

# 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

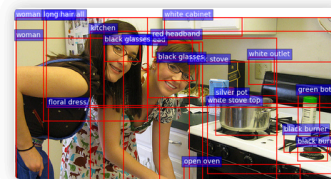
✉ Email

🐦 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

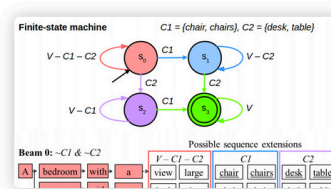


### Tips and Tricks for Visual Question Answering: Learnings from the 2017 Challenge

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

preprint arXiv:1708.02711, 2017.

PDF Slides

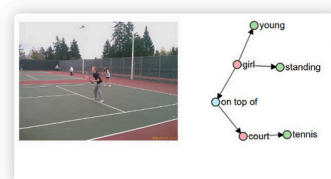


### Guided Open Vocabulary Image Captioning with Constrained Beam Search

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

# Administrativa

- 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.

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→ Cat

Classification

[This image is CC0 public domain](#)

# Supervised vs Unsupervised Learning

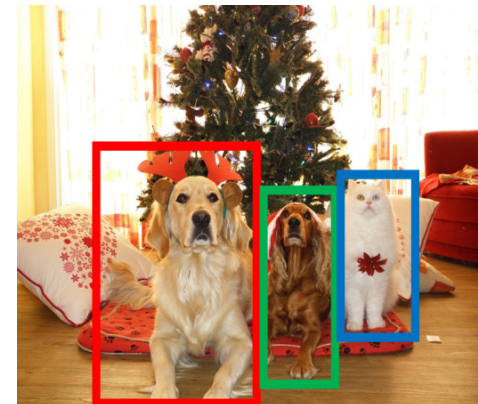
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**DOG, DOG, CAT**

Object Detection

[This image is CC0 public domain](#)

# Supervised vs Unsupervised Learning

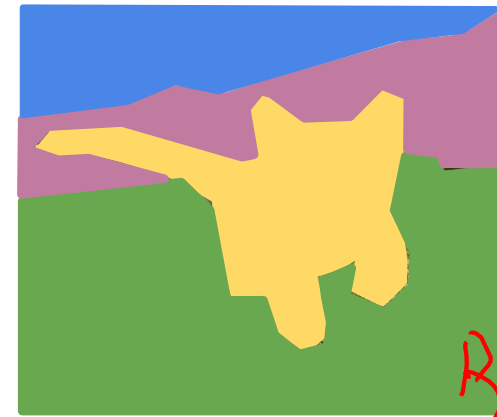
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GRASS, CAT,  
TREE, SKY

Semantic Segmentation

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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

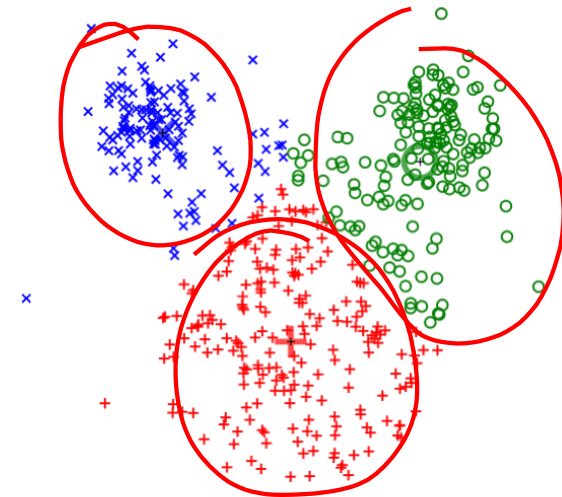
## Unsupervised Learning

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K-means clustering

[This image is CC0 public domain](#)

# Supervised vs Unsupervised Learning

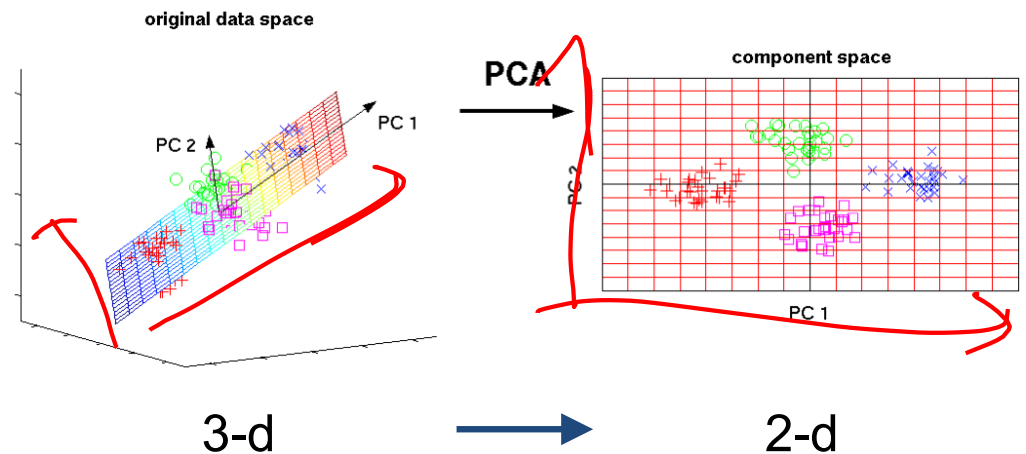
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Principal Component Analysis  
(Dimensionality reduction)

[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!

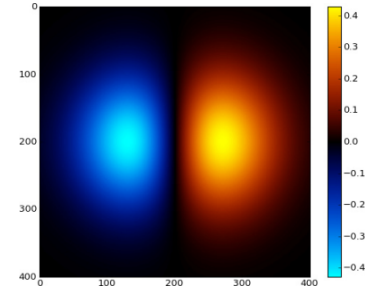
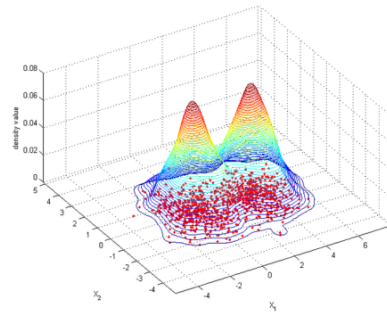
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1-d density estimation



2-d density estimation

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

# Supervised vs Unsupervised Learning

## Supervised Learning

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## Unsupervised Learning

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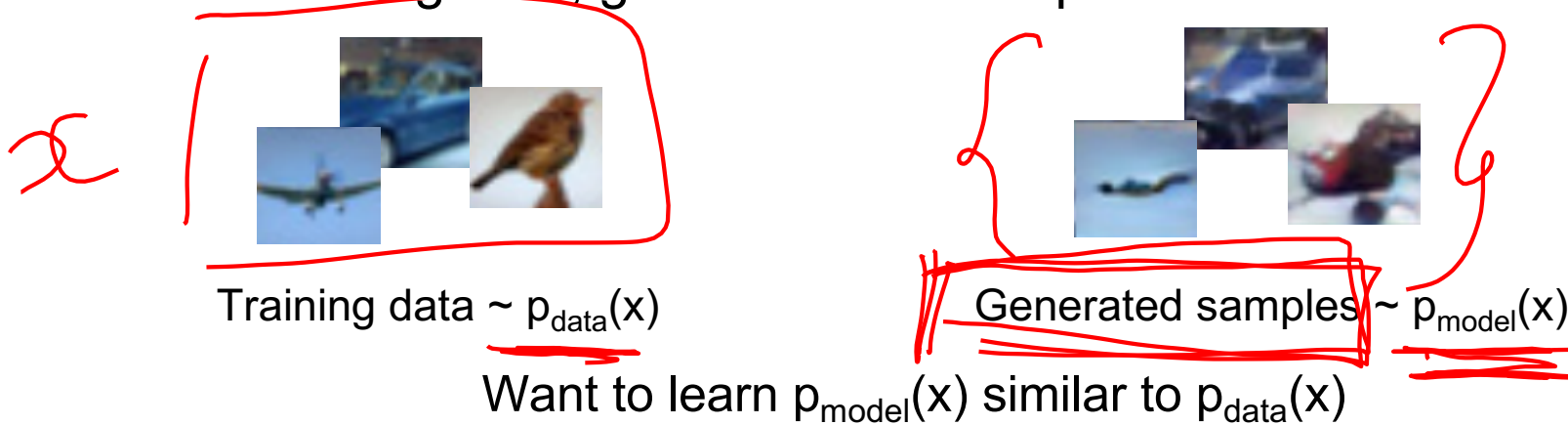
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# Generative Models

Given training data, generate new samples from same distribution



# 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

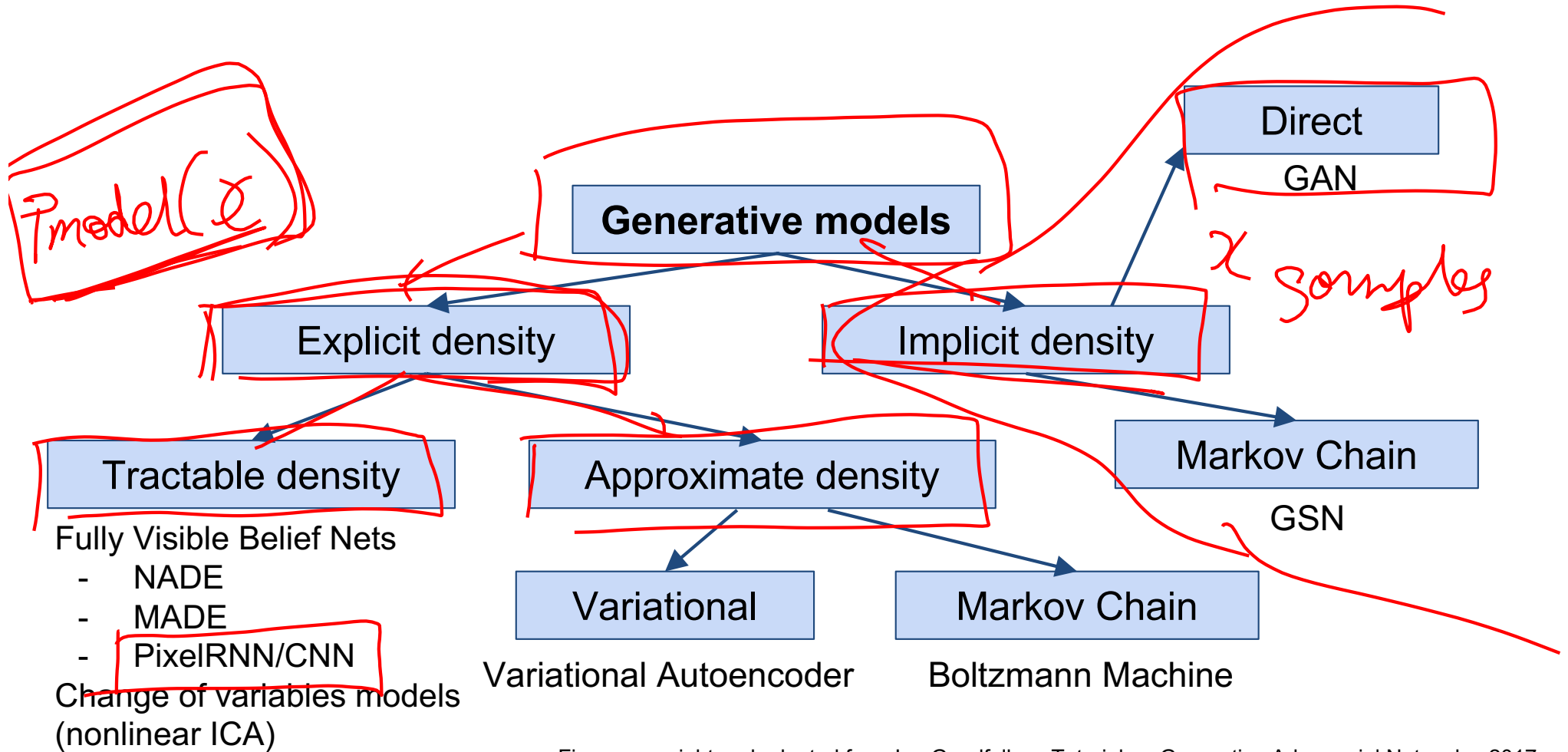


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

# Taxonomy of Generative Models

Today: discuss 3 most popular types of generative models today

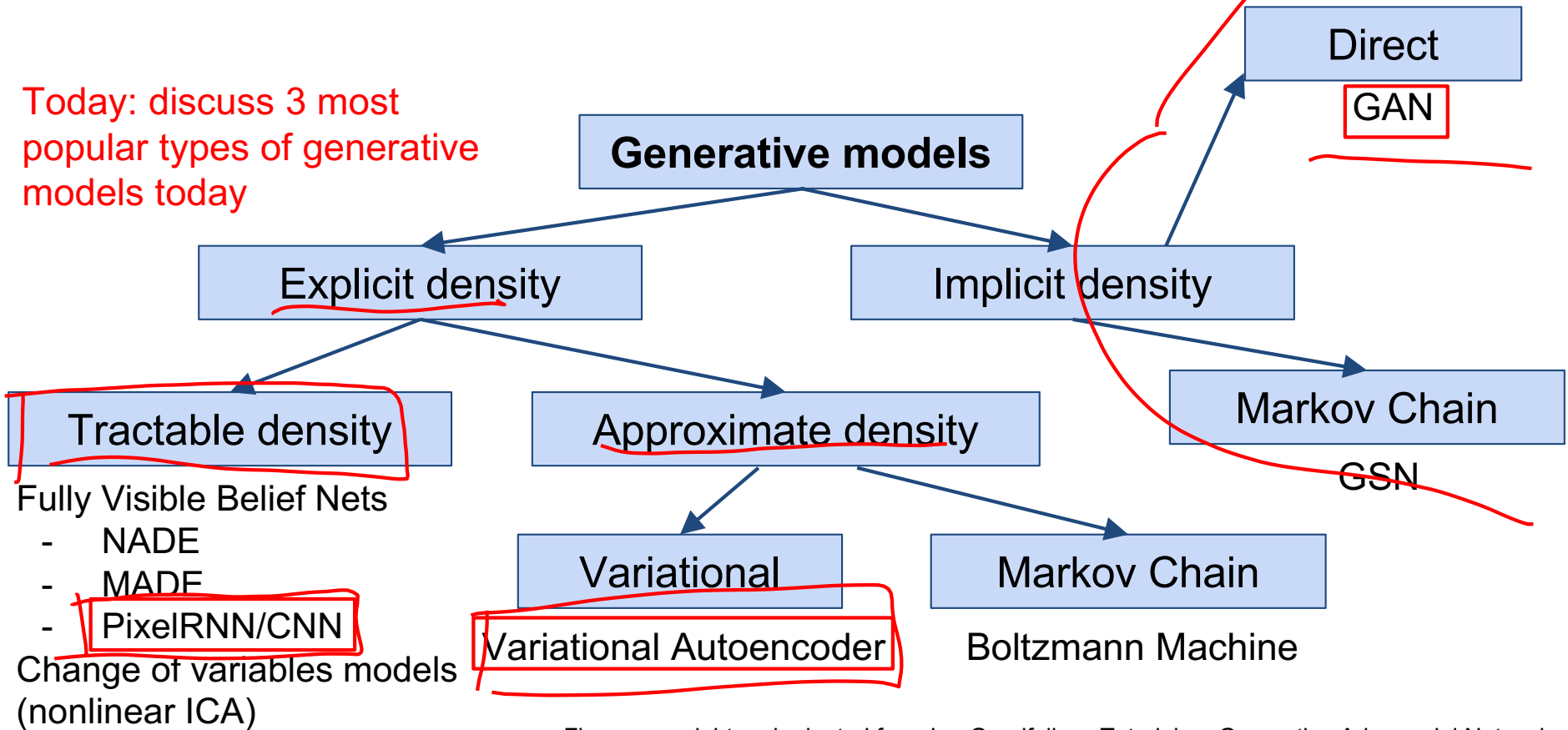
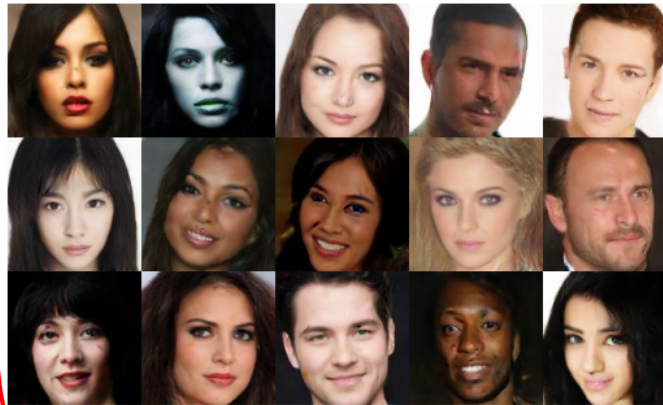


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

# 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

Figures from L-R are copyright: (1) [Alec Radford et al. 2016](#); (2) [David Berthelot et al. 2017](#); [Phillip Isola et al. 2017](#). Reproduced with authors permission.



# PixelRNN and PixelCNN



# Fully Observable Model

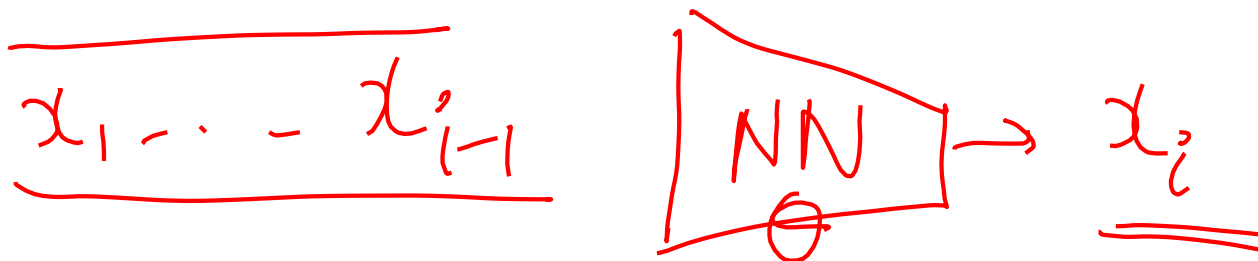
## Explicit density model

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

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↑                                  ↑

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

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

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↑ Likelihood of image  $x$

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

Will need to define ordering of "previous pixels"

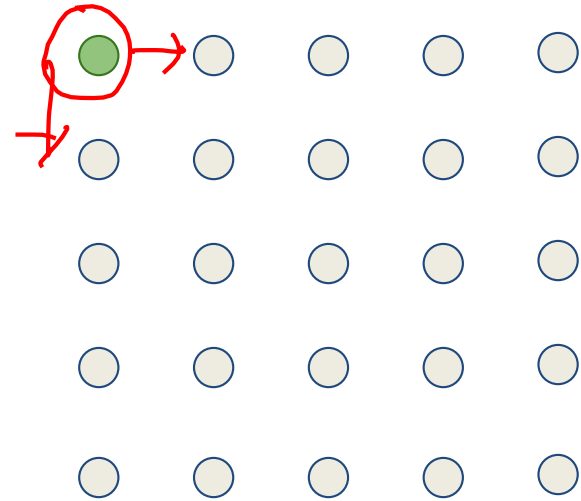
Complex distribution over pixel values  
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Then maximize likelihood of training data

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

Generate image pixels starting from corner

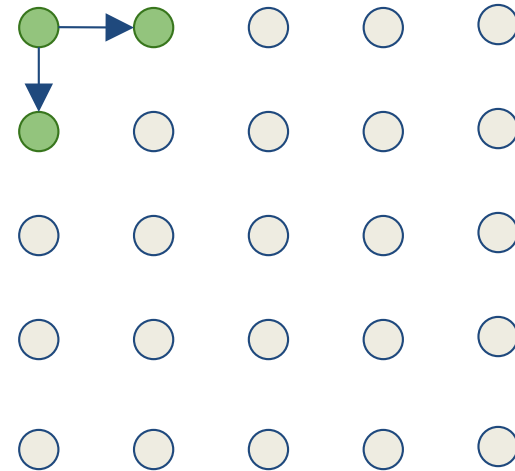
Dependency on previous pixels modeled using an RNN (LSTM)



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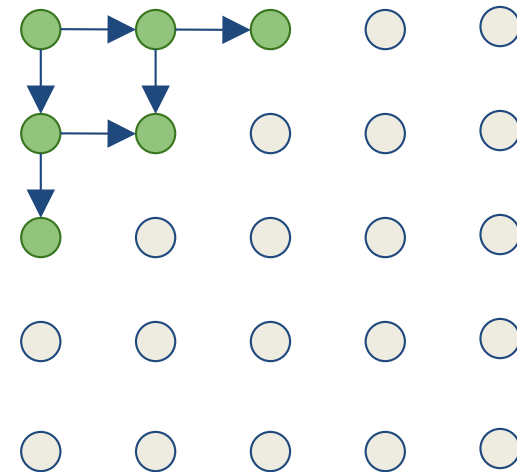
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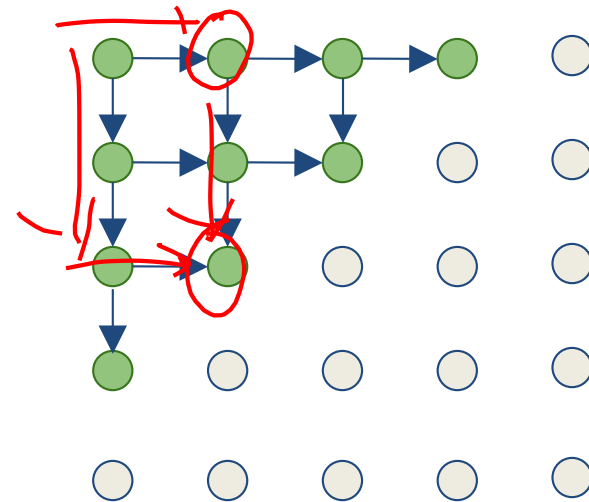


# PixelRNN [van der Oord et al. 2016]

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow!



$$P(x_i | \langle \rangle) \sim \text{RNN}(\text{Softmax}(\cdot | h_i))$$

# 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

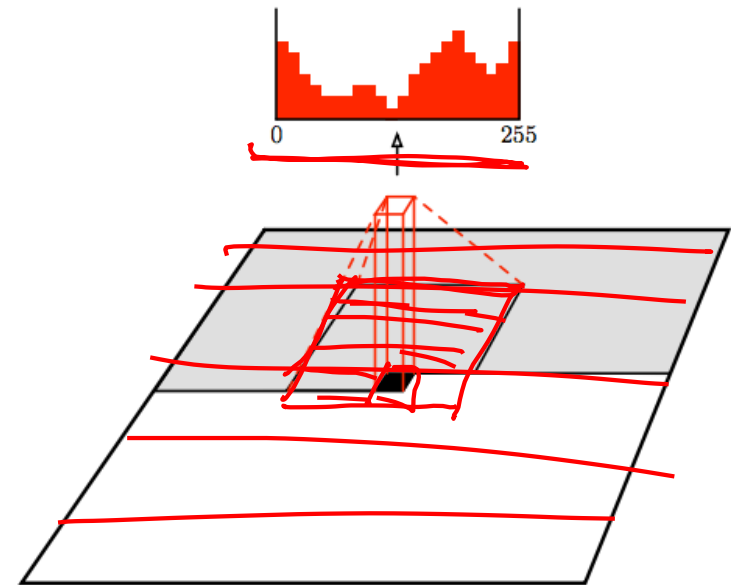


Figure copyright van der Oord et al., 2016. Reproduced with permission.



# PixelCNN [van der Oord et al. 2016]

$D = \{x_1, \dots, x_n\}$

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

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

Softmax loss at each pixel

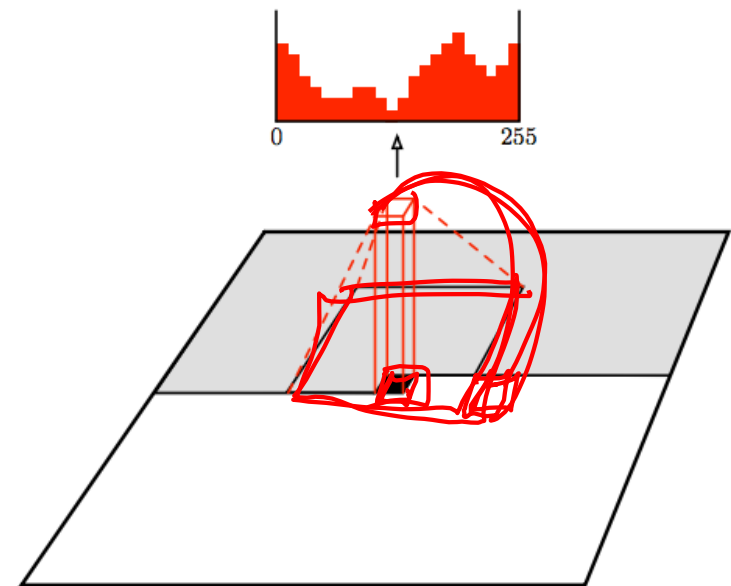


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# PixelCNN [van der Oord et al. 2016]

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

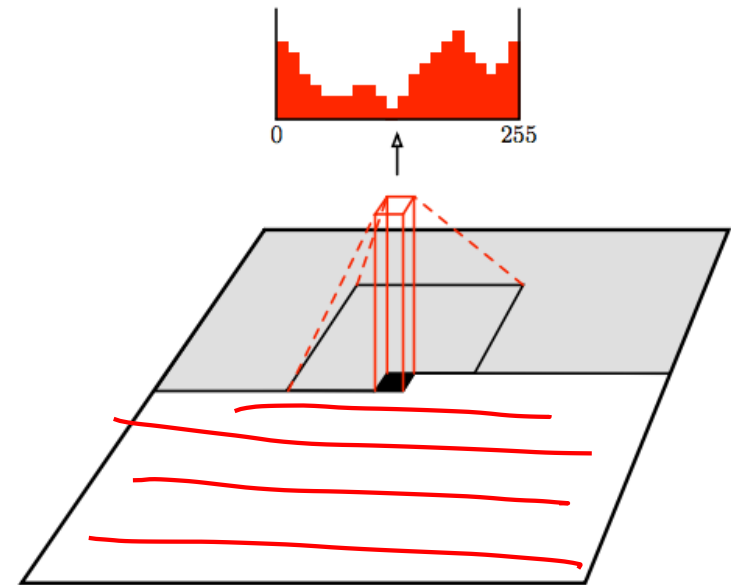
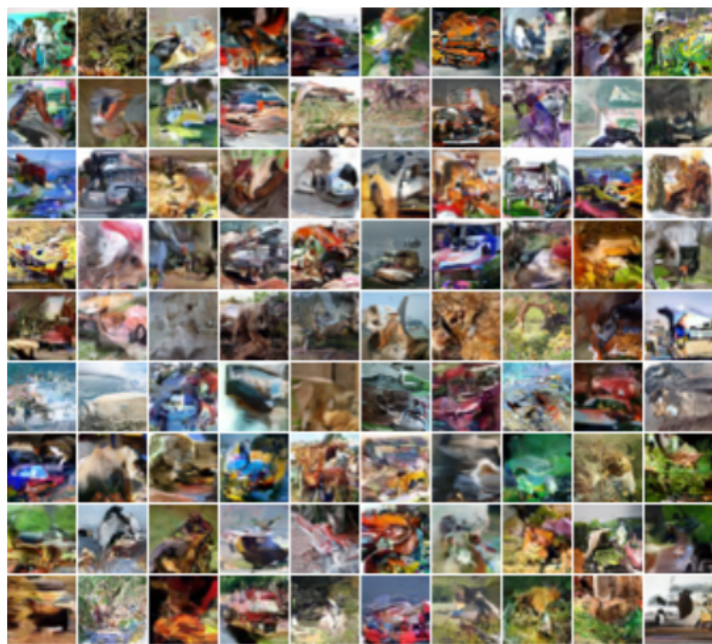
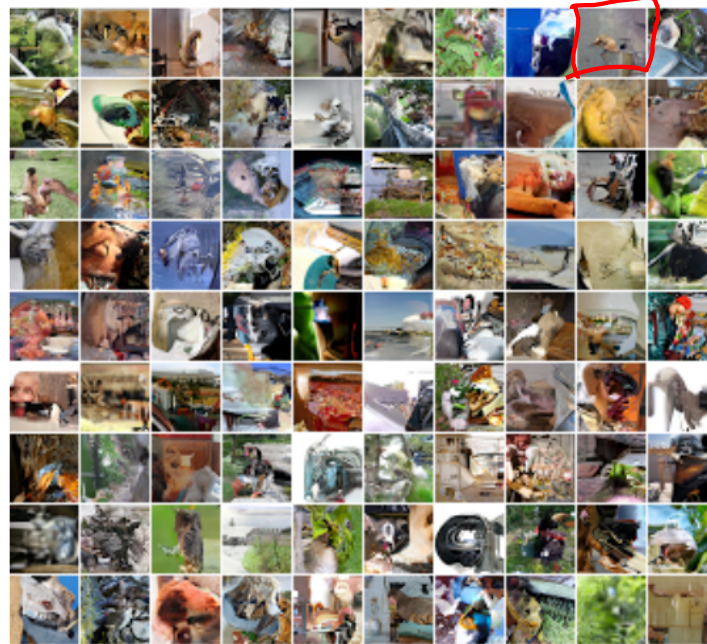


Figure copyright van der Oord et al., 2016. Reproduced with permission.

# 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:

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

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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  $\mathbf{z}$ :

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

*(Handwritten red annotations: a box around the integral, a box around the integrand, and a red arrow pointing to the integral symbol with the label  $\frac{\partial}{\partial \theta}$ )*



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

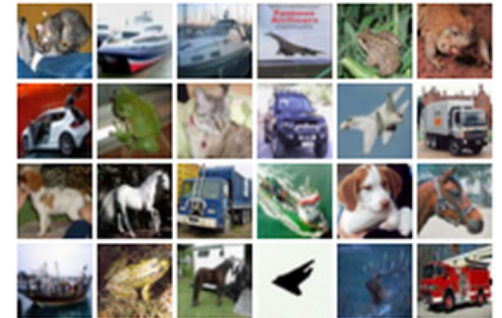
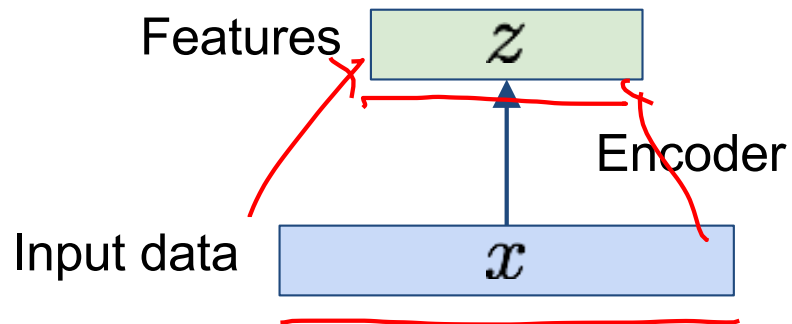
3. Amortized Inference Neural Networks

4. “Reparameterization” Trick



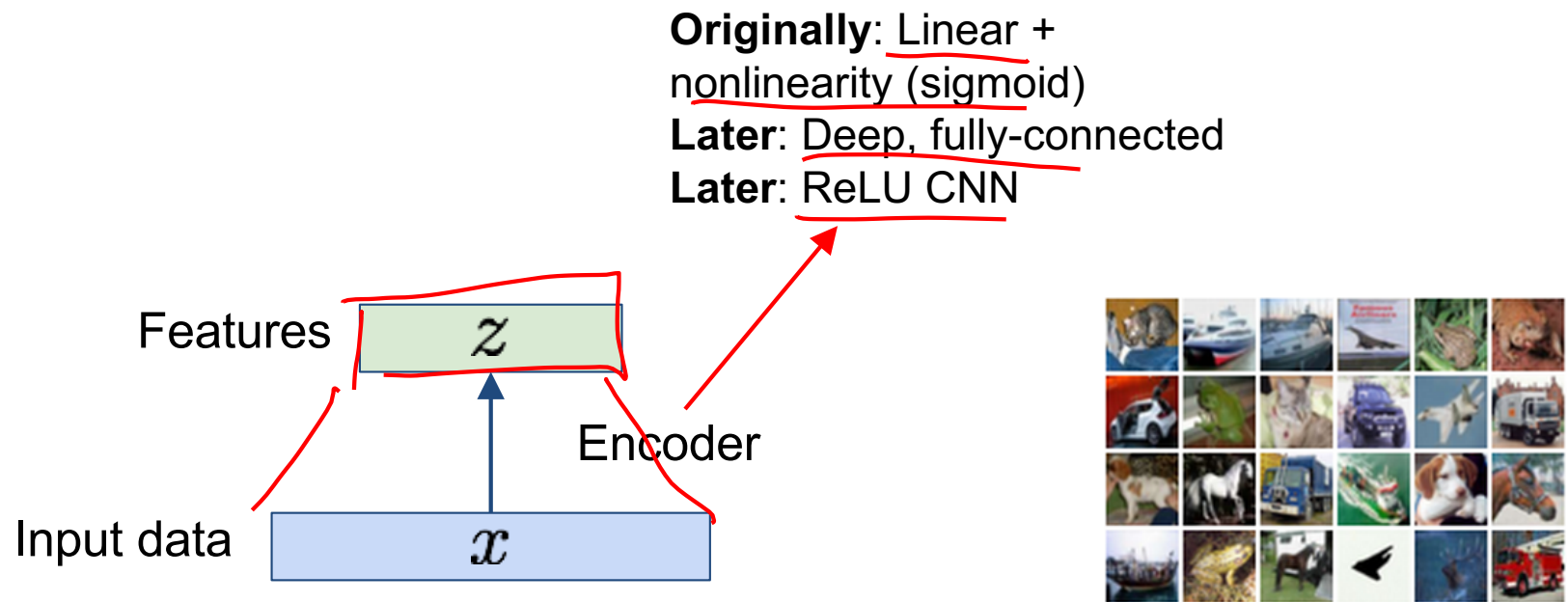
# Autoencoders

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



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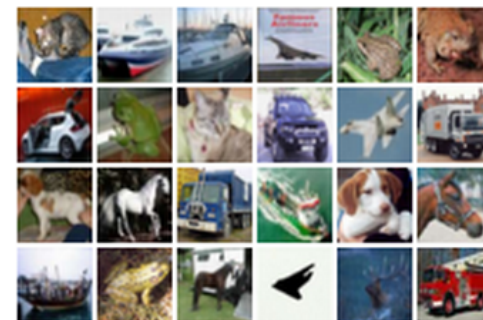
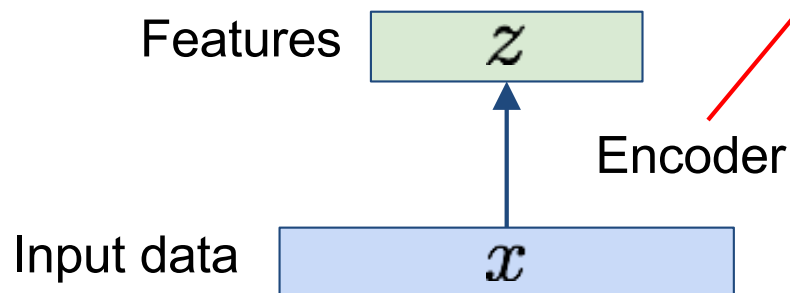
$z$  usually smaller than  $x$   
(dimensionality reduction)

Q: Why dimensionality reduction?

**Originally:** Linear + nonlinearity (sigmoid)

**Later:** Deep, fully-connected

**Later:** ReLU CNN



# Autoencoders

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

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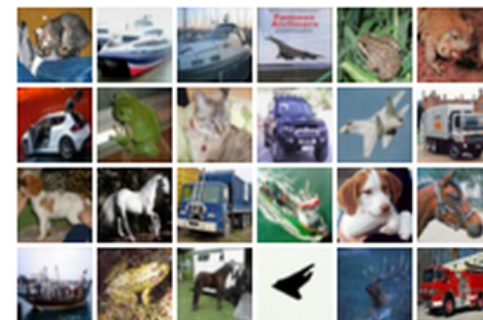
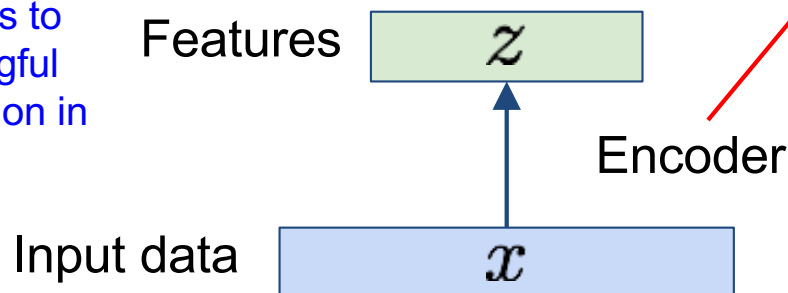
Q: Why dimensionality reduction?

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

**Originally:** Linear + nonlinearity (sigmoid)

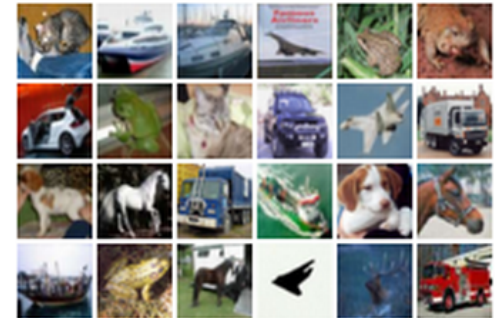
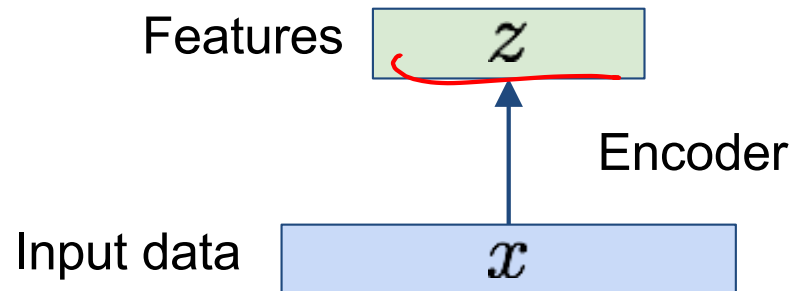
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# Autoencoders

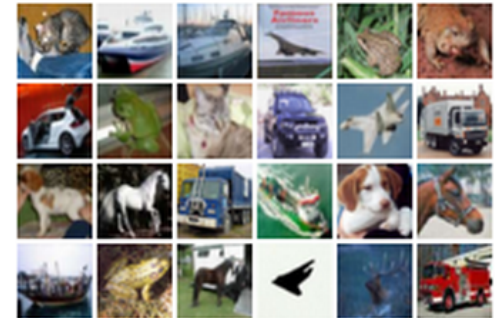
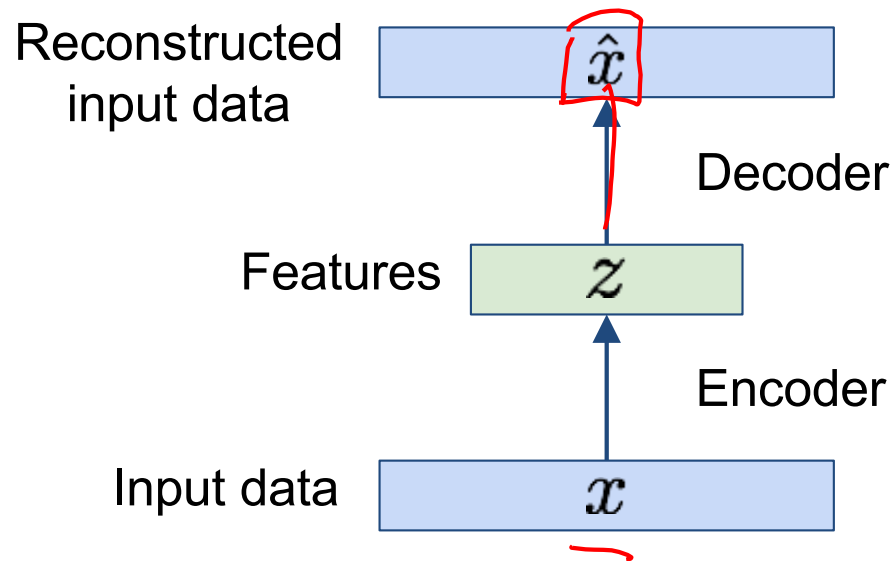
How to learn this feature representation?



# Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data  
“Autoencoding” - encoding itself

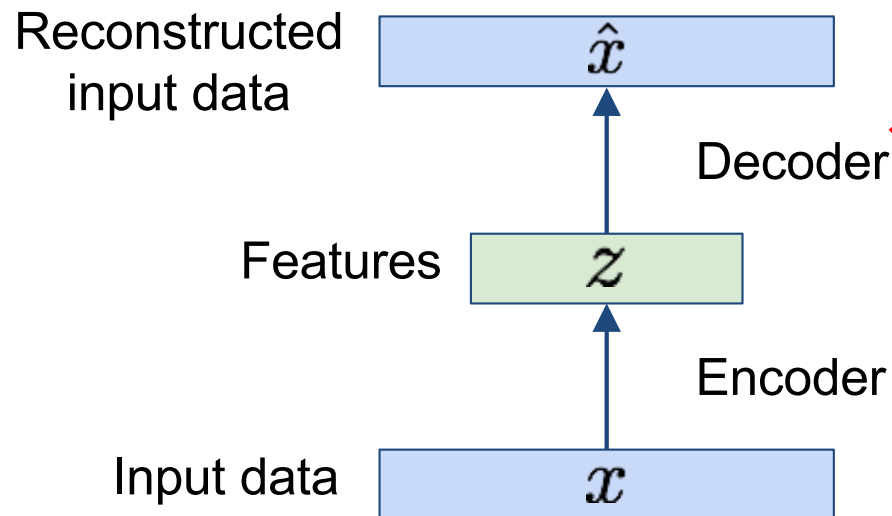


# Autoencoders

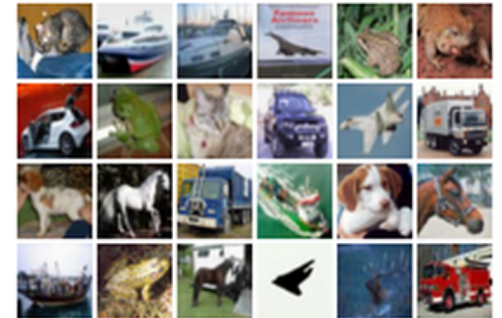
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**Originally:** Linear + nonlinearity (sigmoid)  
**Later:** Deep, fully-connected  
**Later:** ReLU CNN (upconv)

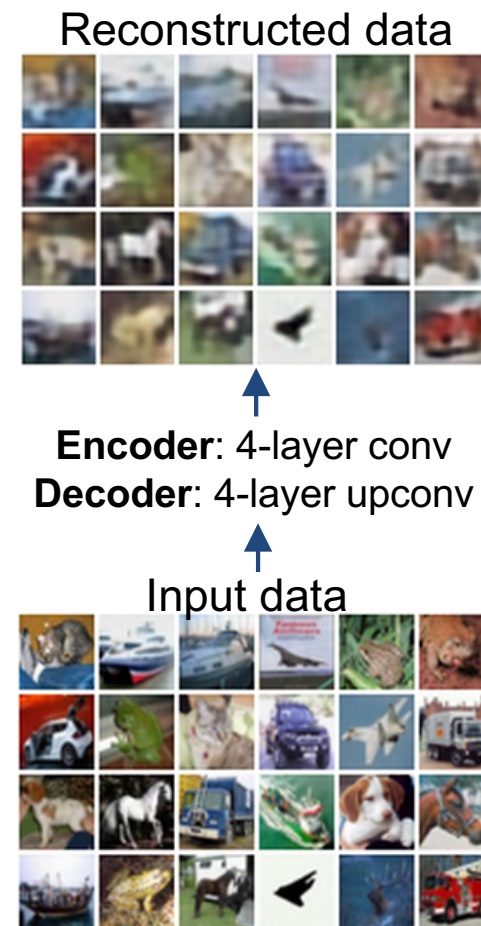
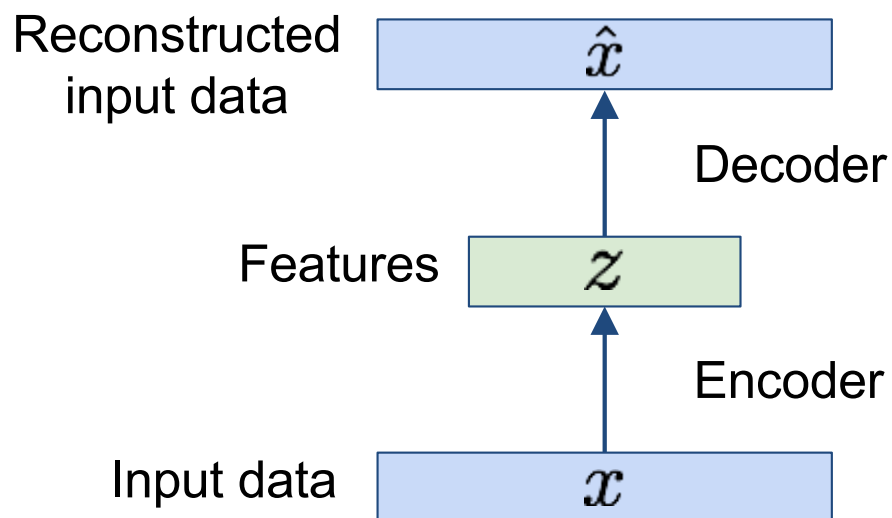


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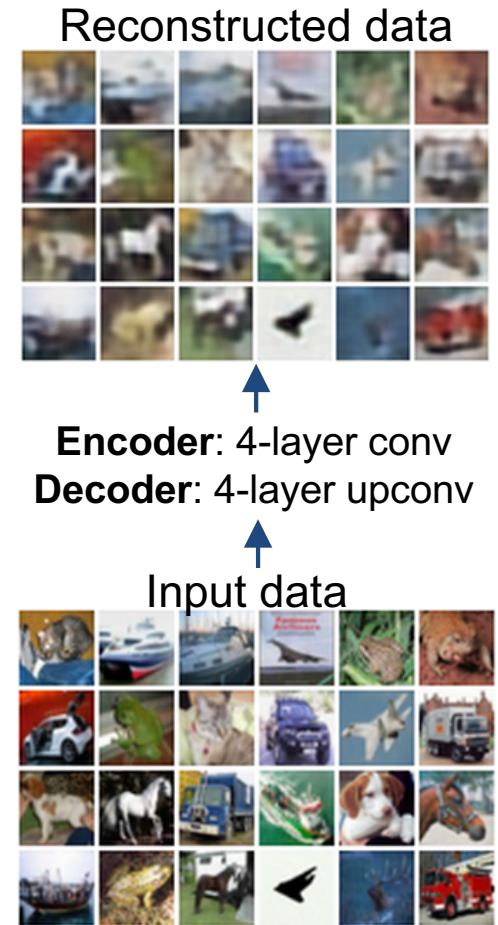
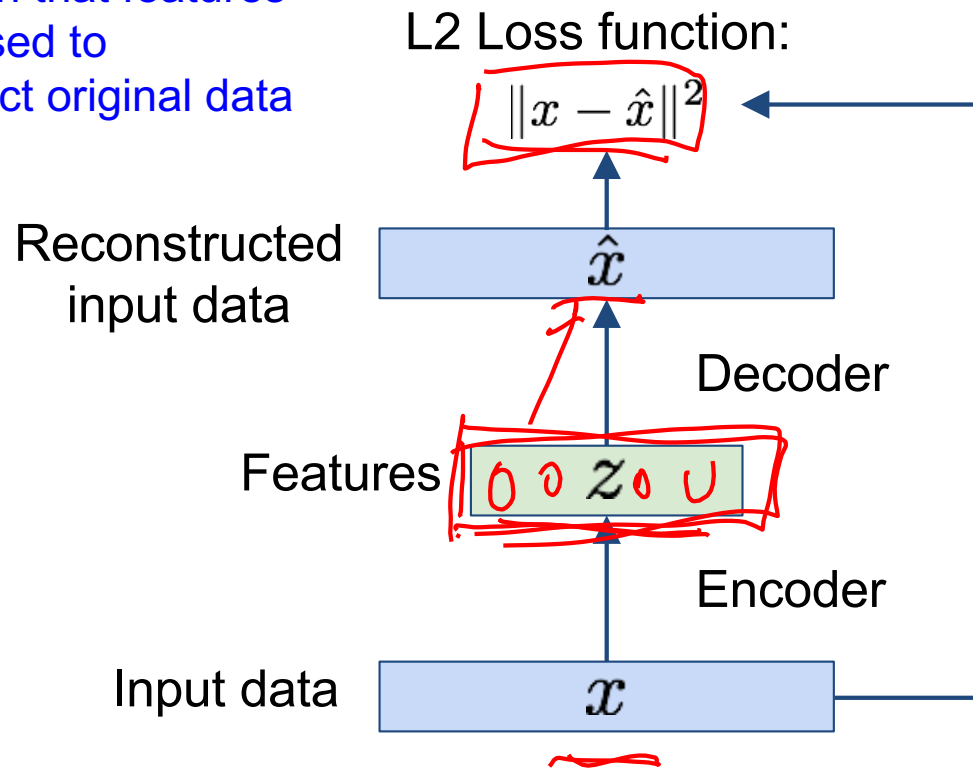
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# Autoencoders

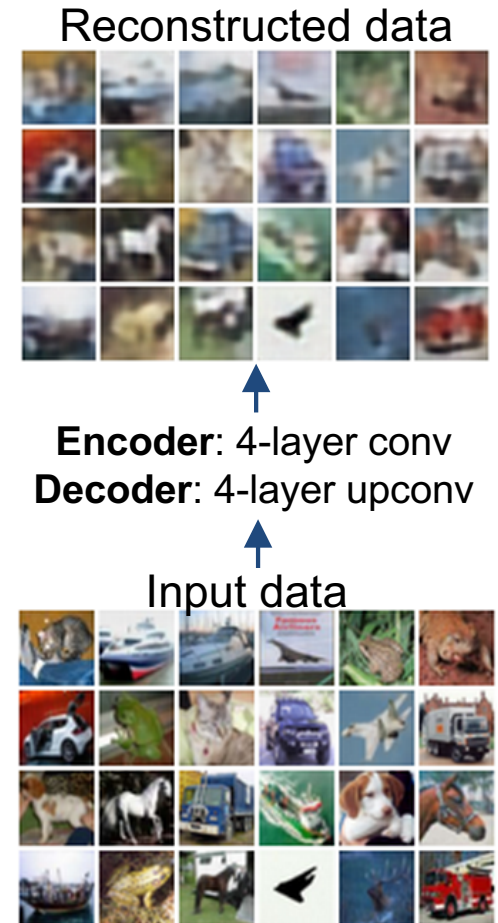
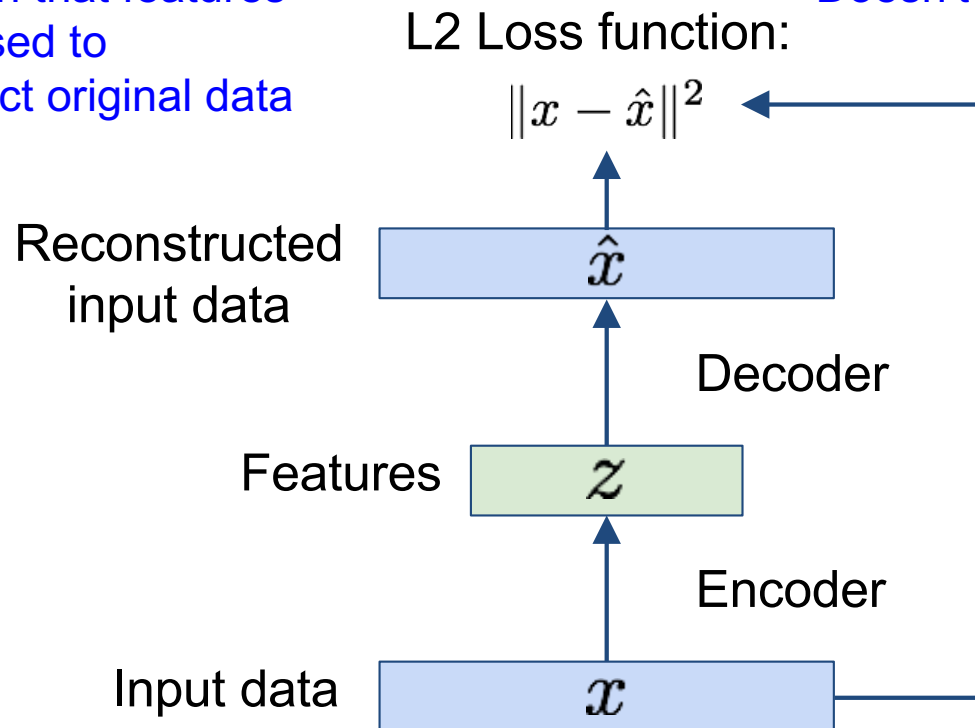
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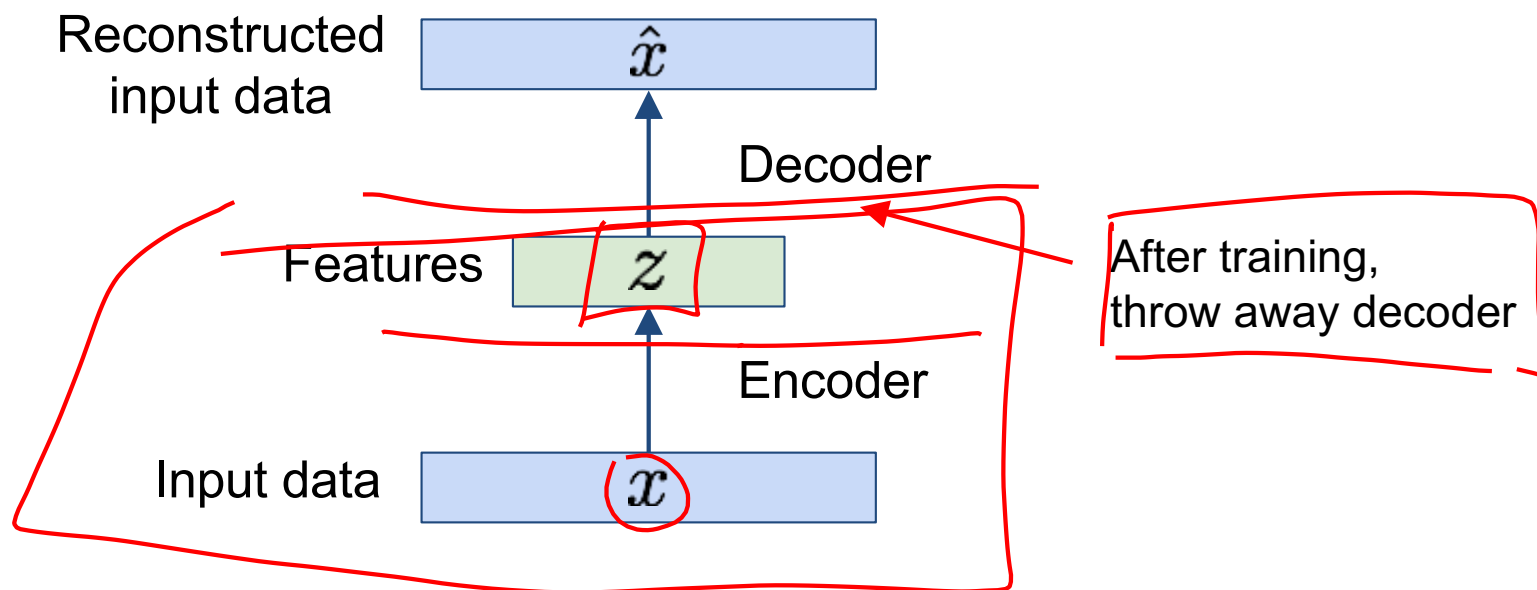
# Autoencoders

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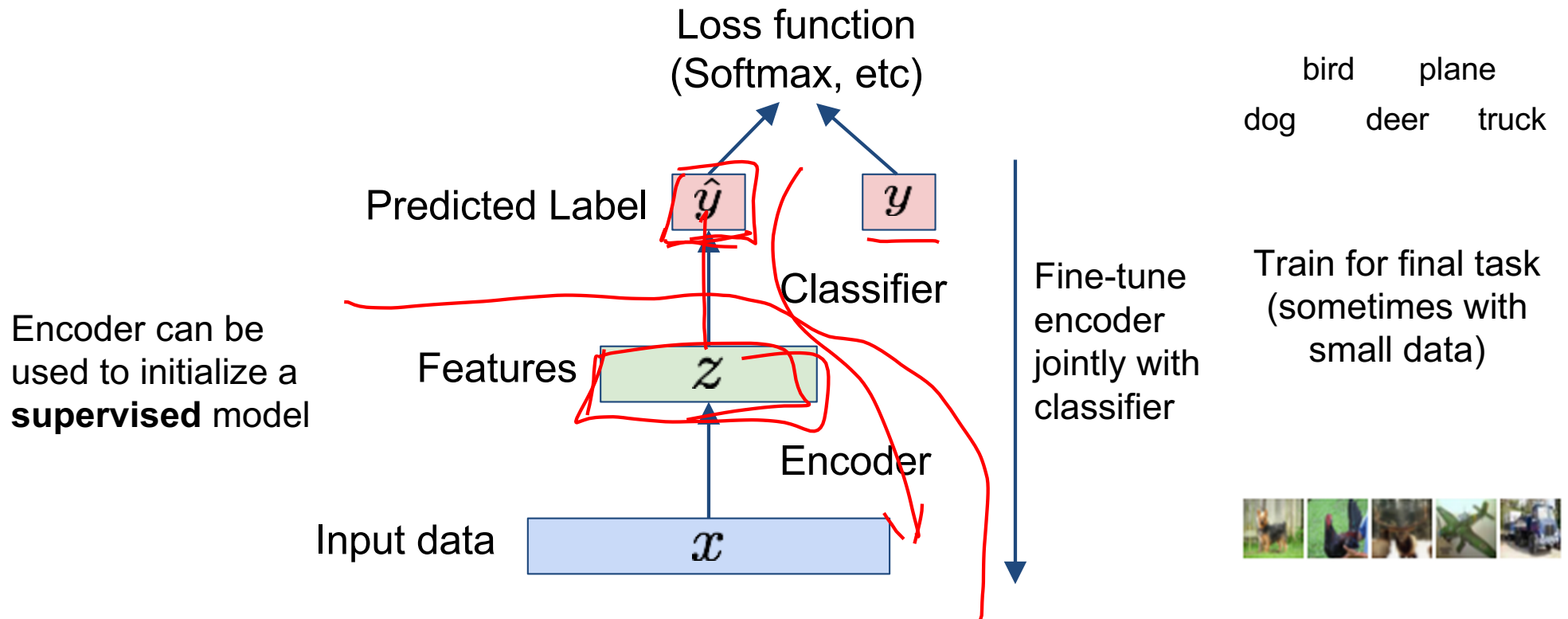
Doesn't use labels!



# Autoencoders



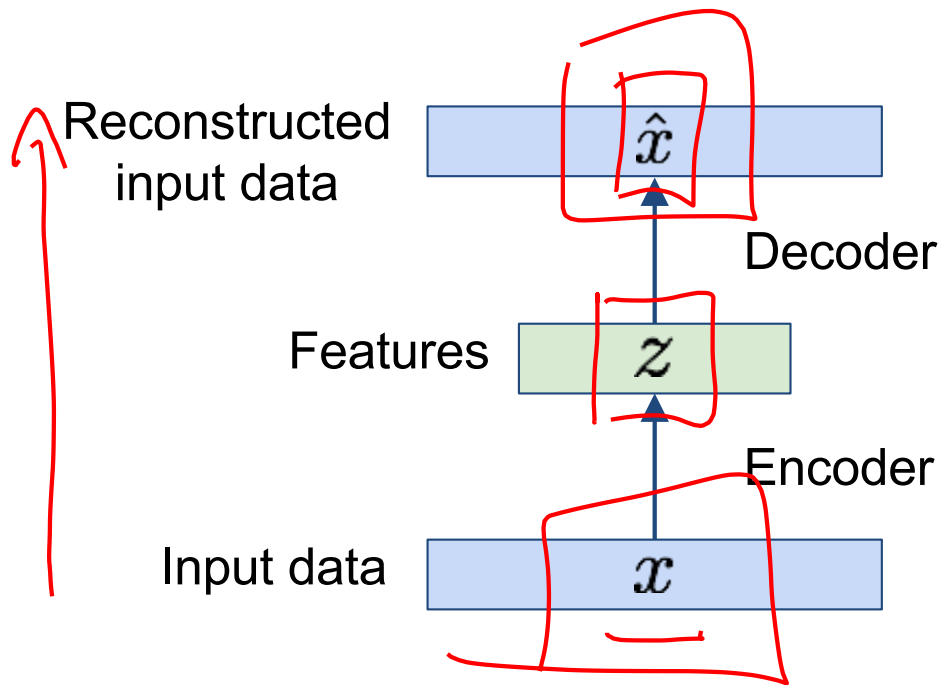
# Autoencoders



# Autoencoders

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

$x_i$



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:

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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:

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

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

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



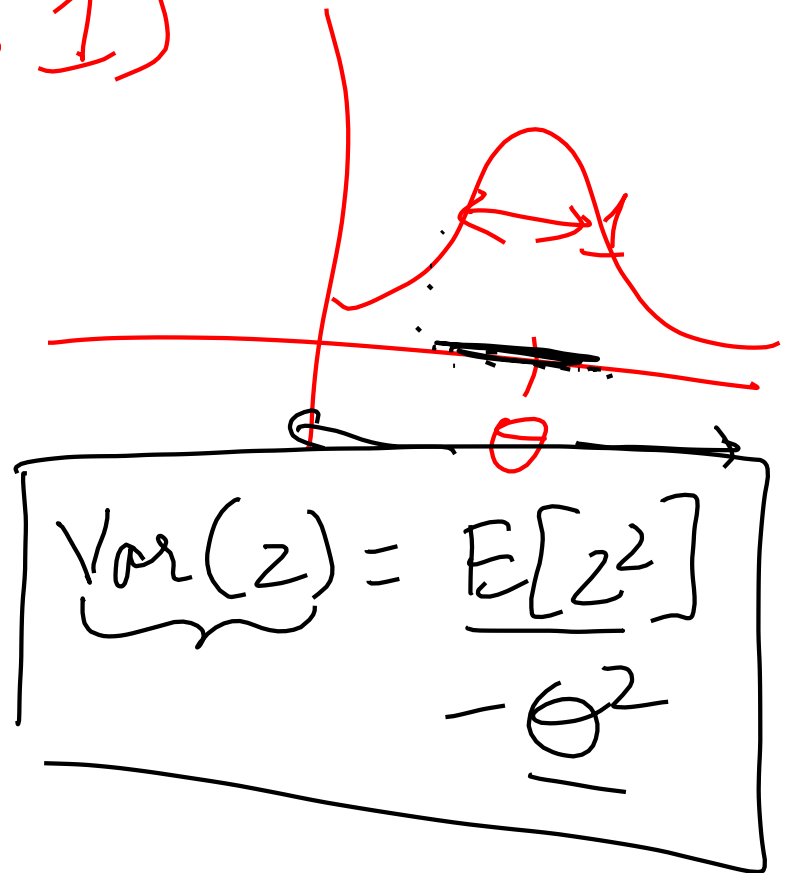
# Example

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

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

$$\min_{\theta} E[z^2]$$

$$\min_{\theta} \int_{-\infty}^{\infty} p(z) z^2 dz$$
$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{(z-\theta)^2}{2}} z^2 dz$$



# Example

# 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”

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

# Option 1

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

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

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

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

$\frac{f}{N}$

$\approx$

# Example

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

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

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

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

# 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”

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

# Option 2

- Path Derivative Gradient Estimator  
aka "reparameterization trick"

$$\frac{\partial}{\partial \theta} \mathbb{E}_{z \sim p_{\theta}} [f(z)] = \frac{\partial}{\partial \theta} \mathbb{E}_{\epsilon} [f(g(\theta, \epsilon))] = \mathbb{E}_{\epsilon \sim p_{\epsilon}} \left[ \frac{\partial f}{\partial g} \frac{\partial g}{\partial \theta} \right] \frac{1}{\sqrt{2}} \Sigma$$

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

$$z = g(\theta, \epsilon)$$

$$\epsilon \sim \mathcal{N}(0, 1)$$

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

# Example

$$Z \sim N(\theta, \sigma^2)$$

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

$$Z = \theta + \sigma \varepsilon$$

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

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

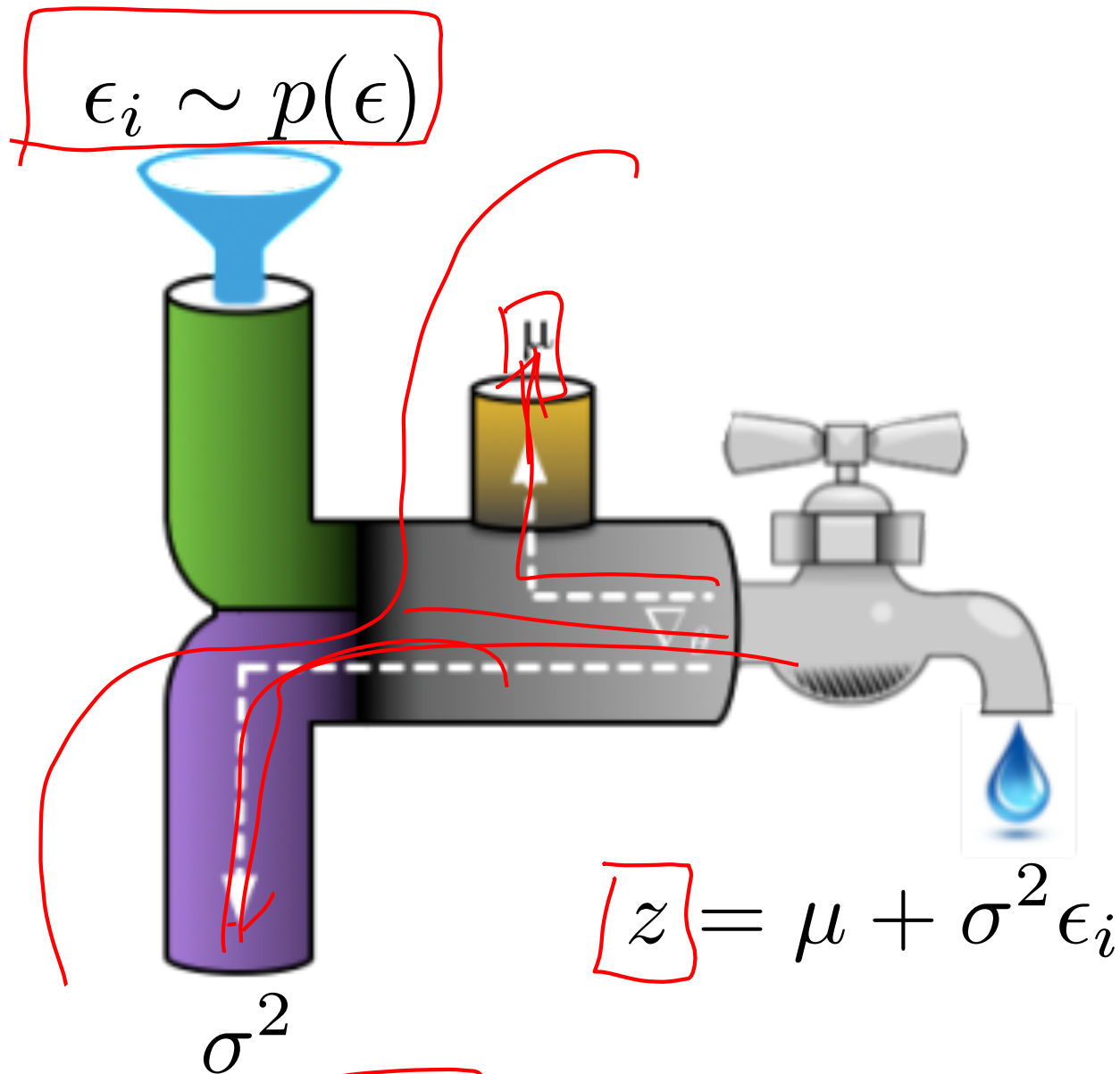
$$\frac{\partial f}{\partial g} = \underline{2z}$$

$$E_{\varepsilon \sim p(\varepsilon)} [2z] = E_{\varepsilon} [2(\theta + \varepsilon)]$$

$$= \frac{1}{N} \sum (\dots)$$



# Reparameterization Intuition



# Two Options

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

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

- Path Derivative Gradient Estimator  
aka “reparameterization trick”

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

# 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
```

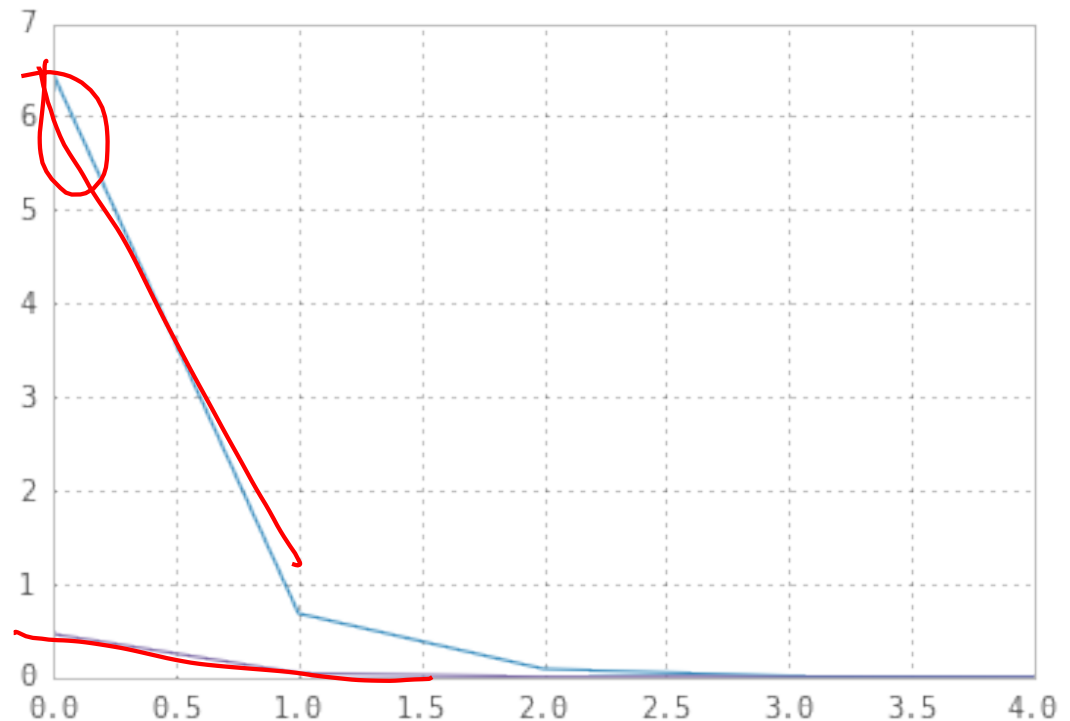
# Example

```
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
```

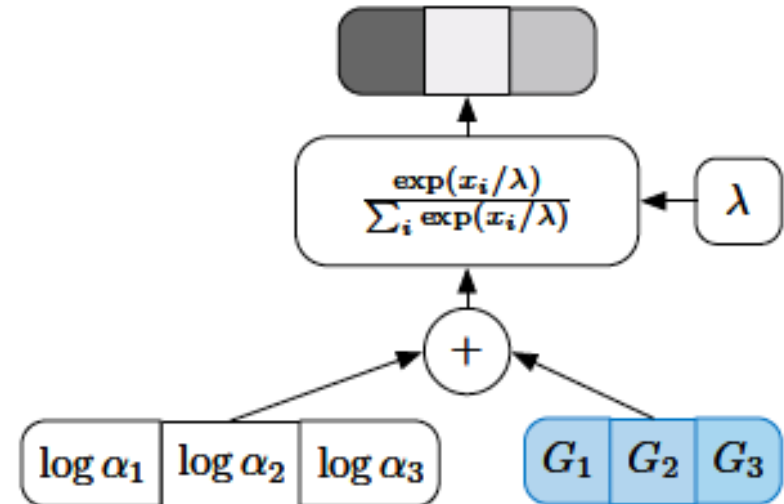
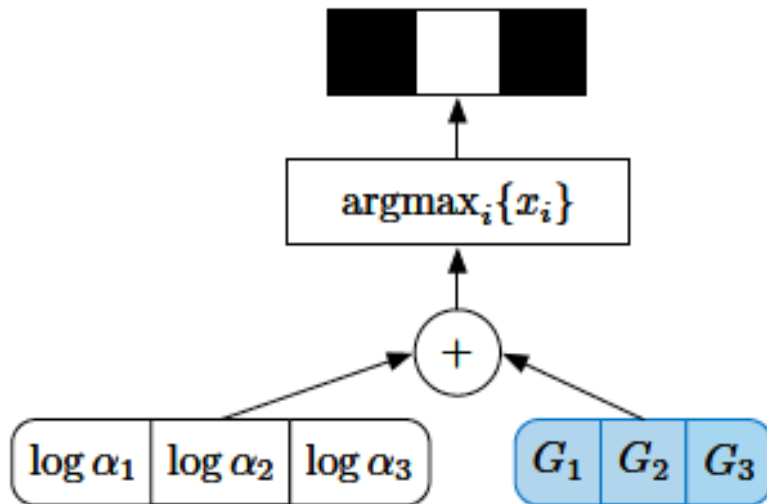


```
[ 3.8409546  3.97298803  4.03007634  3.98531095  3.99579423]
[ 3.97775271  4.00232825  3.99894536  4.00353734  3.99995899]

[ 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

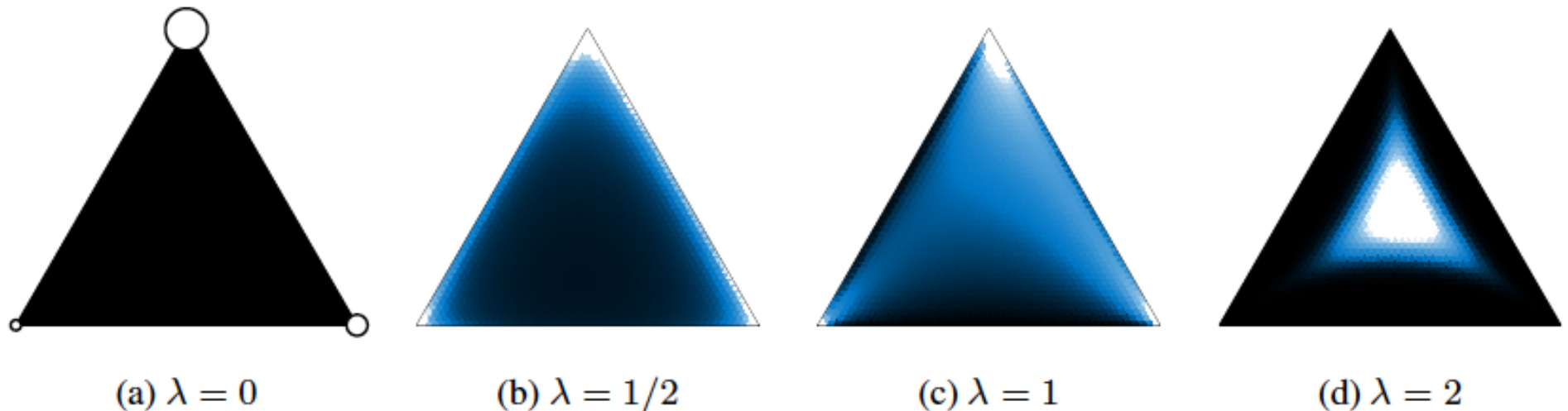


Figure 2: A discrete distribution with unnormalized probabilities  $(\alpha_1, \alpha_2, \alpha_3) = (2, 0.5, 1)$  and three corresponding Concrete densities at increasing temperatures  $\lambda$ . Each triangle represents the set of points  $(y_1, y_2, y_3)$  in the simplex  $\Delta^2 = \{(y_1, y_2, y_3) \mid y_k \in (0, 1), y_1 + y_2 + y_3 = 1\}$ . 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

VAEs are a combination of the following ideas:

1. Auto Encoders

2. Variational Approximation

- Variational Lower Bound / ELBO

3. Amortized Inference Neural Networks

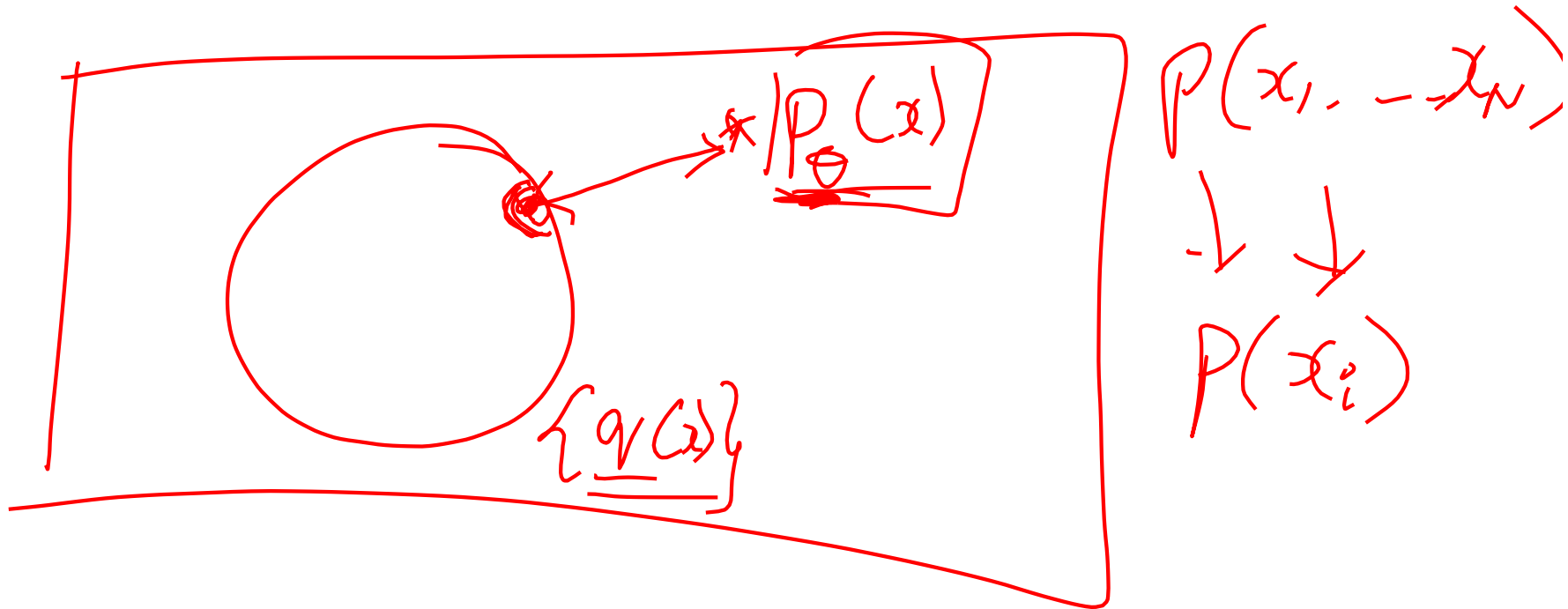
4. “Reparameterization” Trick

# 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:

$$D(p||q)$$

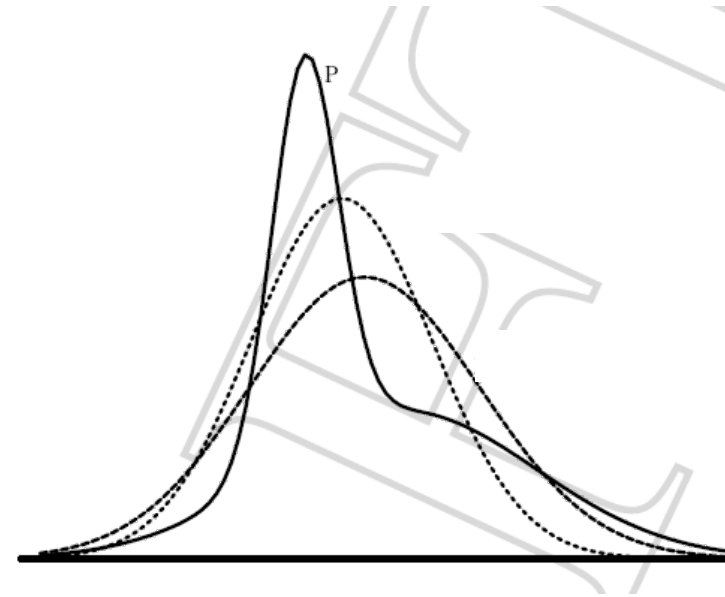
$$\sum_x p(x) \log \frac{p(x)}{q(x)}$$

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

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

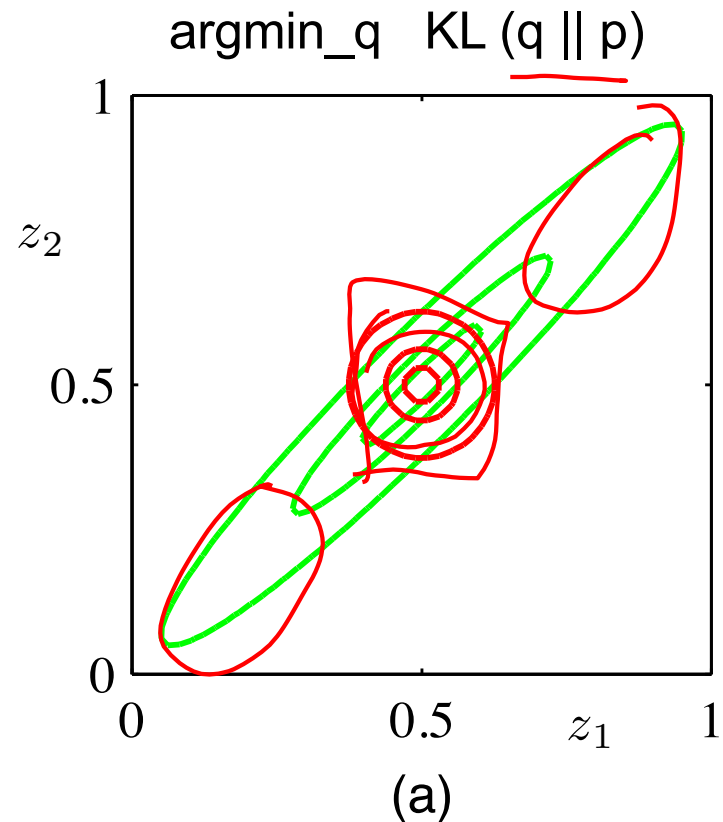
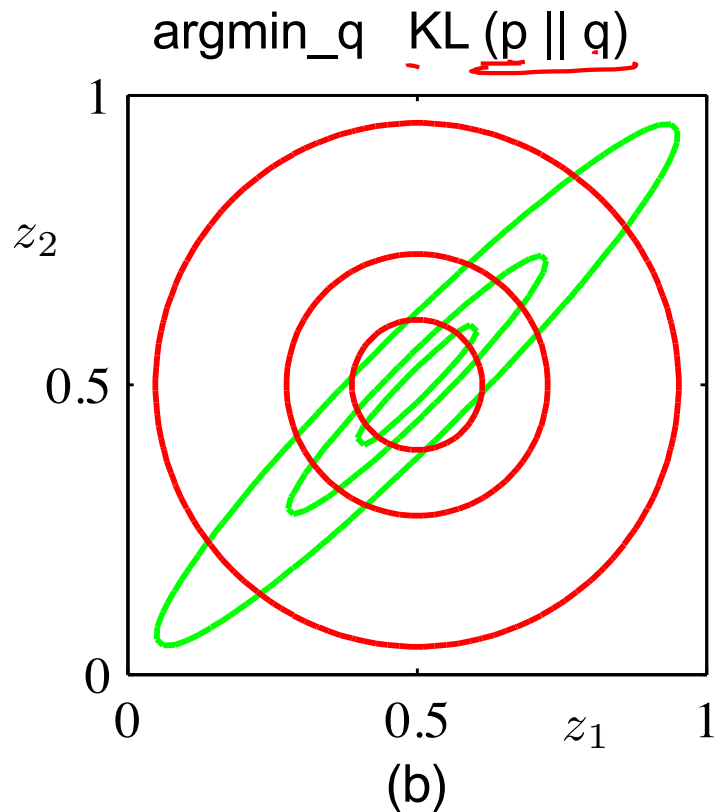
# Find simple approximate distribution

- 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
- $D(q||p)$ 
  - approximate distribution defines support
  - tends to give overconfident results
  - will be tractable



# Example 1

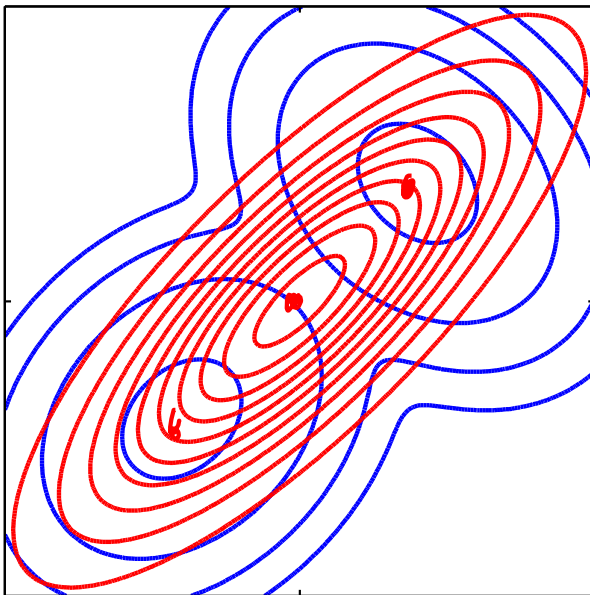
- $p = 2D$  Gaussian with arbitrary co-variance
- $q = 2D$  Gaussian with diagonal co-variance



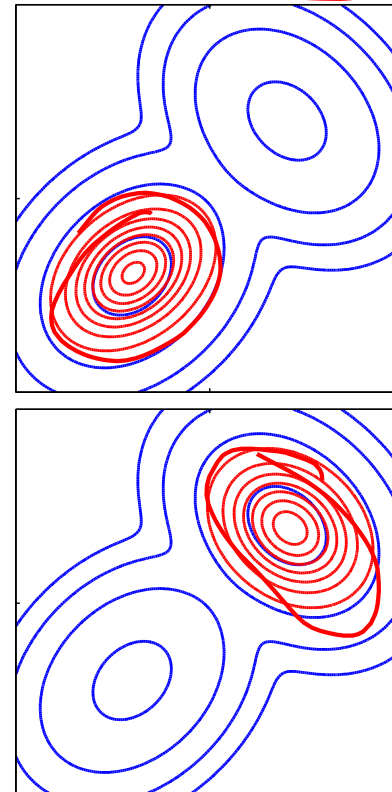
# Example 2

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

argmin<sub>q</sub> KL (p || q)



argmin<sub>q</sub> KL (q || p)



# The general learning problem with missing data

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

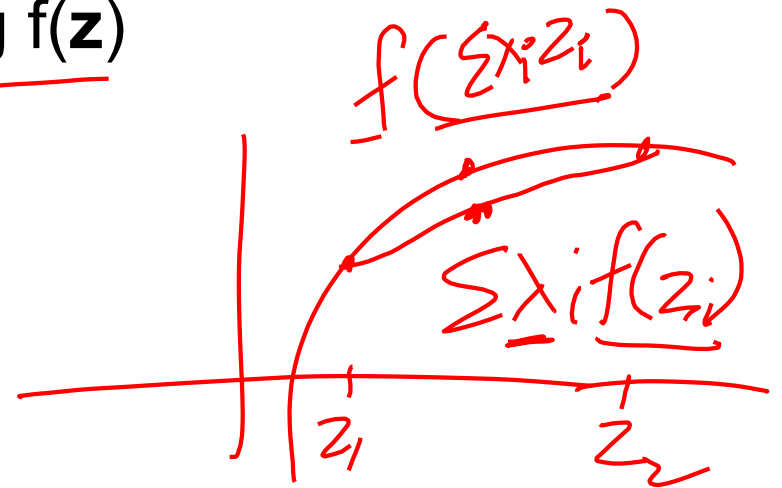
$$\begin{aligned} \underline{ll(\theta : \mathcal{D})} &= \log \prod_{i=1}^N \underline{P(\mathbf{x}_i | \theta)} \\ &= \sum_{i=1}^N \log P(\mathbf{x}_i | \theta) \\ &= \sum_{i=1}^N \log \sum_{\mathbf{z}} P(\mathbf{x}_i, \mathbf{z} | \theta) \end{aligned}$$



# Applying Jensen's inequality

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

$\log(\cdot)$



# Applying Jensen's inequality

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

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



# Evidence Based Lower Bound

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

$$P(x_i | z, \theta) P(z | \theta)$$

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

$$\max_{Q_i, \theta}$$

$$\sum_{\mathbf{z}} Q_i(\mathbf{z}) \log P(x_i | z, \theta)$$

$$E_{z \sim Q_i(z)} [\log P(x_i | z, \theta)]$$

$$+ \sum_{\mathbf{z}} Q_i(\mathbf{z}) \log \frac{P(z | \theta)}{Q_i(\mathbf{z})}$$

$$- |KL(Q_i(z) || P_{\theta}(z))|$$

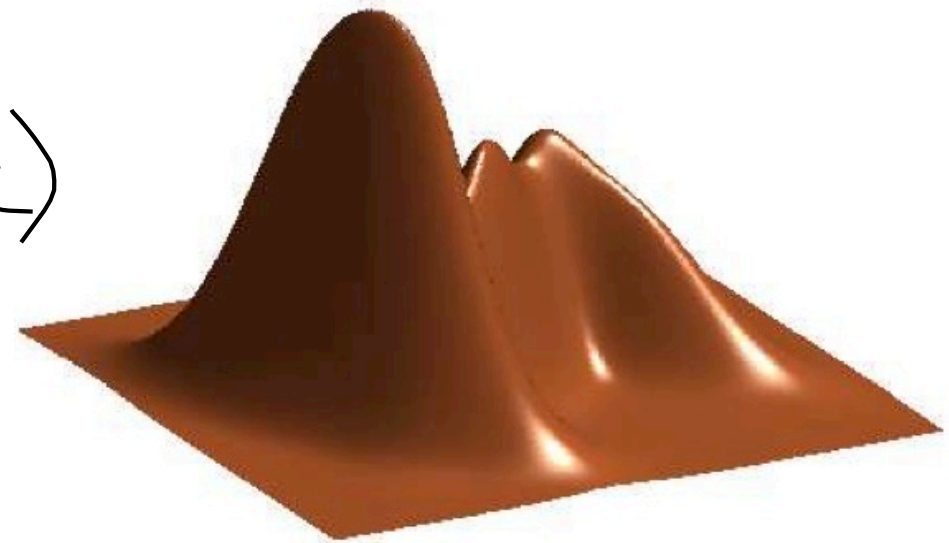
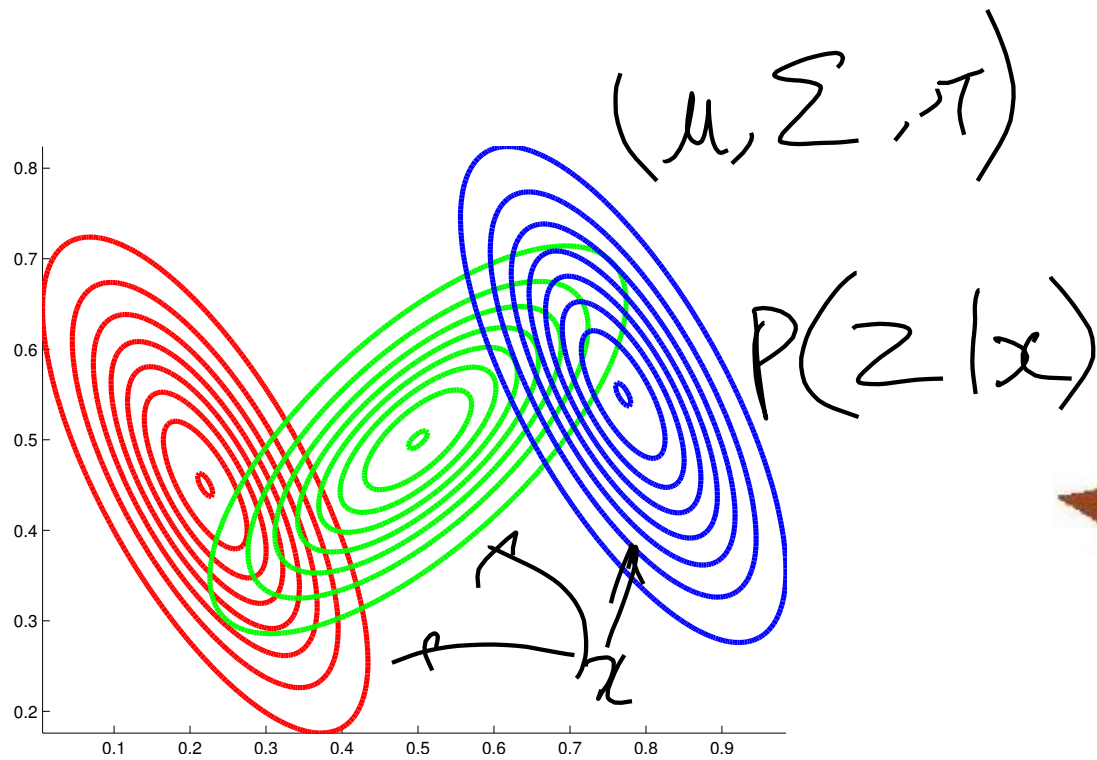
# Evidence Based Lower Bound

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

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

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

# GMM

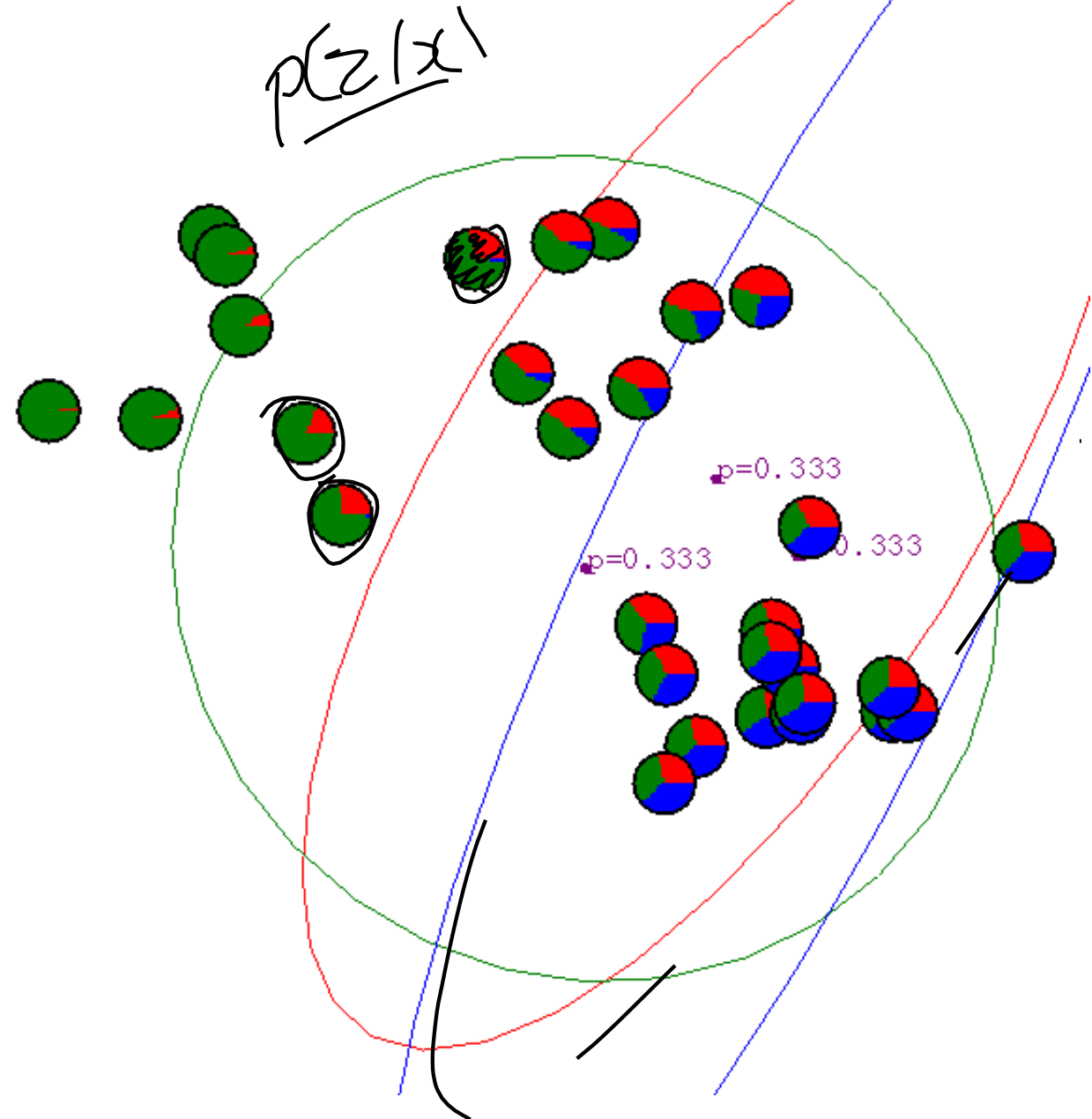




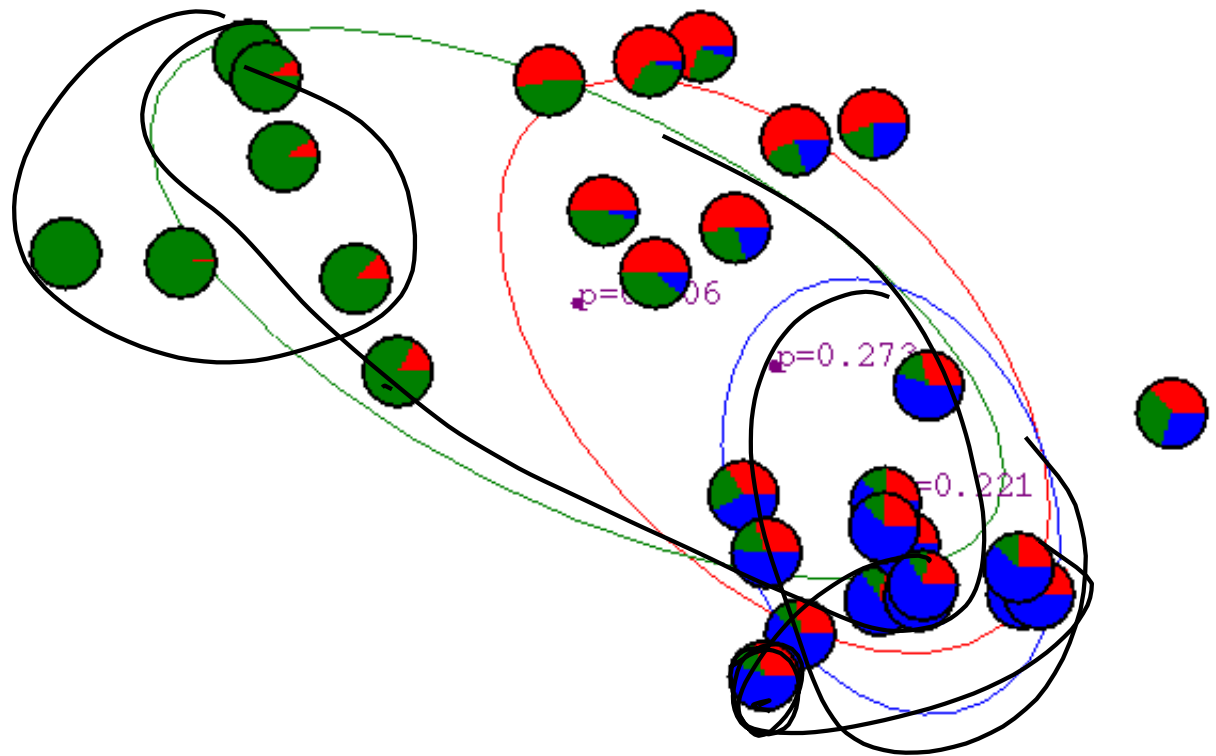
# EM for Learning GMMs

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

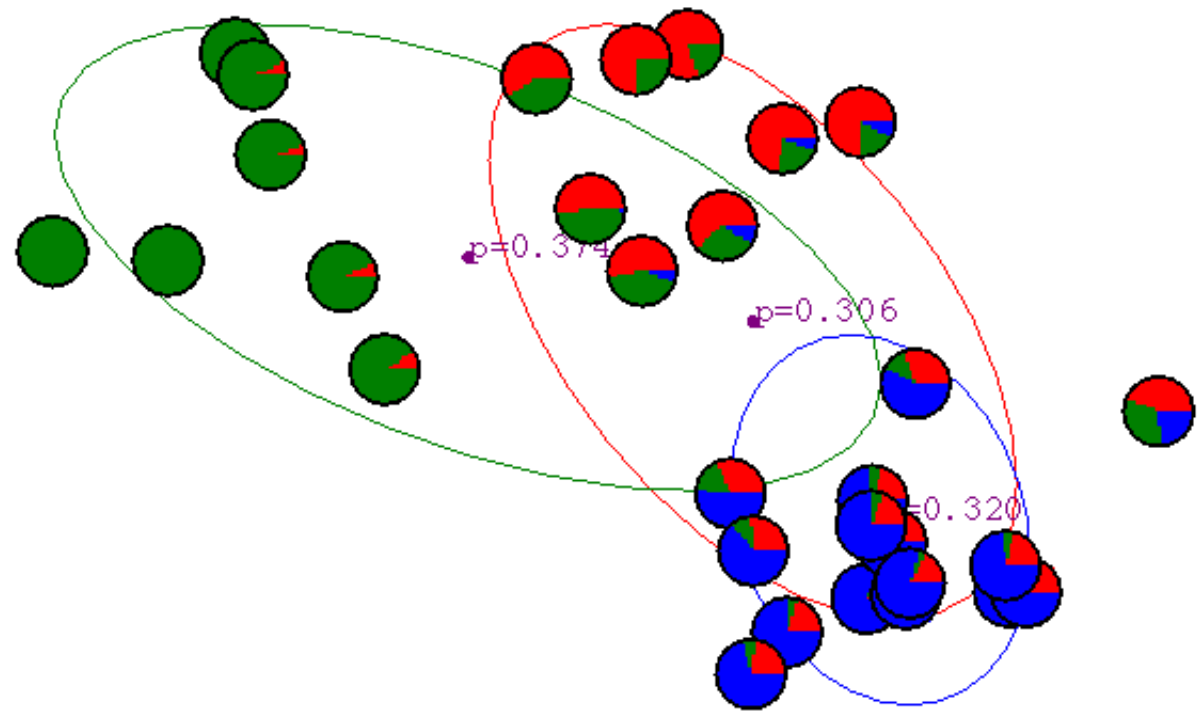
# Gaussian Mixture Example: Start



# After 1st iteration

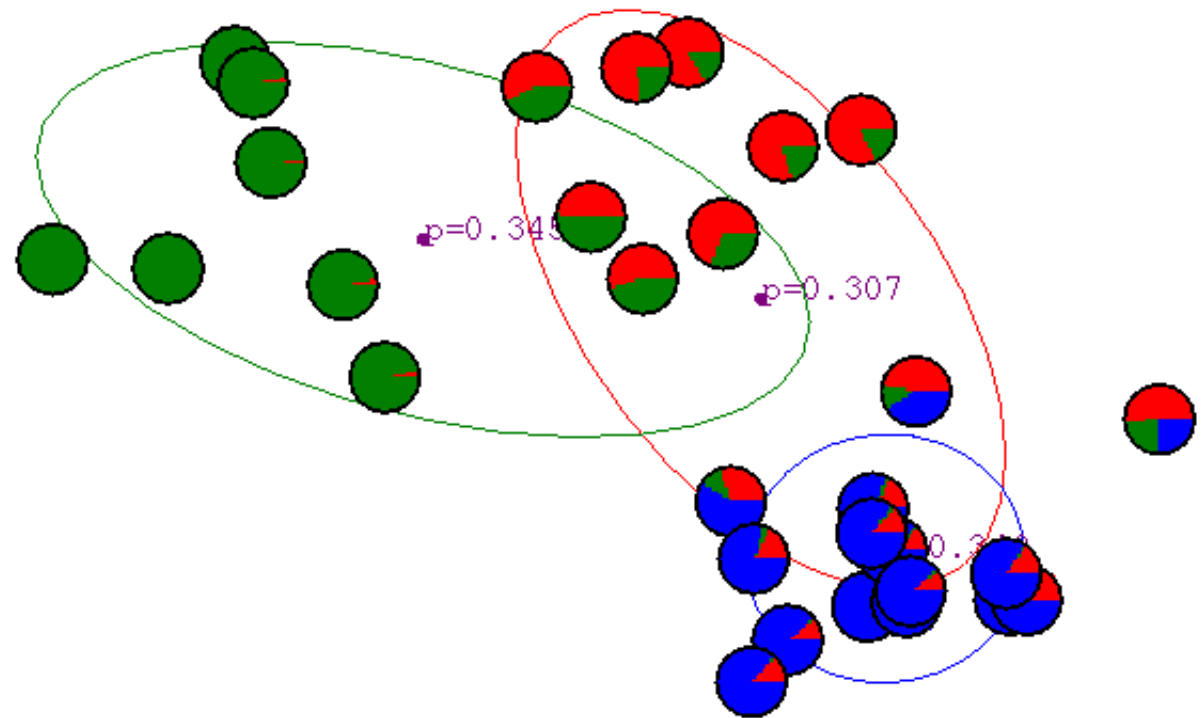


# After 2nd iteration

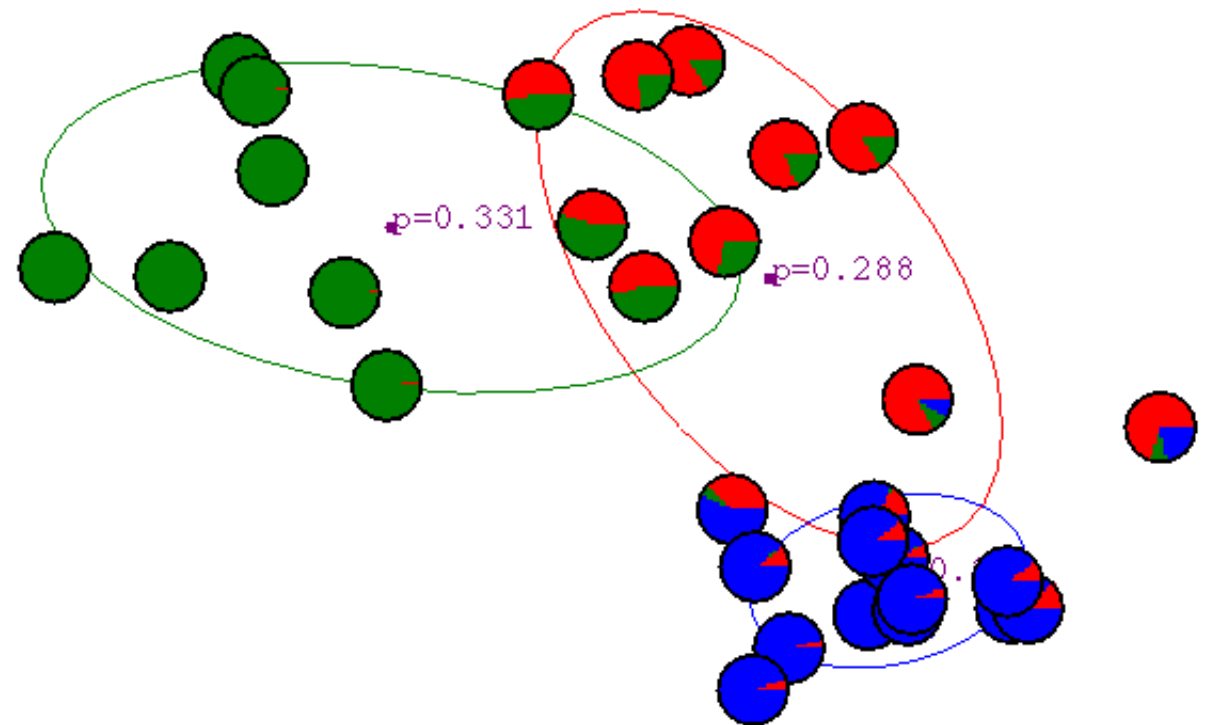




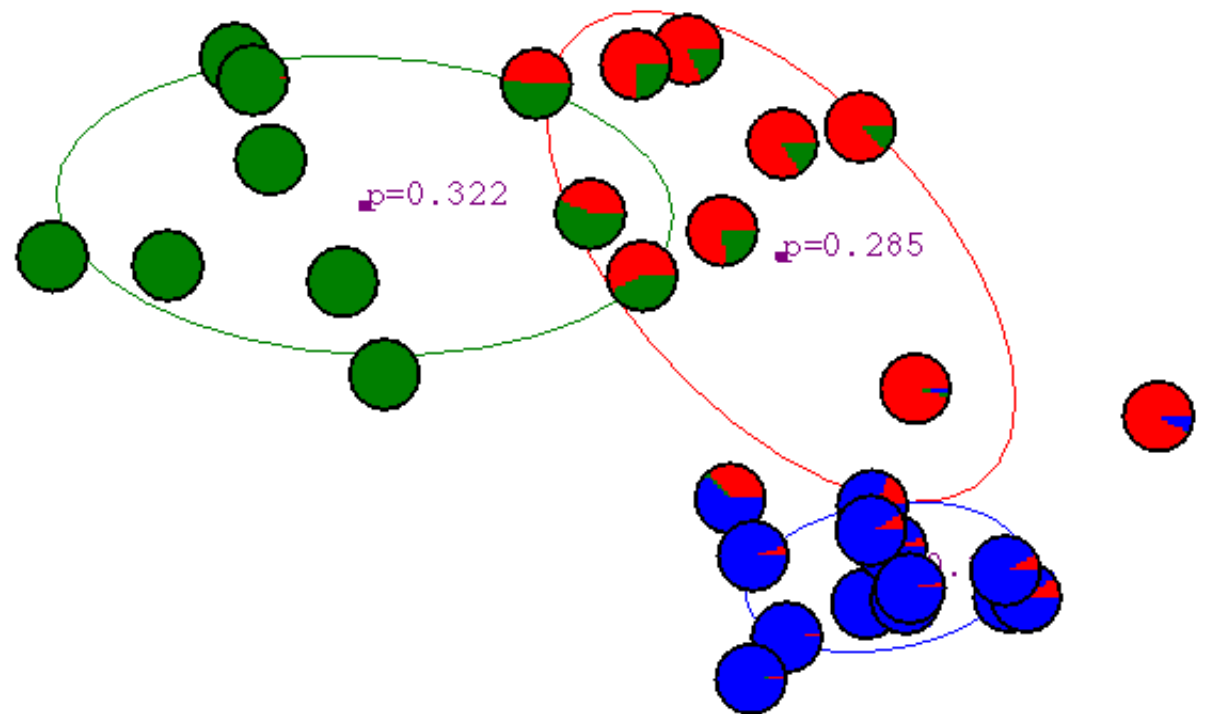
# After 3rd iteration



# After 4th iteration

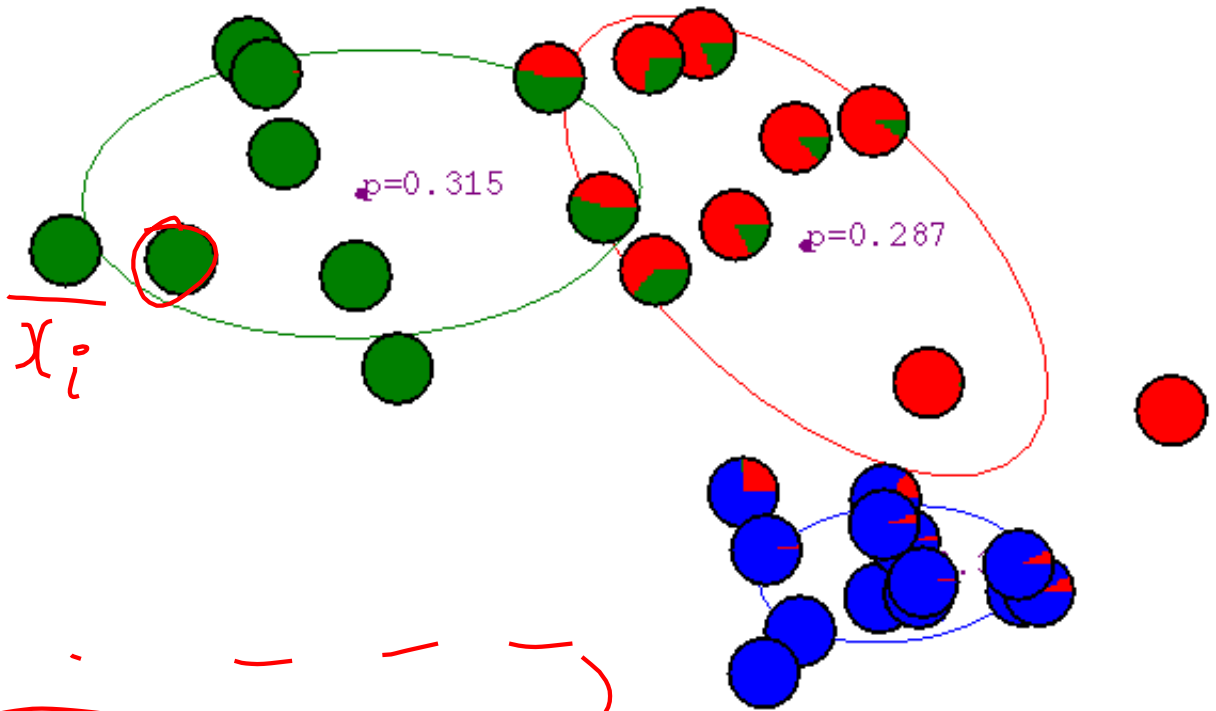


# After 5th iteration

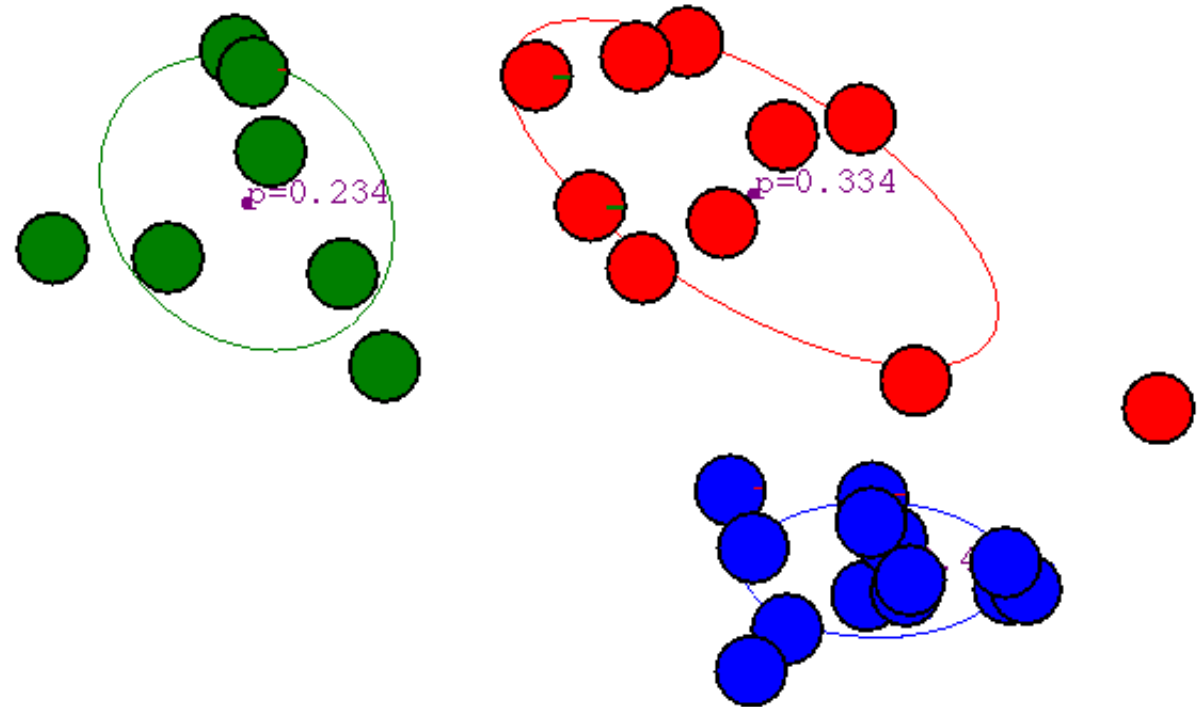


# After 6th iteration

$$P(z|x_i)$$



# After 20th iteration



# Variational Auto Encoders

VAEs are a combination of the following ideas:

1. Auto Encoders

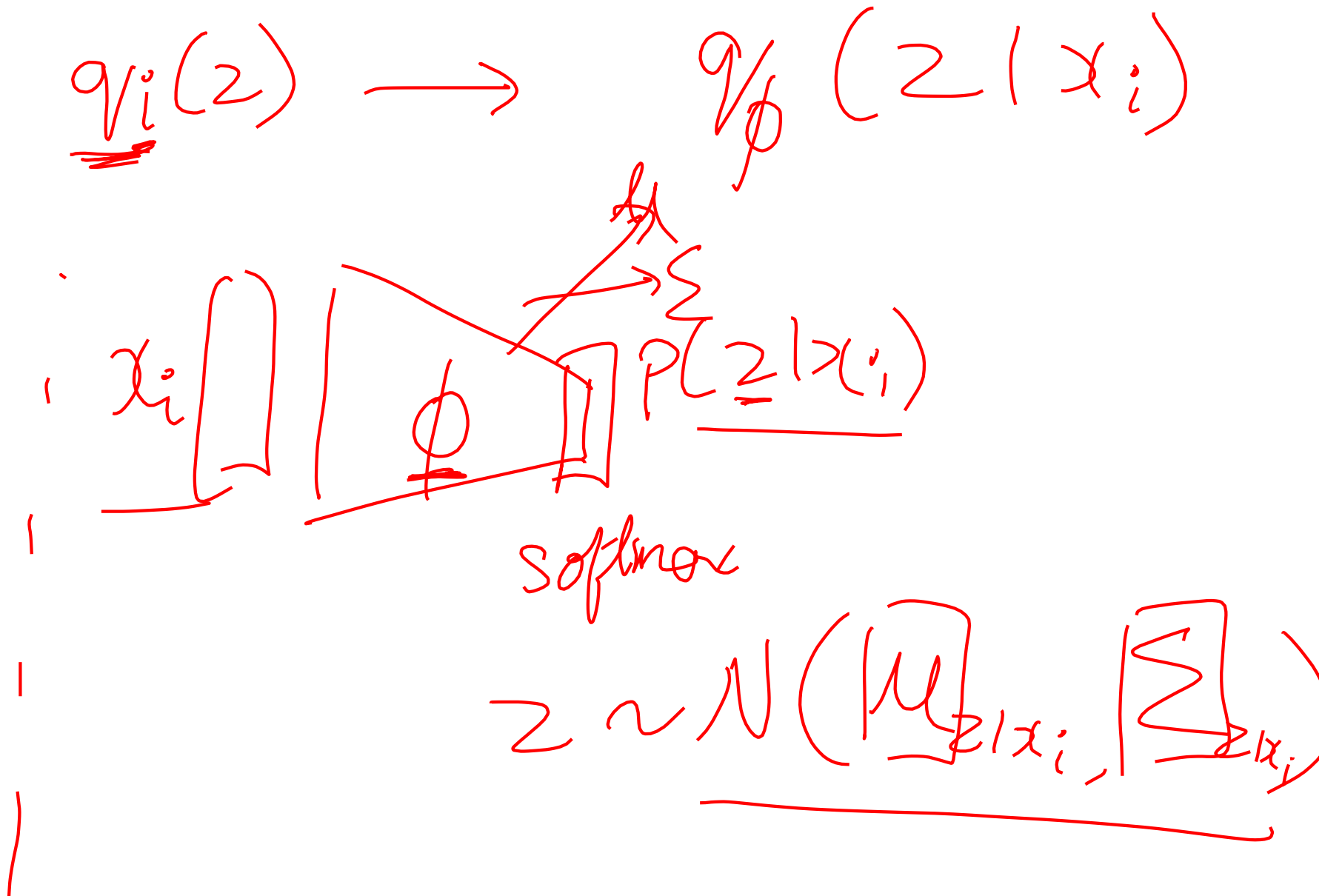
2. Variational Approximation

- Variational Lower Bound / ELBO

3. Amortized Inference Neural Networks

4. “Reparameterization” Trick

# 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

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

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

Input Data

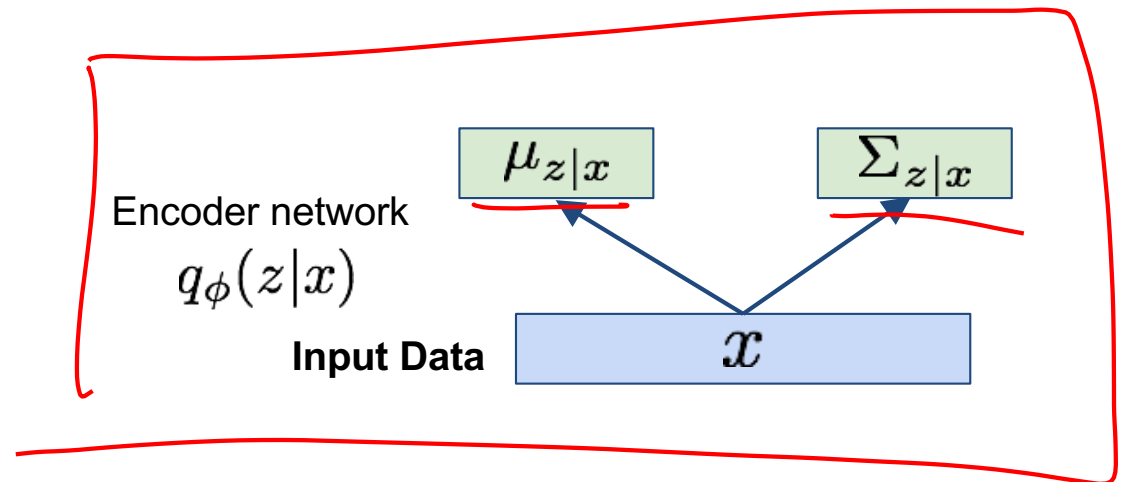
$\mathcal{X}$



# 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

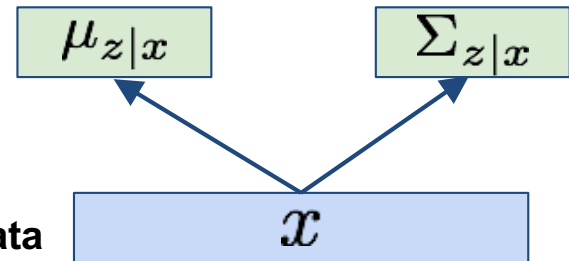
$$\underbrace{\mathbf{E}_z \left[ \log p_\theta(x^{(i)} | z) \right] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}$$

Make approximate posterior distribution close to prior

Encoder network

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

Input Data

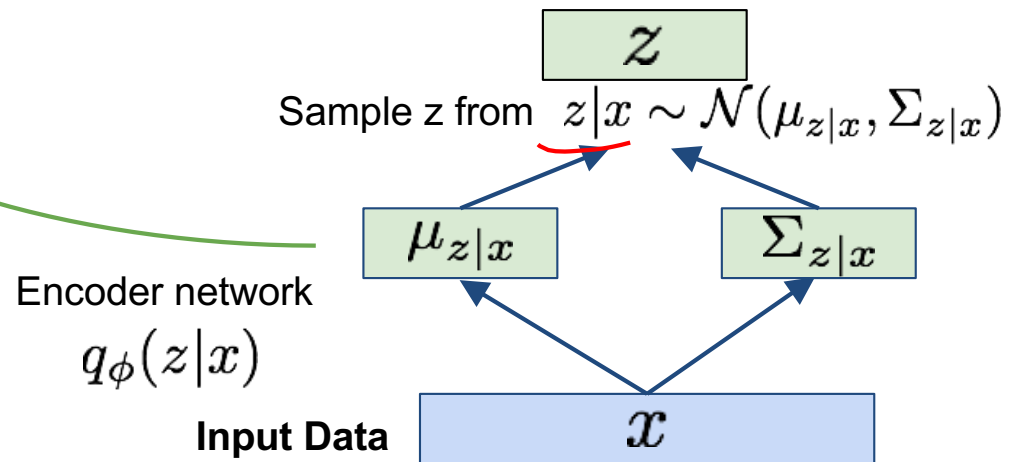


# Variational Auto Encoders

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

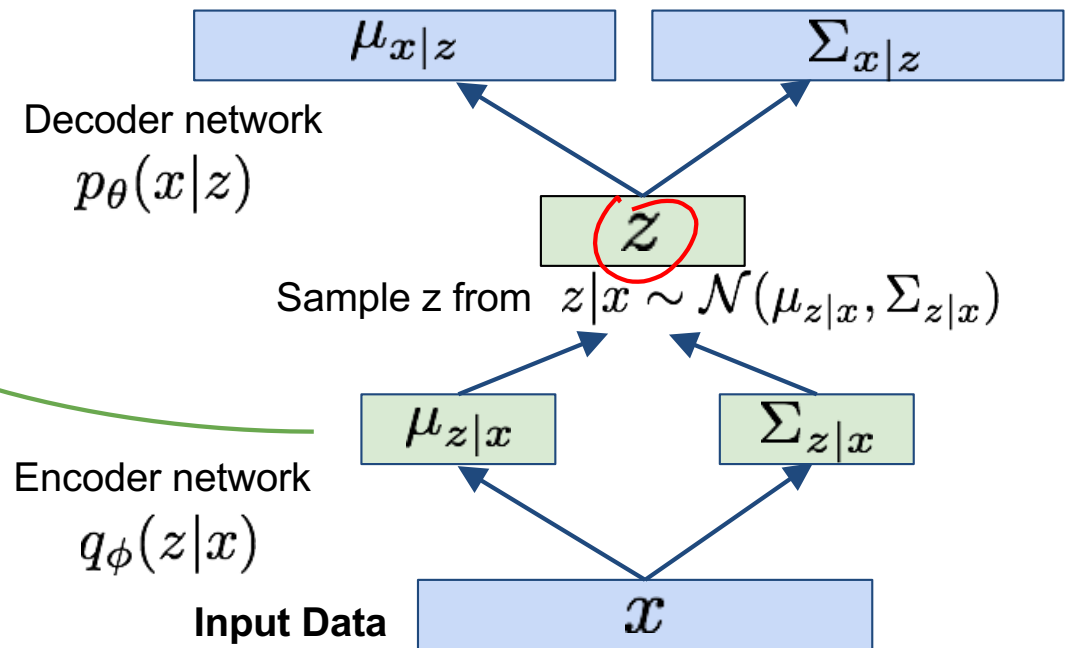


# Variational Auto Encoders

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



# Variational Auto Encoders

Putting it all together: maximizing the likelihood lower bound

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

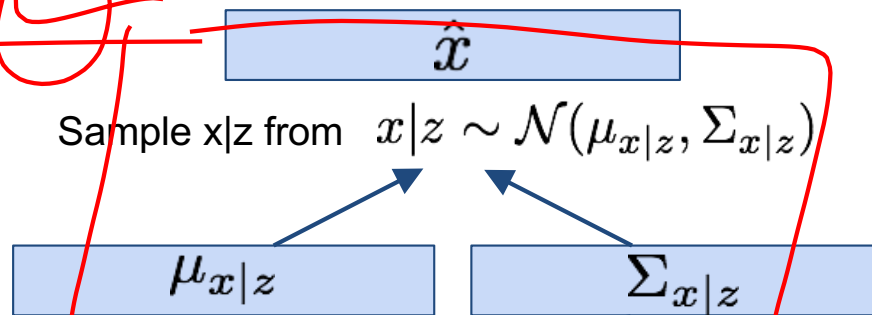
$\mathcal{L}(x^{(i)}, \theta, \phi)$

Make approximate posterior distribution close to prior

Maximize likelihood of original input being reconstructed

Decoder network  
 $p_\theta(x|z)$

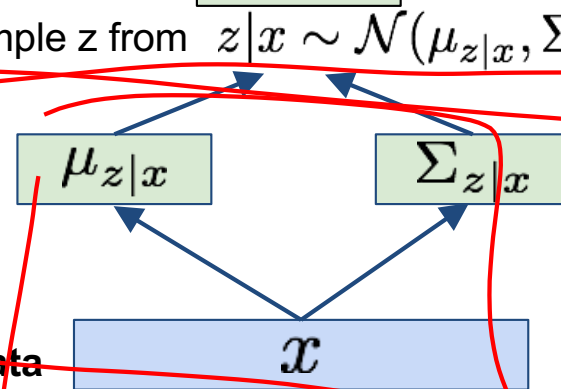
Sample  $x|z$  from  $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$



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

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

Input Data



# Variational Auto Encoders

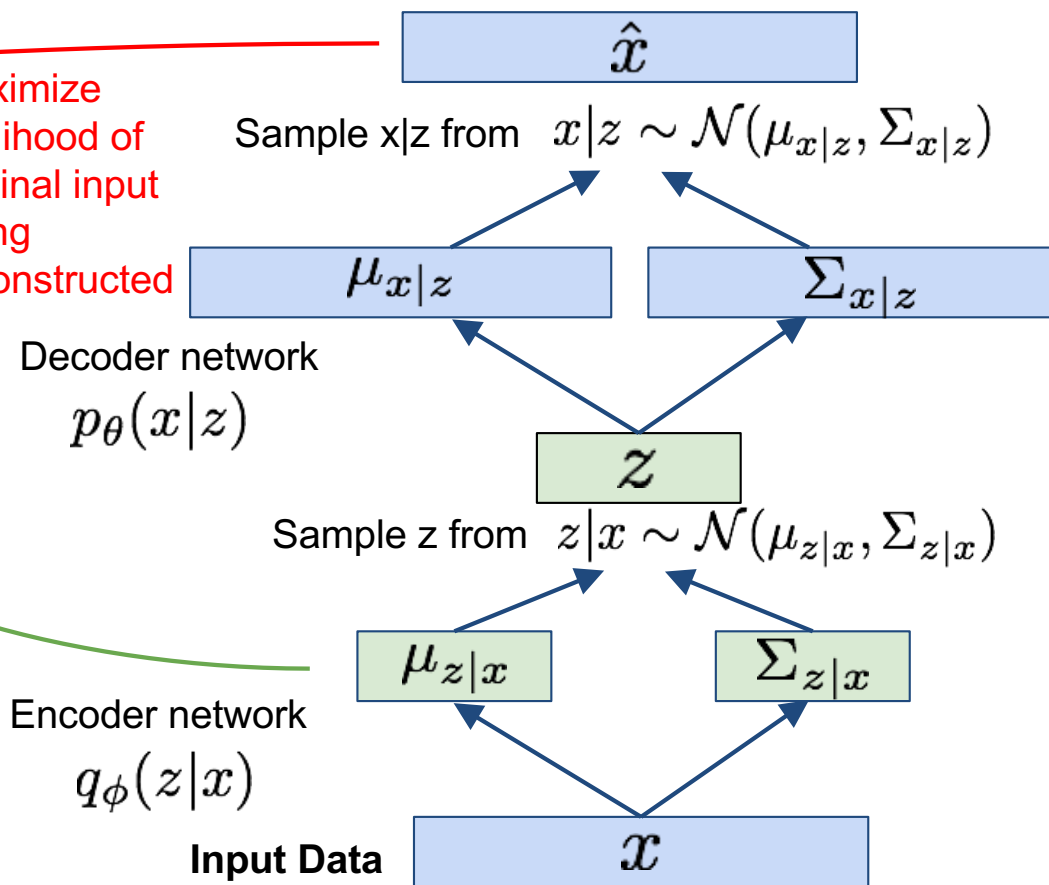
Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

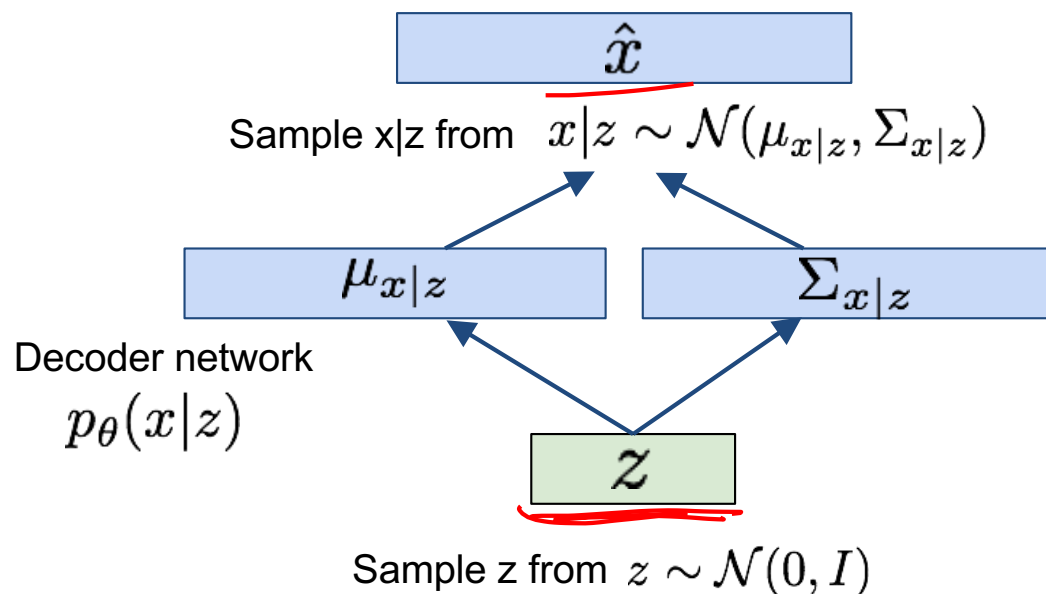
For every minibatch of input data: compute this forward pass, and then backprop!

Maximize likelihood of original input being reconstructed



# Variational Auto Encoders: Generating Data

Use decoder network. Now sample  $z$  from prior!

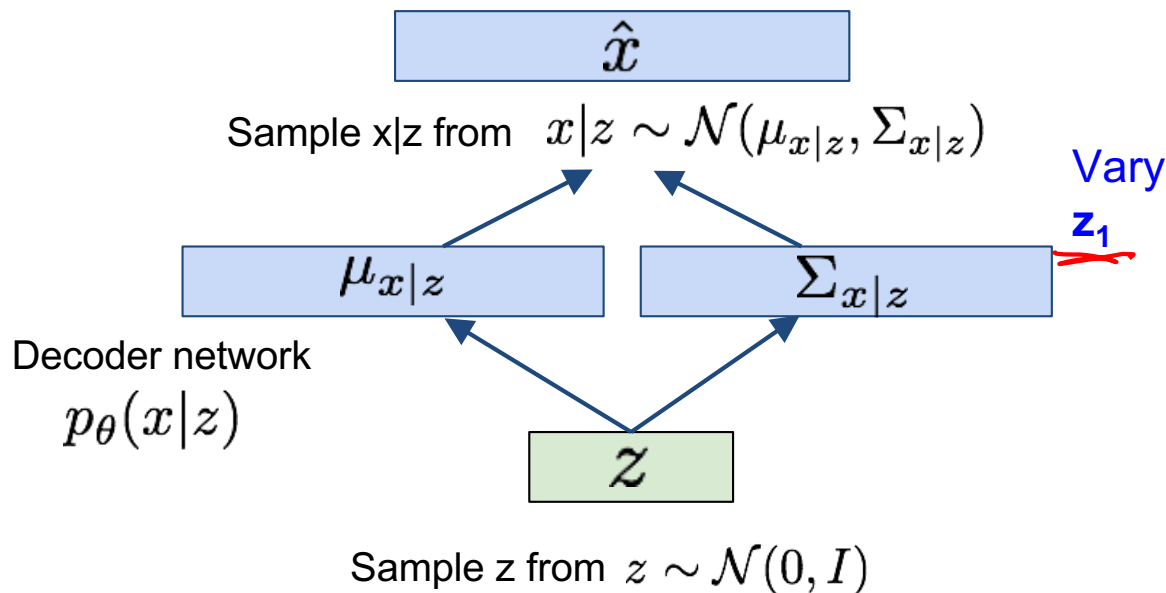






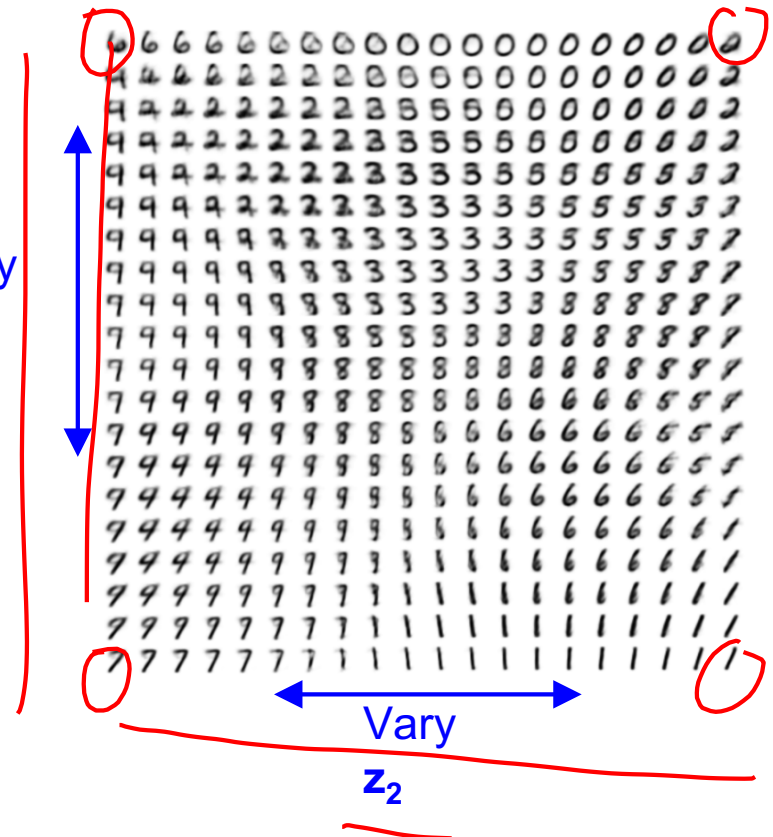
# Variational Auto Encoders: Generating Data

Use decoder network. Now sample  $z$  from prior!



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

Data manifold for 2-d  $z$



# Variational Auto Encoders: Generating Data

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

Different  
dimensions of  $\mathbf{z}$   
encode  
interpretable factors  
of variation

Degree of smile

Vary  
 $z_1$



Vary  
 $z_2$

Head pose

# Variational Auto Encoders: Generating Data

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

Different  
dimensions of  $\mathbf{z}$   
encode  
interpretable factors  
of variation

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

Degree of smile

Vary  
 $z_1$



Head pose

Vary  
 $z_2$

# 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



## 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

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

## So far...

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

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

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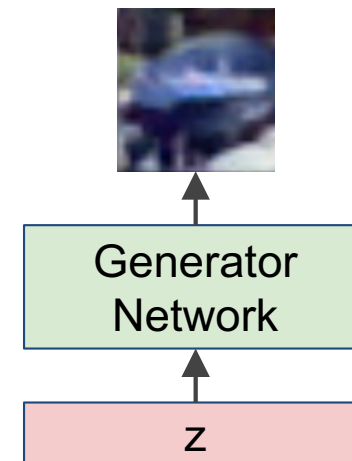
Solution: Sample from a simple distribution, e.g. random noise. Learn transformation to training distribution.

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

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

**Generator network:** try to fool the discriminator by generating real-looking images

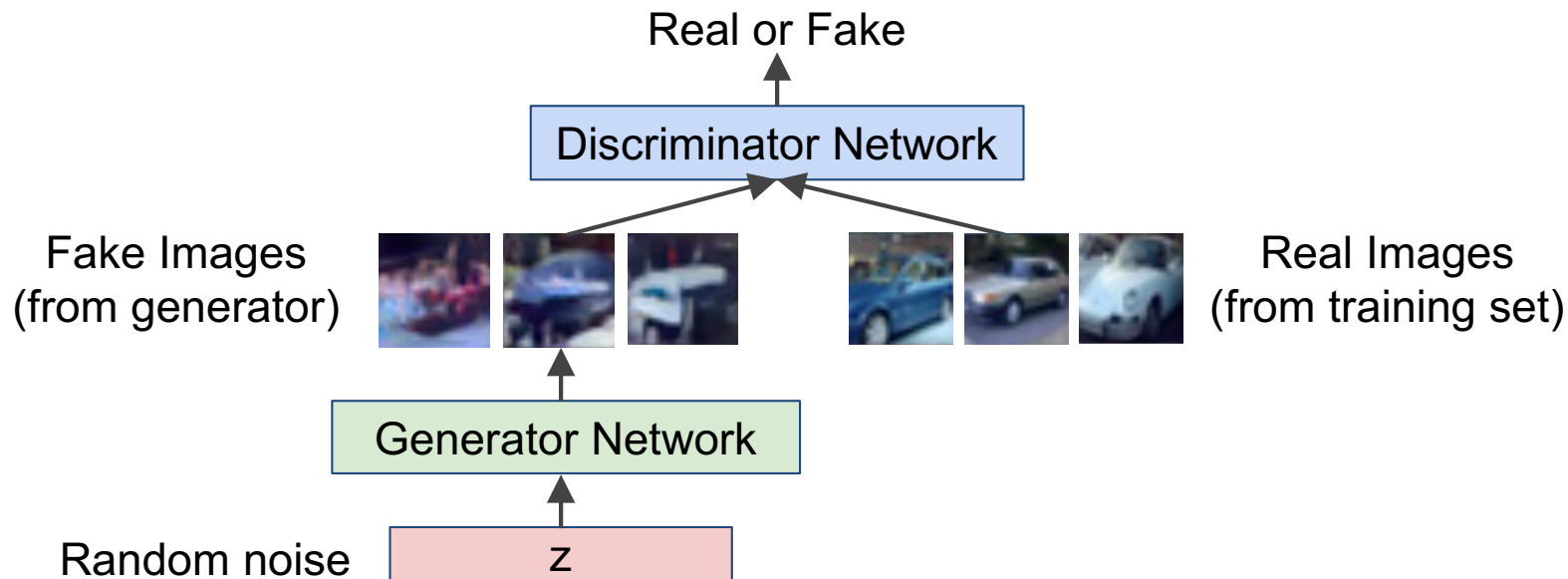
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**Discriminator network:** try to distinguish between real and fake images

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

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

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

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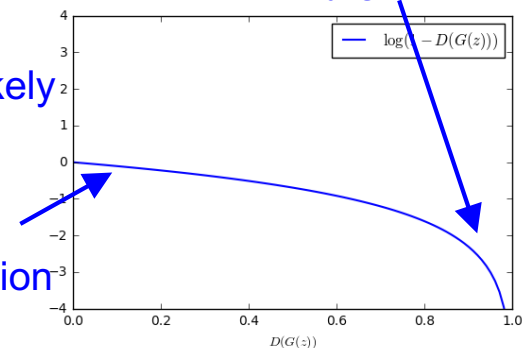
2. **Gradient descent** on generator

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

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

When sample is likely fake, want to learn from it to improve generator. But gradient in this region is relatively flat!

Gradient signal dominated by region where sample is already good



# Training GANs: Two-player game

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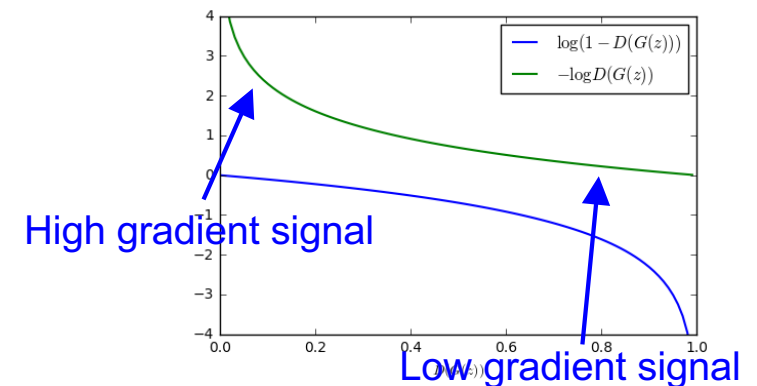
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2. **Instead: Gradient ascent** on generator, **different objective**

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

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.

