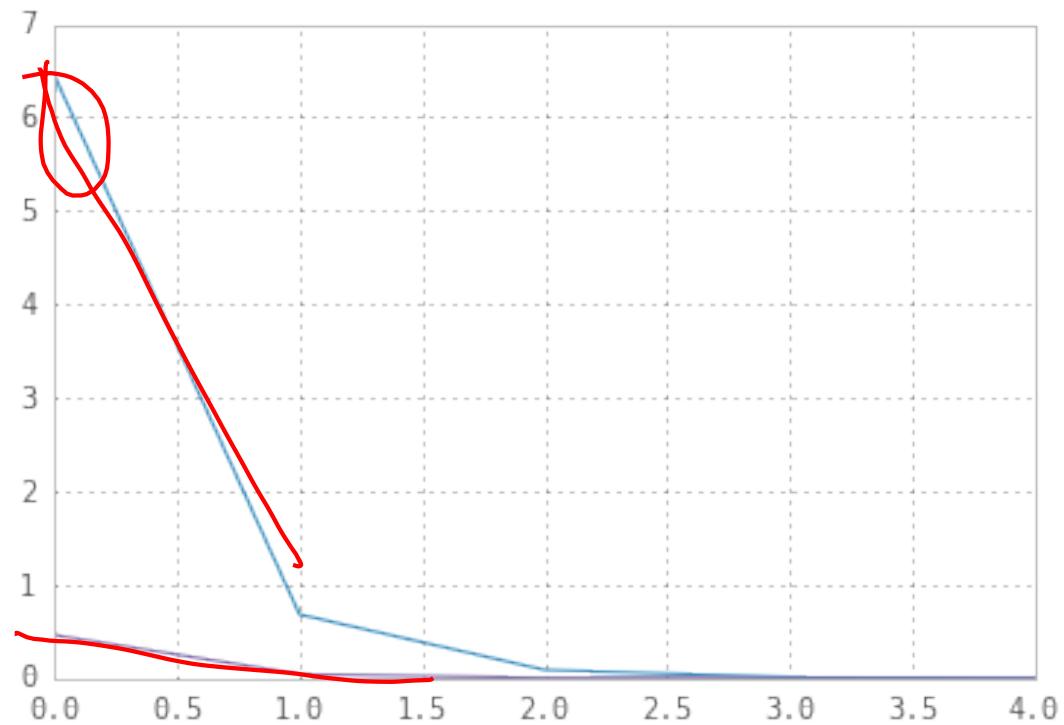
means1 = np.zeros(len(Ns))
vars1 = np.zeros(len(Ns))
means2 = np.zeros(len(Ns))
vars2 = np.zeros(len(Ns))

est1 = np.zeros(reps)
est2 = np.zeros(reps)
for i, N in enumerate(Ns):
    for r in range(reps):
        x = np.random.randn(N) + theta
        est1[r] = grad1(x)
        eps = np.random.randn(N)
        est2[r] = grad2(eps)
    means1[i] = np.mean(est1)
    means2[i] = np.mean(est2)
    vars1[i] = np.var(est1)
    vars2[i] = np.var(est2)

print means1
print means2
print
print vars1
print vars2
```

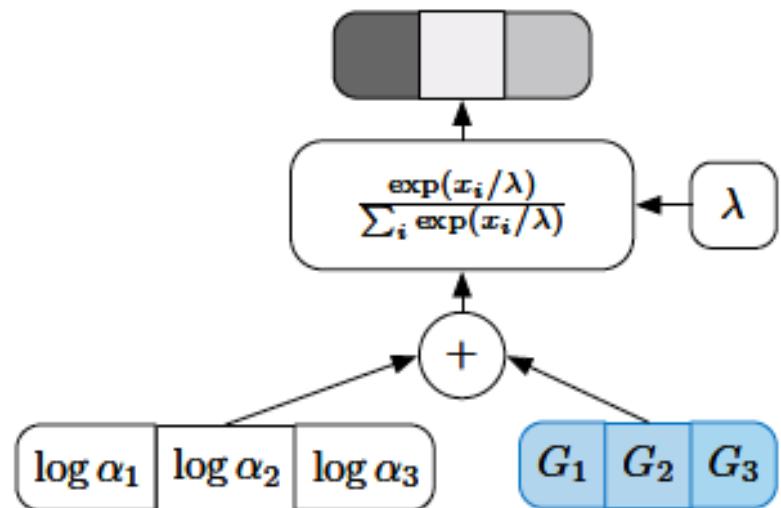
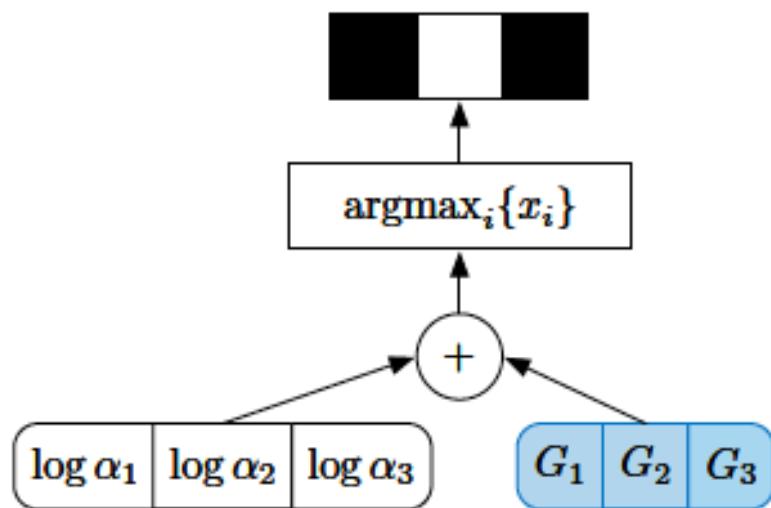
```
[ 3.8409546  3.97298803  4.03007634  3.98531095  3.99579423]
[ 3.97775271  4.00232825  3.99894536  4.00353734  3.99995899]

[ 6.45307927e+00   6.80227241e-01   8.69226368e-02   1.00489791e-02
 8.62396526e-04]
[ 4.59767676e-01   4.26567475e-02   3.33699503e-03   5.17148975e-04
 4.65338152e-05]
```



# Aside: Gumbel Softmax

- Meet the Gumbel Softmax “trick”



# Aside: Gumbel Softmax

- Sampling on the Simplex

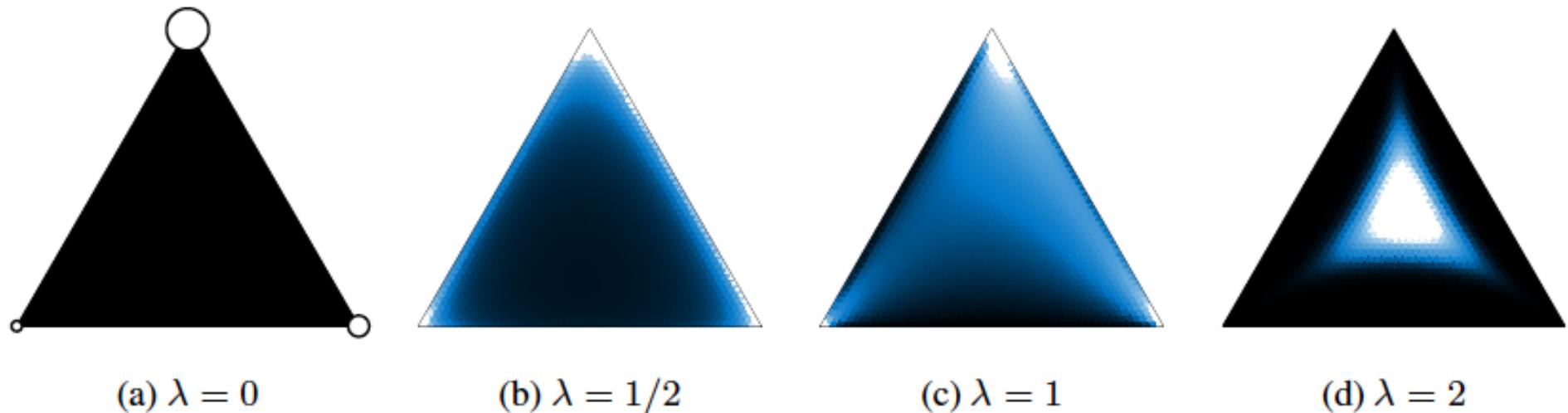


Figure 2: A discrete distribution with unnormalized probabilities  $(\alpha_1, \alpha_2, \alpha_3) = (2, 0.5, 1)$  and three corresponding Concrete densities at increasing temperatures  $\lambda$ . Each triangle represents the set of points  $(y_1, y_2, y_3)$  in the simplex  $\Delta^2 = \{(y_1, y_2, y_3) \mid y_k \in (0, 1), y_1 + y_2 + y_3 = 1\}$ . For  $\lambda = 0$  the size of white circles represents the mass assigned to each vertex of the simplex under the discrete distribution. For  $\lambda \in \{2, 1, 0.5\}$  the intensity of the shading represents the value of  $p_{\alpha, \lambda}(y)$ .

# Variational Auto Encoders

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- Variational Lower Bound / ELBO

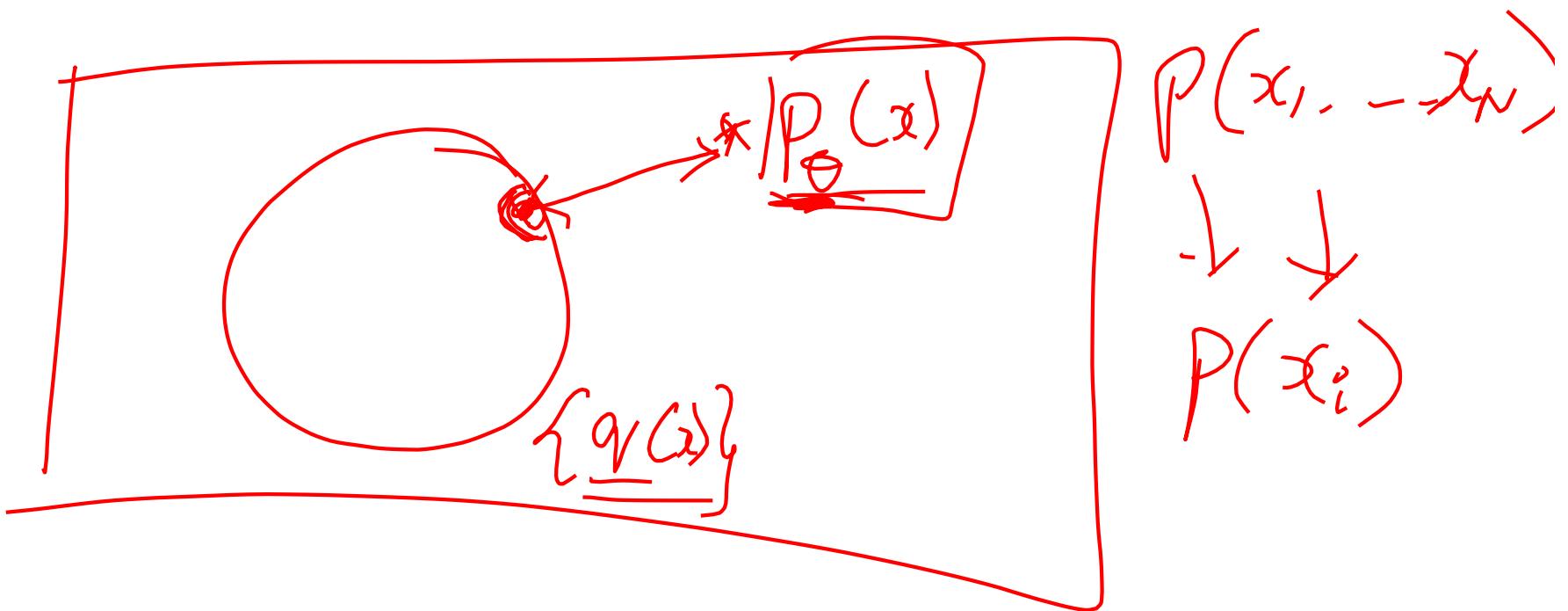
3. Amortized Inference Neural Networks

4. “Reparameterization” Trick

# What is Variational Inference?

- A class of methods for
  - approximate inference, parameter learning
  - And approximating integrals basically..
- Key idea
  - Reality is complex
  - Instead of performing approximate computation in something complex,
  - Can we perform exact computation in something “simple”?
  - Just need to make sure the simple thing is “close” to the complex thing.

# Intuition



# KL divergence: Distance between distributions

- Given two distributions  $p$  and  $q$  KL divergence:

$$D(p||q)$$

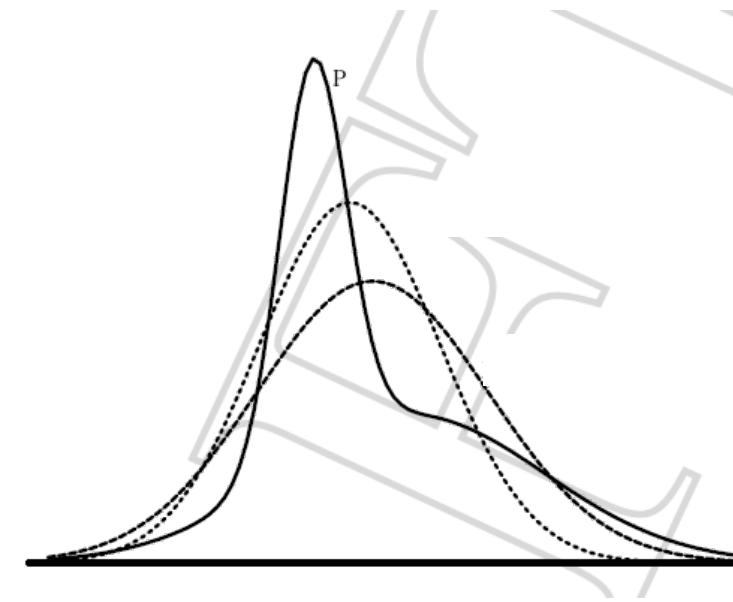
$$\sum_x p(x) \log \frac{p(x)}{q(x)}$$

- $D(p||q) = 0$  iff  $p=q$

- Not symmetric –  $p$  determines where difference is important

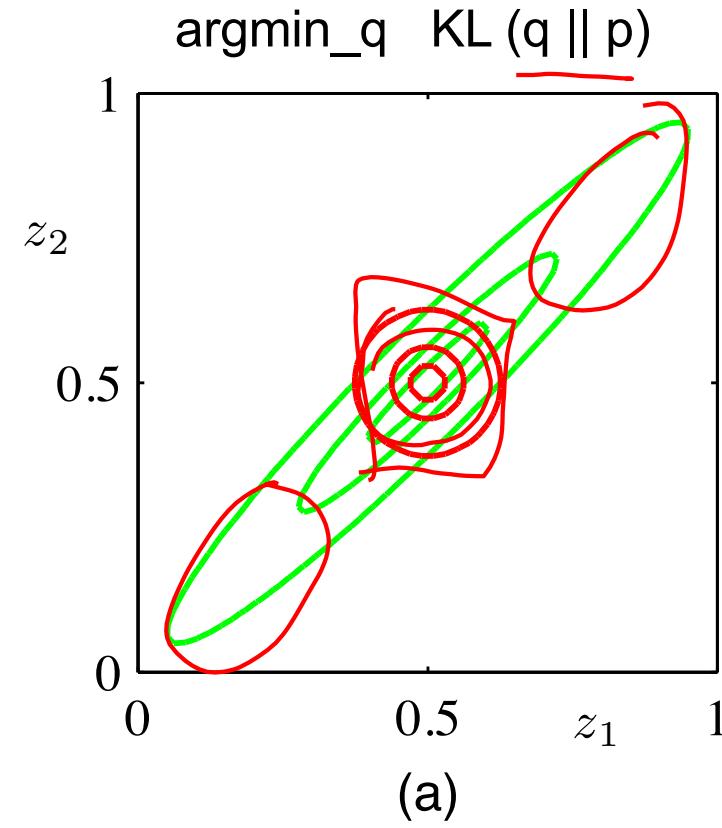
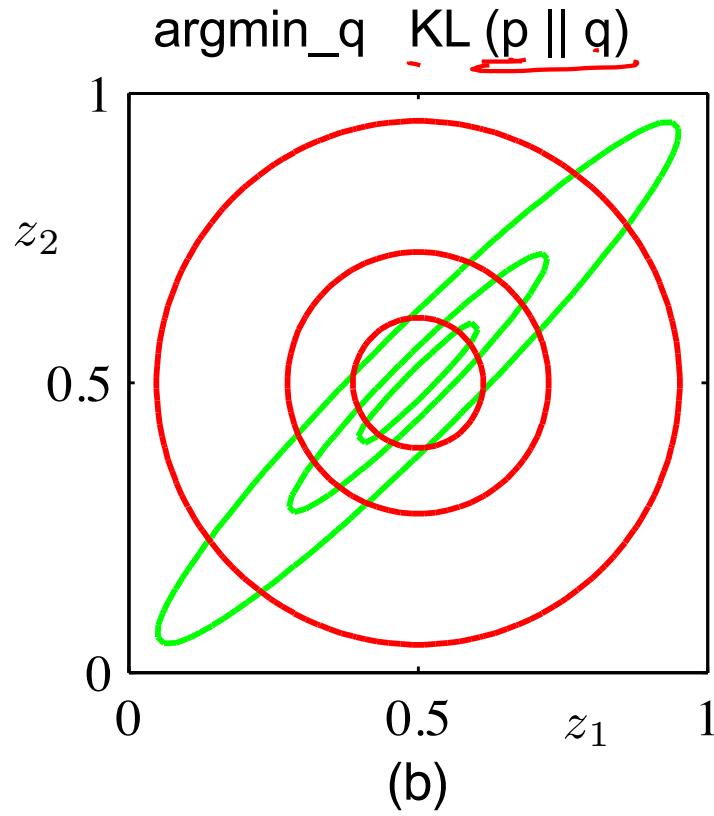
# Find simple approximate distribution

- Suppose  $p$  is intractable posterior
- Want to find simple  $q$  that approximates  $p$
- KL divergence not symmetric
- $D(p||q)$ 
  - true distribution  $p$  defines support of diff.
  - the “correct” direction
  - will be intractable to compute
- $\underline{D(q||p)}$ 
  - approximate distribution defines support
  - tends to give overconfident results
  - will be tractable



# Example 1

- $p = 2D$  Gaussian with arbitrary co-variance
- $q = 2D$  Gaussian with diagonal co-variance

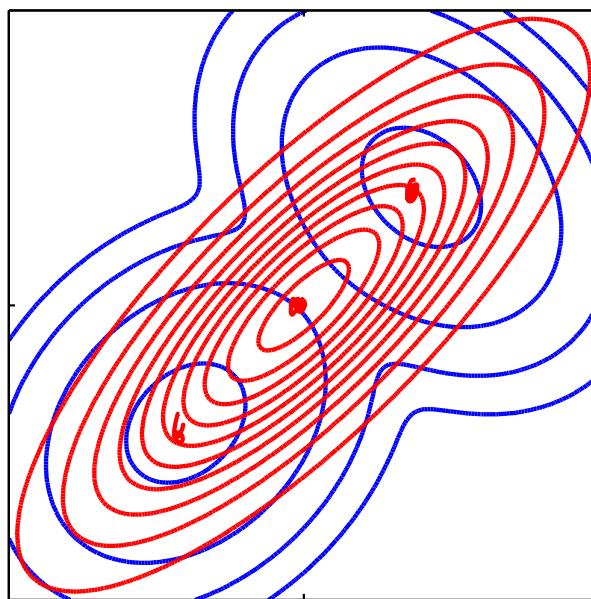


$p = \text{Green}; q = \text{Red}$

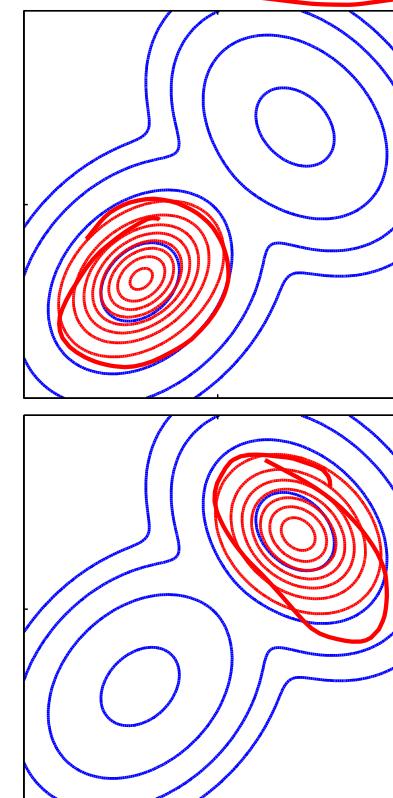
# Example 2

- p = Mixture of Two Gaussians
- q = Single Gaussian

$\text{argmin}_q \text{ KL}(p \parallel q)$



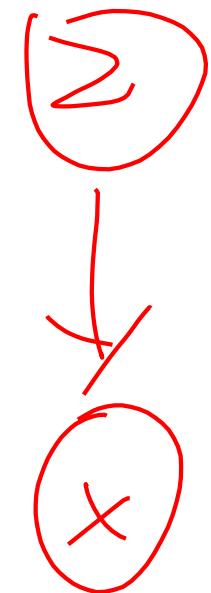
$\text{argmin}_q \text{ KL}(q \parallel p)$



# The general learning problem with missing data

- Marginal likelihood –  $\mathbf{x}$  is observed,  $\mathbf{z}$  is missing:

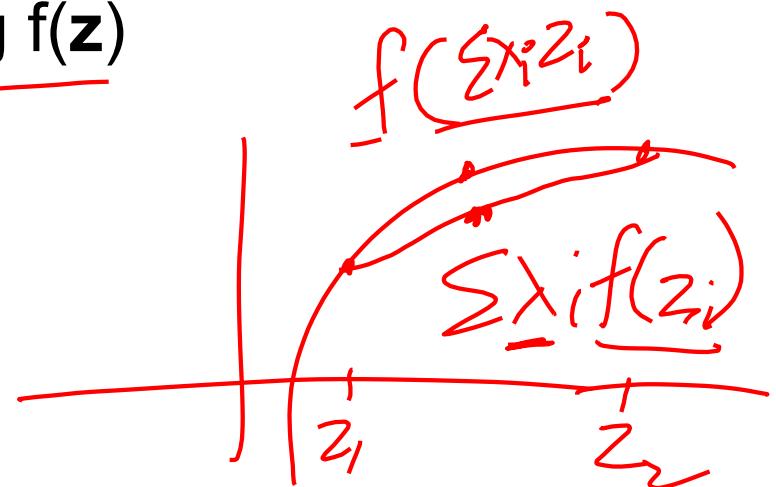
$$\begin{aligned} \underline{ll(\theta : \mathcal{D})} &= \log \prod_{i=1}^N P(\underline{\mathbf{x}_i} | \theta) \\ &= \sum_{i=1}^N \log P(\underline{\mathbf{x}_i} | \theta) \\ &= \sum_{i=1}^N \left[ \log \sum_{\mathbf{z}} P(\mathbf{x}_i, \mathbf{z} | \theta) \right] \end{aligned}$$



# Applying Jensen's inequality

- Use:  $\underline{\log \sum_z P(z) f(z)} \geq \underline{\sum_z P(z) \log f(z)}$

$\log(\cdot)$



# Applying Jensen's inequality

- Use:  $\log \underbrace{\sum_{\mathbf{z}} P(\mathbf{z})}_{\text{red}} f(\mathbf{z}) \geq \sum_{\mathbf{z}} P(\mathbf{z}) \underbrace{\log f(\mathbf{z})}_{\text{red}}$

$$ll(\theta : \mathcal{D}) = \sum_{i=1}^N \log \sum_{\mathbf{z}} Q_i(\mathbf{z}) \frac{P(\mathbf{x}_i, \mathbf{z} \mid \theta)}{Q_i(\mathbf{z})}$$

The equation shows the log-likelihood function for a dataset  $\mathcal{D}$ . It consists of a sum over  $i$  from 1 to  $N$ , where each term is the log of a sum over  $\mathbf{z}$  of the ratio  $P(\mathbf{x}_i, \mathbf{z} \mid \theta) / Q_i(\mathbf{z})$ . Red annotations highlight the terms  $\sum_{\mathbf{z}} Q_i(\mathbf{z})$  and  $P(\mathbf{x}_i, \mathbf{z} \mid \theta) / Q_i(\mathbf{z})$ .

# Evidence Based Lower Bound

- Define potential function  $F(\theta, Q)$ :

$$\max_{\theta} \boxed{ll(\theta : \mathcal{D})} \geq \boxed{F(\theta, Q_i)} = \sum_{i=1}^N \sum_{\mathbf{z}} Q_i(\mathbf{z}) \log \frac{\overbrace{P(\mathbf{x}_i, \mathbf{z} | \theta)}^{\text{P}(\mathbf{x}_i | \mathbf{z}, \theta) P(\mathbf{z} | \theta)}}{\overbrace{Q_i(\mathbf{z})}^{Q_i(\mathbf{z})}}$$

$$\begin{aligned} & \max_{\theta} \boxed{Q_i(\mathbf{z}), \theta} \quad \left| \sum_{\mathbf{z}} Q_i(\mathbf{z}) \log \overbrace{P(\mathbf{x}_i | \mathbf{z}, \theta)}^{\mathbb{E}_{\mathbf{z} \sim Q_i(\mathbf{z})} [\log P(\mathbf{x}_i | \mathbf{z}, \theta)]} \right. \\ & + \left. \sum_{\mathbf{z}} Q_i(\mathbf{z}) \log \frac{\overbrace{P(\mathbf{z} | \theta)}^{\log P(\mathbf{z} | \theta)}}{Q_i(\mathbf{z})} \right. \\ & - \left. \boxed{-KL(Q_i(\mathbf{z}) || P_\theta(\mathbf{z}))} \right. \end{aligned}$$

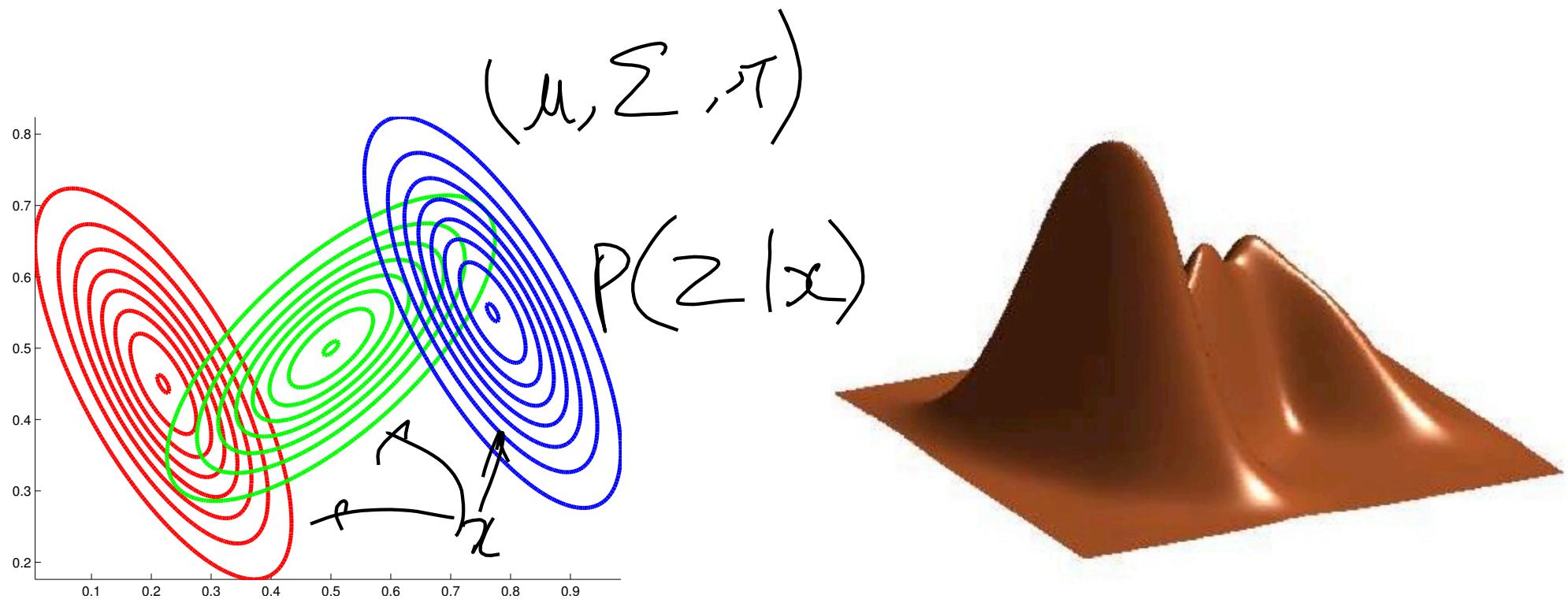
# Evidence Based Lower Bound

- Define potential function  $F(\theta, Q)$ :

$$ll(\theta : \mathcal{D}) \geq F(\theta, Q_i) = \sum_{i=1}^N \sum_{\mathbf{z}} Q_i(\mathbf{z}) \log \frac{P(\mathbf{x}_i, \mathbf{z} \mid \theta)}{Q_i(\mathbf{z})}$$

- EM corresponds to coordinate ascent on  $F$ 
  - Thus, maximizes lower bound on marginal log likelihood

# GMM

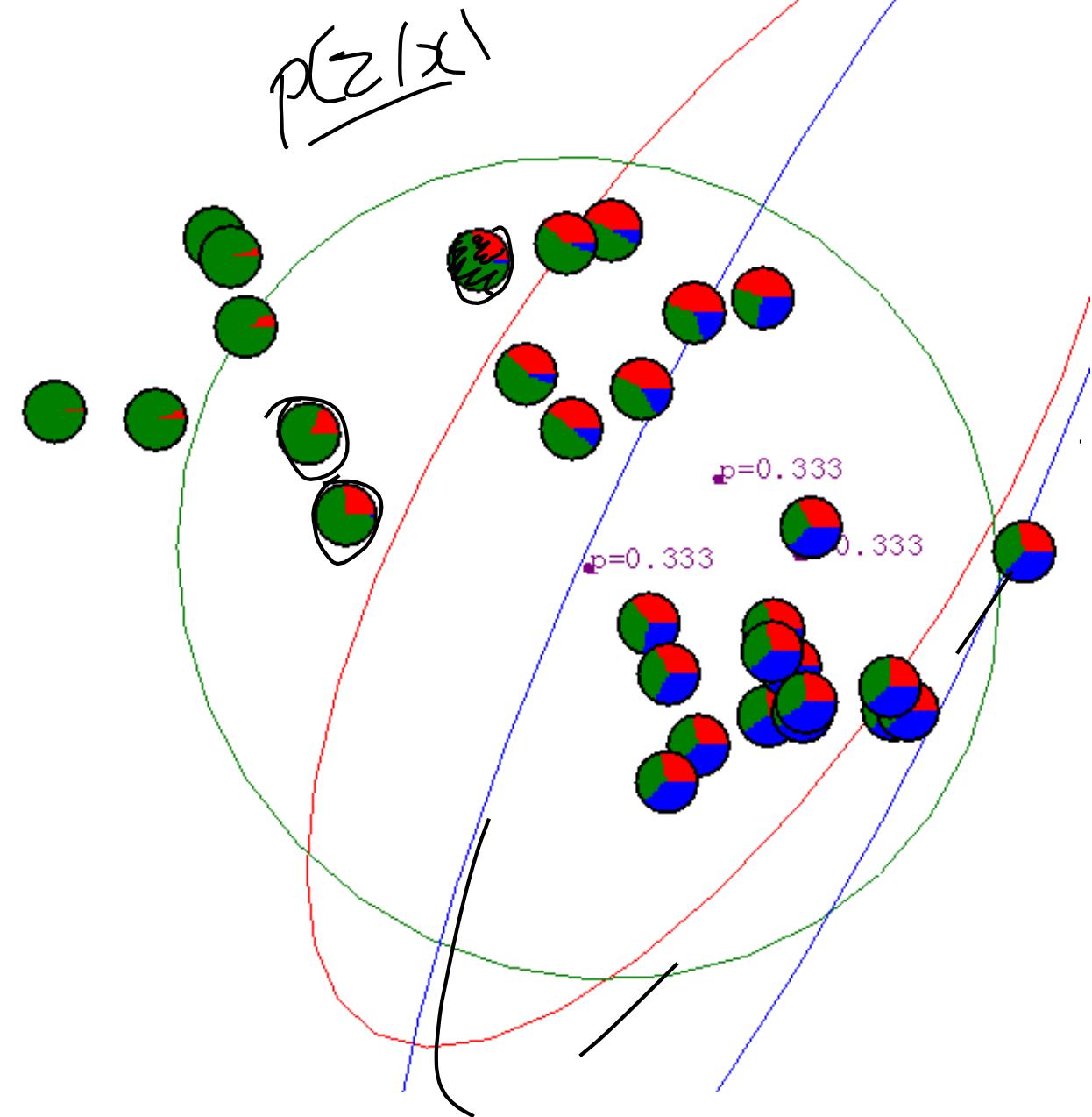




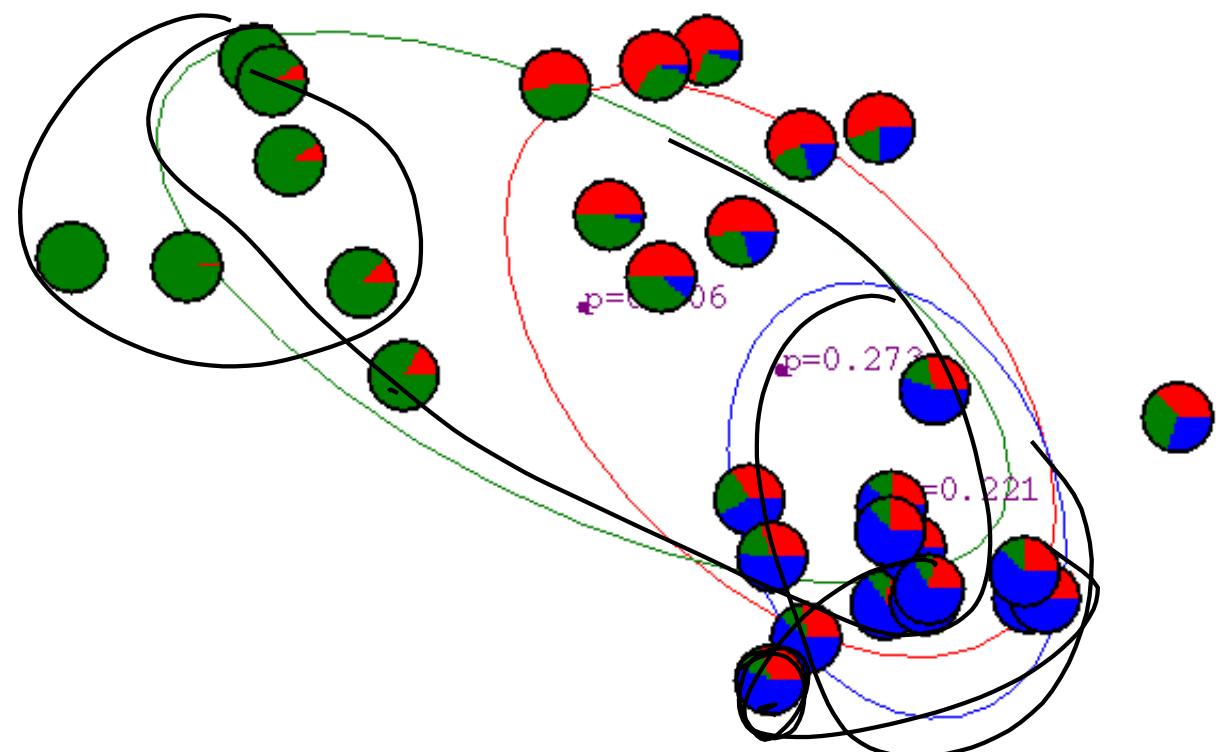
# EM for Learning GMMs

- Simple Update Rules
  - E-Step: estimate  $Q_i(z) = \Pr(z = j | x_i)$
  - M-Step: maximize full likelihood weighted by posterior

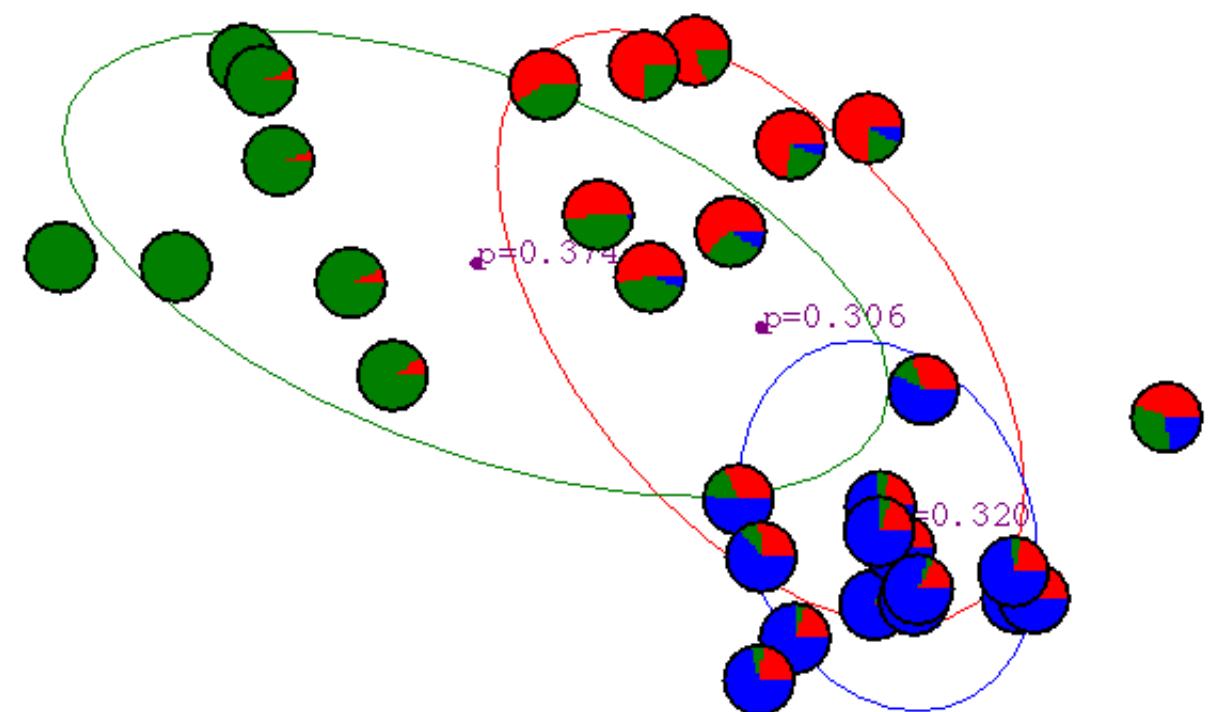
# Gaussian Mixture Example: Start



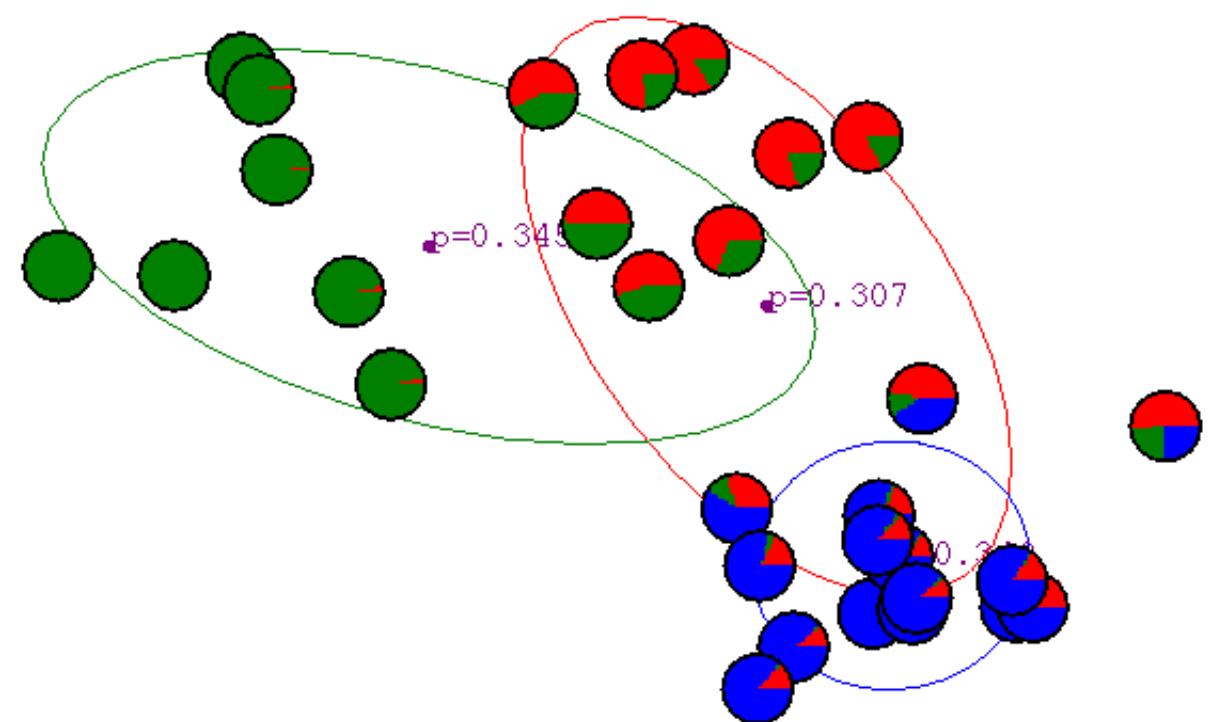
# After 1st iteration



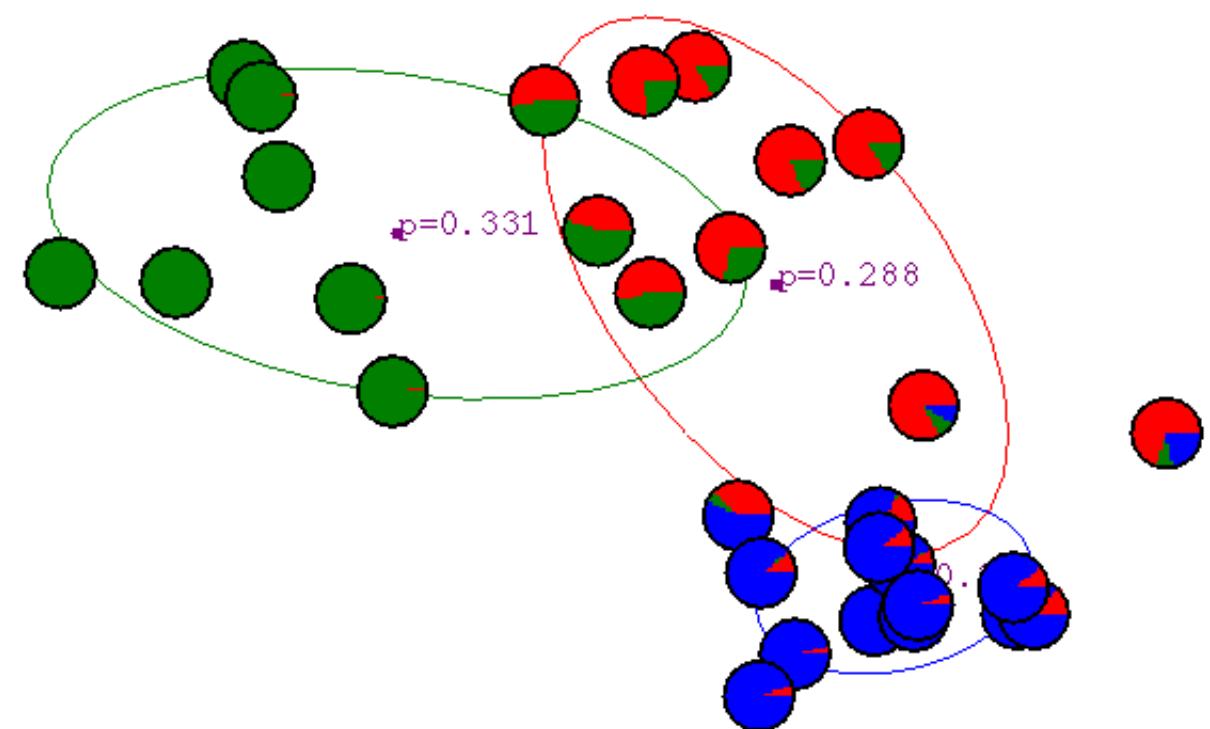
# After 2nd iteration



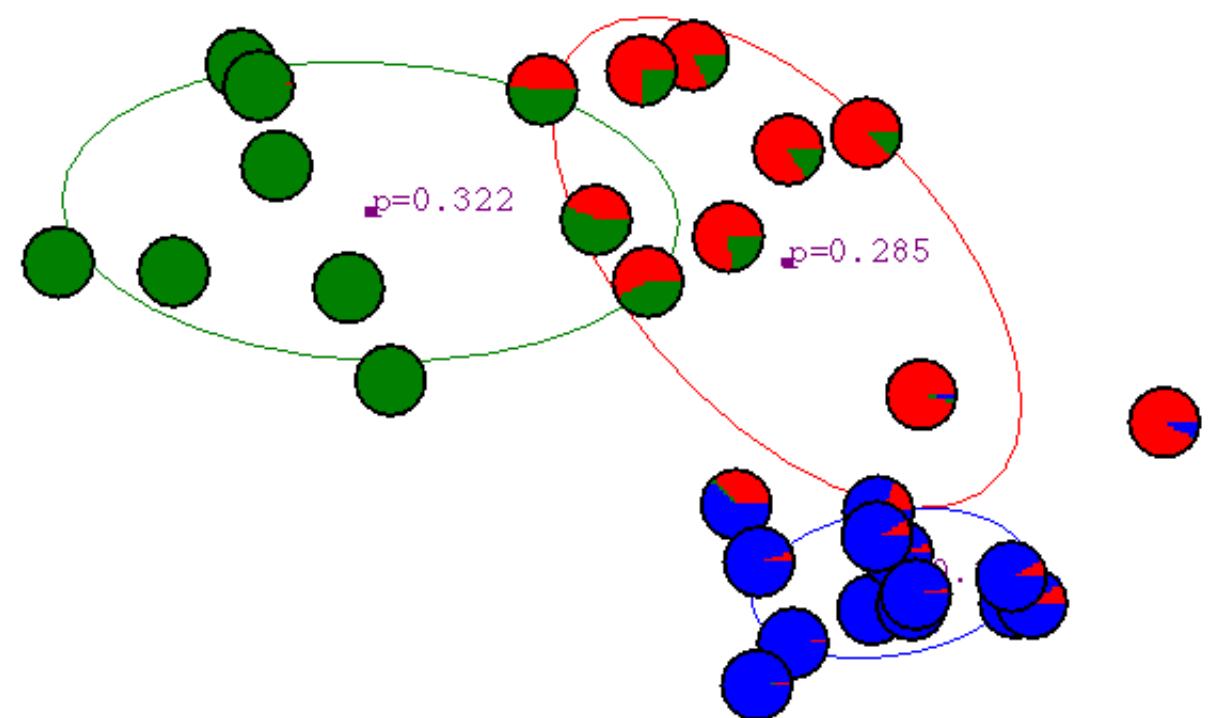
# After 3rd iteration



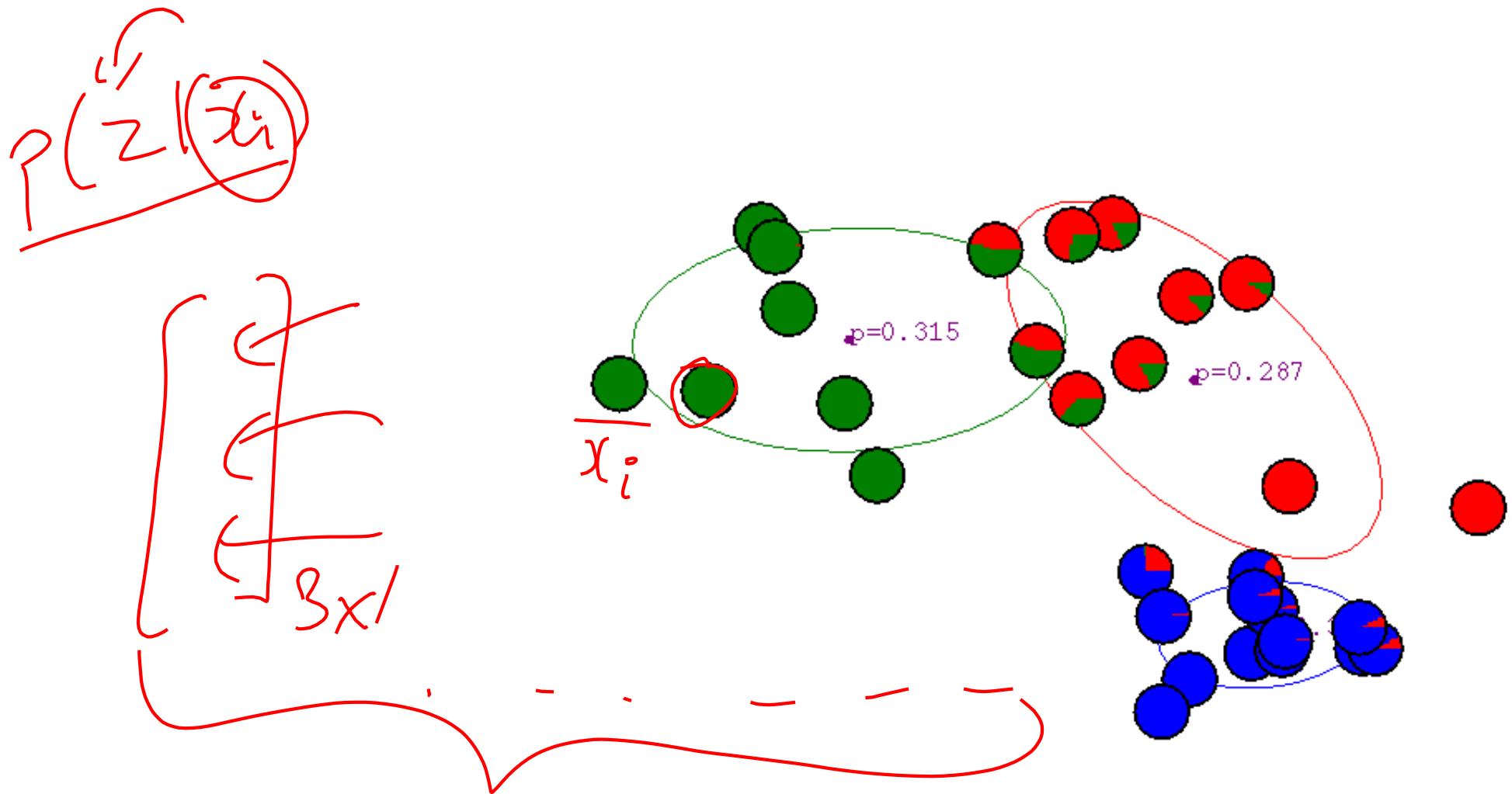
# After 4th iteration



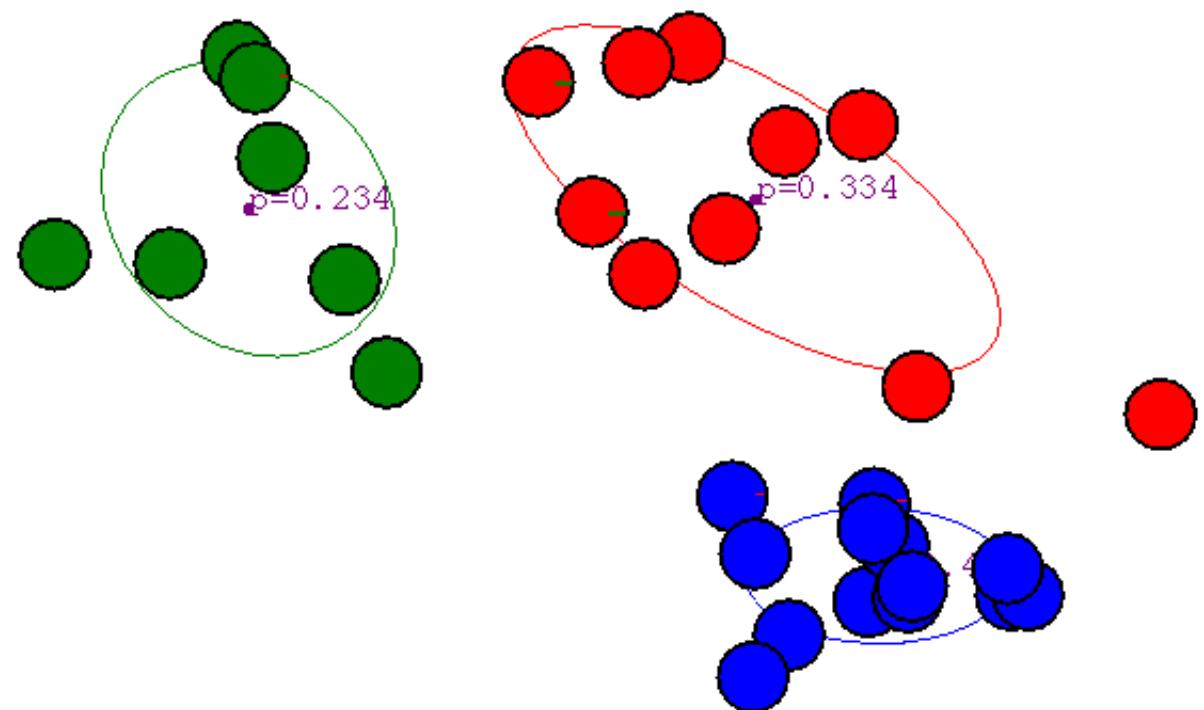
# After 5th iteration



# After 6th iteration



# After 20th iteration



# Variational Auto Encoders

VAEs are a combination of the following ideas:

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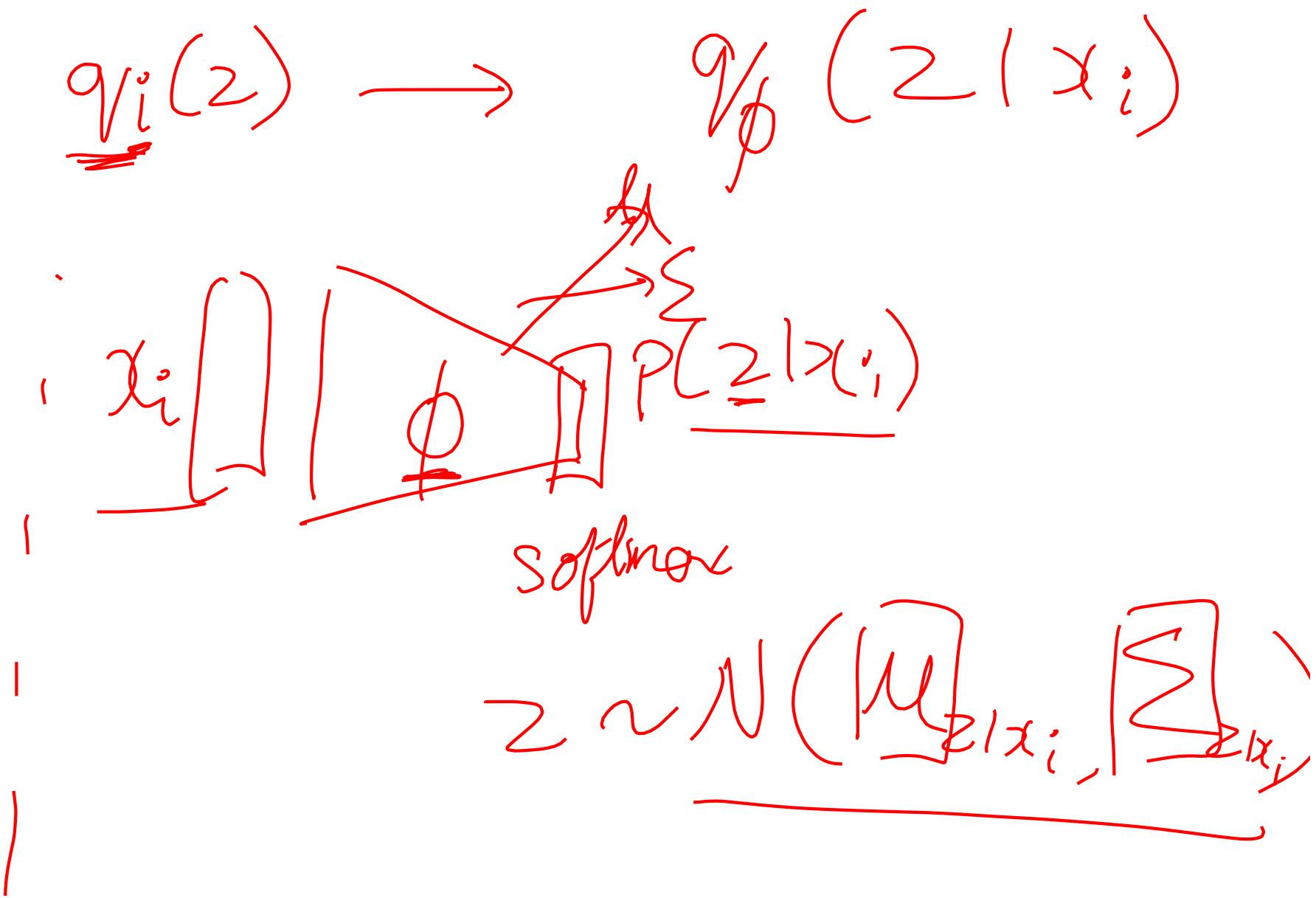
2. Variational Approximation

- Variational Lower Bound / ELBO

3. Amortized Inference Neural Networks

4. “Reparameterization” Trick

# Amortized Inference Neural Networks



# Variational Auto Encoders

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 Auto Encoders

Putting it all together: maximizing the likelihood lower bound

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

Let's look at computing the bound (forward pass) for a given minibatch of input data

Input Data

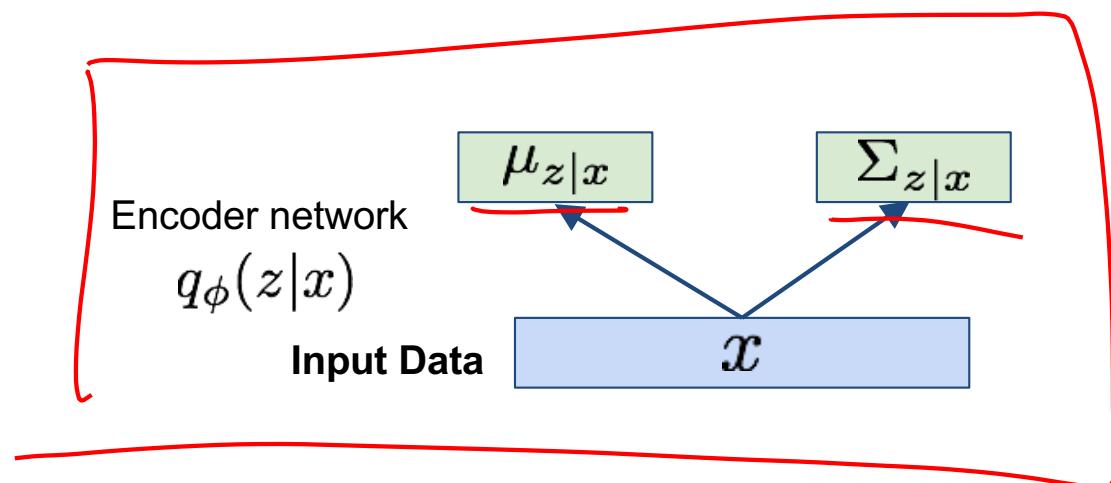
$x$



# Variational Auto Encoders

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 Auto Encoders

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

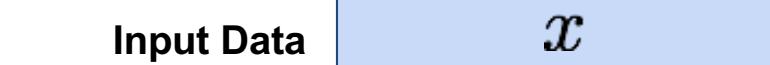
Encoder network

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

Input Data

$$\mu_{z|x}$$

$$\Sigma_{z|x}$$

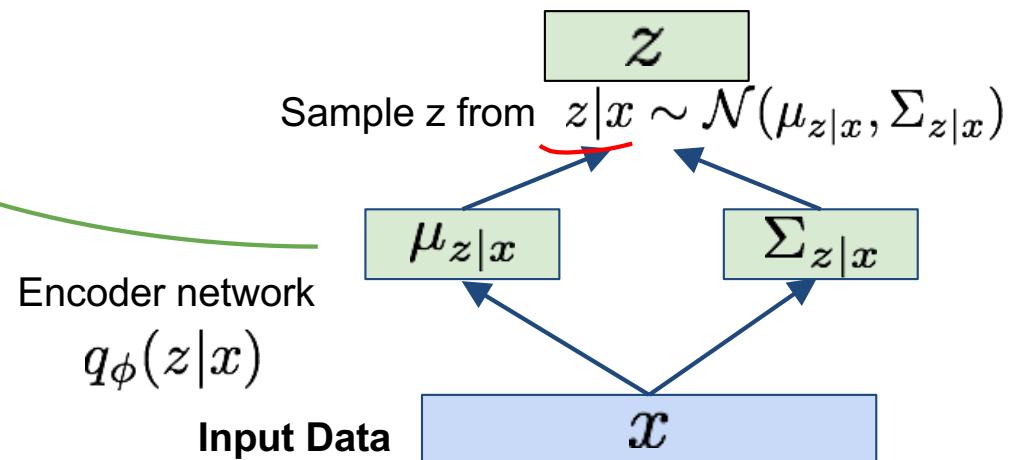


# Variational Auto Encoders

Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

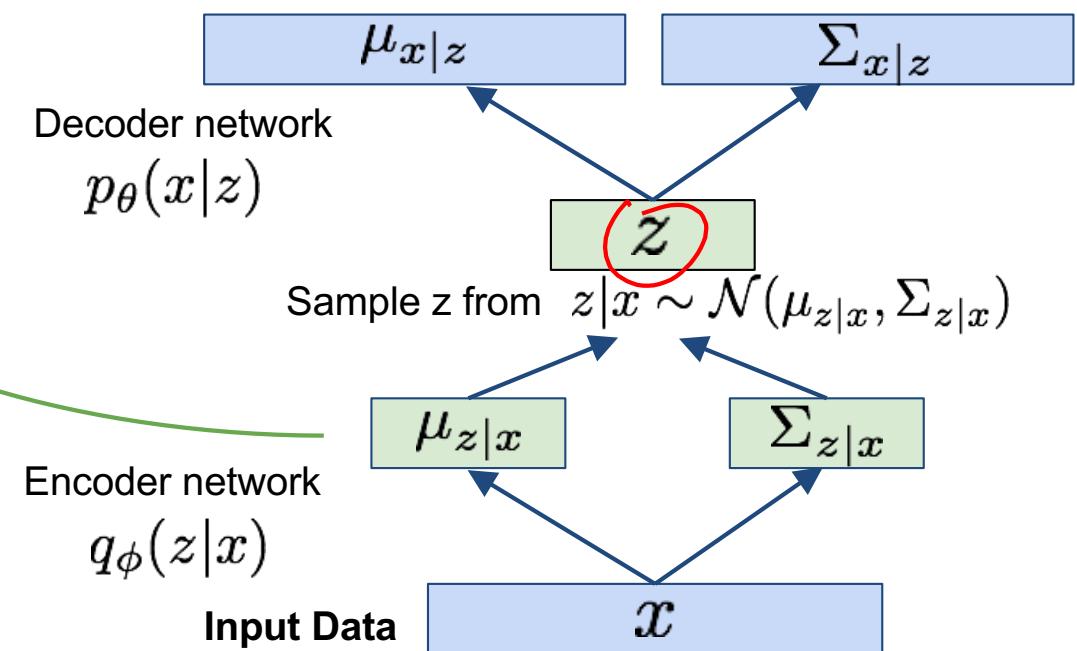


# Variational Auto Encoders

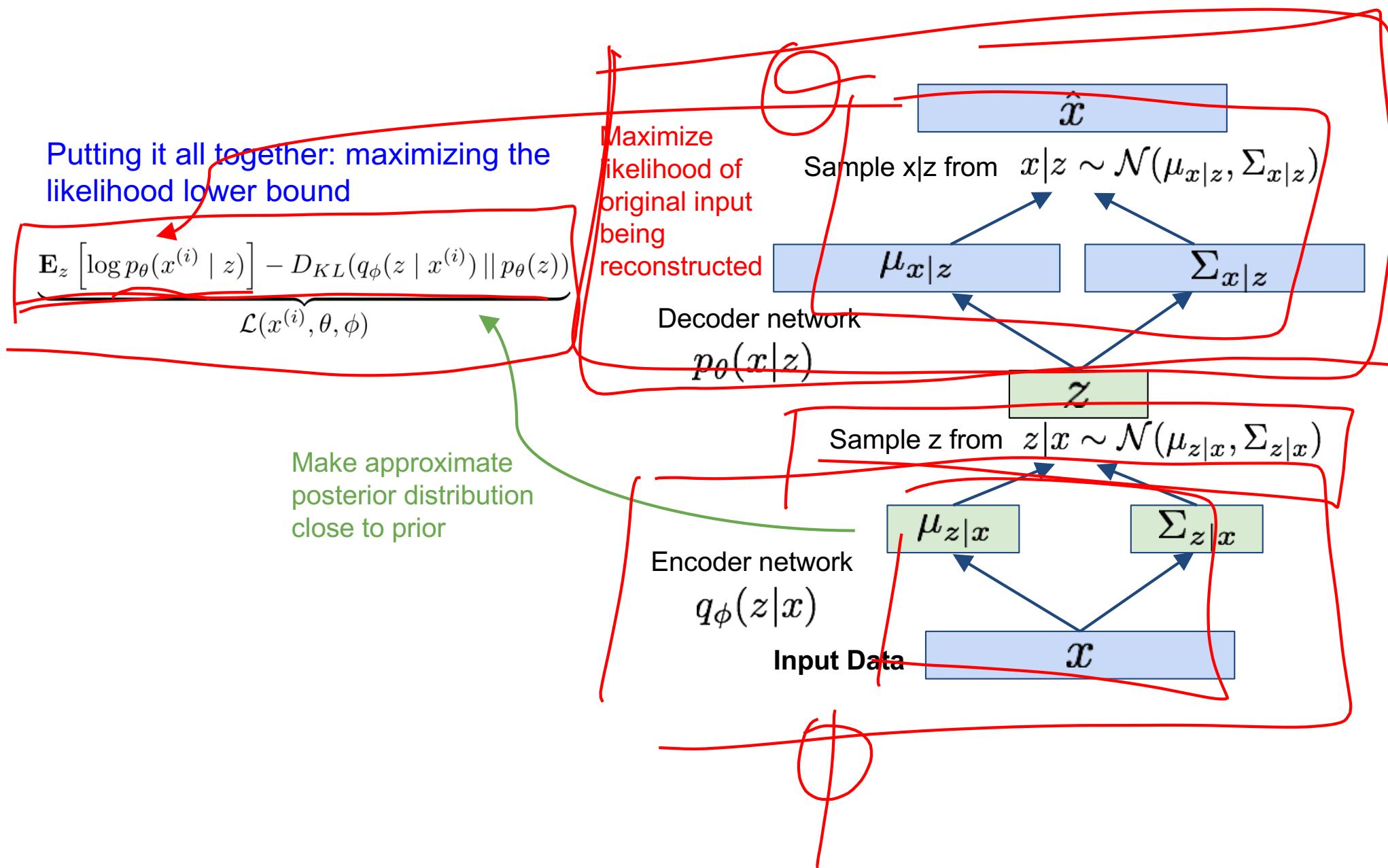
Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior



# Variational Auto Encoders

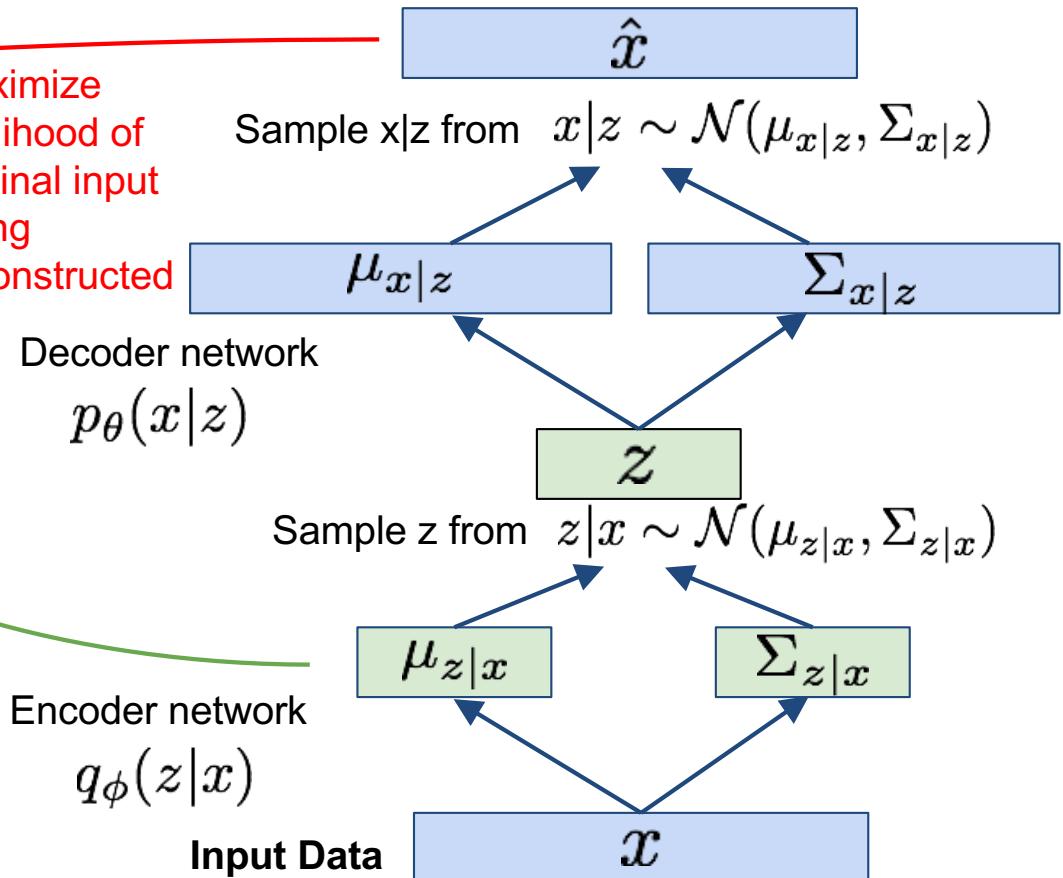


# Variational Auto Encoders

Putting it all together: maximizing the likelihood lower bound

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

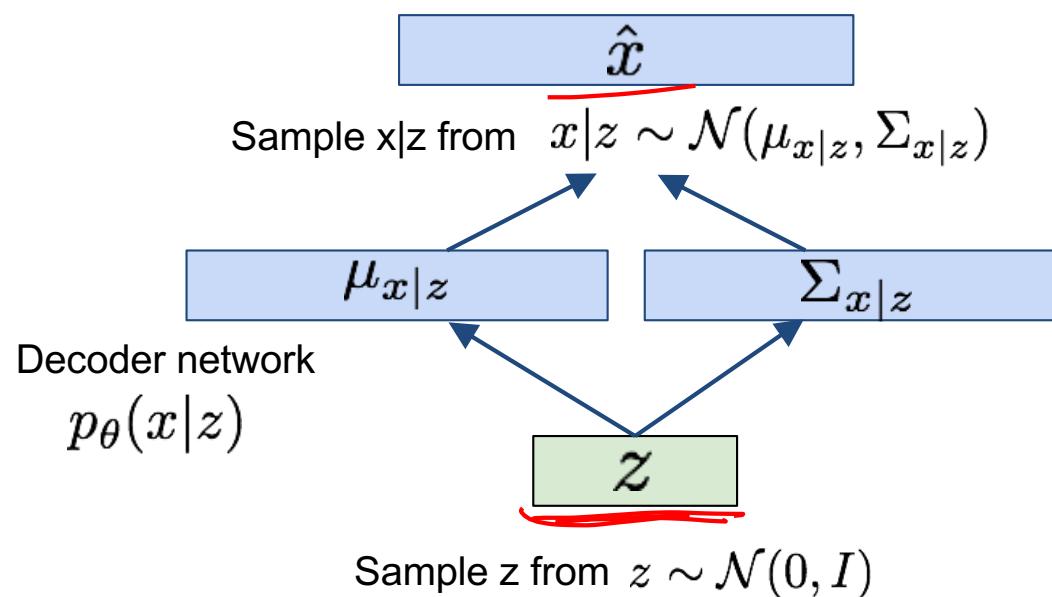
Maximize likelihood of original input being reconstructed



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

# Variational Auto Encoders: Generating Data

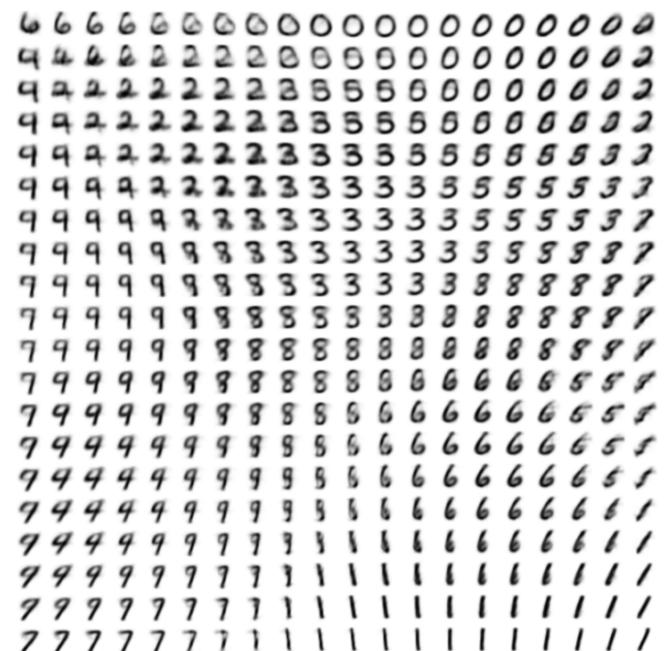
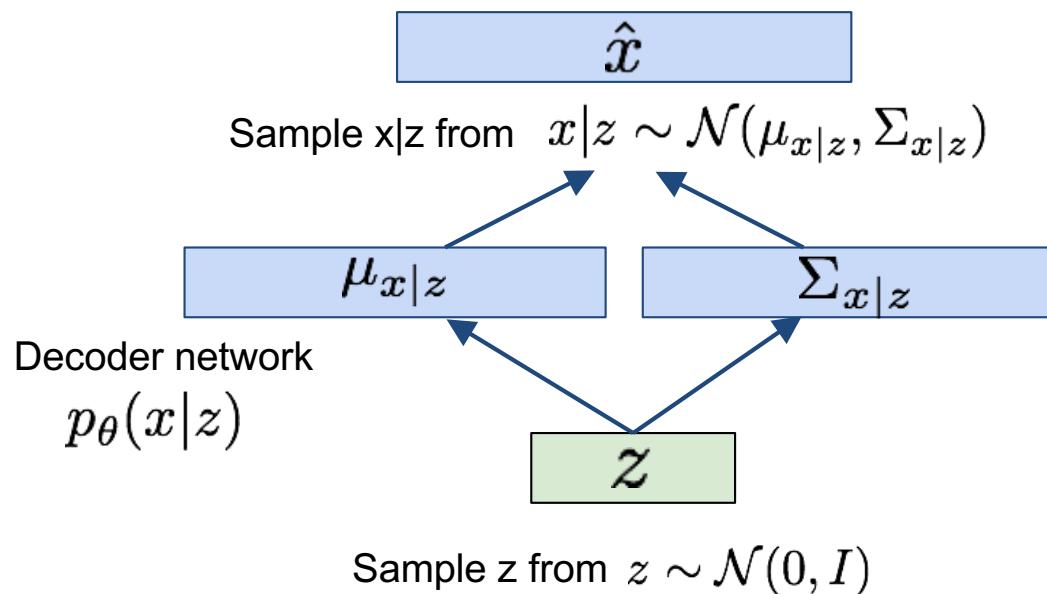
Use decoder network. Now sample z from prior!



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

# Variational Auto Encoders: Generating Data

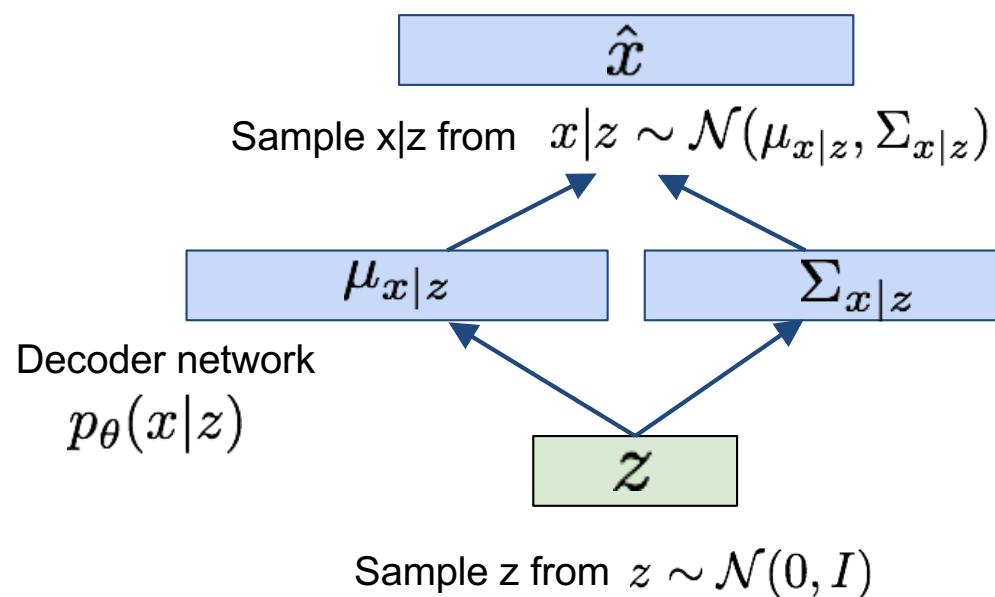
Use decoder network. Now sample z from prior!



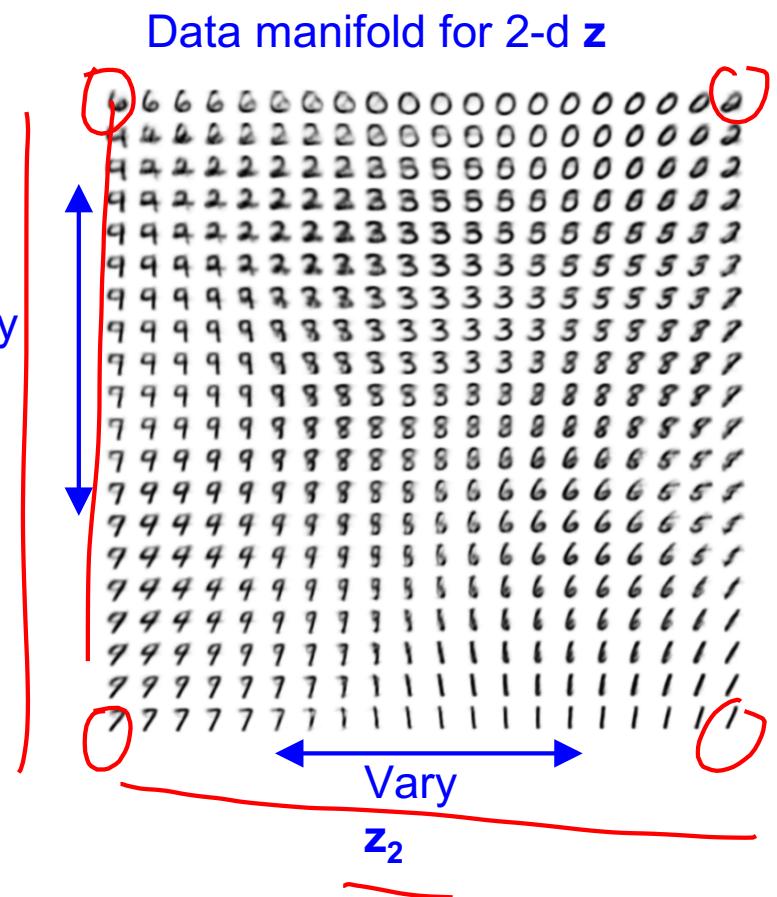
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

# Variational Auto Encoders: Generating Data

Use decoder network. Now sample z from prior!



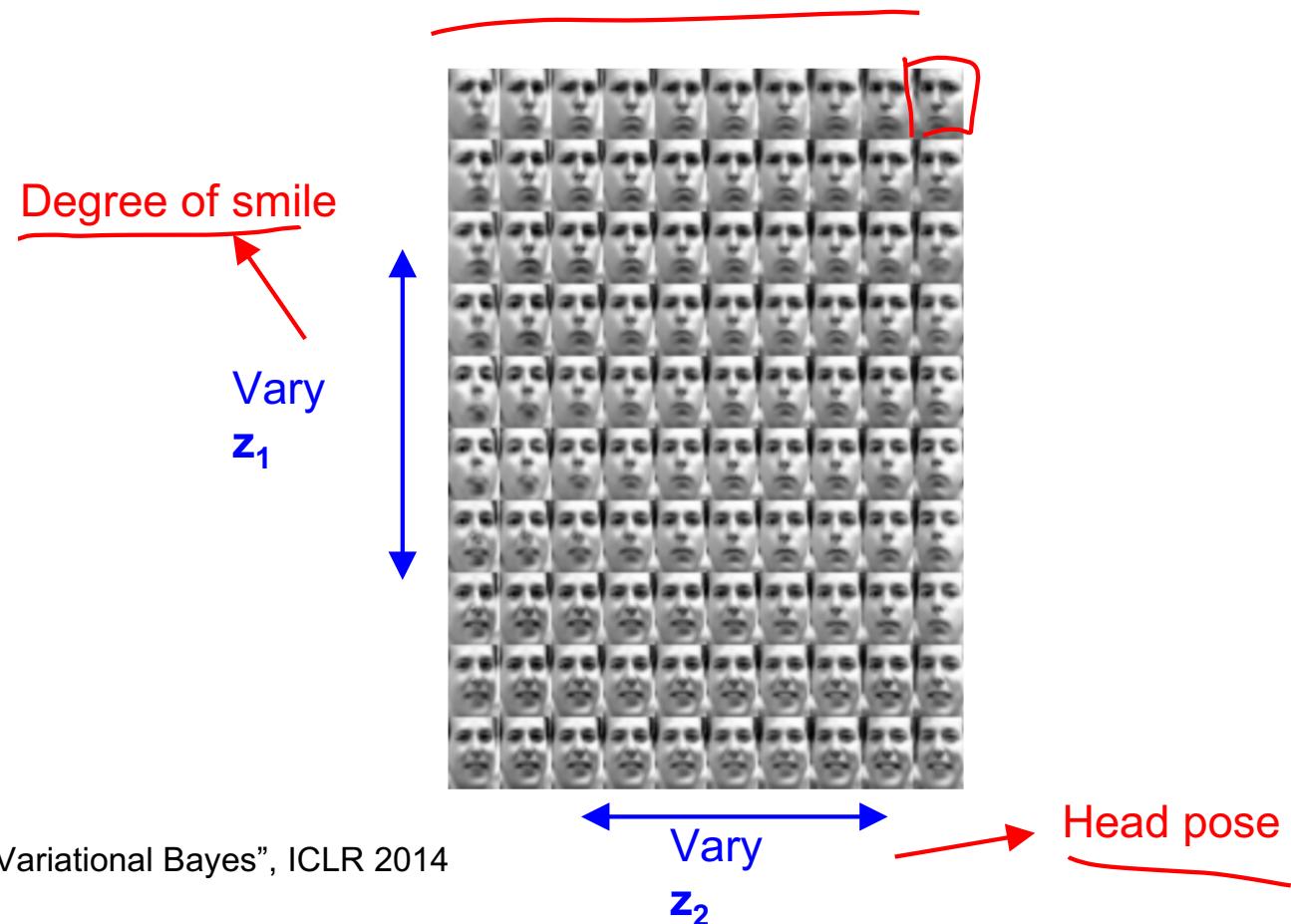
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014



# Variational Auto Encoders: Generating Data

Diagonal prior on  $\mathbf{z}$   
=> independent  
latent variables

Different  
dimensions of  $\mathbf{z}$   
encode  
interpretable factors  
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Also good feature representation that  
can be computed using  $q_\phi(\mathbf{z}|\mathbf{x})$ !

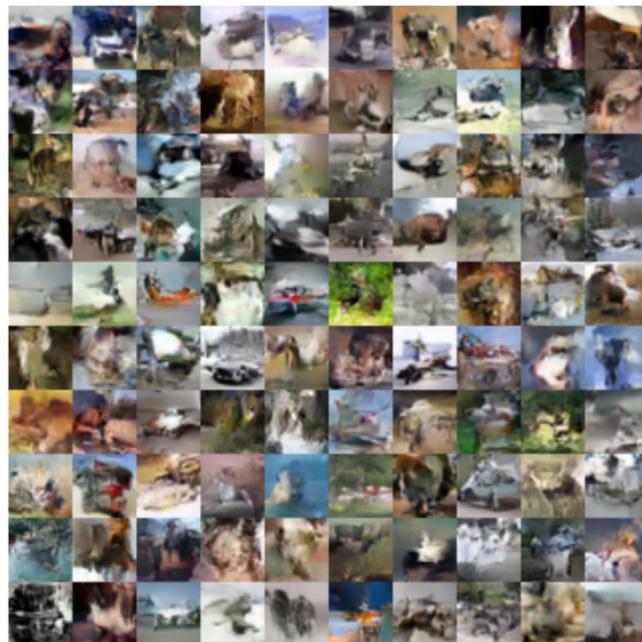
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Degree of smile  
Vary  $\mathbf{z}_1$

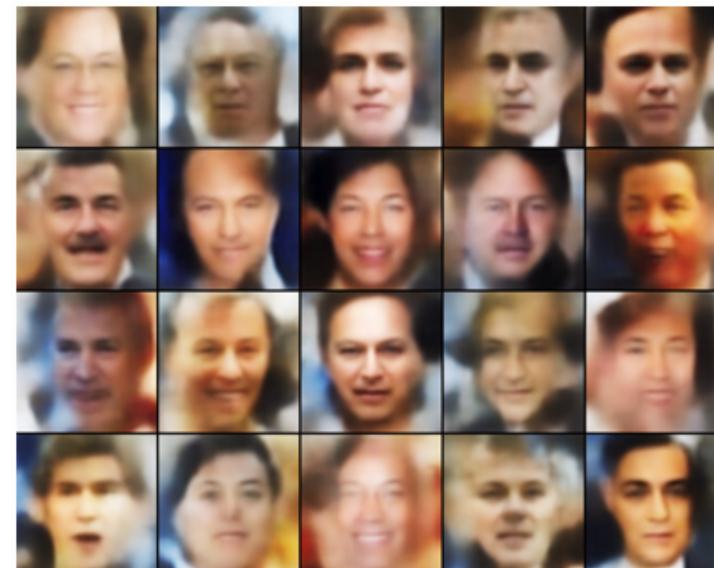


Vary  $\mathbf{z}_2$  Head pose

# Variational Auto Encoders: Generating Data



32x32 CIFAR-10



Labeled Faces in the Wild

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# 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
- 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
- Incorporating structure in latent variables

$$P(\underline{x_{\text{high}}} | \underline{x_{\text{low}}})$$

# Generative Adversarial Networks (GAN)

# So far...

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

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

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

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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: don't work with 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, e.g. random noise. Learn transformation to training distribution.

Q: What can we use to represent this complex transformation?

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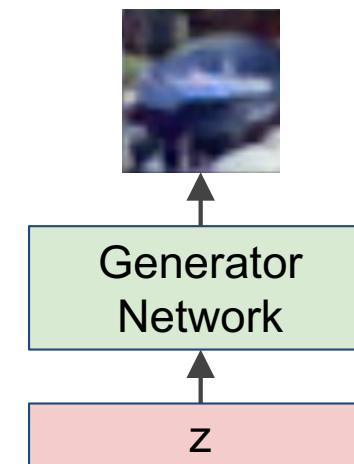
Solution: Sample from a simple distribution, e.g. random noise. Learn transformation to training distribution.

Q: What can we use to represent this complex transformation?

A: A neural network!

Output: Sample from training distribution

Input: Random noise



# Training GANs: Two-player game

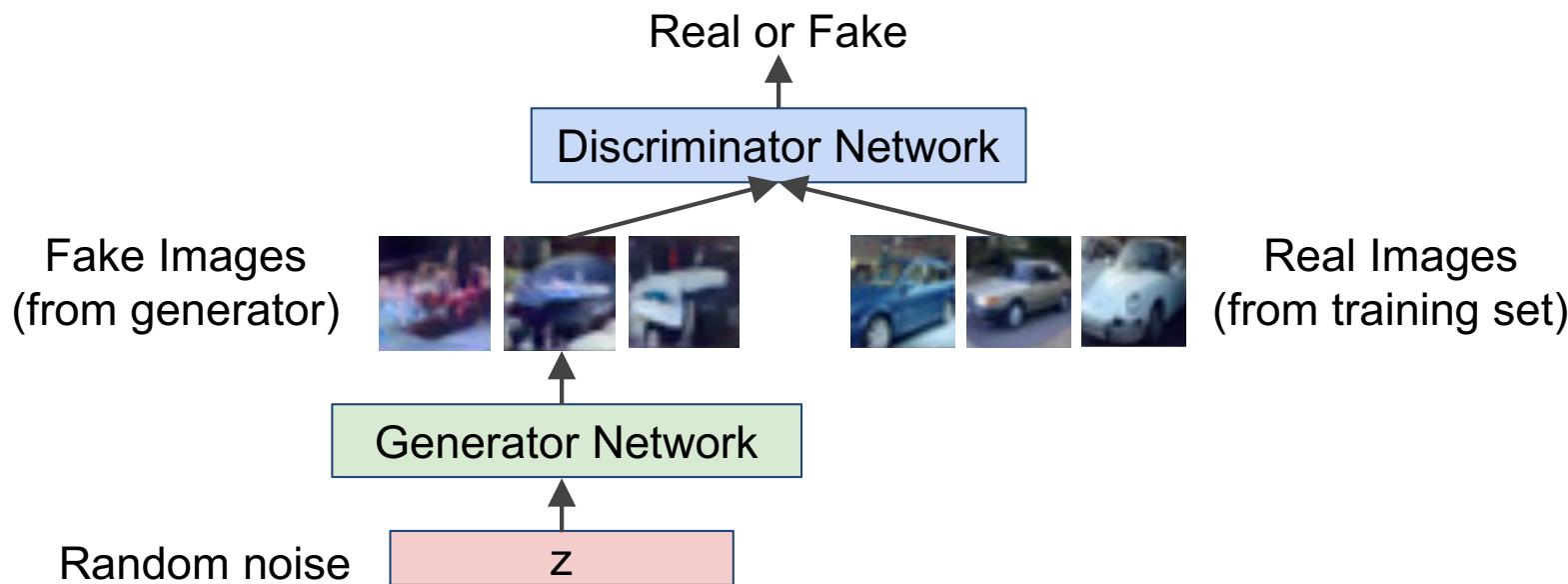
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**Generator network:** try to fool the discriminator by generating real-looking images  
**Discriminator network:** try to distinguish between real and fake images

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Fake and real images copyright Emily Denton et al. 2015. Reproduced with permission.

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**Generator network:** try to fool the discriminator by generating real-looking images  
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Train jointly in **minimax game**

Minimax objective function:

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

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

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- Discriminator ( $\theta_d$ ) wants to **maximize objective** such that  $D(x)$  is close to 1 (real) and  $D(G(z))$  is close to 0 (fake)
- Generator ( $\theta_g$ ) 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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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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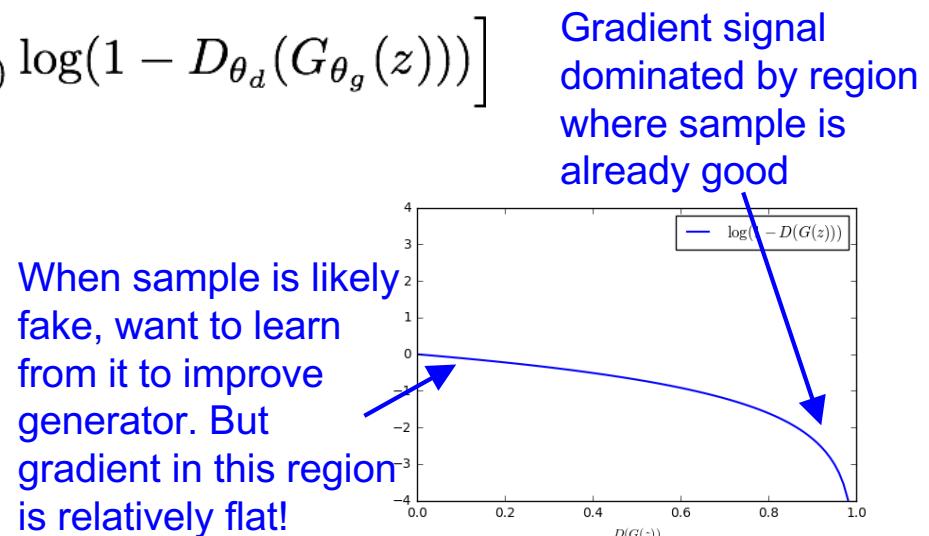
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In practice, optimizing this generator objective does not work well!



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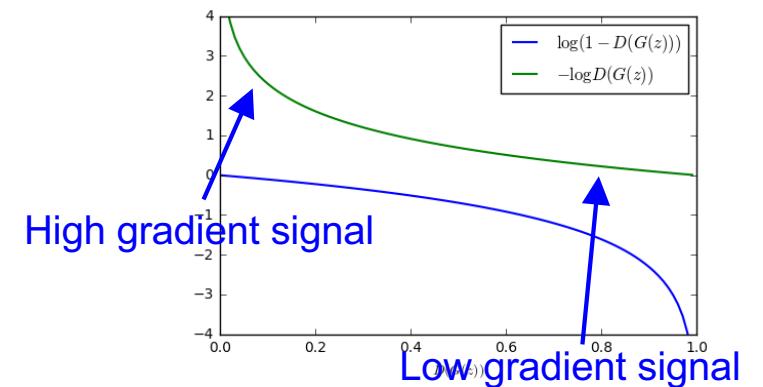
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2. Instead: **Gradient ascent** on generator, different objective

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

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.



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Aside: Jointly training two networks is challenging, can be unstable. Choosing objectives with better loss landscapes helps training, is an active area of research.

