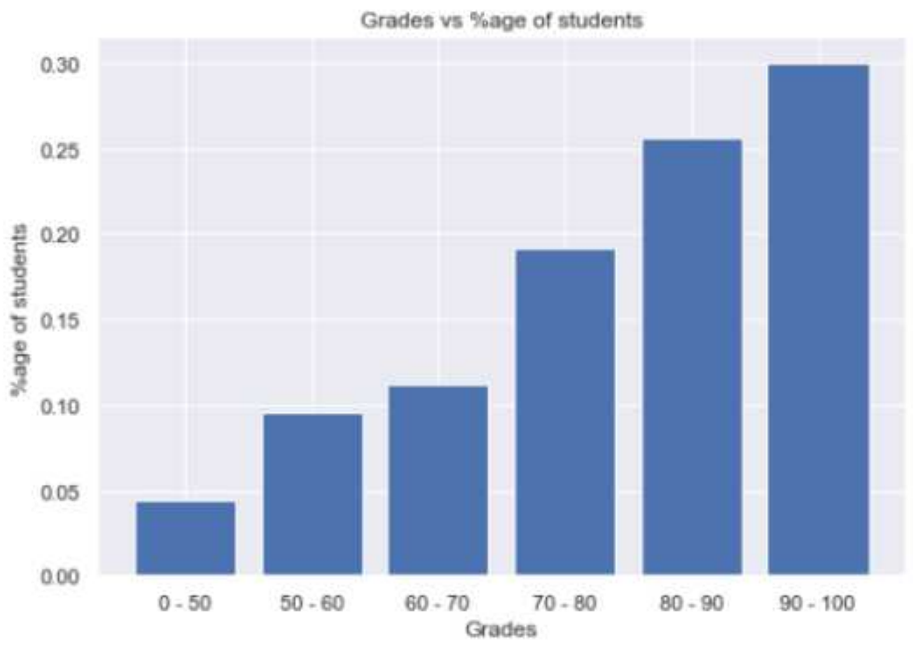
Lecture 19:
Generative Models, Part 1

Admin: Midterm grades

Many students did worse on midterm than homework; this is typical!

Overall course will be curved if needed (but only to your benefit)

WI2022 Midterm Grade Distribution



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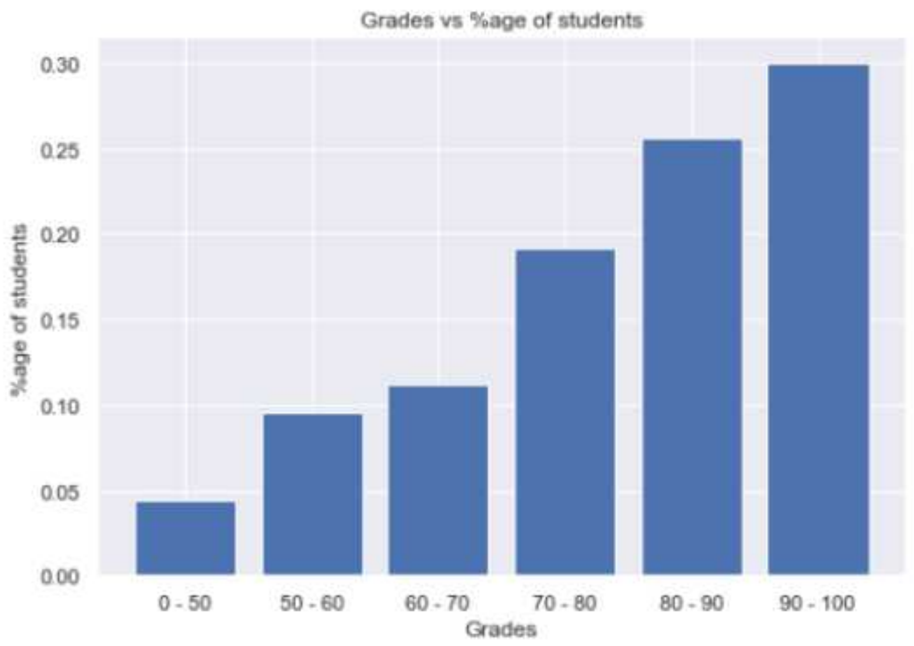


FA2020 Course Grade Cutoffs / Distribution

A+: 98% / 5.8%
A: 90.5% / 58.7%
A-: 88.5% / 11.6%
B+: 86 / 11.6%
B: 81 / 5.8%

Admin: A4

Object Detection: FCOS, Faster R-CNN

Due Tuesday, 3/29/2022, 11:59pm ET

See Piazza for updates to Faster R-CNN:
- Small changes to improve mAP
- Hand-grading rubric

Admin: A5

Recurrent networks, Transformers

Should be out tonight, due Monday April 11, 11:59pm ET

Last Time: Vision Transformer (ViT)

Linear projection to C-dim vector of predicted class scores

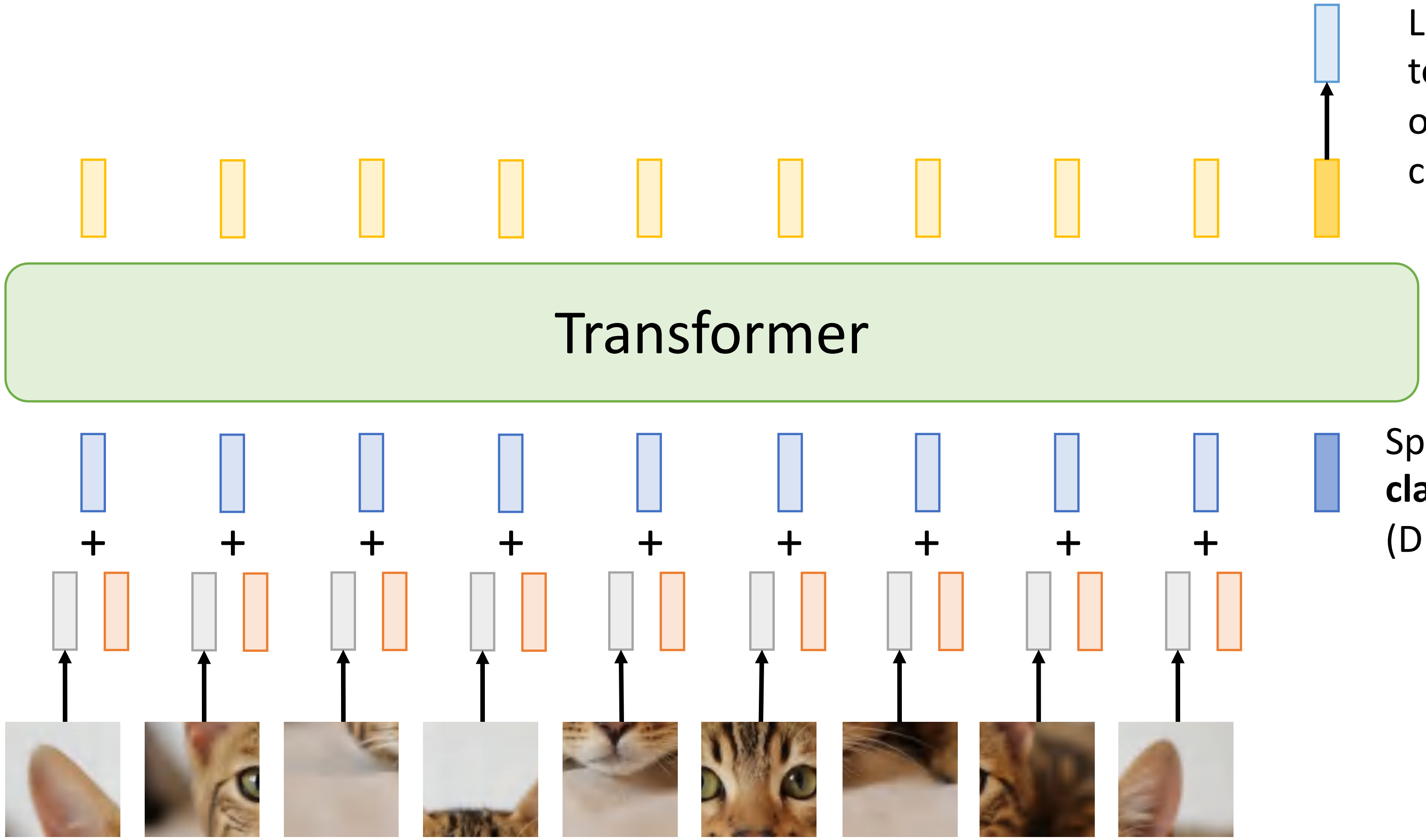
Output vectors

Exact same as NLP Transformer!

Add positional embedding: learned D-dim vector per position

Linear projection to D-dimensional vector

N input patches, each of shape 3x16x16



Special extra input: **classification token** (D dims, learned)

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021

Today:
Generative Models, Part 1

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)

x is data, y is label

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

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

Classification

Cat

Supervised vs Unsupervised Learning

Supervised Learning

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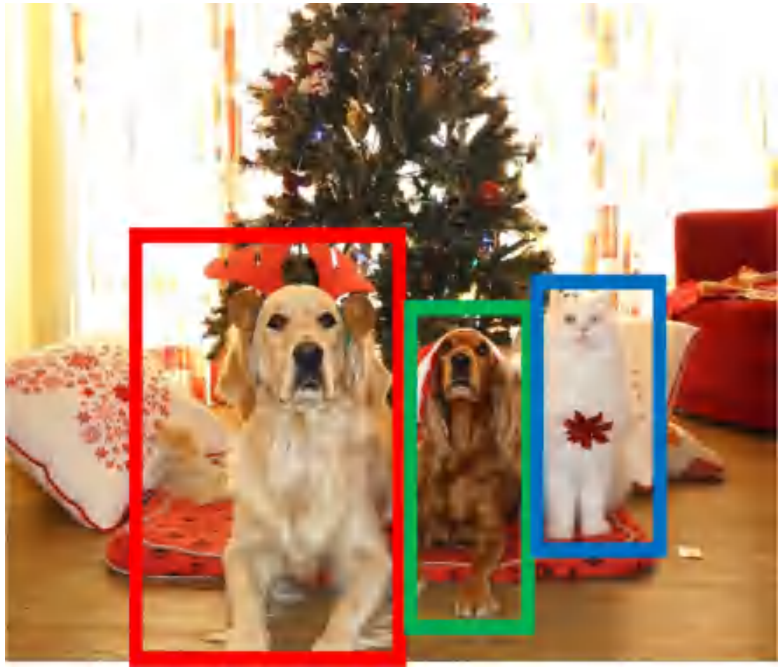
Object Detection



DOG, DOG, CAT

Supervised vs Unsupervised Learning

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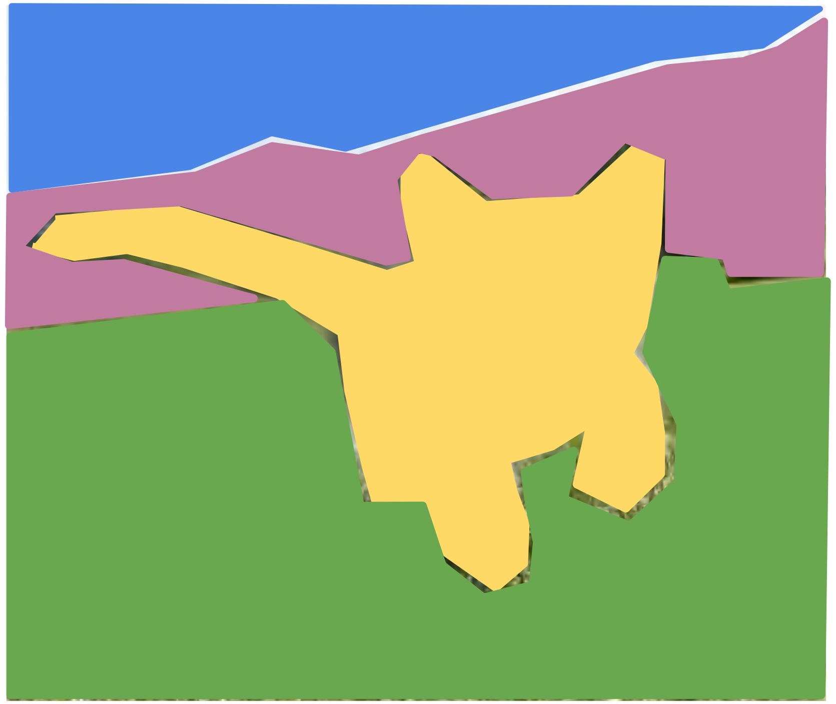
Semantic Segmentation



GRASS, CAT, TREE, SKY

Supervised vs Unsupervised Learning

Supervised Learning

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

Image captioning

A cat sitting on a suitcase on the floor

Caption generated using neuraltalk2
Image is CC0 Public domain.

Supervised vs Unsupervised Learning

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Unsupervised Learning

Data: x

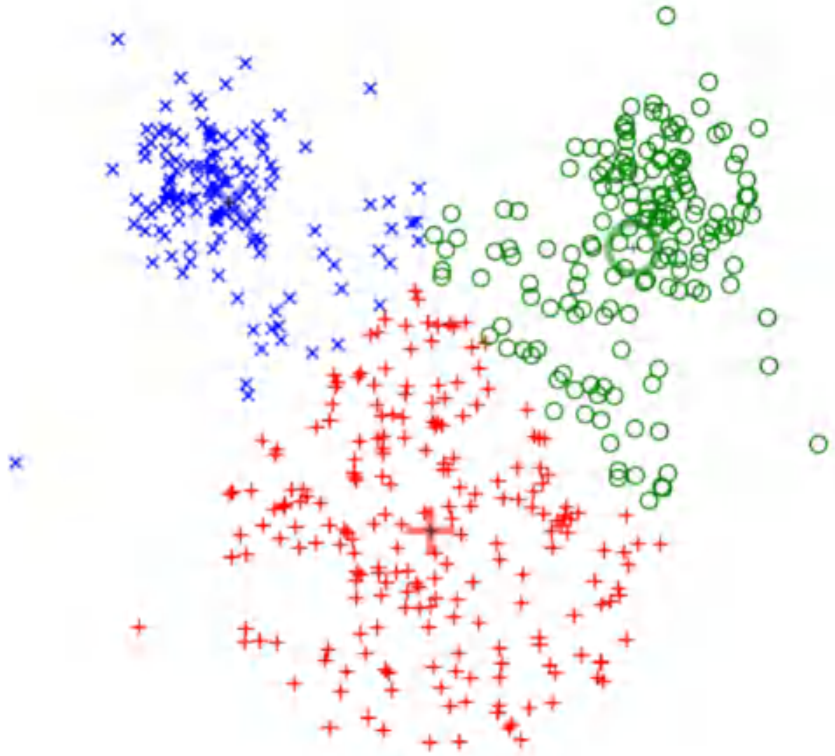
Just data, no labels!

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

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

Supervised vs Unsupervised Learning

Clustering
(e.g. K-Means)



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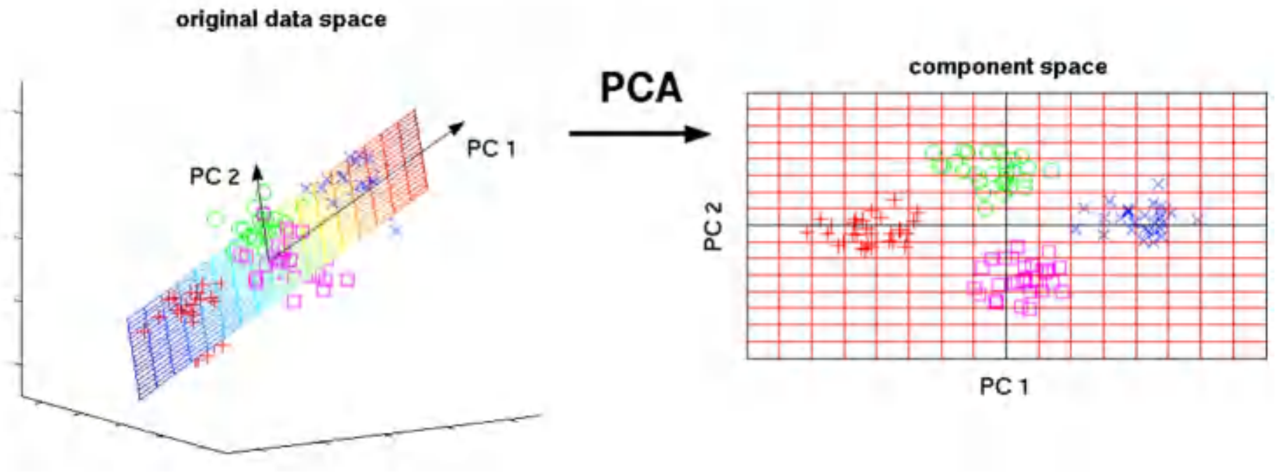
Supervised vs Unsupervised Learning

Dimensionality Reduction
(e.g. Principal Components Analysis)



3D → 2D

This image from Matthias Scholz is CC0 public domain

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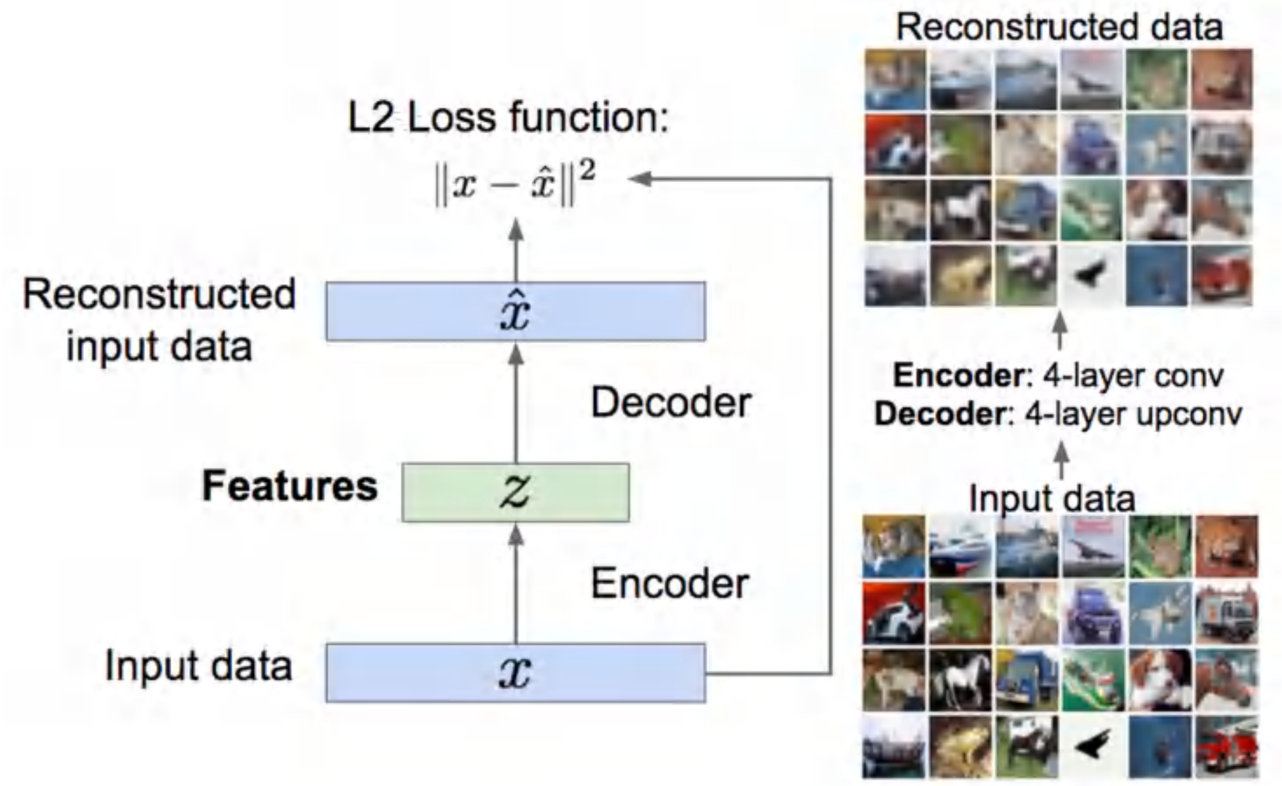
Supervised vs Unsupervised Learning

Feature Learning
(e.g. autoencoders)



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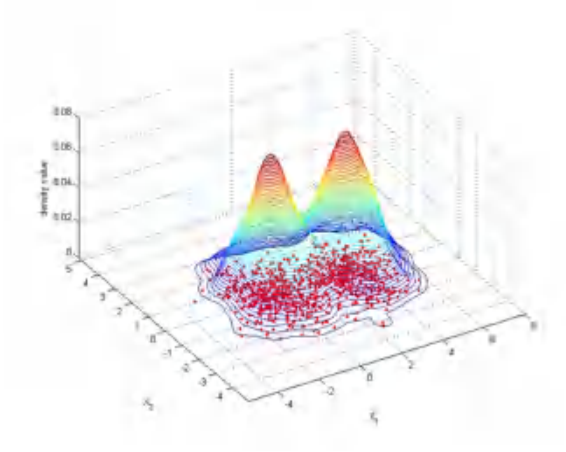
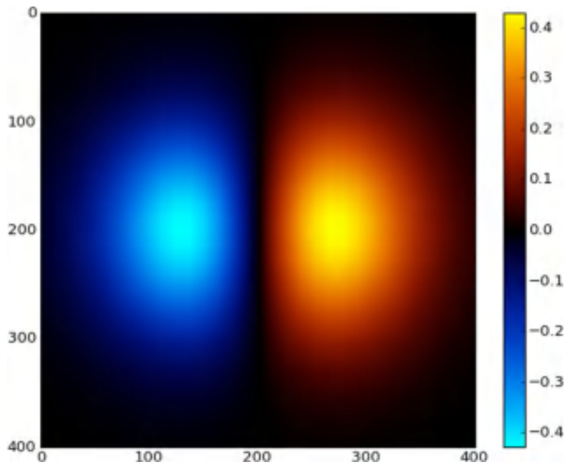
Supervised vs Unsupervised Learning

Density Estimation





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Discriminative vs Generative Models

Discriminative Model:
Learn a probability distribution p(y|x)

Generative Model:
Learn a probability distribution p(x)

Conditional Generative Model: Learn p(x|y)

Data: x

Label: y

Cat

Discriminative vs Generative Models

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Probability Recap:

Density Function
p(x) assigns a positive number to each possible x; higher numbers mean x is more likely

Density functions are **normalized**:

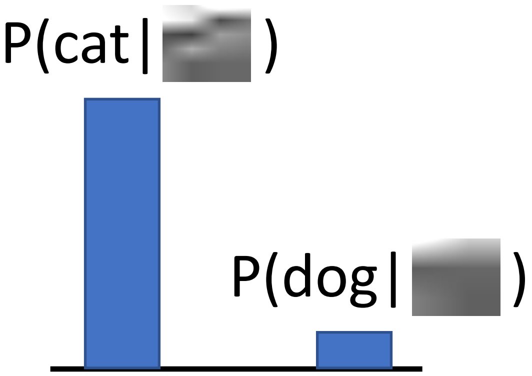
$$\int_X p(x)dx = 1$$

Different values of x **compete** for density

Discriminative vs Generative Models

Discriminative Model: Learn a probability distribution p(y|x)

Data: x



Generative Model: Learn a probability distribution p(x)

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Conditional Generative Model: Learn p(x|y)

Discriminative vs Generative Models

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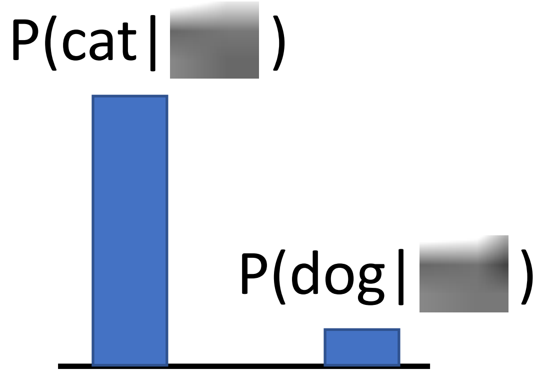
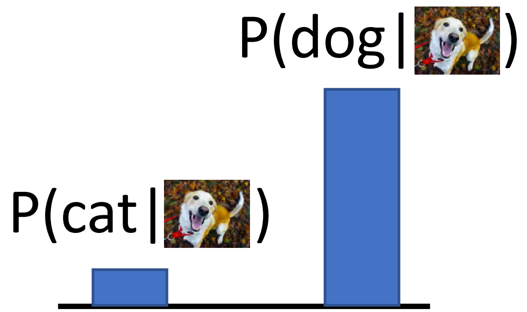


Generative Model: Learn a probability distribution p(x)



Conditional Generative Model: Learn p(x|y)

Discriminative model: the possible labels for each input "compete" for probability mass. But no competition between **images**

Discriminative vs Generative Models

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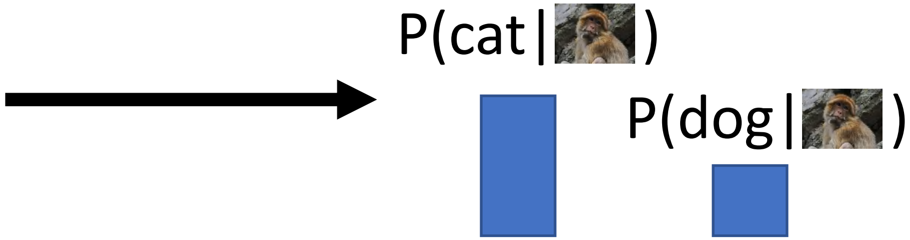
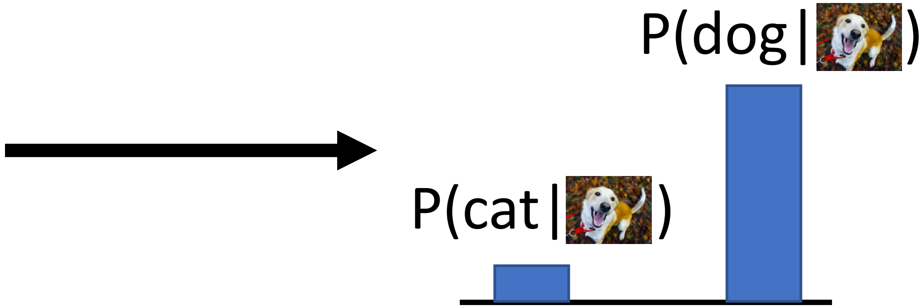
Conditional Generative Model: Learn p(x|y)

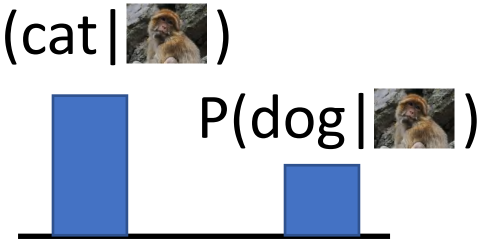




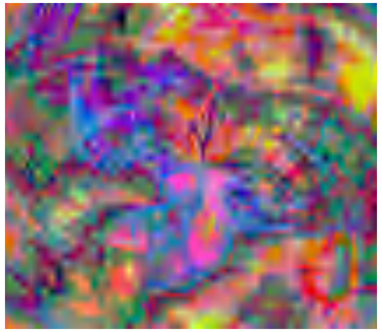
Discriminative model: No way for the model to handle unreasonable inputs; it must give label distributions for all images

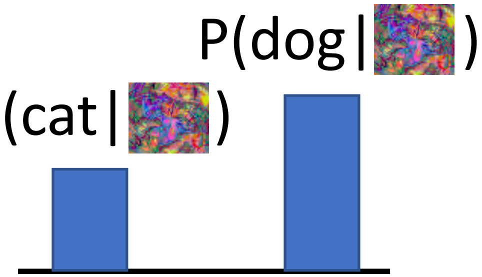
Discriminative vs Generative Models

Discriminative Model: Learn a probability distribution p(y|x)



Generative Model: Learn a probability distribution p(x)





Conditional Generative Model: Learn p(x|y)

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Discriminative vs Generative Models

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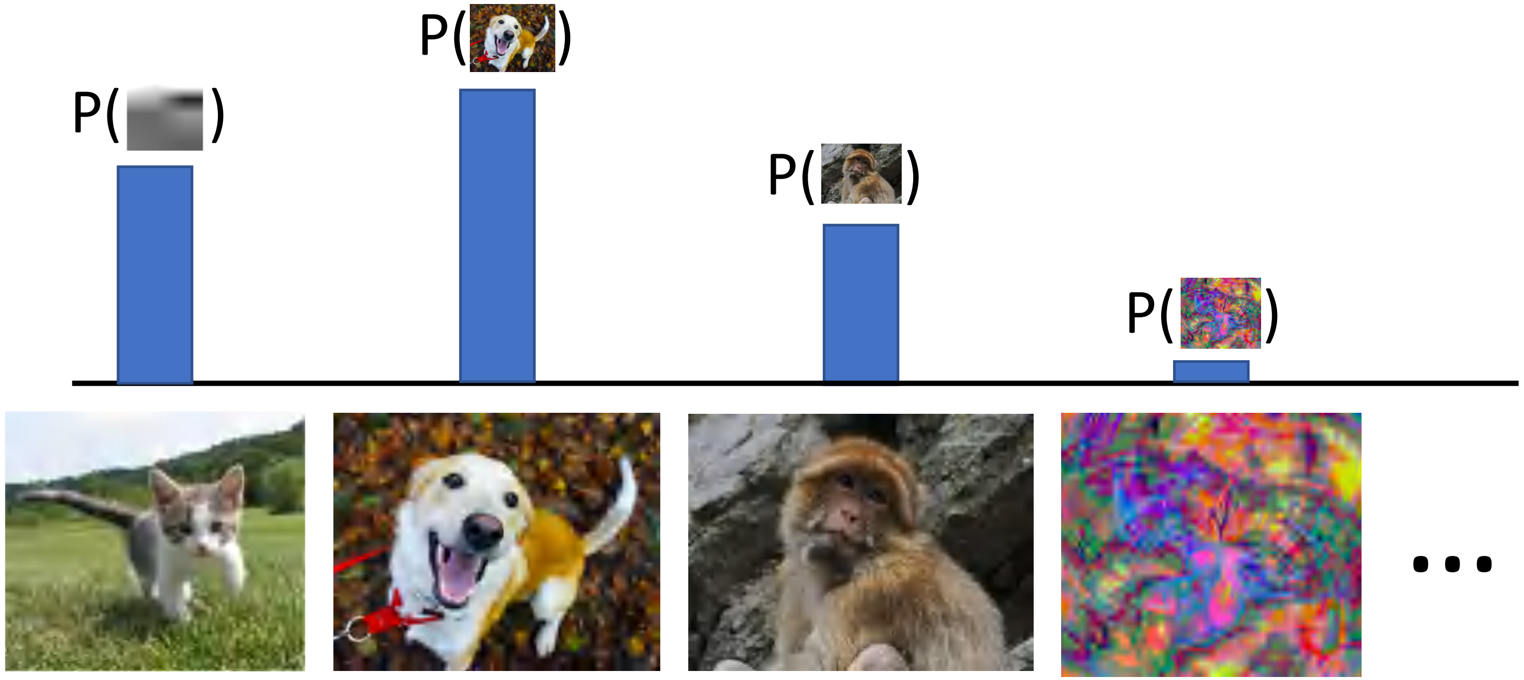

Generative model: All possible images compete with each other for probability mass

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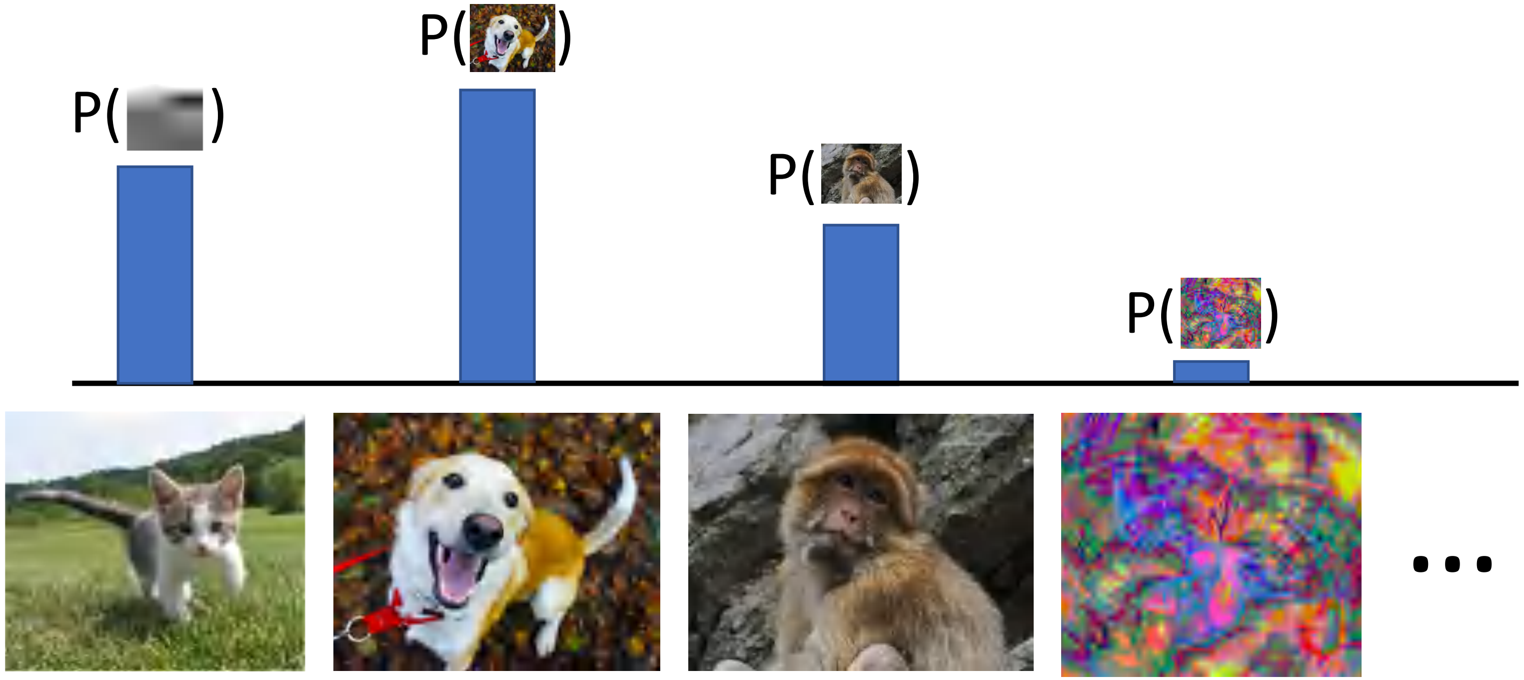


Generative model: All possible images compete with each other for probability mass

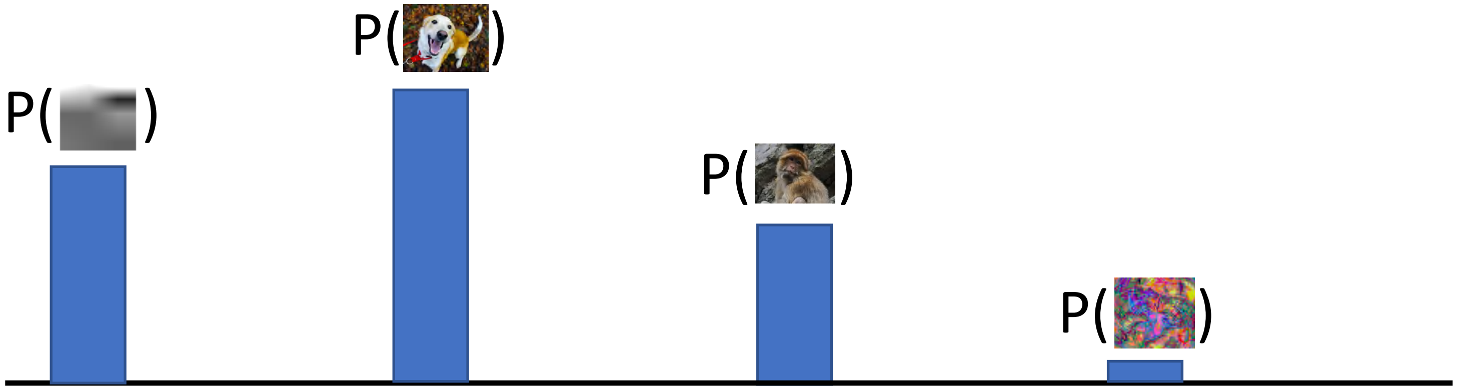
Requires deep image understanding! Is a dog more likely to sit or stand? How about 3-legged dog vs 3-armed monkey?

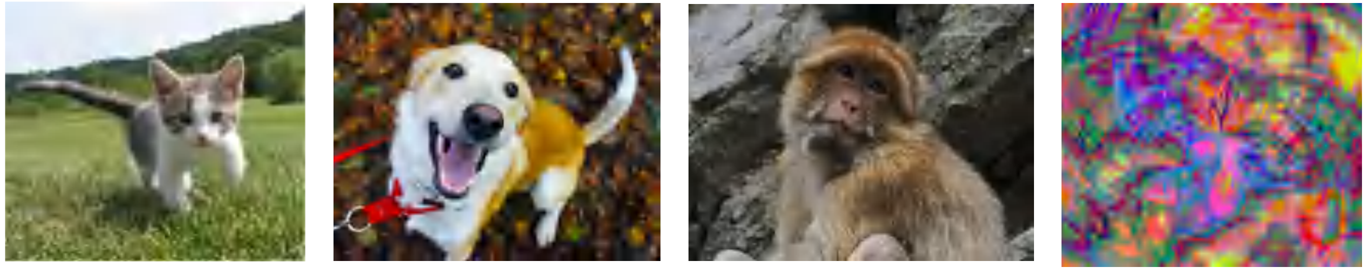
Discriminative vs Generative Models

Discriminative Model: Learn a probability distribution p(y|x)

Generative Model: Learn a probability distribution p(x)

Conditional Generative Model: Learn p(x|y)





...

Generative model: All possible images compete with each other for probability mass

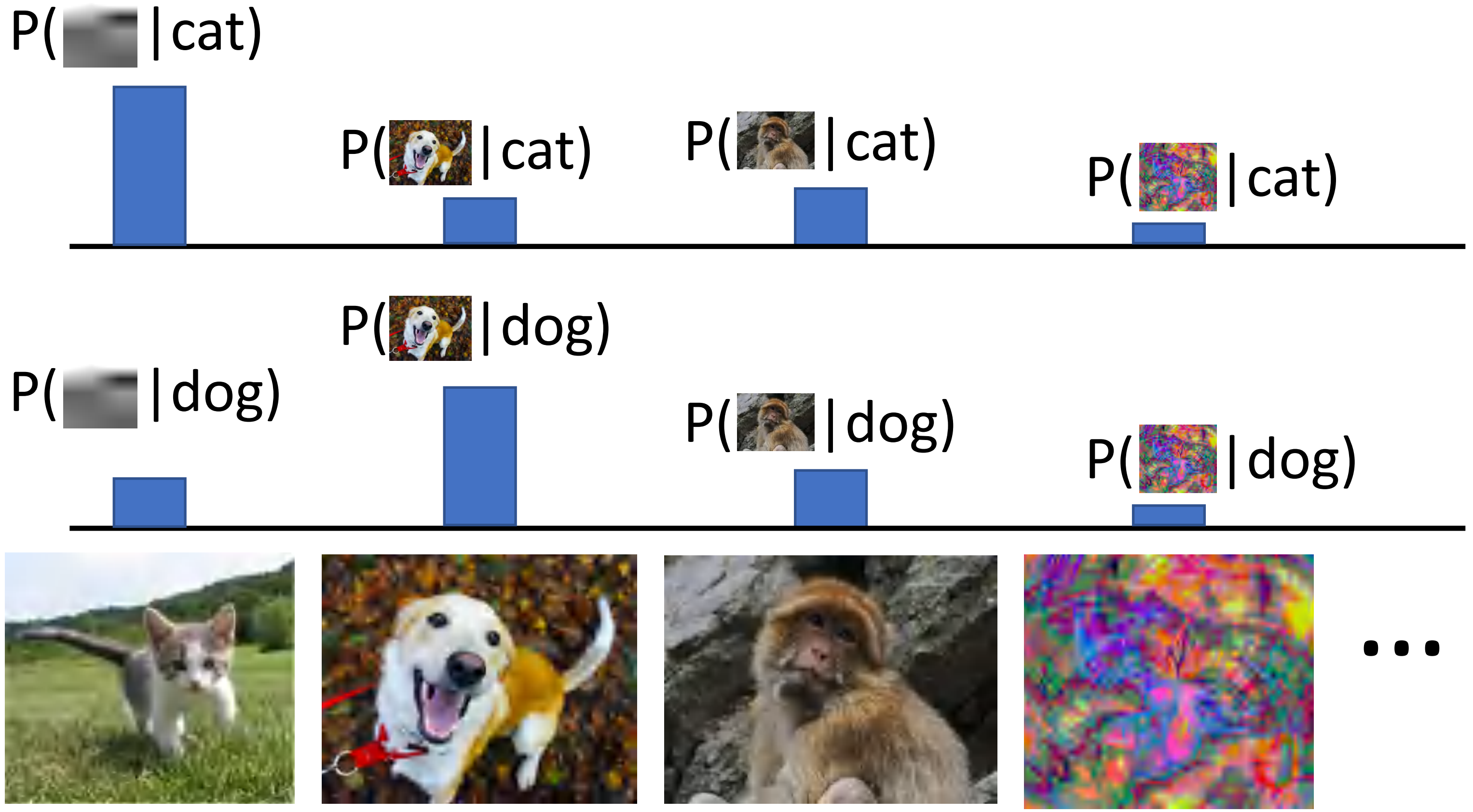
Model can "reject" unreasonable inputs by assigning them small values

Discriminative vs Generative Models

Discriminative Model: Learn a probability distribution p(y|x)

Generative Model: Learn a probability distribution p(x)

Conditional Generative Model: Learn p(x|y)



Conditional Generative Model: Each possible label induces a competition among all images

Discriminative vs Generative Models

Discriminative Model:
Learn a probability distribution p(y|x)

Generative Model:
Learn a probability distribution p(x)

Conditional Generative Model: Learn p(x|y)

Recall **Bayes' Rule:**

$$P(x \mid y) = \frac{P(y \mid x)}{P(y)} P(x)$$

Discriminative vs Generative Models

Discriminative Model: Learn a probability distribution p(y|x)

Generative Model: Learn a probability distribution p(x)

Conditional Generative Model: Learn p(x|y)

Recall **Bayes' Rule:**

$$\underbrace{\boxed{P(x \mid y)}}_{\text{Conditional Generative Model}} = \frac{\overbrace{\boxed{P(y \mid x)}}^{\text{Discriminative Model}}}{\underbrace{\boxed{P(y)}}_{\text{Prior over labels}}} \overbrace{\boxed{P(x)}}^{\text{(Unconditional) Generative Model}}$$

We can build a conditional generative model from other components!

What can we do with a discriminative model?

Discriminative Model:
Learn a probability distribution $p(y|x)$

→ Assign labels to data
Feature learning (with labels)

Generative Model:
Learn a probability distribution $p(x)$

Conditional Generative Model: Learn $p(x|y)$

What can we do with a generative model?

Discriminative Model:
Learn a probability distribution p(y|x) → Assign labels to data
Feature learning (with labels)

Generative Model:
Learn a probability distribution p(x) → Detect outliers
Feature learning (without labels)
Sample to **generate** new data

Conditional Generative Model: Learn p(x|y)

What can we do with a generative model?

Discriminative Model:
Learn a probability distribution $p(y|x)$ → Assign labels to data; Feature learning (with labels)

Generative Model:
Learn a probability distribution $p(x)$ → Detect outliers; Feature learning (without labels); Sample to **generate** new data

Conditional Generative Model: Learn $p(x|y)$ → Assign labels, while rejecting outliers!; Generate new data conditioned on input labels

Taxonomy of Generative Models

Generative models

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

Taxonomy of Generative Models

Model can compute p(x)

Generative models

Model does not explicitly compute p(x), but can sample from p(x)

Explicit density

Implicit density

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

Taxonomy of Generative Models

Model can compute p(x)

Generative models

Model does not explicitly compute p(x), but can sample from p(x)

Explicit density

Implicit density

Can compute approximation to p(x)

Tractable density

Approximate density

Can compute p(x)
- Autoregressive
- NADE / MADE
- NICE / RealNVP
- Glow
- Ffjord

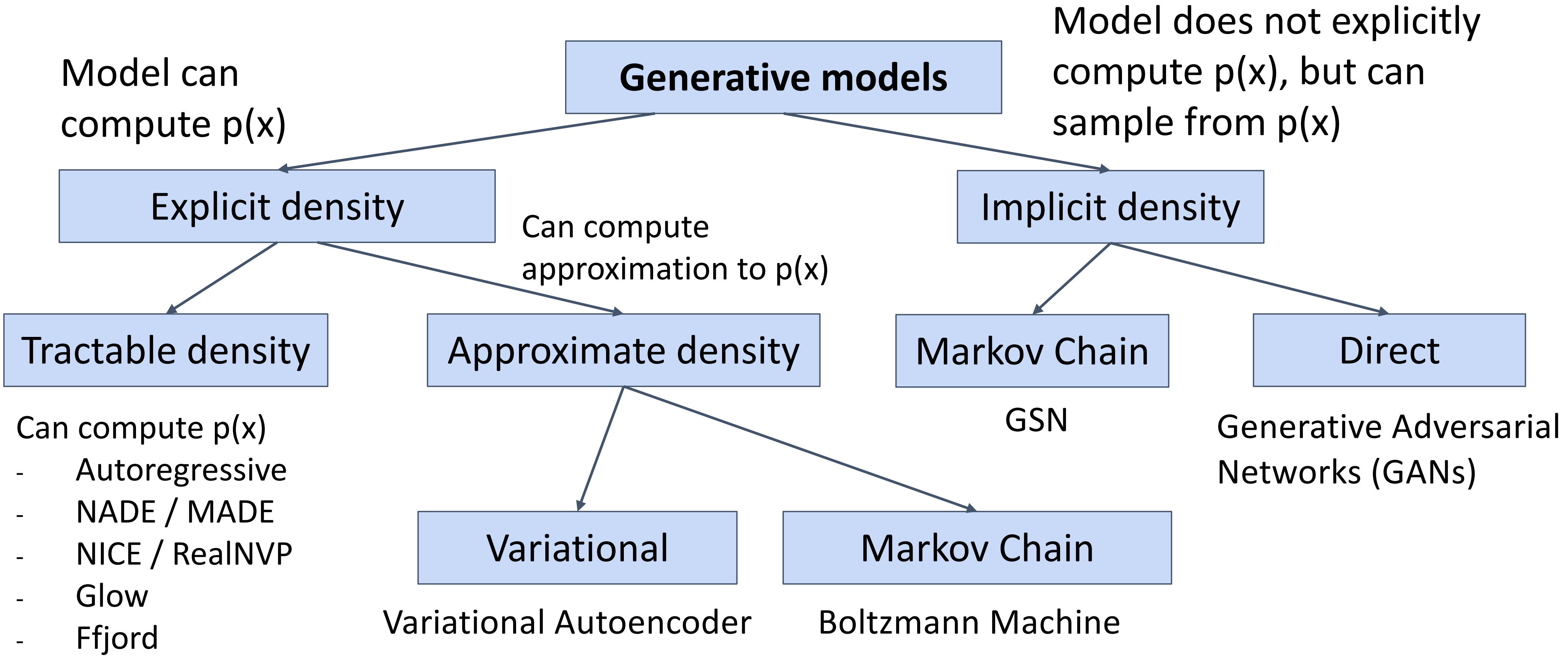
Figure adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Taxonomy of Generative Models

- **Generative models**
  - Explicit density — Model can compute p(x)
    - Tractable density — Can compute p(x)
      - Autoregressive
      - NADE / MADE
      - NICE / RealNVP
      - Glow
      - Ffjord
    - Approximate density — Can compute approximation to p(x)
      - Variational — Variational Autoencoder
      - Markov Chain — Boltzmann Machine
  - Implicit density — Model does not explicitly compute p(x), but can sample from p(x)

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

Taxonomy of Generative Models



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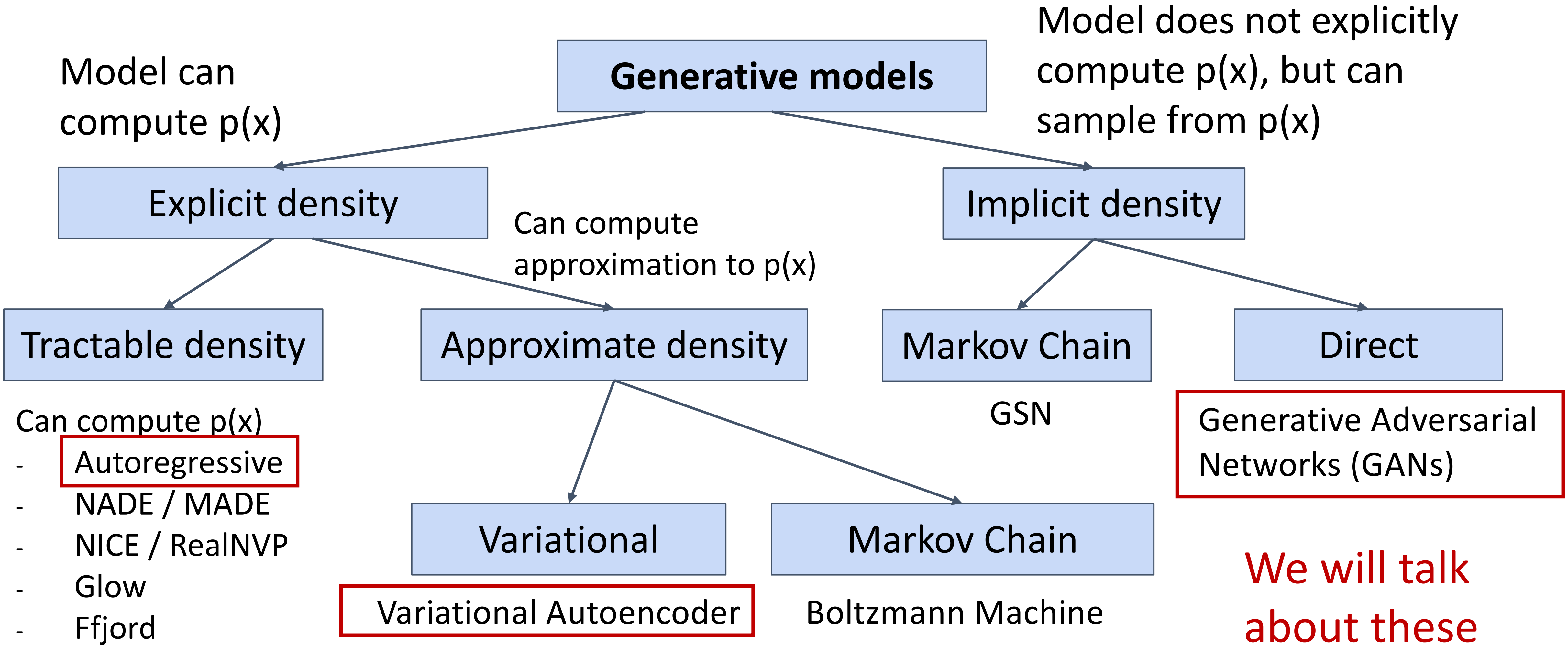

Figure adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Autoregressive models

Explicit Density Estimation

Goal: Write down an explicit function for $p(x) = f(x, W)$

Explicit Density Estimation

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Given dataset $x^{(1)}, x^{(2)}, \dots x^{(N)}$, train the model by solving:

$$W^* = \arg\max_{W} \prod_i p(x^{(i)})$$

Maximize probability of training data
(Maximum likelihood estimation)

Explicit Density Estimation

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Maximize probability of training data (Maximum likelihood estimation)

$$= \arg\max_{W} \sum_i \log p(x^{(i)})$$

Log trick to exchange product for sum

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Log trick to exchange product for sum

$$= \arg\max_{W} \sum_i \log f(x^{(i)}, W)$$

This will be our loss function!
Train with gradient descent

Explicit Density: Autoregressive Models

Goal: Write down an explicit function for $p(x) = f(x, W)$

Assume x consists of multiple subparts:

$$x = (x_1, x_2, x_3, \ldots, x_T)$$

Explicit Density: Autoregressive Models

Goal: Write down an explicit function for $p(x) = f(x, W)$

Assume x consists of multiple subparts:

$$x = (x_1, x_2, x_3, \ldots, x_T)$$

Break down probability using the chain rule:

$$\begin{aligned} p(x) &= p(x_1, x_2, x_3, \ldots, x_T) \\ &= p(x_1)p(x_2 \mid x_1)p(x_3 \mid x_1, x_2) \ldots \end{aligned}$$

Explicit Density: Autoregressive Models

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Probability of the next subpart given all the previous subparts

Explicit Density: Autoregressive Models

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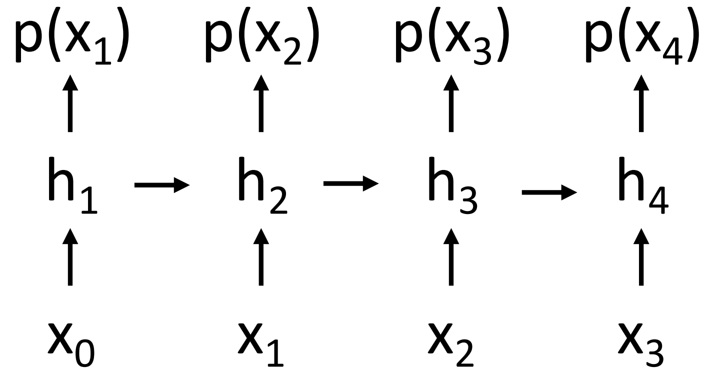
Probability of the next subpart given all the previous subparts



We've already seen this! Language modeling with an RNN!

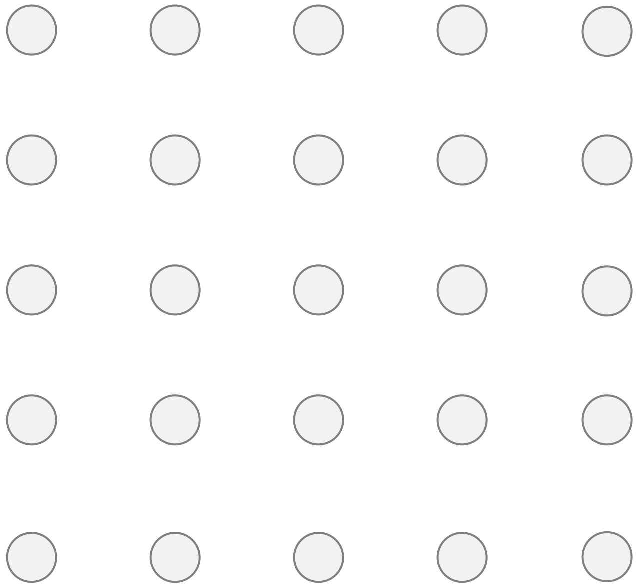
PixelRNN

Generate image pixels one at a time, starting at the upper left corner

Compute a hidden state for each pixel that depends on hidden states and RGB values from the left and from above (LSTM recurrence)

$$h_{x,y} = f(h_{x-1,y}, h_{x,y-1}, W)$$

At each pixel, predict red, then blue, then green: softmax over [0, 1, …, 255]



Van den Oord et al, “Pixel Recurrent Neural Networks”, ICML 2016

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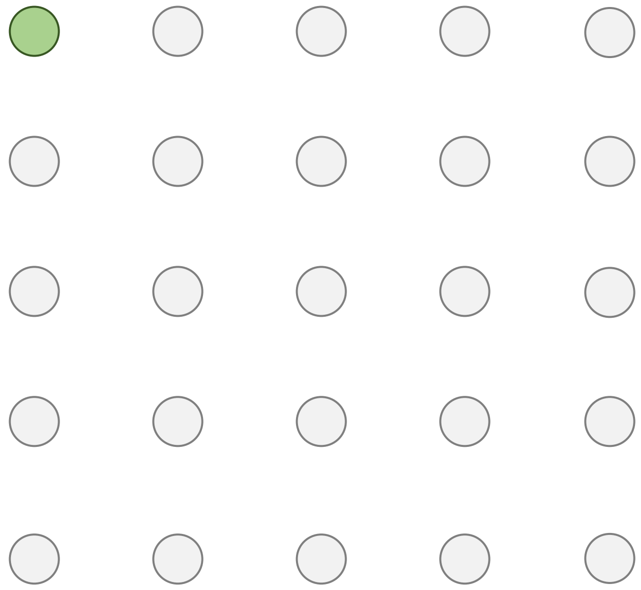

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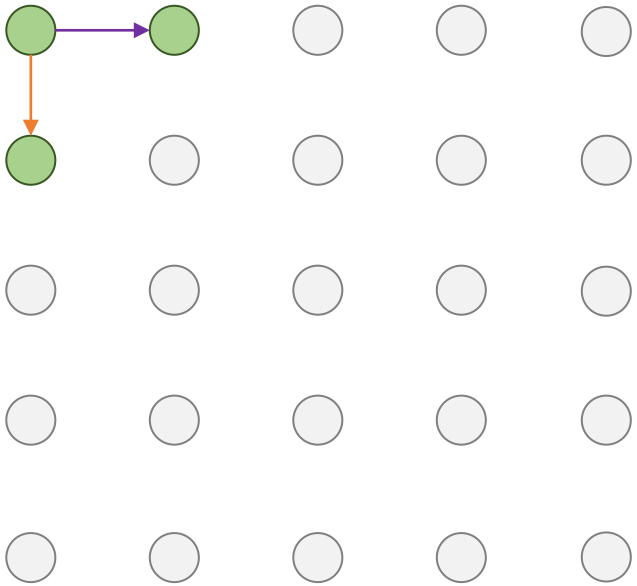

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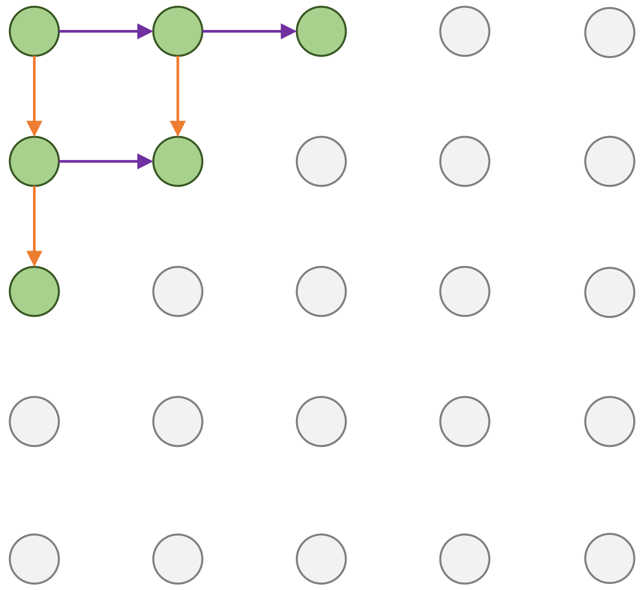

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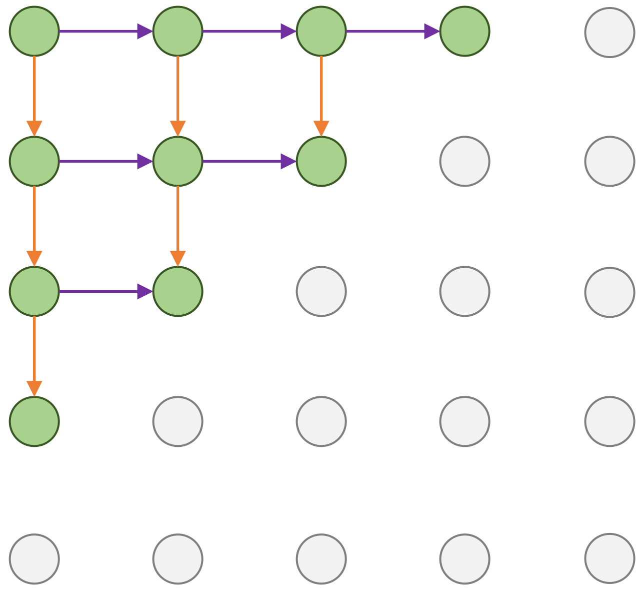

Van den Oord et al, “Pixel Recurrent Neural Networks”, ICML 2016

PixelRNN

Generate image pixels one at a time, starting at the upper left corner

Compute a hidden state for each pixel that depends on hidden states and RGB values from the left and from above (LSTM recurrence)

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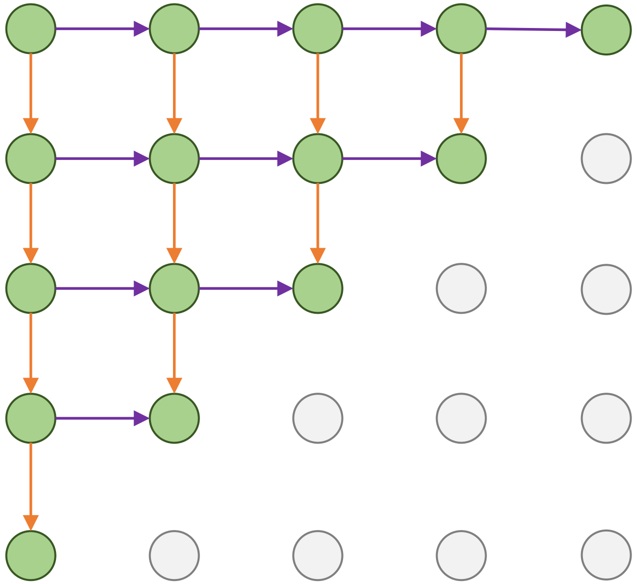

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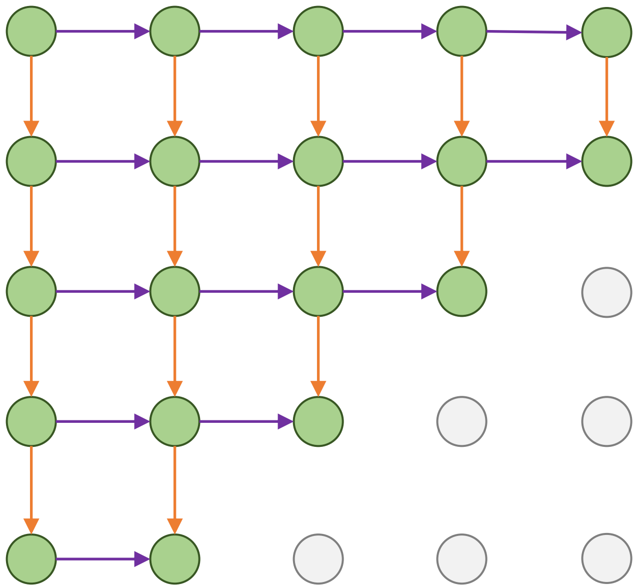

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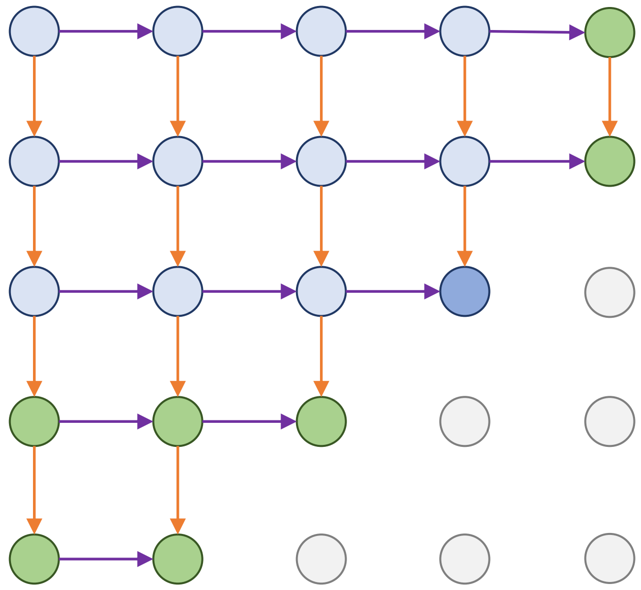

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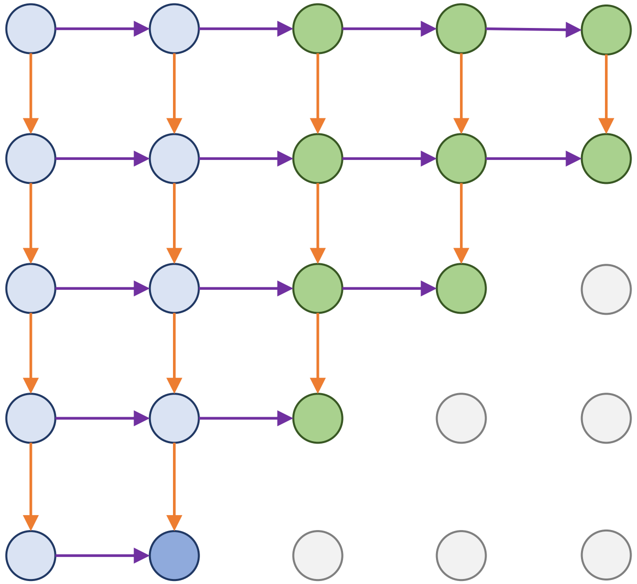

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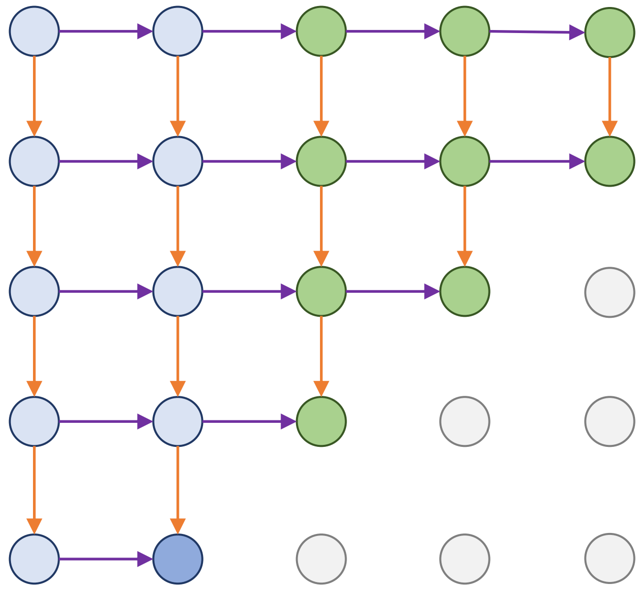
Problem: Very slow during both training and testing; N x N image requires 2N-1 sequential steps

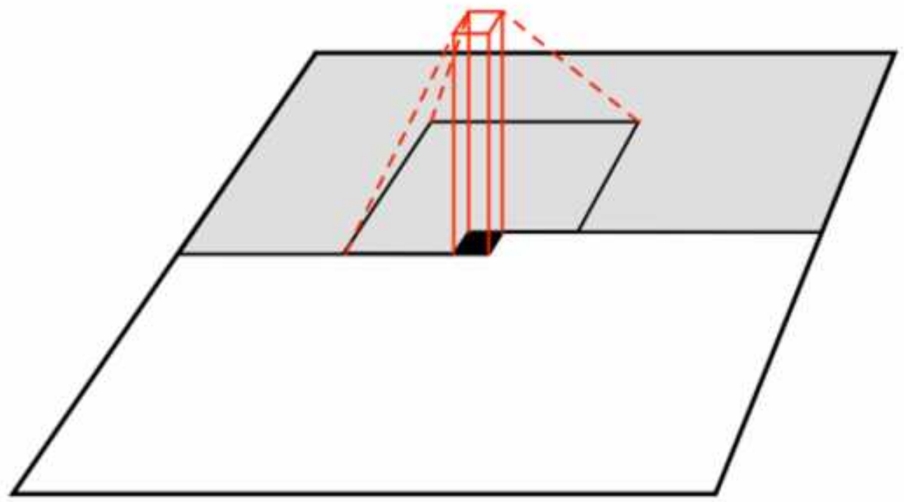


Van den Oord et al, “Pixel Recurrent Neural Networks”, ICML 2016

PixelCNN

Still generate image pixels starting from corner

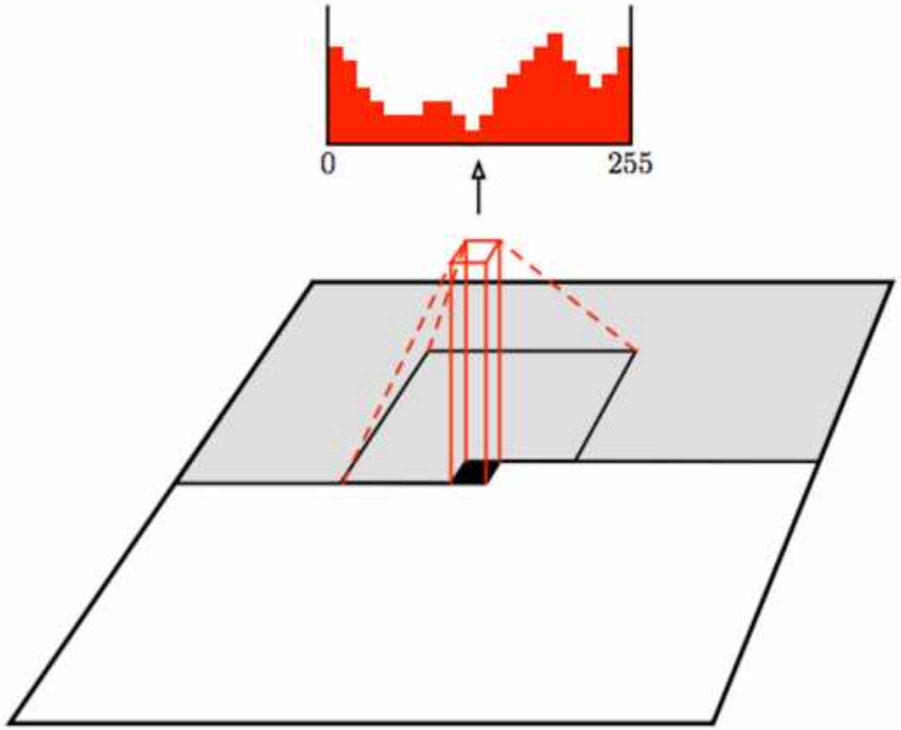
Dependency on previous pixels now modeled using a CNN over context region



Van den Oord et al, "Conditional Image Generation with PixelCNN Decoders", NeurIPS 2016

PixelCNN

Softmax loss at each pixel



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

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

Van den Oord et al, "Conditional Image Generation with PixelCNN Decoders", NeurIPS 2016

PixelCNN

Still generate image pixels starting from corner

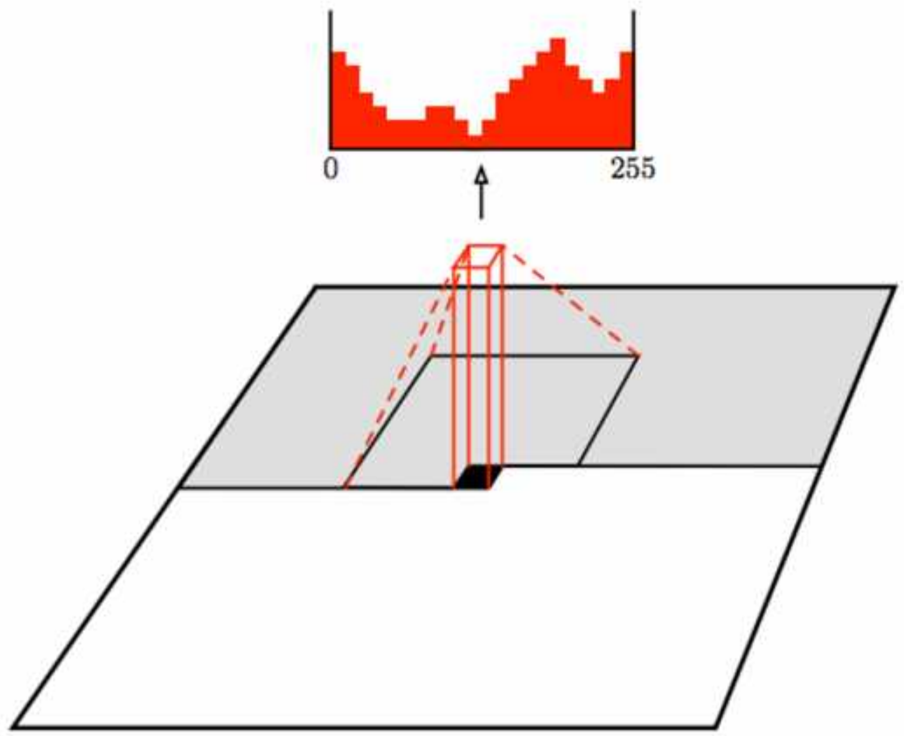
Dependency on previous pixels now modeled using a CNN over context region

Training: maximize likelihood of training images

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

Generation must still proceed sequentially
=> still slow

Softmax loss
at each pixel



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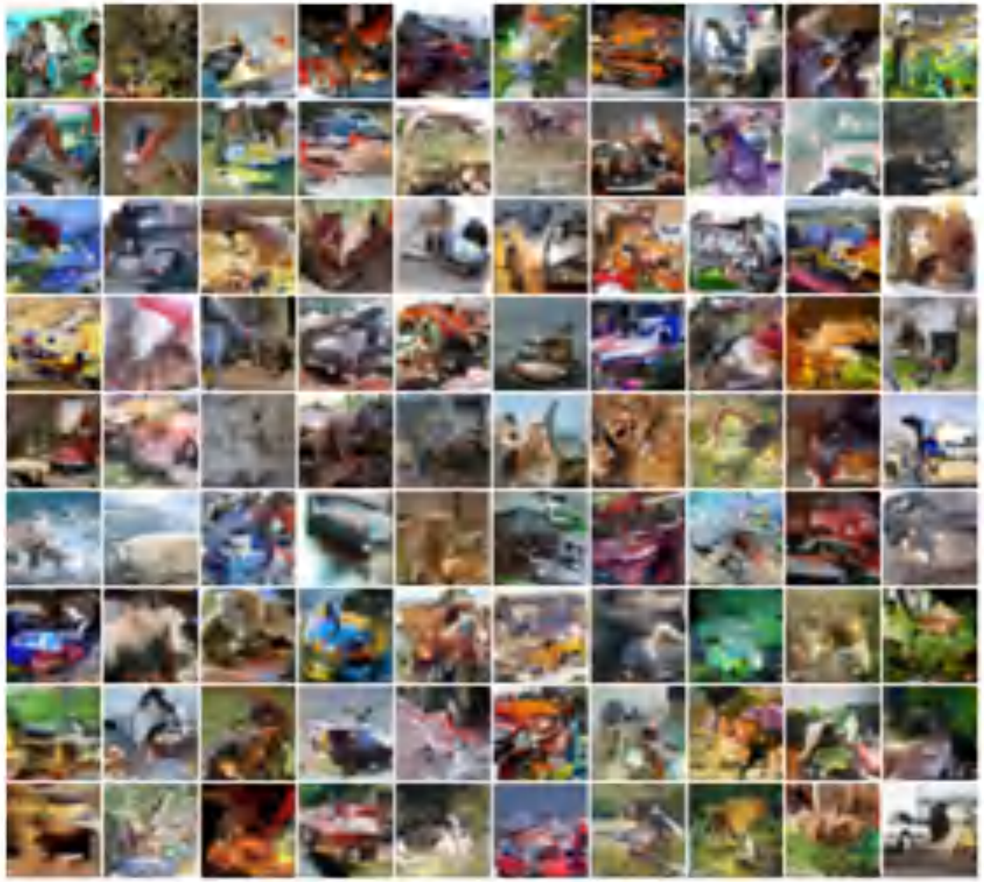
PixelRNN: Generated Samples



32x32 CIFAR-10

32x32 ImageNet

Van den Oord et al, “Pixel Recurrent Neural Networks”, ICML 2016

Autoregressive Models: 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

Variational Autoencoders

PixelRNN / PixelCNN explicitly parameterizes density function with a neural network, so we can train to maximize likelihood of training data:

$$\mathrm{p}_W(x) = \prod_{t=1}^{T} p_W(x_t \mid x_1, \ldots, x_{t-1})$$

Variational Autoencoders (VAE) define an **intractable density** that we cannot explicitly compute or optimize

But we will be able to directly optimize a **lower bound** on the density

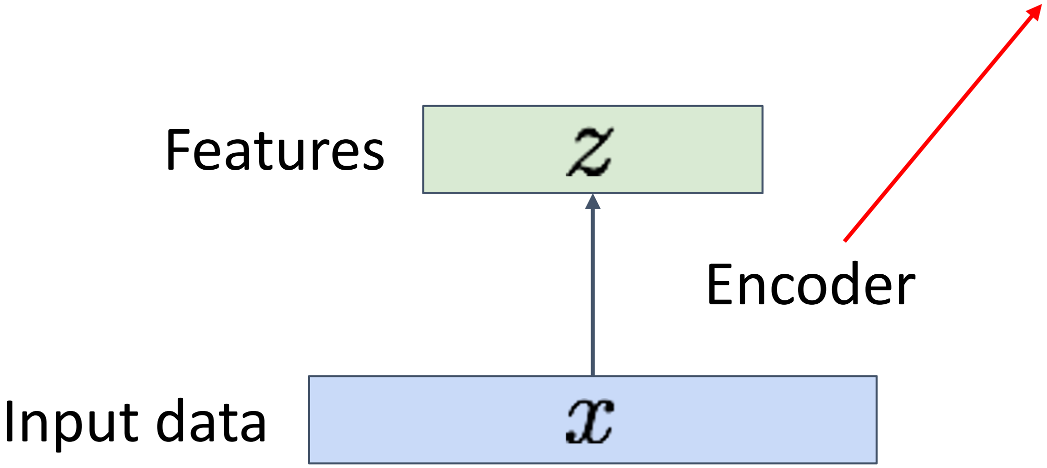
Variational Autoencoders

(Regular, non-variational) Autoencoders

Unsupervised method for learning feature vectors from raw data x, without any labels

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

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



Input Data

(Regular, non-variational) Autoencoders

Problem: How can we learn this feature transform from raw data?

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

But we can't observe features!

Originally: Linear + nonlinearity (sigmoid)
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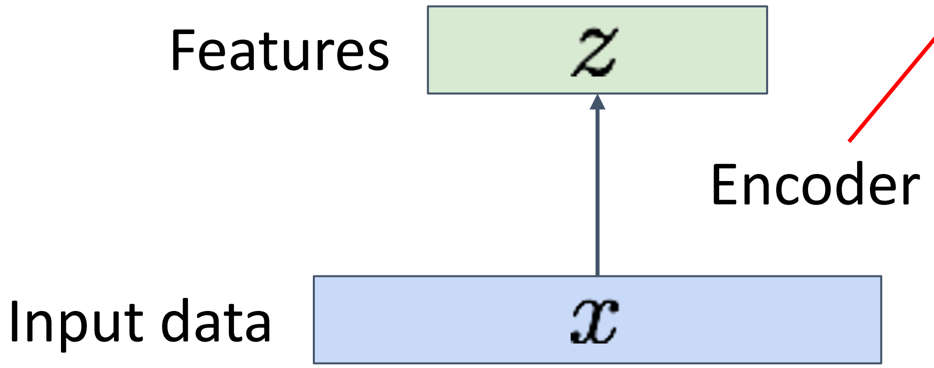
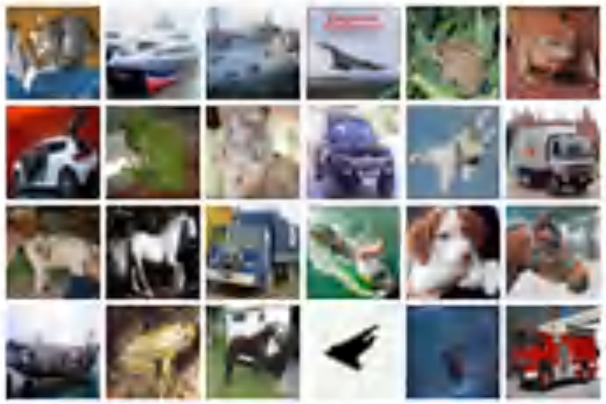
Later: ReLU CNN





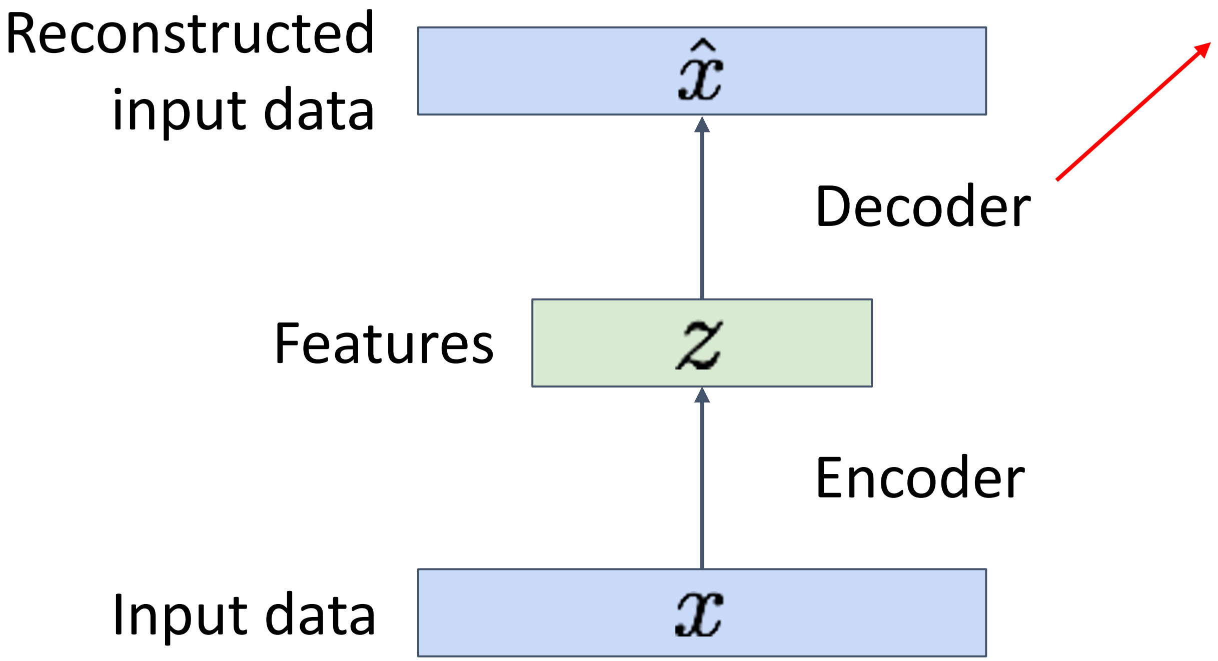
Input Data

(Regular, non-variational) Autoencoders

Problem: How can we learn this feature transform from raw data?

Idea: Use the features to reconstruct the input data with a **decoder**

"Autoencoding" = encoding itself



Originally: Linear + nonlinearity (sigmoid)

Later: Deep, fully-connected

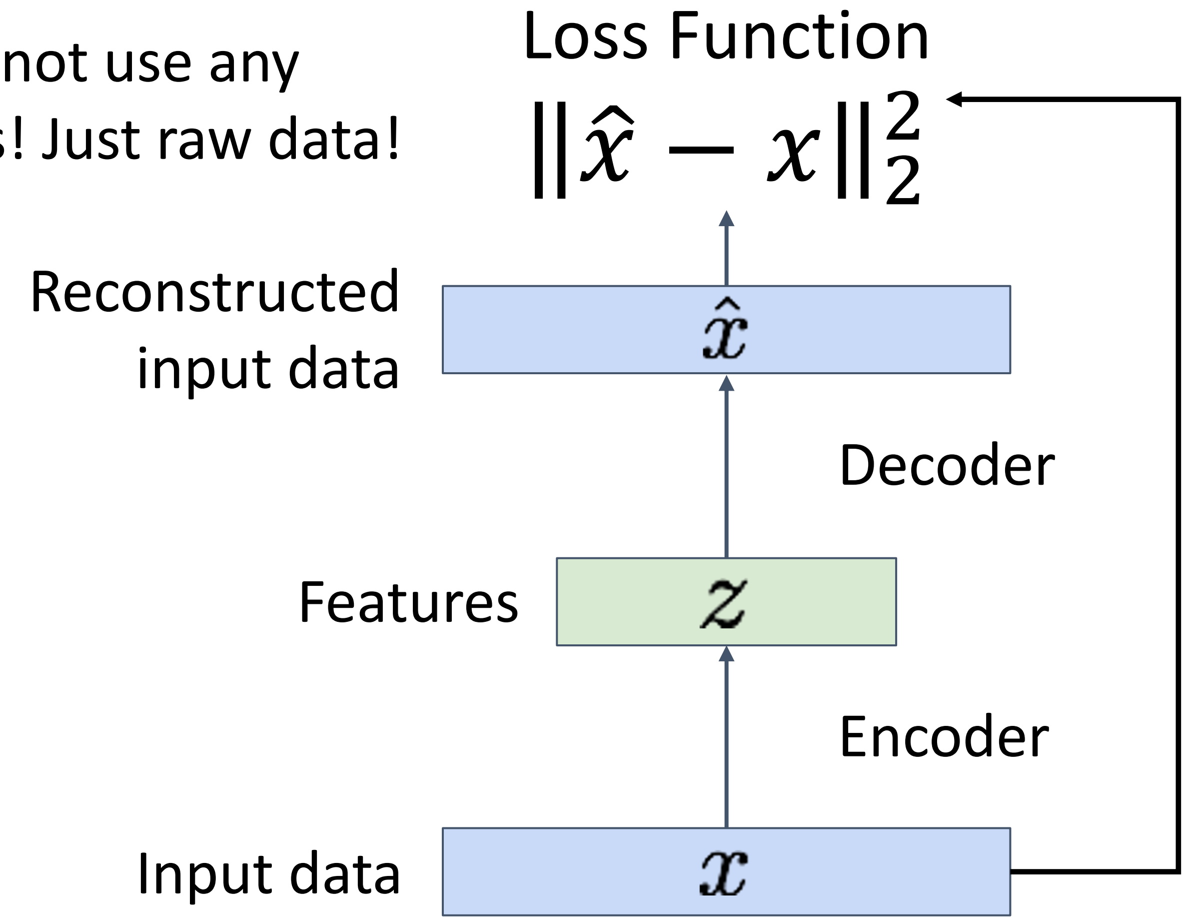
Later: ReLU CNN (upconv)

Input Data

(Regular, non-variational) Autoencoders

Loss: L2 distance between input and reconstructed data.

Does not use any labels! Just raw data!



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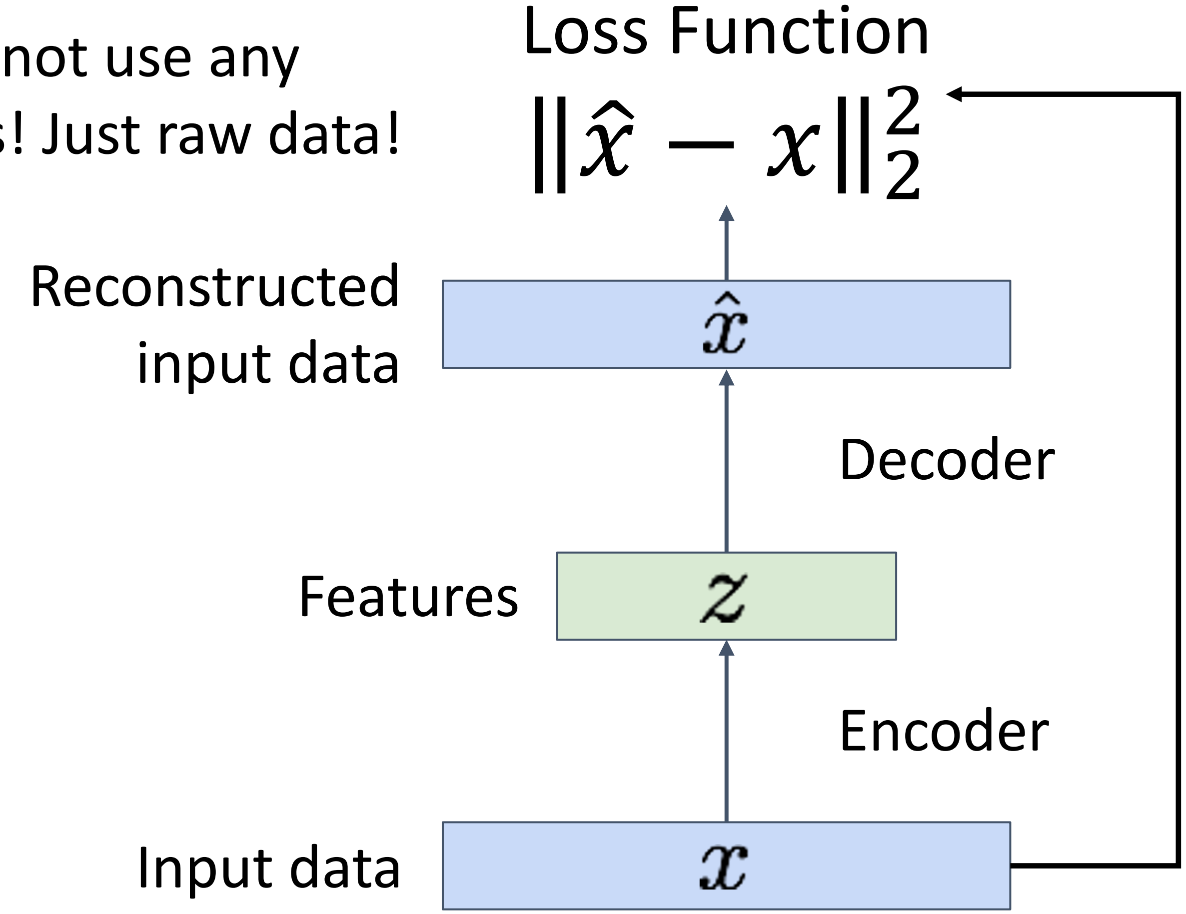
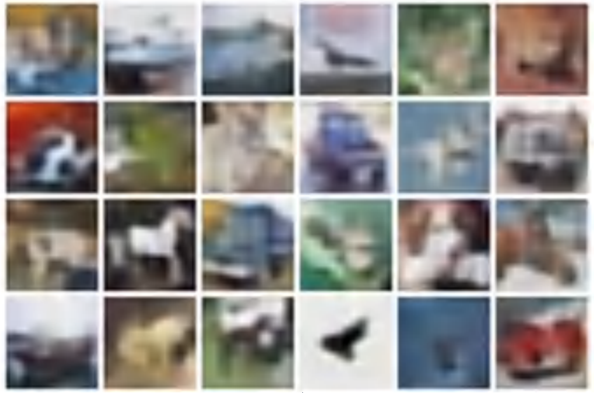
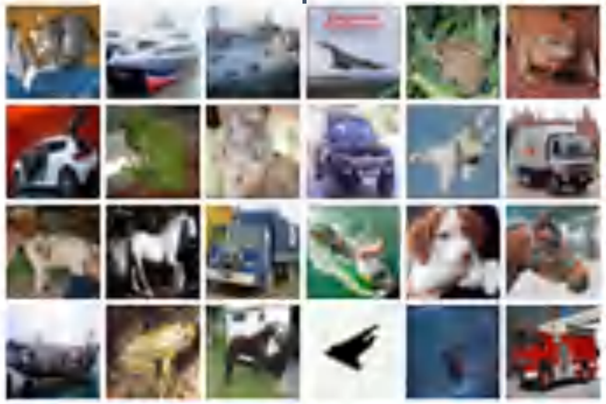


Reconstructed data



Decoder:
4 tconv layers

Encoder:
4 conv layers



Input Data

(Regular, non-variational) Autoencoders

Loss: L2 distance between input and reconstructed data.

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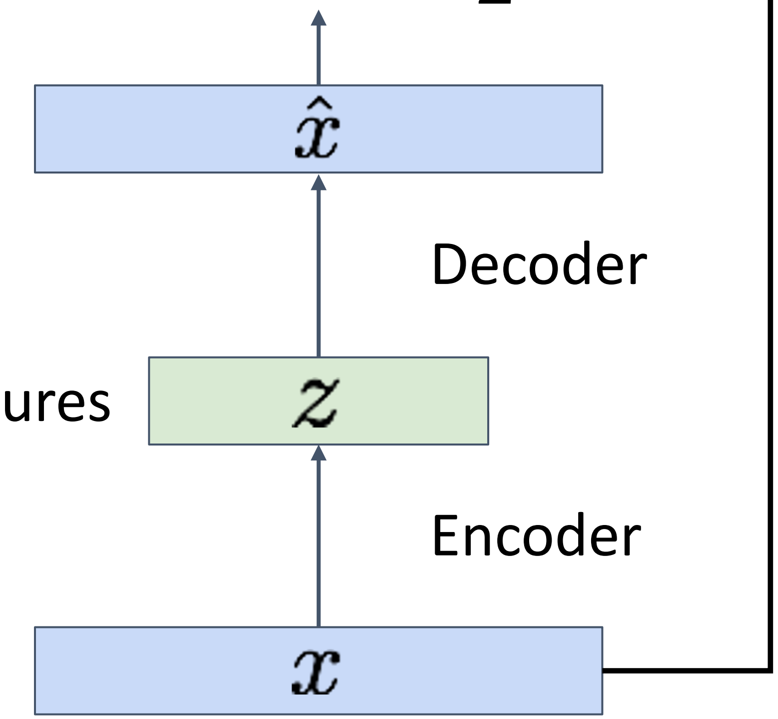
Loss Function

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

Reconstructed input data

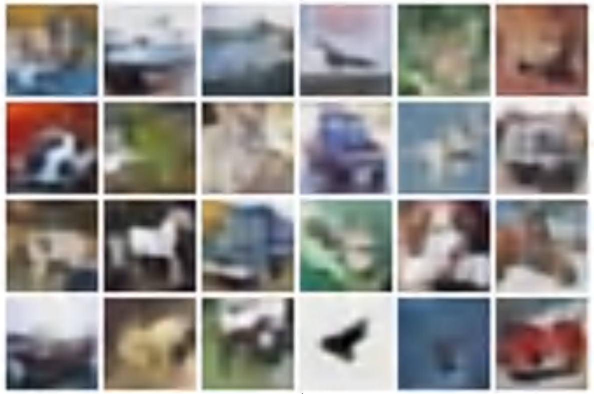


Features need to be **lower dimensional** than the data

Features

Input data

Reconstructed data



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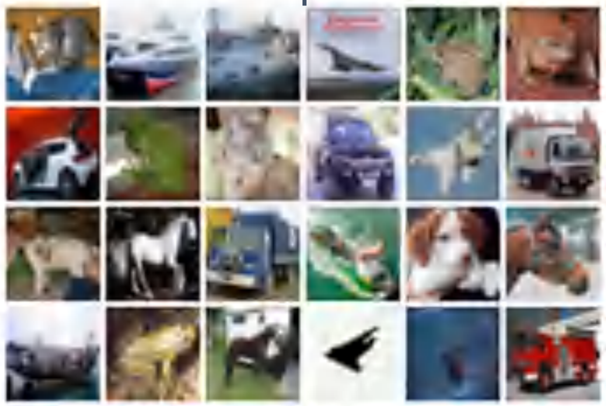
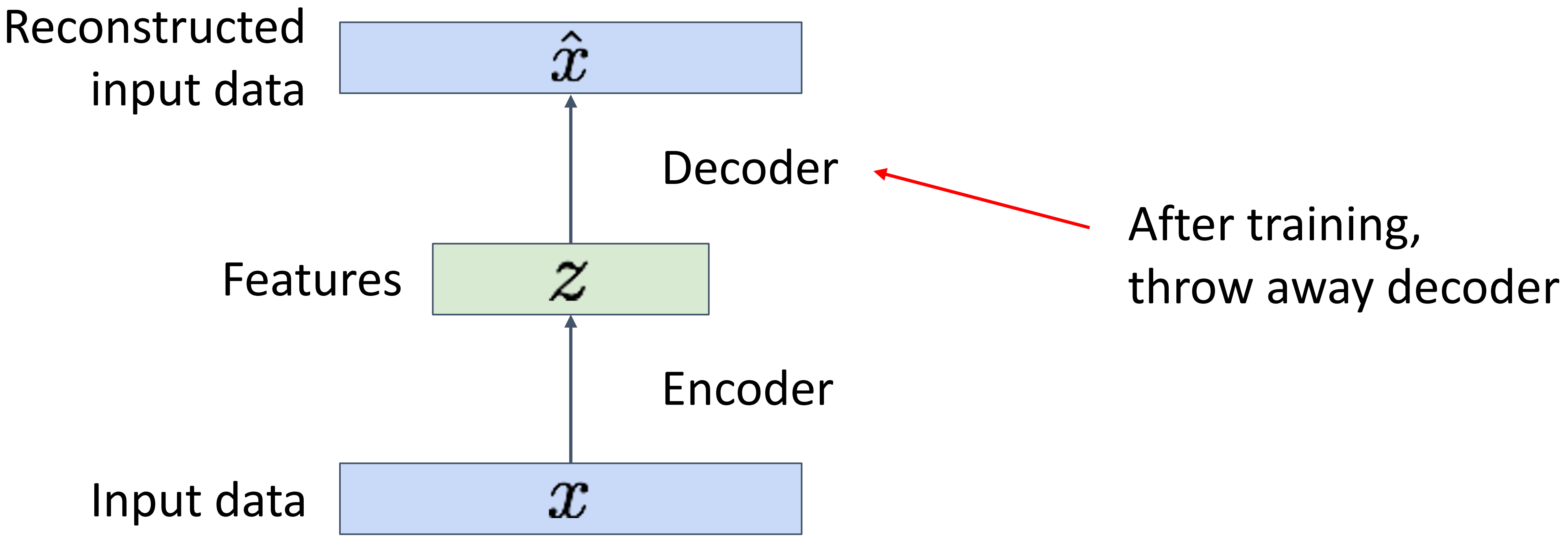


Input Data

(Regular, non-variational) Autoencoders

After training, **throw away decoder** and use encoder for a downstream task



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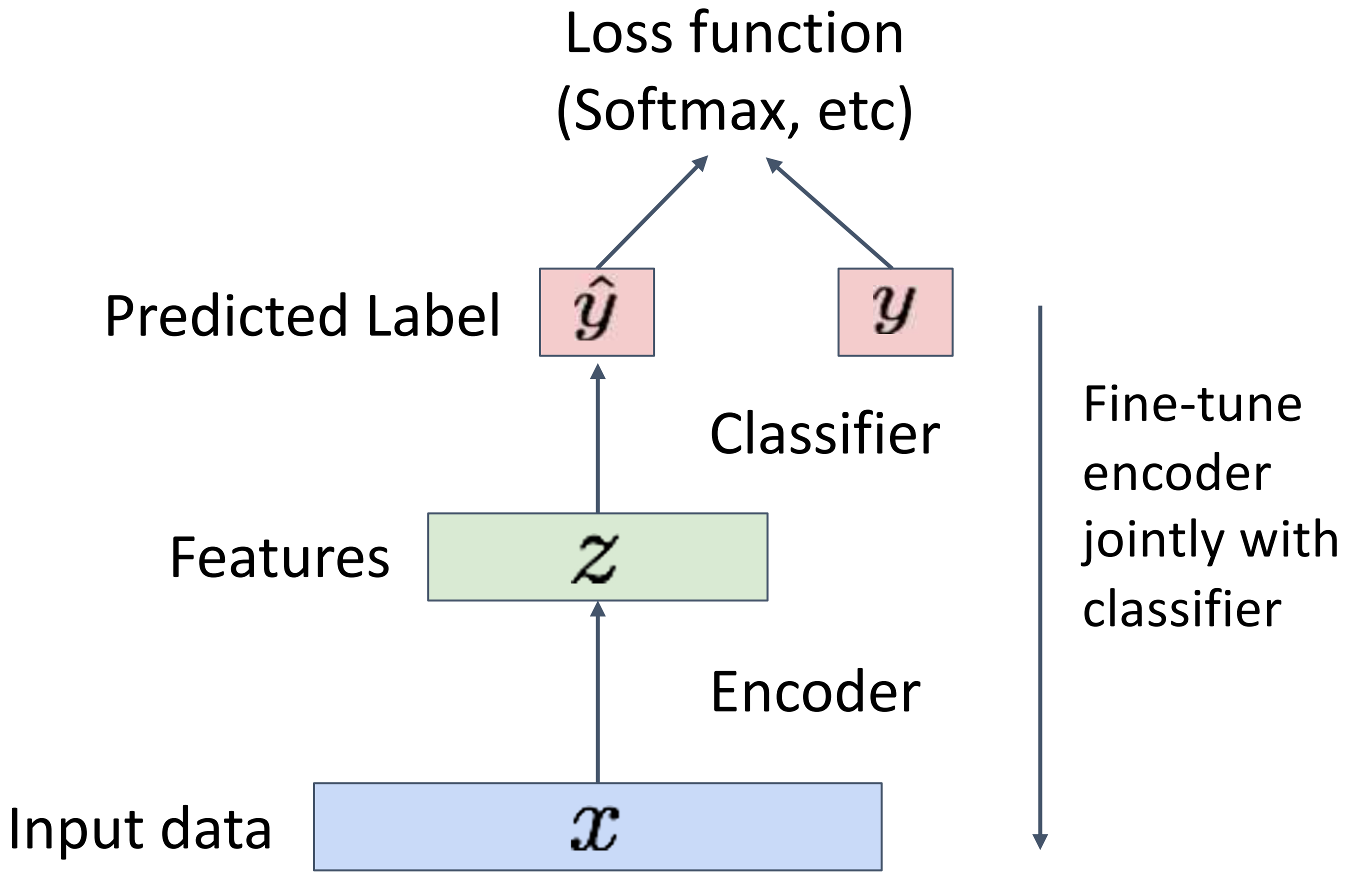


Encoder can be used to initialize a **supervised** model

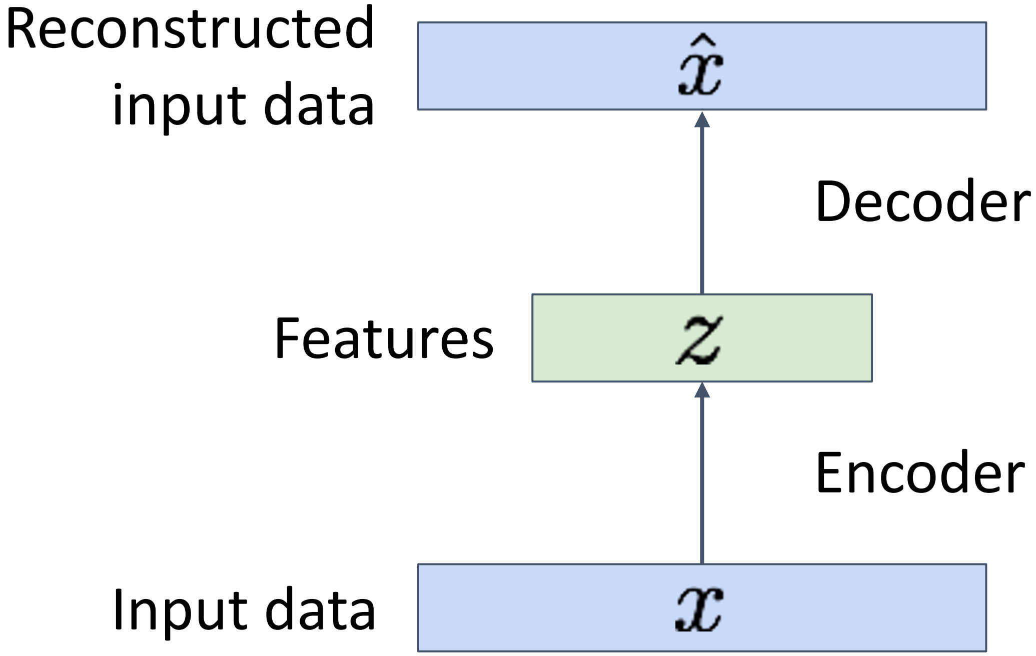
Train for final task (sometimes with small data)

(Regular, non-variational) Autoencoders

Autoencoders learn **latent features** for data without any labels!

Can use features to initialize a **supervised** model

Not probabilistic: No way to sample new data from learned model



Variational Autoencoders

Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

Variational Autoencoders

Probabilistic spin on autoencoders:

1. Learn latent features z from raw data
2. Sample from the model to generate new data

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

Intuition: x is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

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

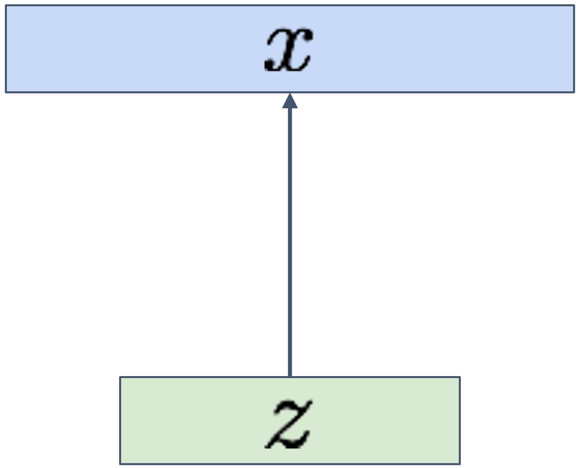
After training, sample new data like this:

Sample from conditional

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

Sample z from prior

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



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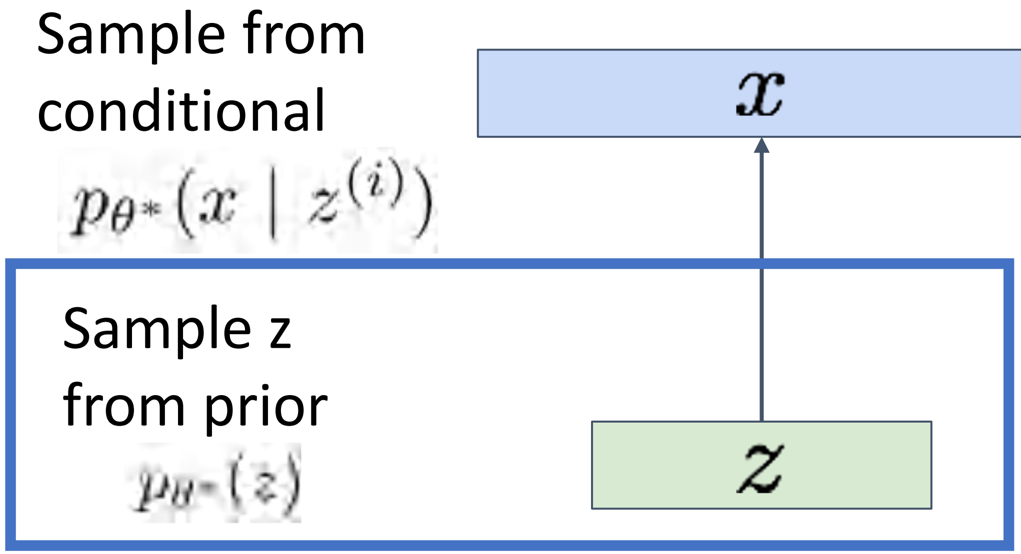

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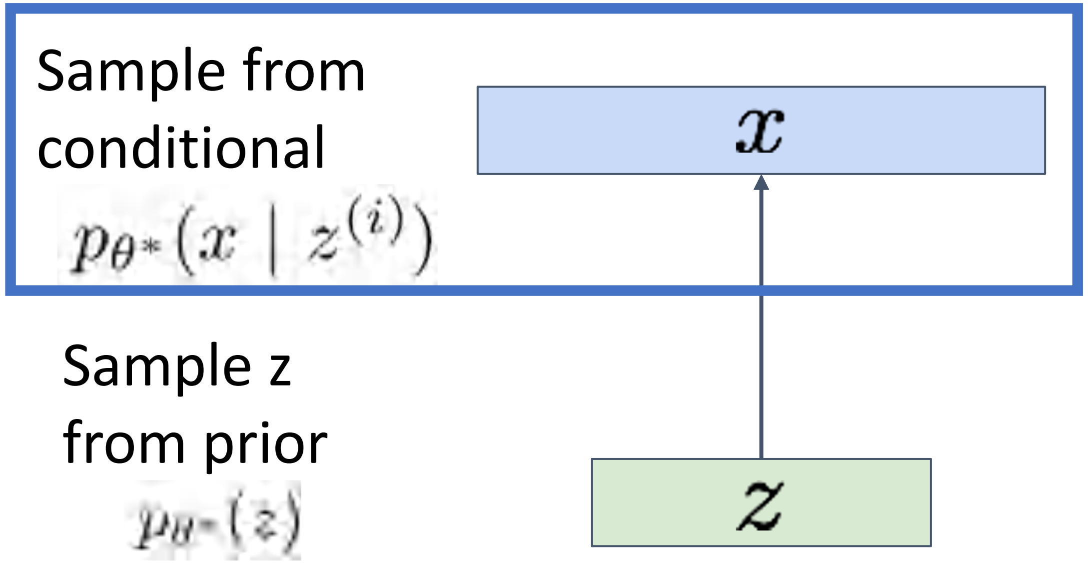

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Represent p(x|z) with a neural network (Similar to **decoder** from autencoder)

Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

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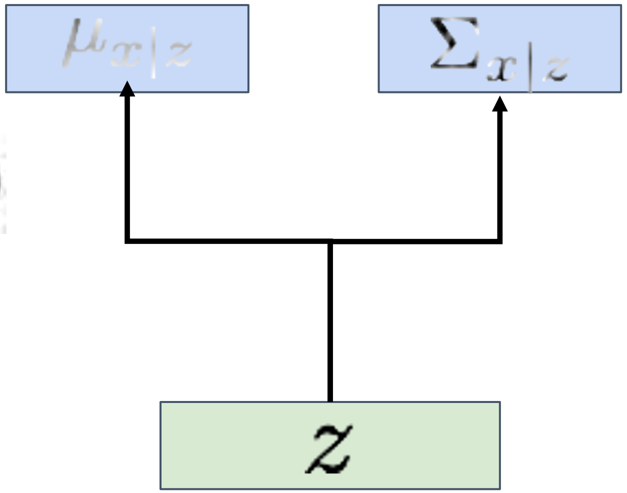

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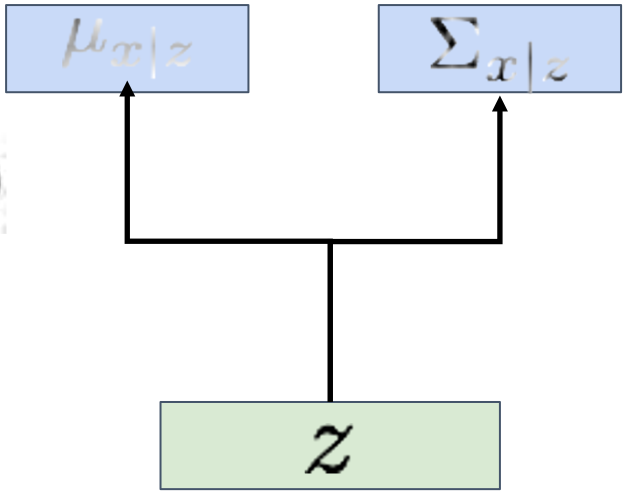

Assume training data $\left\{x^{(i)}\right\}_{i=1}^{N}$ is generated from unobserved (latent) representation **z**

How to train this model?

Basic idea: **maximize likelihood of data**

If we could observe the z for each x, then could train a *conditional generative model* p(x|z)

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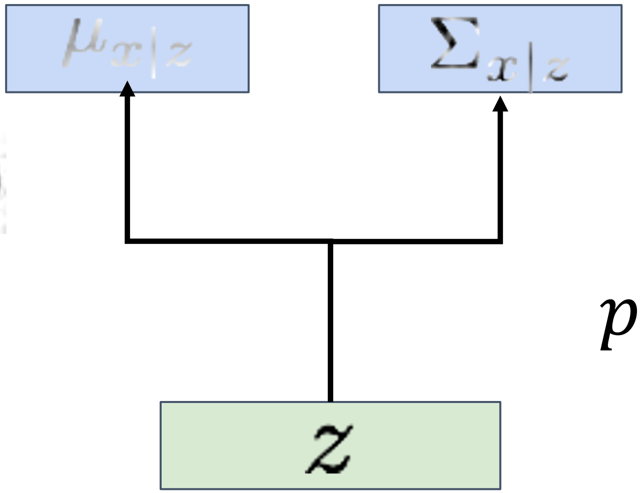

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How to train this model?

Basic idea: **maximize likelihood of data**

We don't observe z, so need to marginalize:

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

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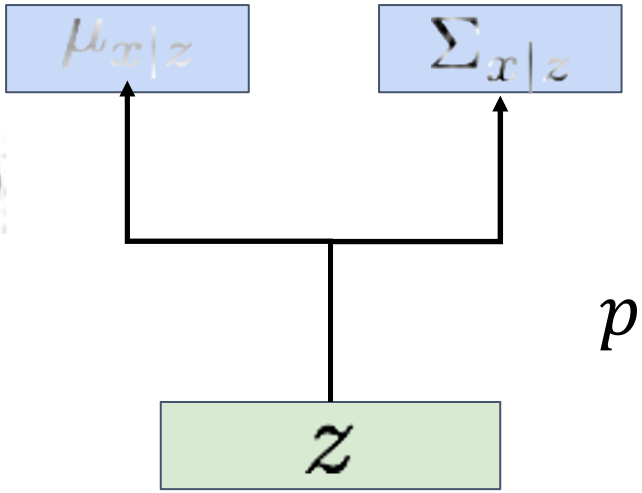

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Ok, can compute this with decoder network

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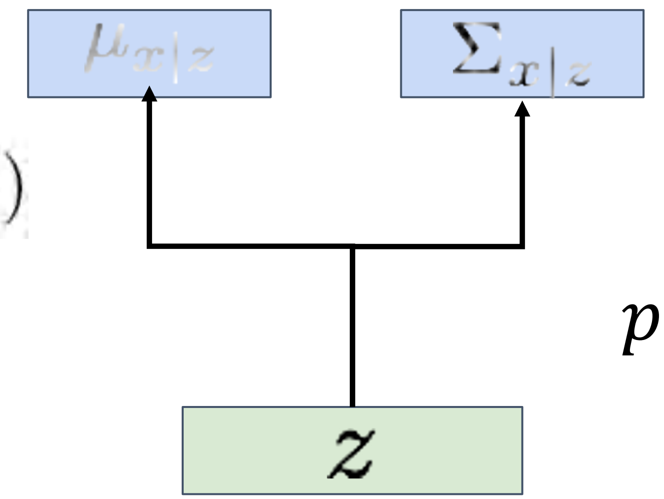

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Ok, we assumed Gaussian prior for z

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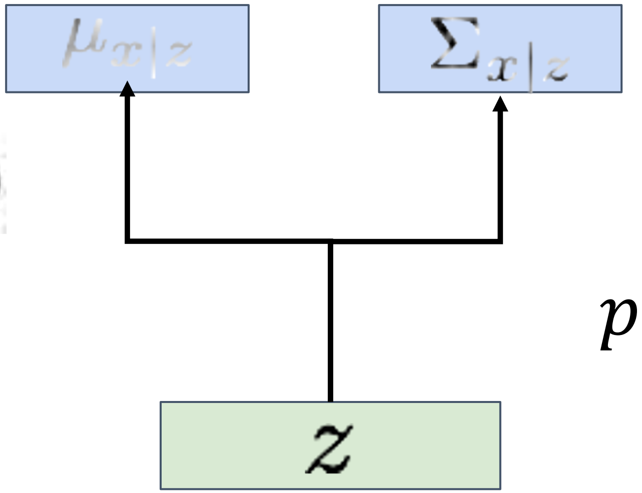

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Problem: Impossible to integrate over all z!

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

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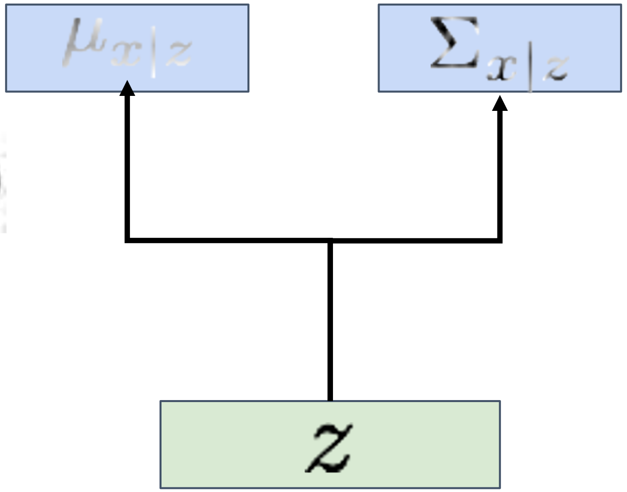

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$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)}$$

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

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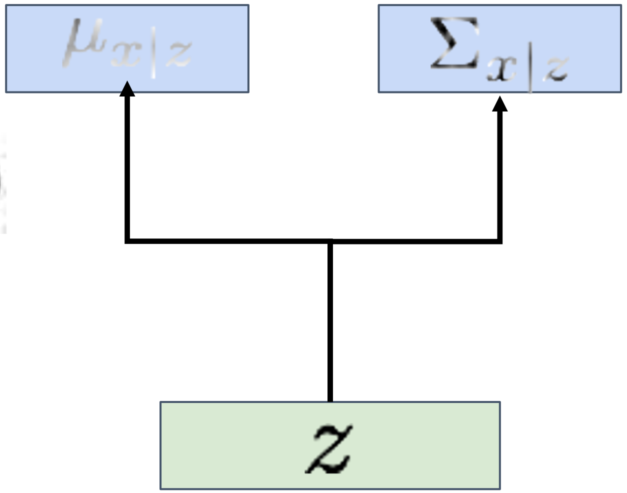

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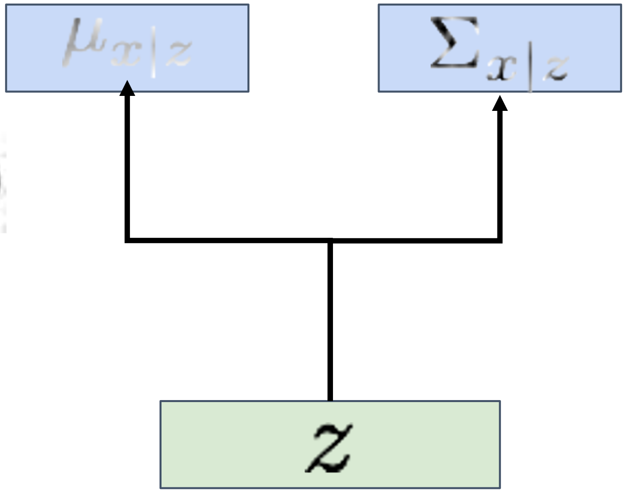
Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample from conditional

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

Sample z from prior

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



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

How to train this model?

Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)\boxed{p_\theta(z)}}{p_\theta(z \mid x)}$$

Ok, we assumed Gaussian prior

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

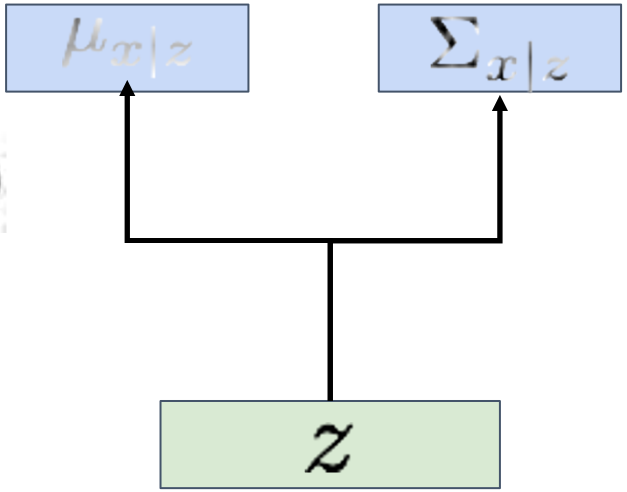
Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

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

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



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Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{\boxed{p_\theta(z \mid x)}}$$

Problem: No way to compute this!

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

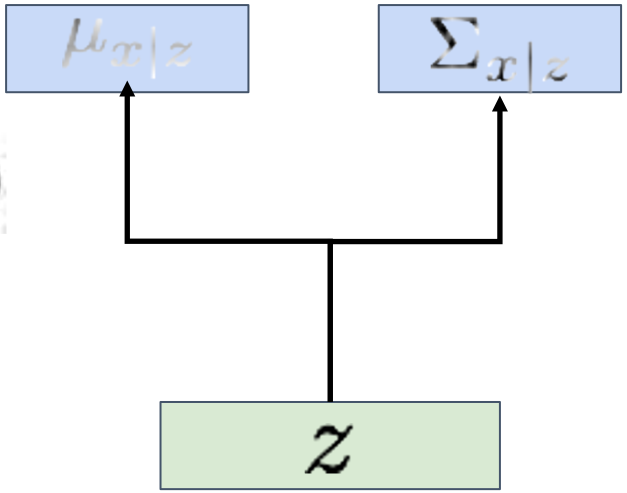
Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

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

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



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Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)}$$

Solution: Train another network **(encoder)** that learns $q_\phi(z \mid x) \approx p_\theta(z \mid x)$

Recall $p(x,z) = p(x \mid z)p(z) = p(z \mid x)p(x)$

Variational Autoencoders

Decoder must be **probabilistic**:
Decoder inputs z, outputs mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

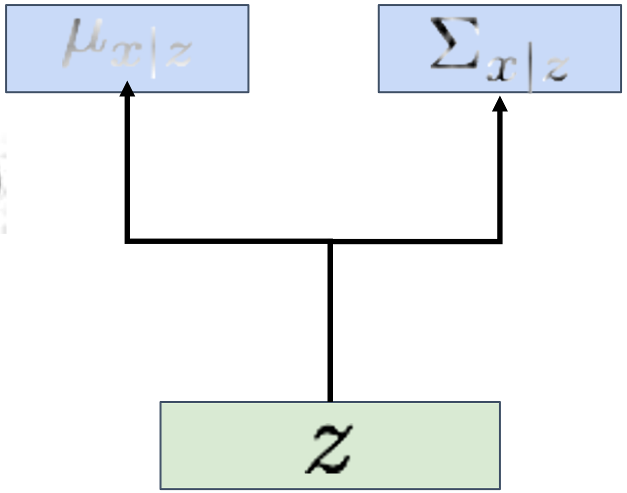
Sample x from Gaussian with mean $\mu_{x|z}$ and (diagonal) covariance $\Sigma_{x|z}$

Sample from conditional

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

Sample z from prior

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



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

How to train this model?

Basic idea: **maximize likelihood of data**

Another idea: Try Bayes' Rule:

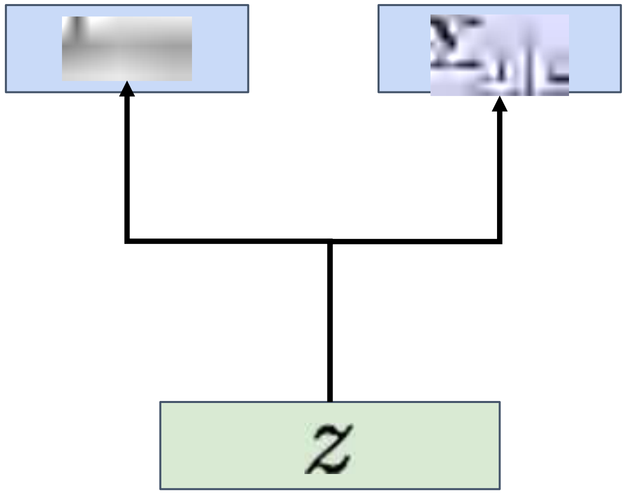
$$p_\theta(x) = \frac{p_\theta(x \mid z)p_\theta(z)}{p_\theta(z \mid x)} \approx \frac{p_\theta(x \mid z)p_\theta(z)}{\boxed{q_\phi(z \mid x)}}$$

Use **encoder** to compute $q_\phi(z \mid x) \approx p_\theta(z \mid x)$

Variational Autoencoders

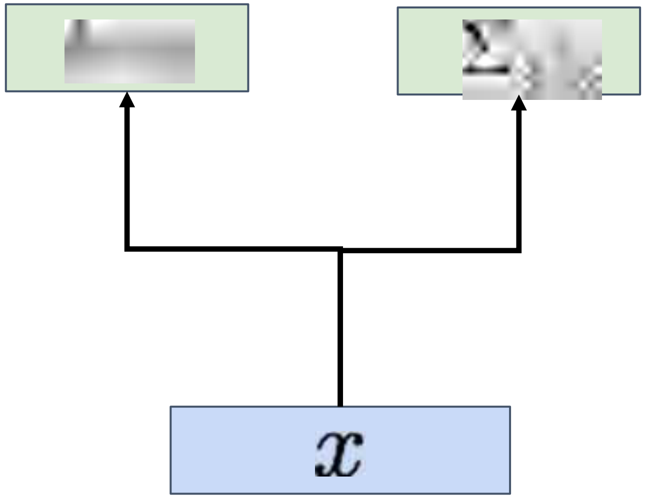
Decoder network inputs latent code z, gives distribution over data x

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



Encoder network inputs data x, gives distribution over latent codes z

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$



If we can ensure that $q_\phi(z \mid x) \approx p_\theta(z \mid x)$,

then we can approximate

$$p_\theta(x) \approx \frac{p_\theta(x \mid z)p(z)}{q_\phi(z \mid x)}$$

Idea: Jointly train both encoder and decoder

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)}$$

Bayes' Rule

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

Multiply top and bottom by $q_\Phi(z|x)$

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= \log p_\theta(x|z) - \log \frac{q_\phi(z|x)}{p(z)} + \log \frac{q_\phi(z|x)}{p_\theta(z|x)}$$

Split up using rules for logarithms

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{\boxed{p_\theta(x|z)}\boxed{p(z)}\boxed{q_\phi(z|x)}}{\boxed{p_\theta(z|x)}\boxed{q_\phi(z|x)}}$$

$$= \log \boxed{p_\theta(x|z)} - \log \frac{\boxed{q_\phi(z|x)}}{\boxed{p(z)}} + \log \frac{\boxed{q_\phi(z|x)}}{\boxed{p_\theta(z|x)}}$$

Split up using rules for logarithms

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= \log p_\theta(x|z) - \log \frac{q_\phi(z|x)}{p(z)} + \log \frac{q_\phi(z|x)}{p_\theta(z|x)}$$

$$\log p_\theta(x) = E_{z \sim q_\phi(z|x)}[\log p_\theta(x)]$$

We can wrap in an expectation since it doesn't depend on z

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$\log p_\theta(x) = E_{z\sim q_\phi(z|x)}[\log p_\theta(x)]$$

We can wrap in an expectation since it doesn't depend on z

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$= E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

Data reconstruction

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$= E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL divergence between prior, and samples from the encoder network

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL divergence between encoder and posterior of decoder

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

KL is >= 0, so dropping this term gives a **lower bound** on the data likelihood:

Variational Autoencoders

$$\log p_\theta(x) = \log \frac{p_\theta(x \mid z)p(z)}{p_\theta(z \mid x)} = \log \frac{p_\theta(x|z)p(z)q_\phi(z|x)}{p_\theta(z|x)q_\phi(z|x)}$$

$$= E_z[\log p_\theta(x|z)] - E_z\left[\log \frac{q_\phi(z|x)}{p(z)}\right] + E_z\left[\log \frac{q_\phi(z|x)}{p_\theta(z|x)}\right]$$

$$= E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right) + D_{KL}(q_\phi(z|x), p_\theta(z|x))$$

$$\log p_\theta(x) \geq E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

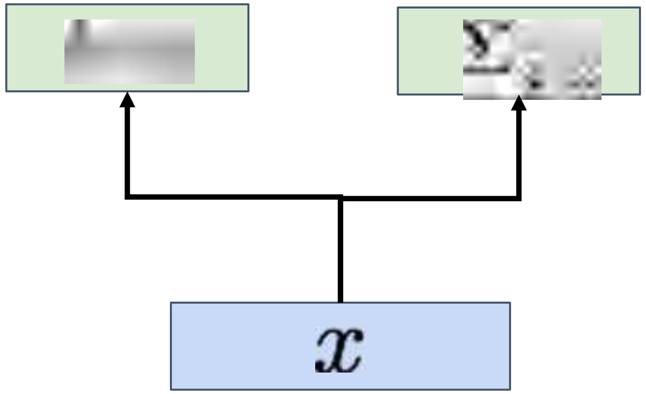
Variational Autoencoders

Jointly train **encoder** q and **decoder** p to maximize the **variational lower bound** on the data likelihood
Also called **Evidence Lower Bound (ELBo)**

$$\log p_\theta(x) \geq E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\Big(q_\phi(z|x), p(z)\Big)$$

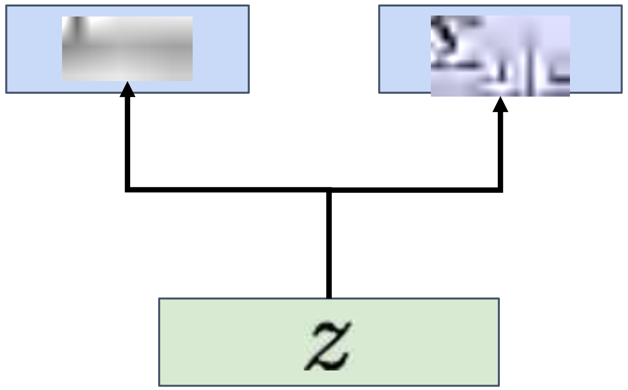
Encoder Network

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$



Decoder Network

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



Example: Fully-Connected VAE

x: 28x28 image, flattened to 784-dim vector

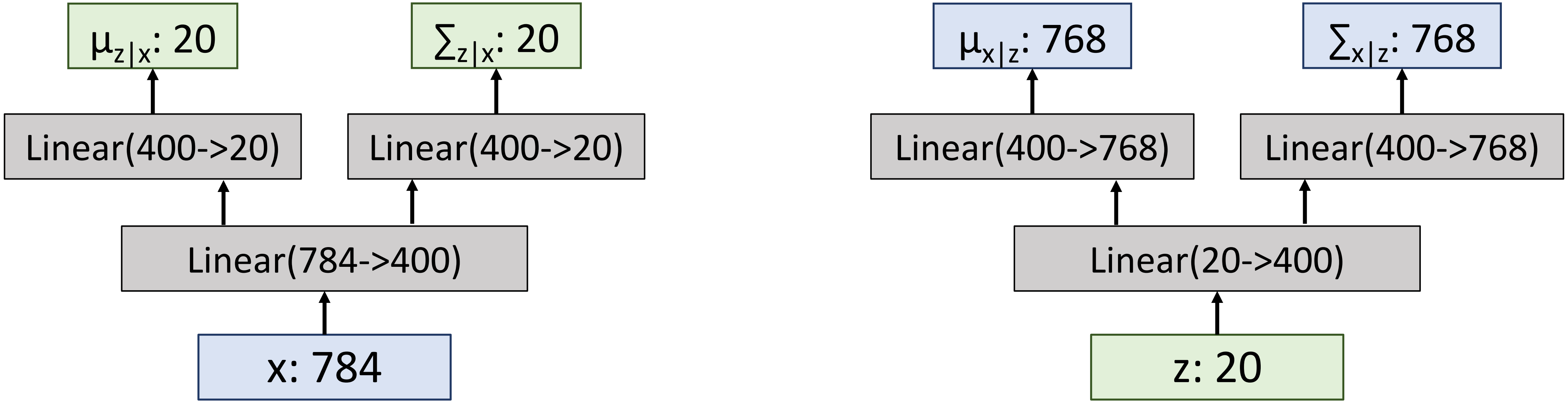
z: 20-dim vector

Encoder Network

$$q_\phi(z \mid x) = N(\mu_{z|x}, \Sigma_{z|x})$$

Decoder Network

$$p_\theta(x \mid z) = N(\mu_{x|z}, \Sigma_{x|z})$$



Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

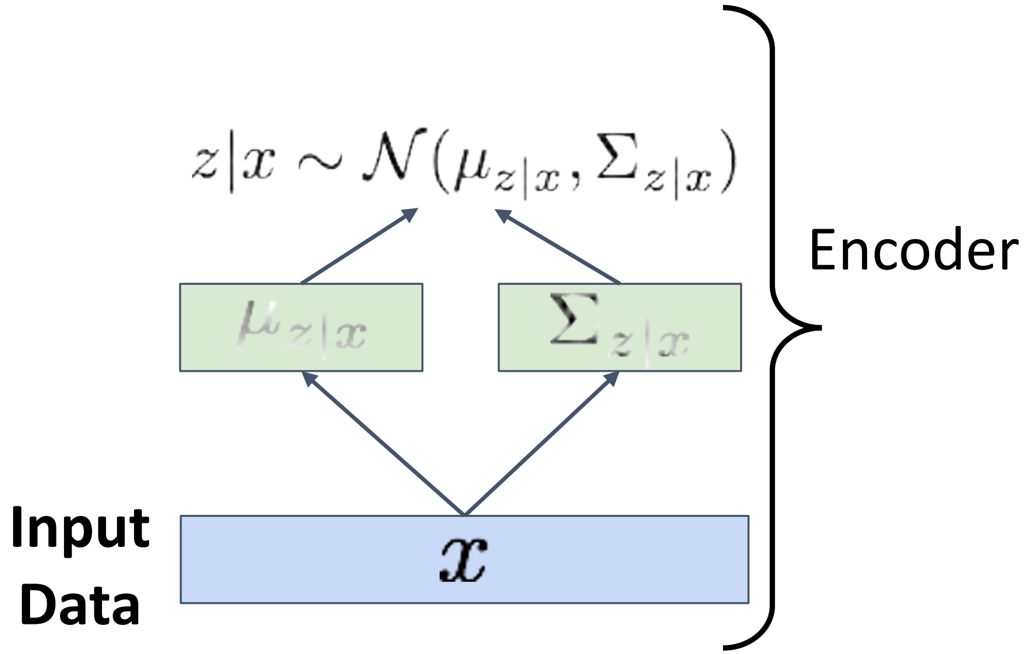
Input Data x

Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - D_{KL}\left(q_\phi(z|x), p(z)\right)$$

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

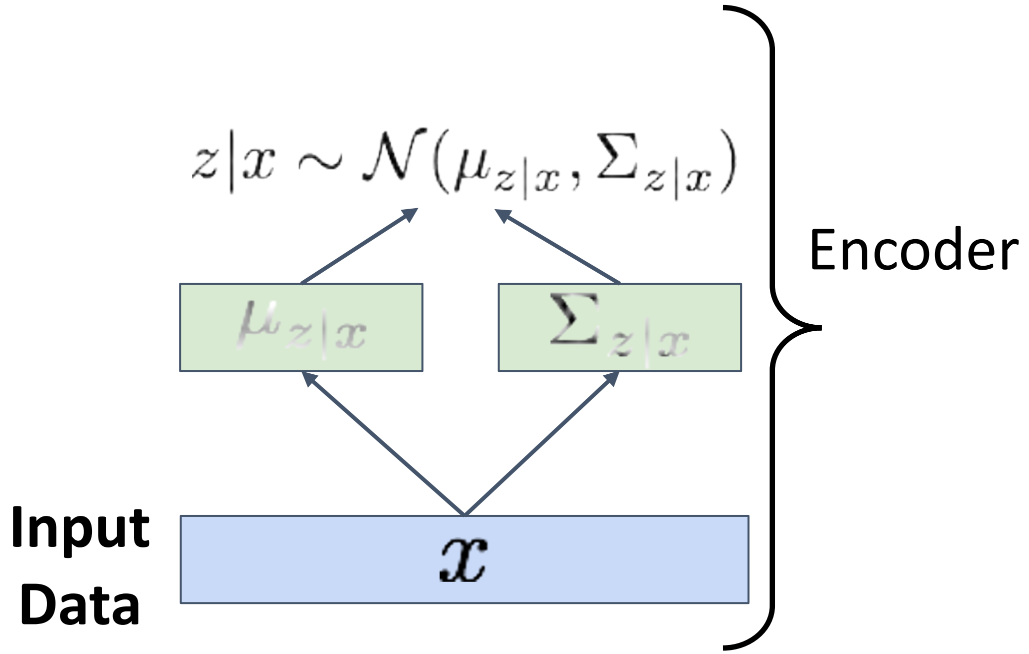


Variational Autoencoders

Train by maximizing the
variational lower bound

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**



Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

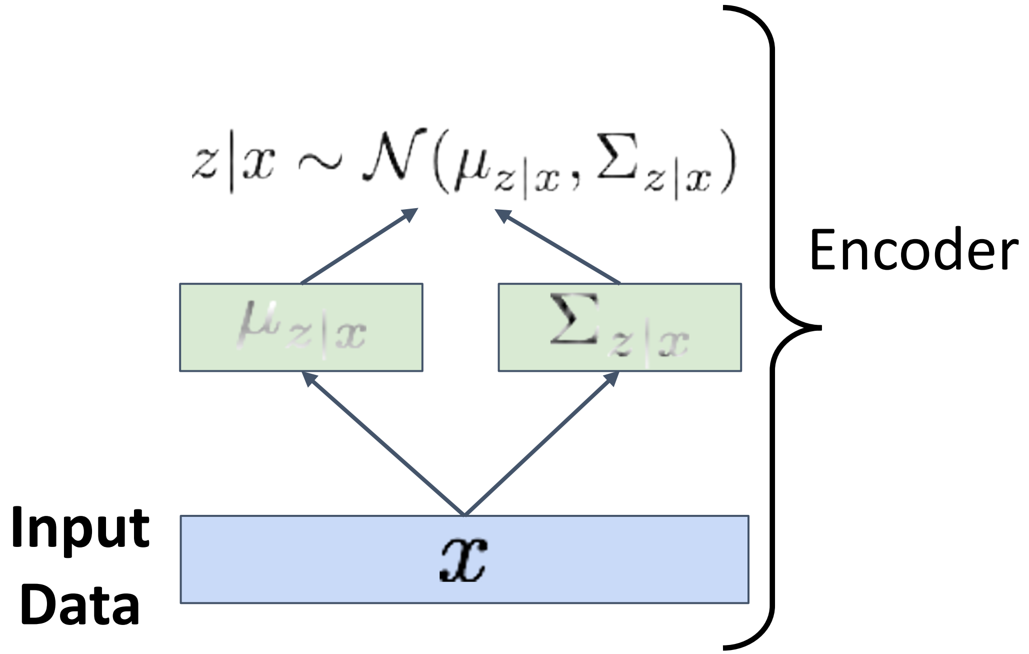
Closed form solution when q_ϕ is diagonal Gaussian and p is unit Gaussian! (Assume z has dimension J)

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**

$$-D_{KL}\left(q_\phi(z|x), p(z)\right) = \int_Z q_\phi(z|x) \log \frac{p(z)}{q_\phi(z|x)} dz$$

$$= \int_Z N\left(z; \mu_{z|x}, \Sigma_{z|x}\right) \log \frac{N(z; 0, I)}{N\left(z; \mu_{z|x}, \Sigma_{z|x}\right)} dz$$

$$= \frac{1}{2} \sum_{j=1}^{J} \left(1 + \log\left(\left(\Sigma_{z|x}\right)_j^2\right) - \left(\mu_{z|x}\right)_j^2 - \left(\Sigma_{z|x}\right)_j^2\right)$$

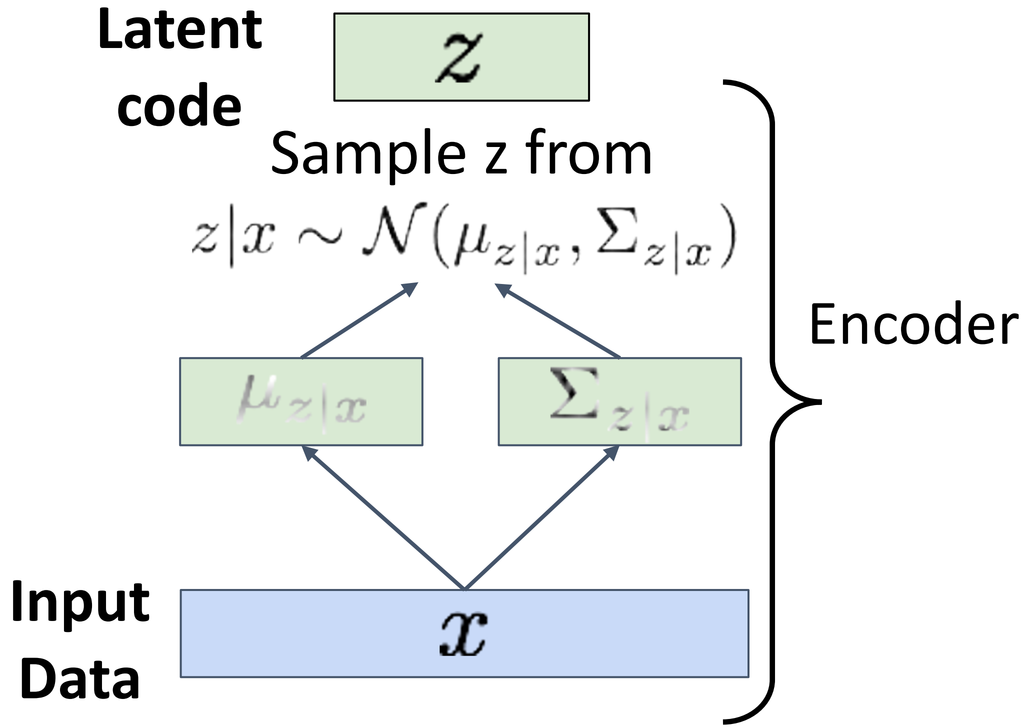


Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output

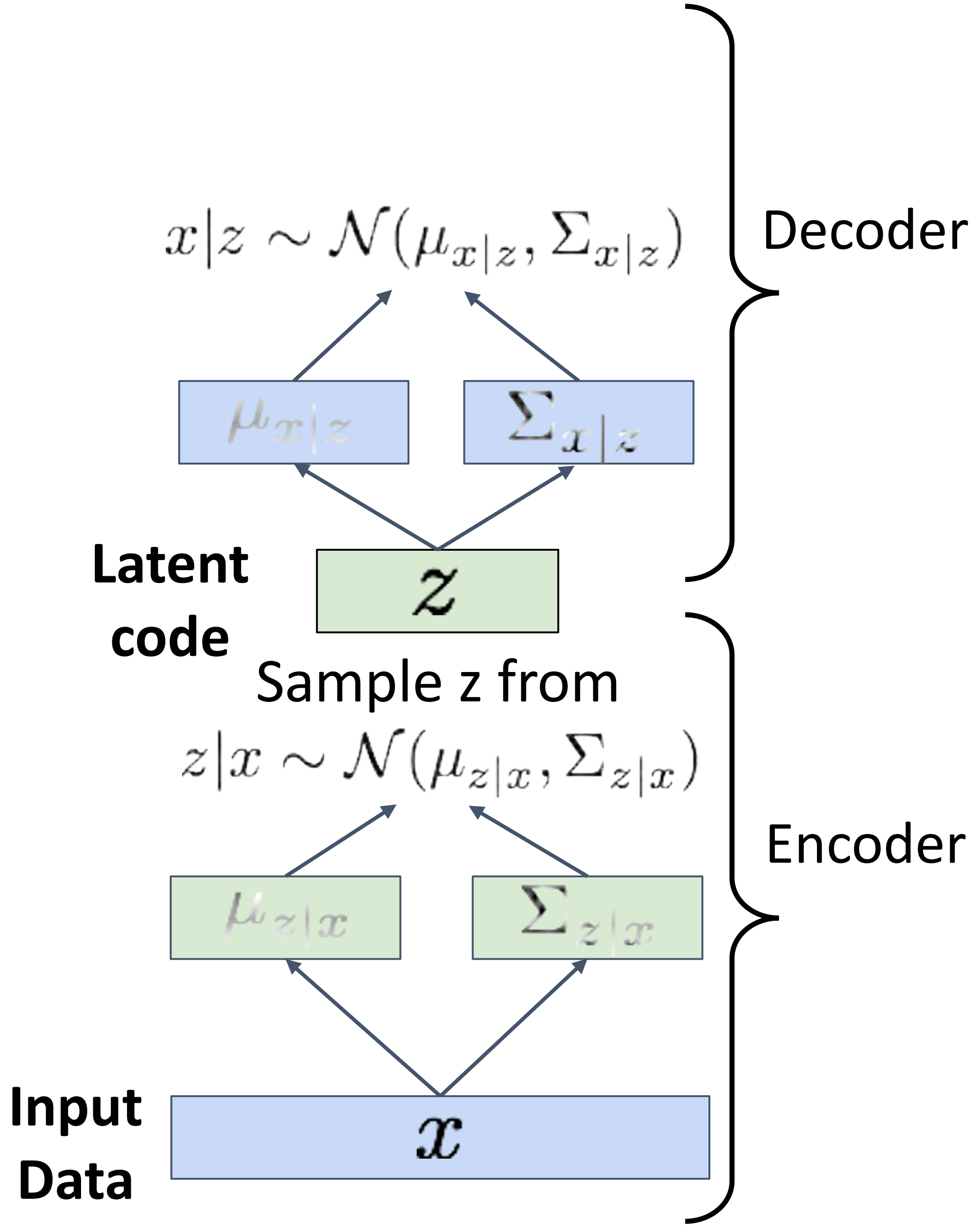


Variational Autoencoders

Train by maximizing the **variational lower bound**

$$E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples

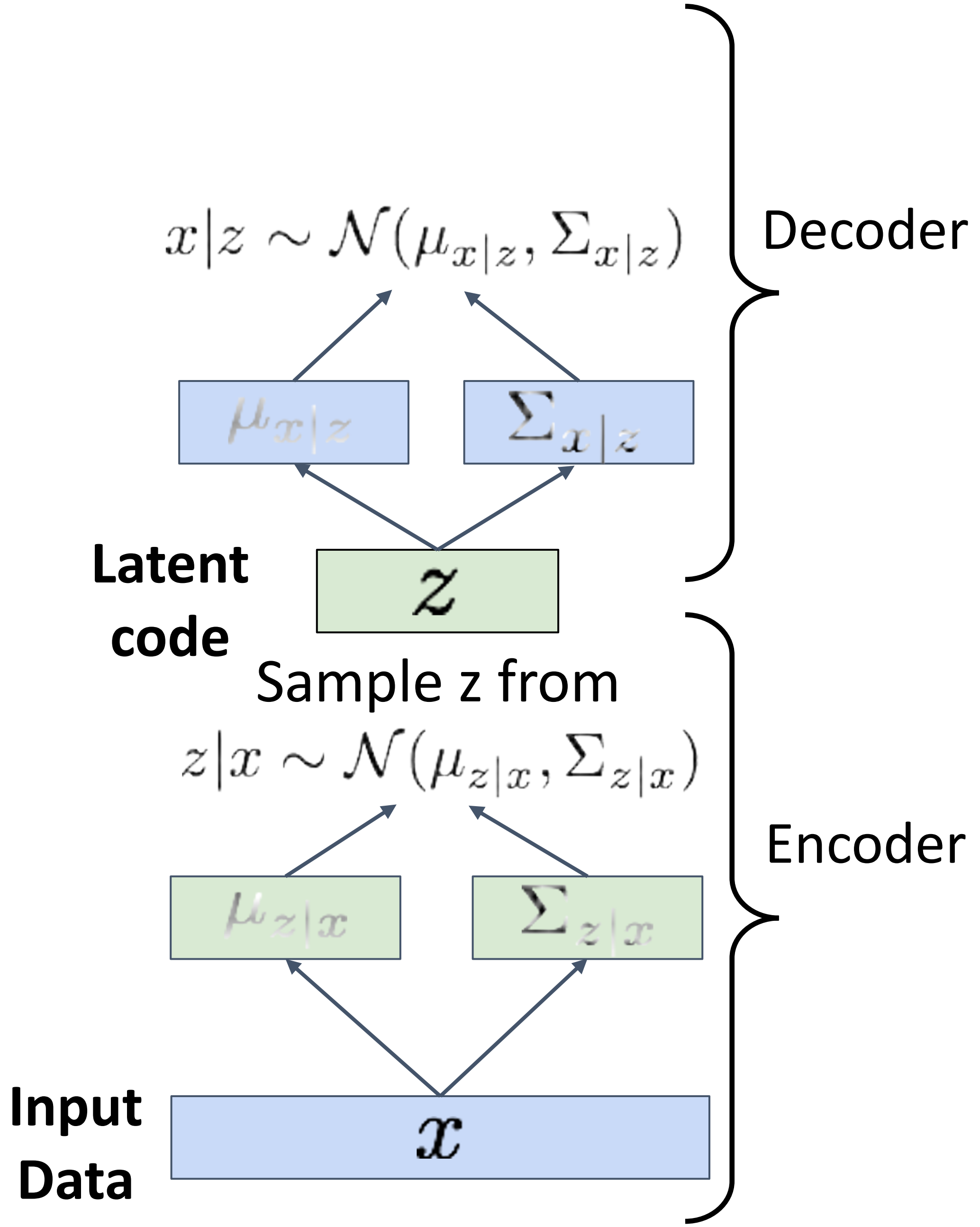


Variational Autoencoders

Train by maximizing the **variational lower bound**

$$\boxed{E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]} - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples
5. **Original input data should be likely under the distribution output from (4)!**

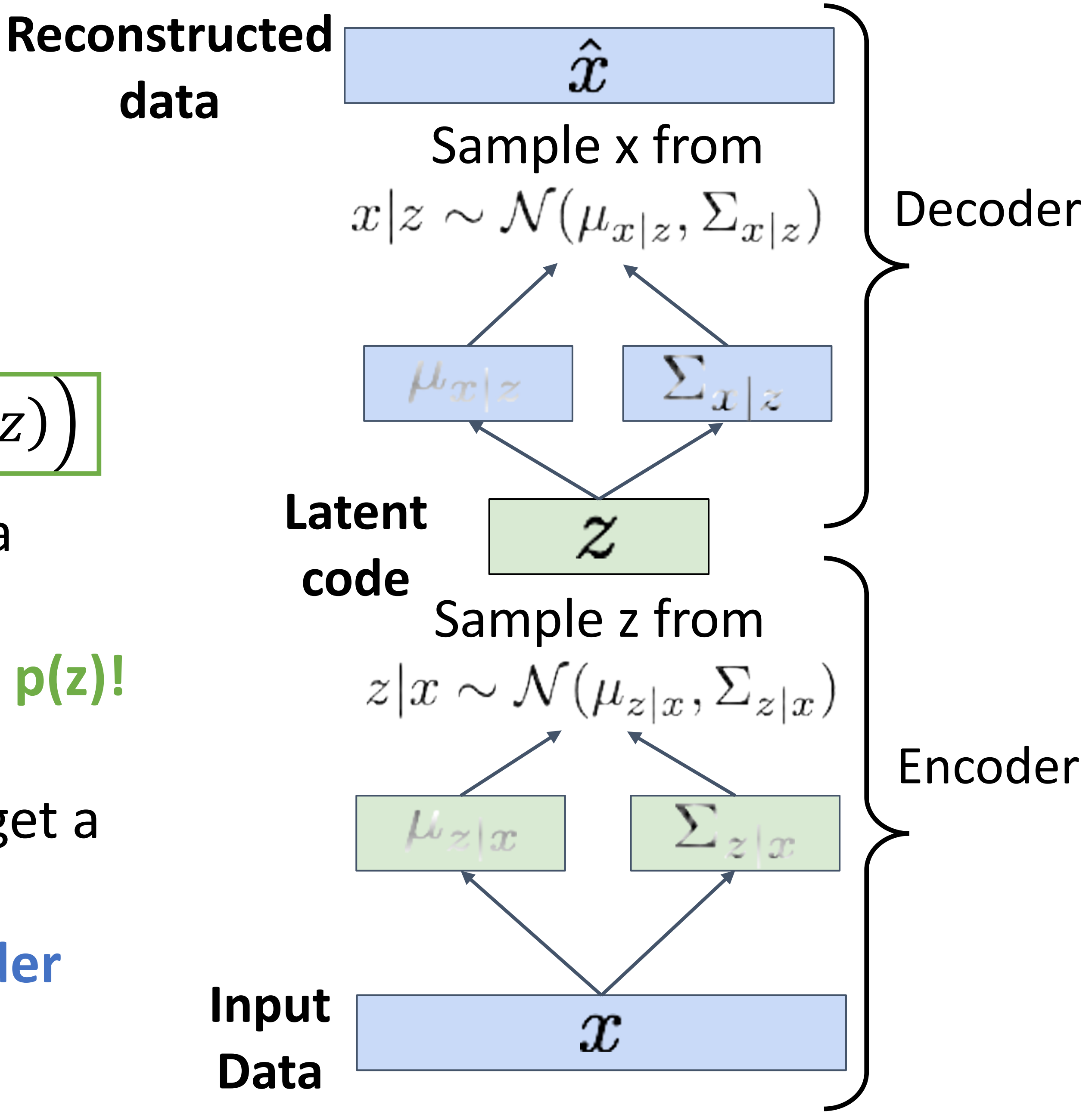


Variational Autoencoders

Train by maximizing the **variational lower bound**

$$\boxed{E_{z \sim q_\phi(z|x)}[\log p_\theta(x|z)]} - \boxed{D_{KL}\left(q_\phi(z|x), p(z)\right)}$$

1. Run input data through **encoder** to get a distribution over latent codes
2. **Encoder output should match the prior p(z)!**
3. Sample code z from encoder output
4. Run sampled code through **decoder** to get a distribution over data samples
5. **Original input data should be likely under the distribution output from (4)!**
6. Can sample a reconstruction from (4)



Variational Autoencoders: Generating Data

After training we can generate new data!

1. Sample z from prior p(z)

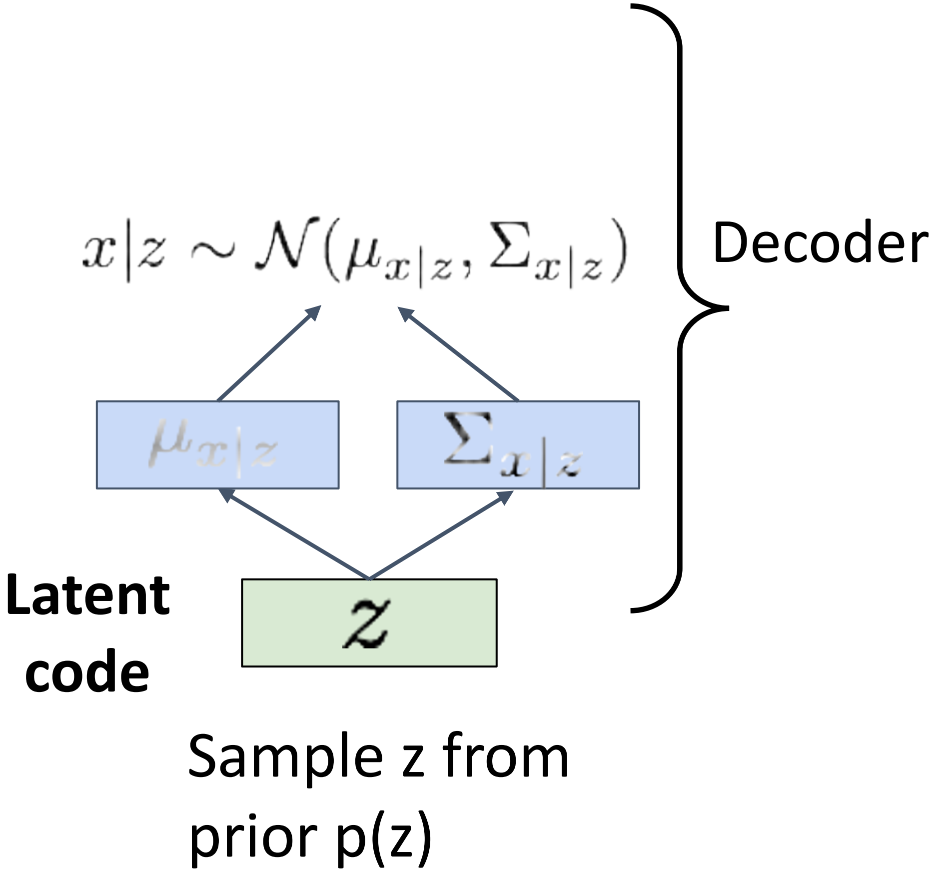
Latent code $\boxed{z}$

Sample z from prior p(z)

Variational Autoencoders: Generating Data

After training we can generate new data!

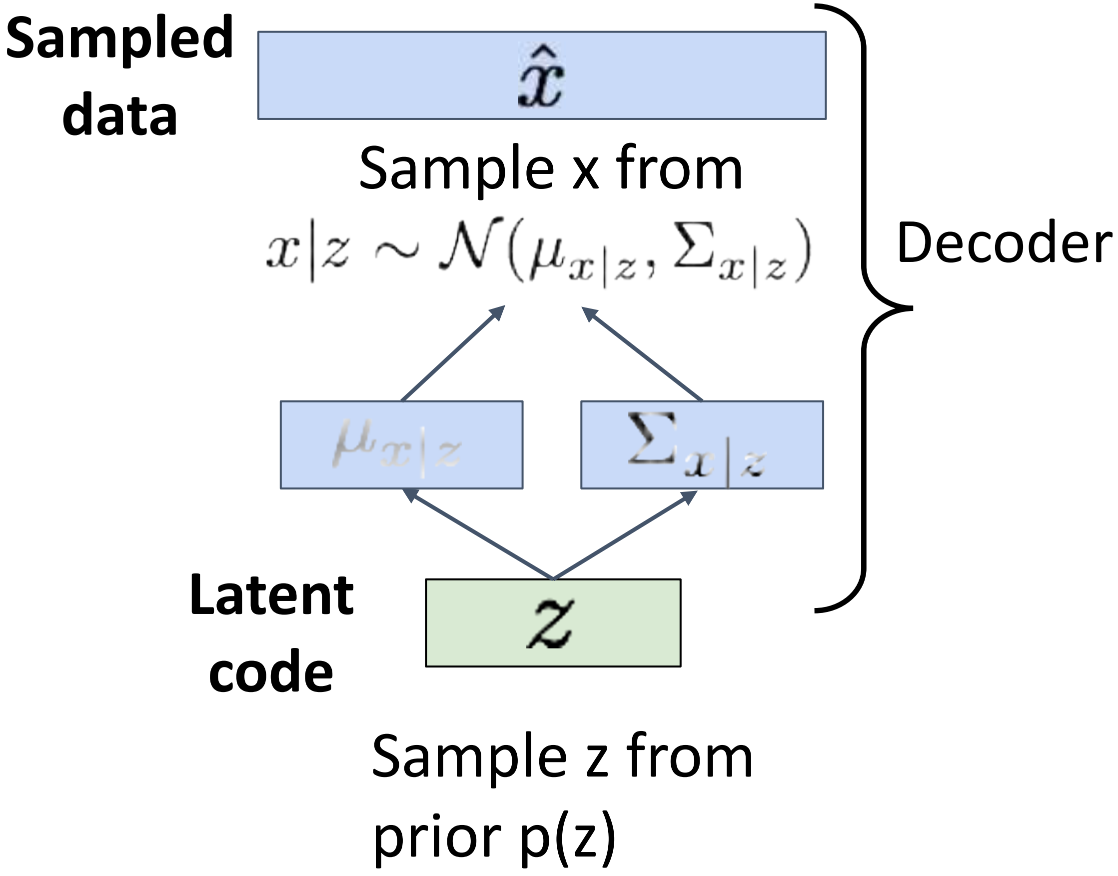
1. Sample z from prior p(z)
2. Run sampled z through decoder to get distribution over data x



Variational Autoencoders: Generating Data

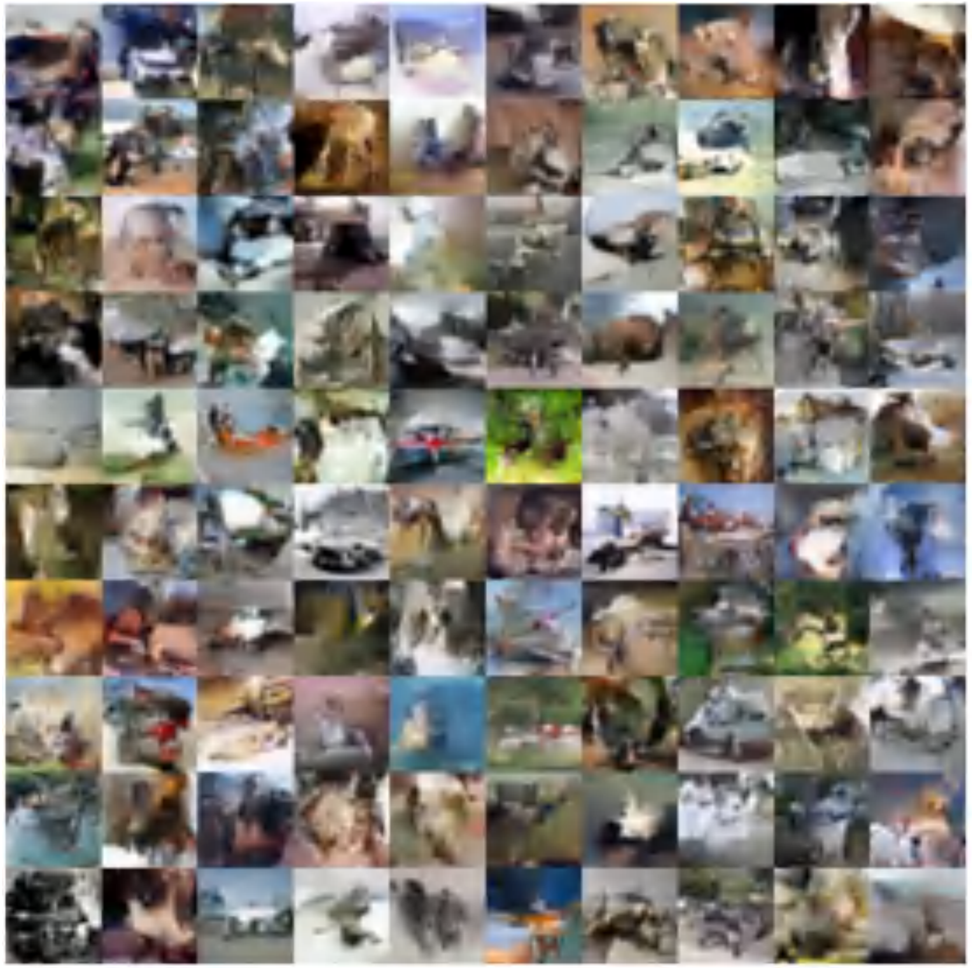
After training we can generate new data!

1. Sample z from prior p(z)
2. Run sampled z through decoder to get distribution over data x
3. Sample from distribution in (2) to generate data



Variational Autoencoders: Generating Data

32x32 CIFAR-10



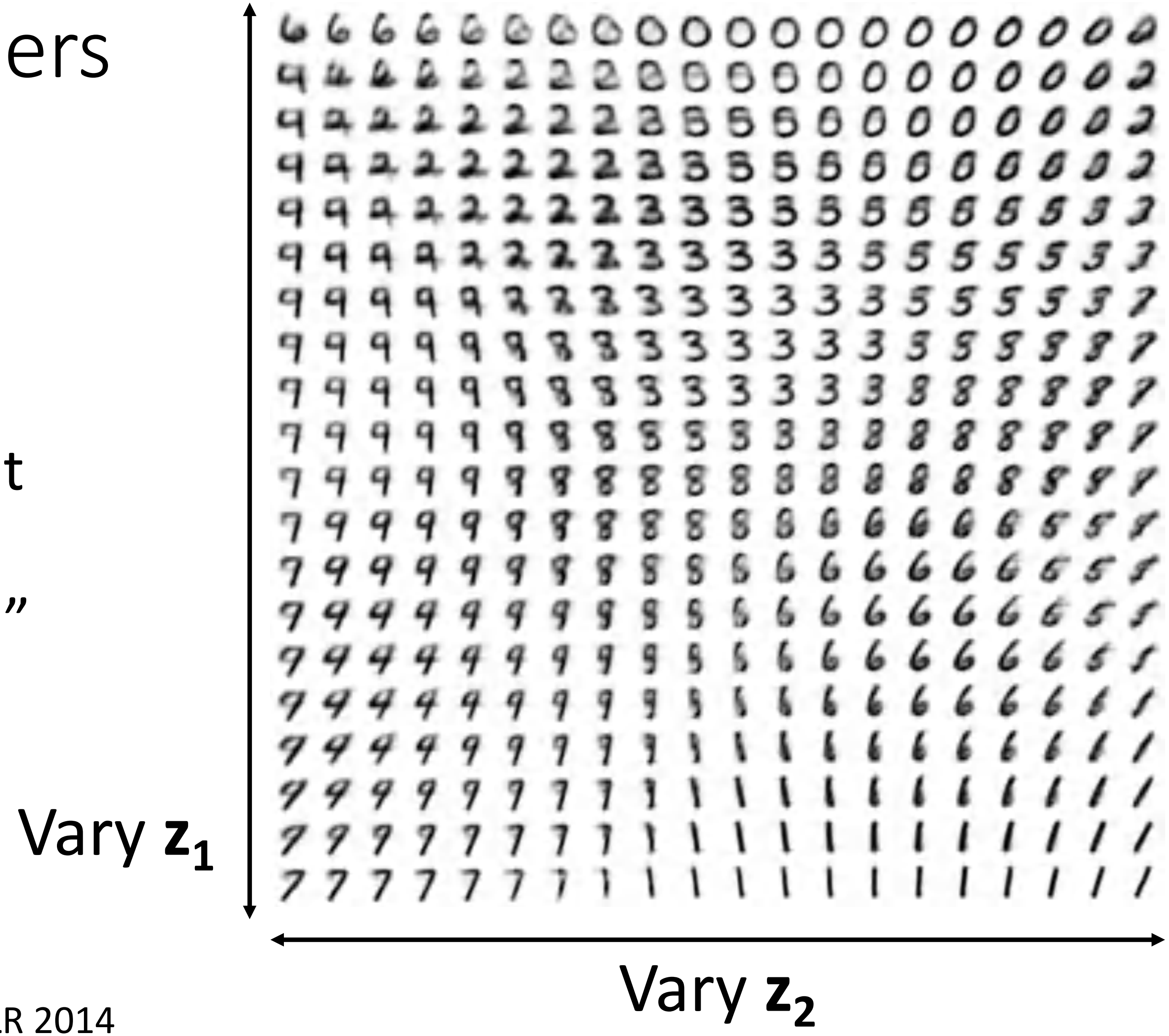
Labeled Faces in the Wild

Figures from (L) Dirk Kingma et al. 2016; (R) Anders Larsen et al. 2017.

Variational Autoencoders

The diagonal prior on p(z) causes dimensions of z to be independent

"Disentangling factors of variation"

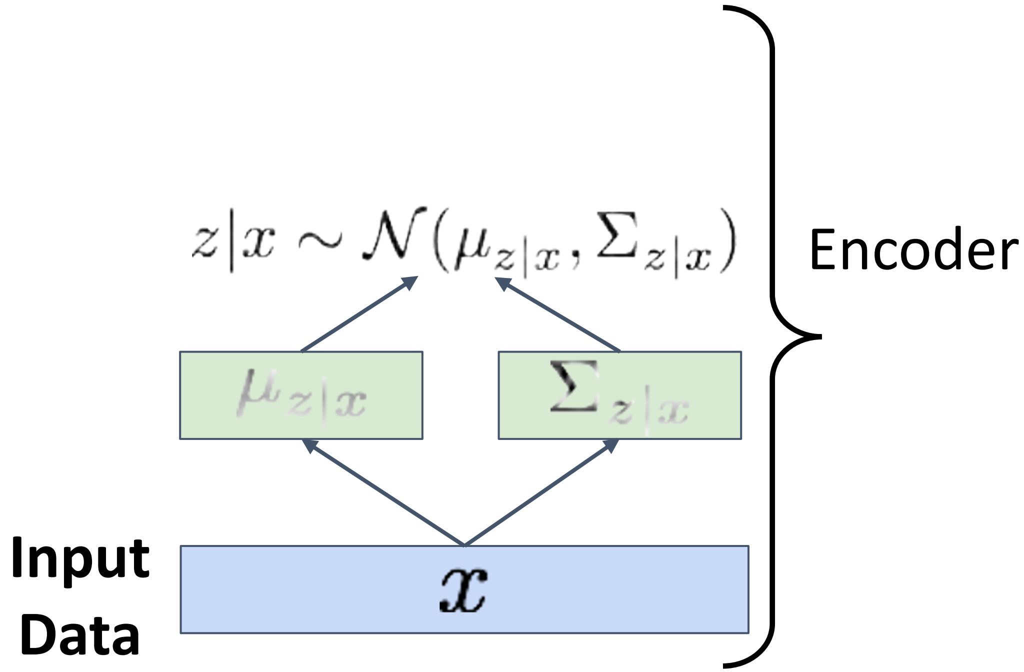


Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

Variational Autoencoders

After training we can **edit images**

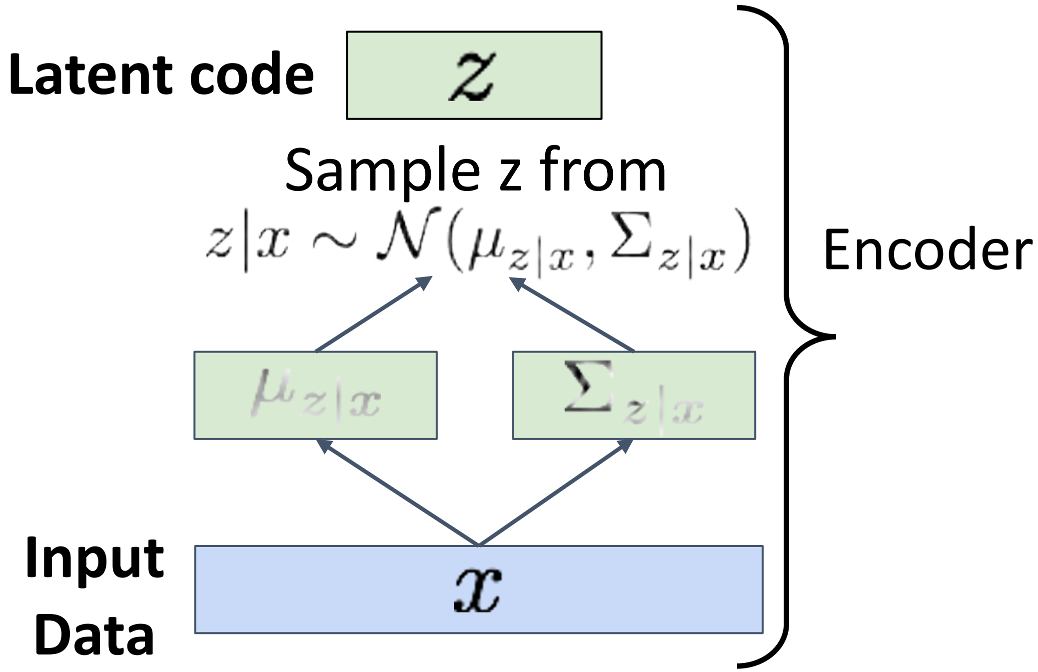
1. Run input data through **encoder** to get a distribution over latent codes



Variational Autoencoders

After training we can **edit images**

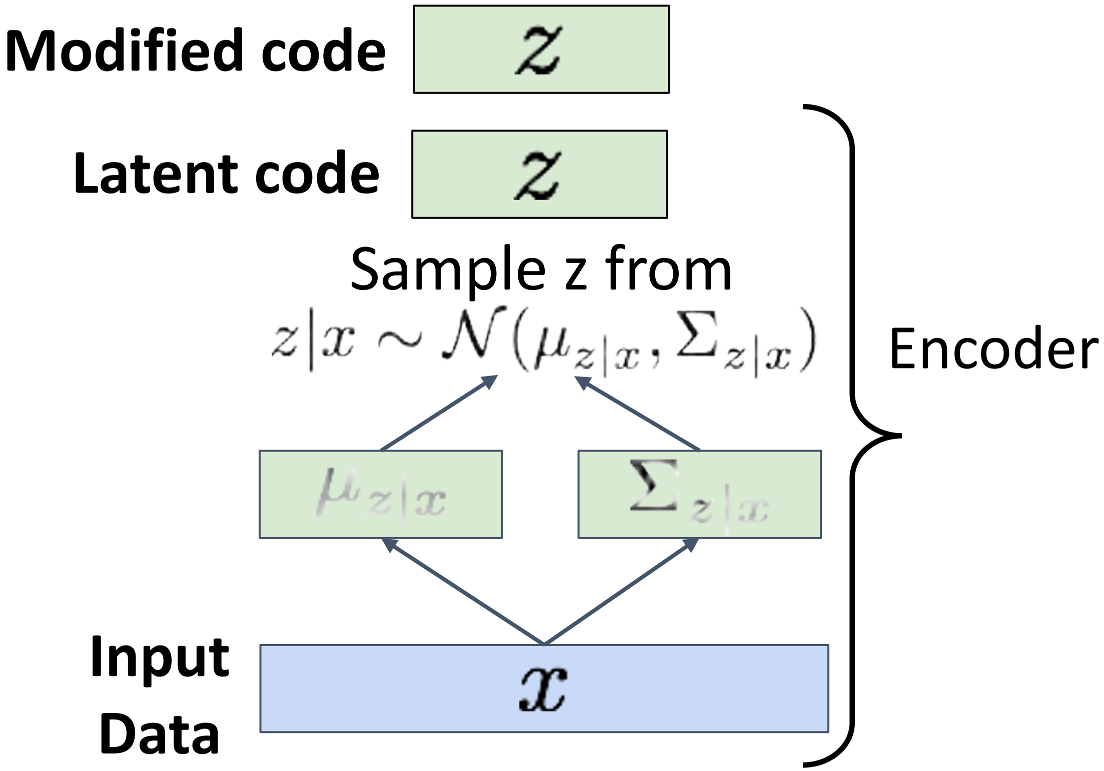
1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output



Variational Autoencoders

After training we can **edit images**

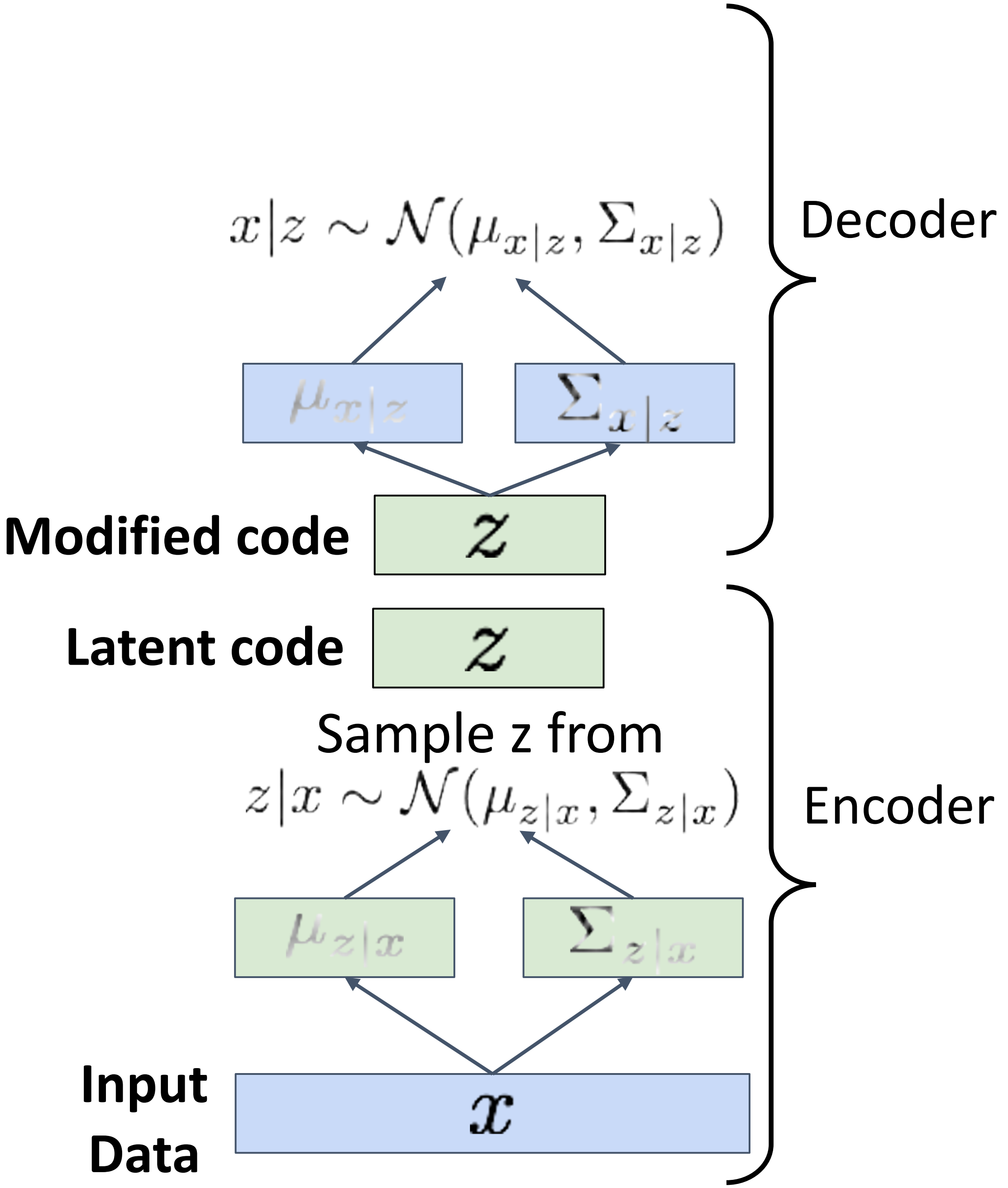
1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code



Variational Autoencoders

After training we can **edit images**

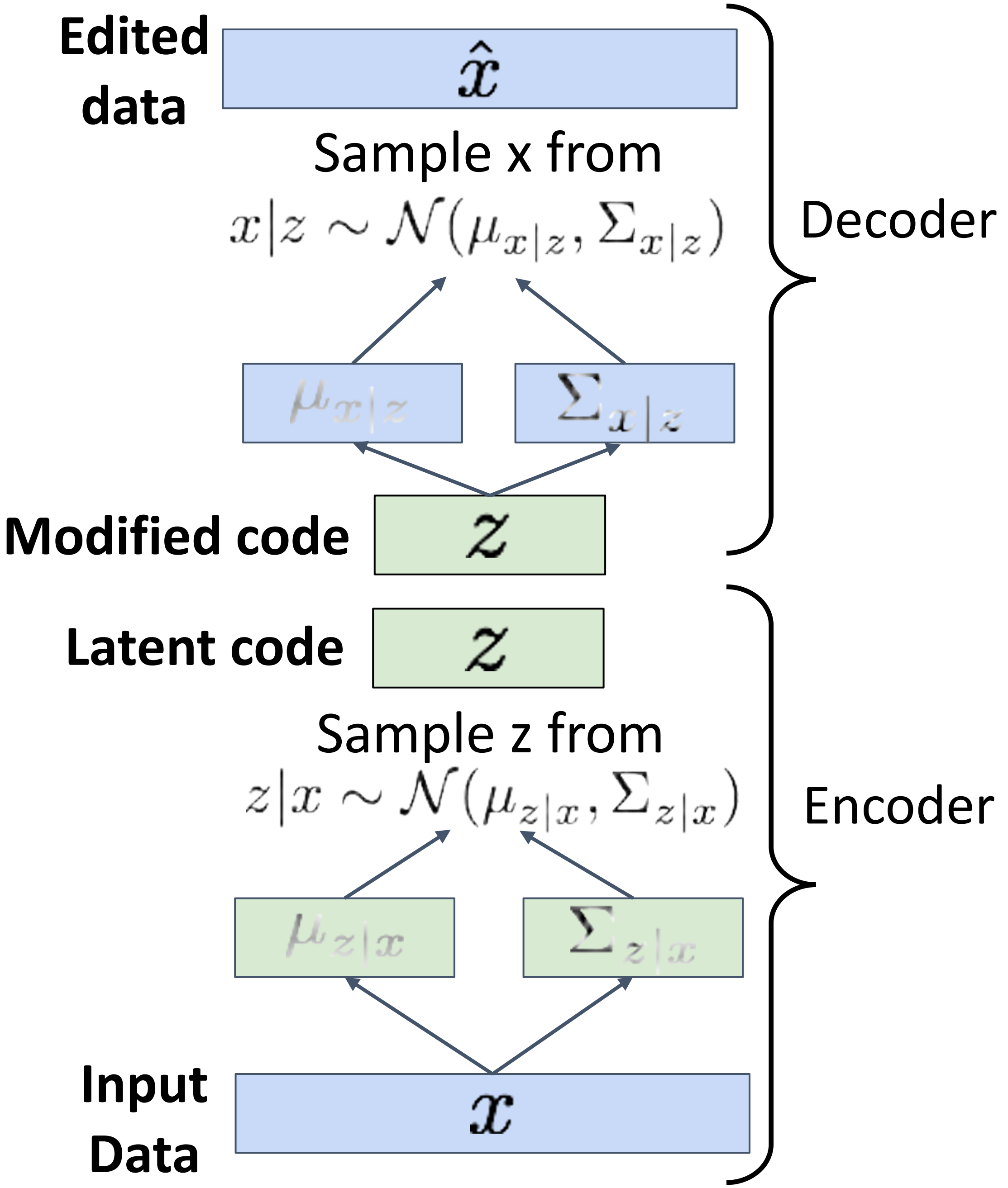
1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code
4. Run modified z through **decoder** to get a distribution over data sample



Variational Autoencoders

After training we can **edit images**

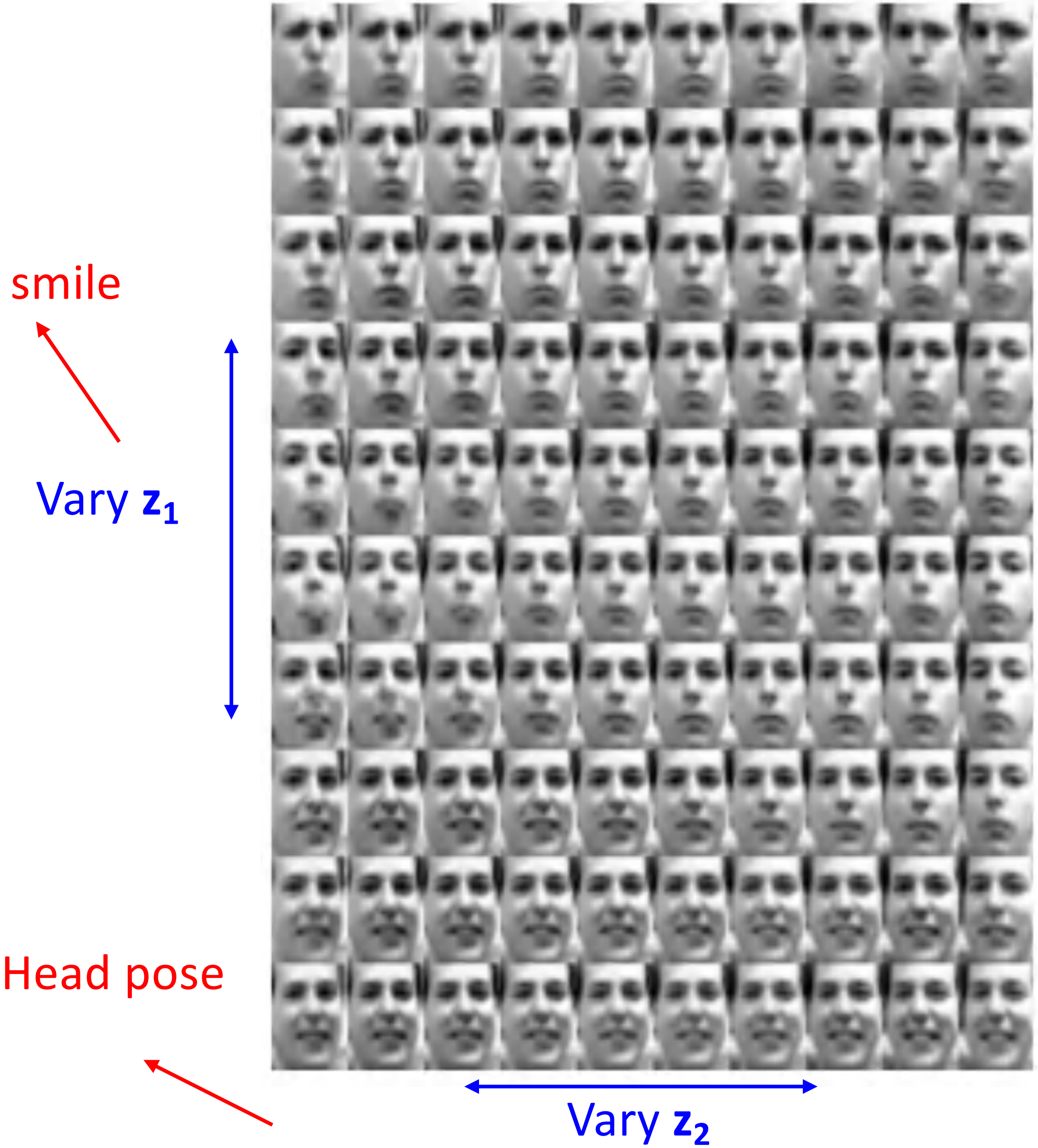
1. Run input data through **encoder** to get a distribution over latent codes
2. Sample code z from encoder output
3. Modify some dimensions of sampled code
4. Run modified z through **decoder** to get a distribution over data samples
5. Sample new data from (4)



Variational Autoencoders

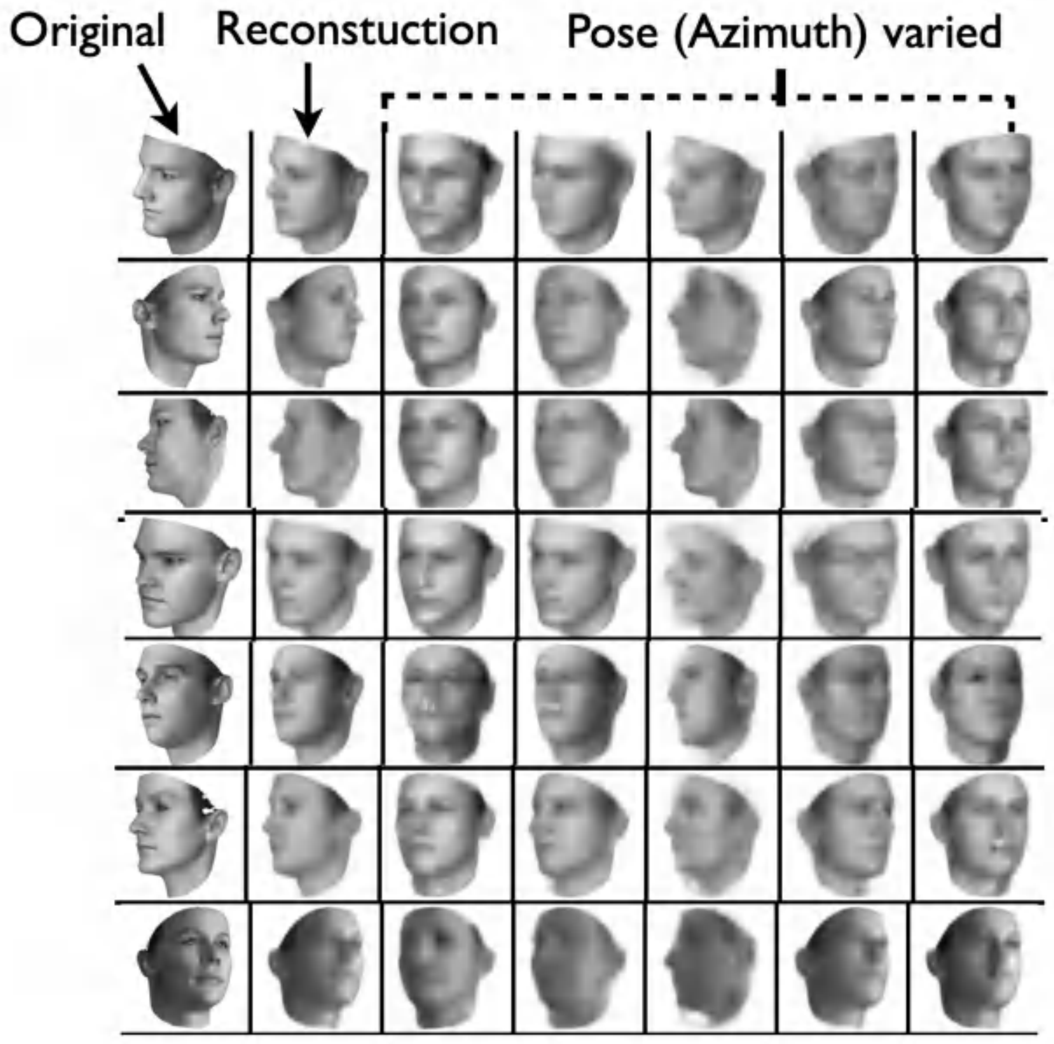
The diagonal prior on p(z) causes dimensions of z to be independent

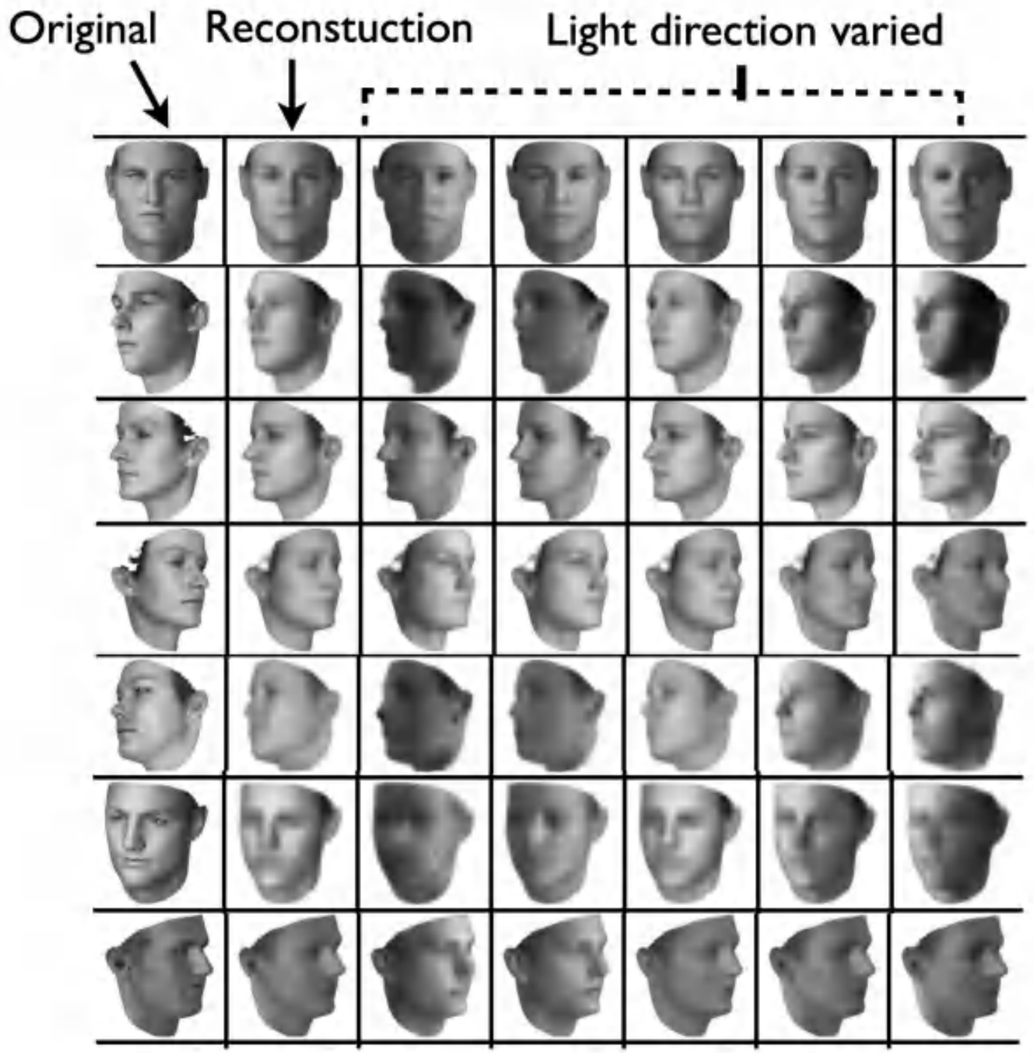
"Disentangling factors of variation"



Kingma and Welling, Auto-Encoding Variational Beyes, ICLR 2014

Variational Autoencoders: Image Editing





Kulkarni et al, “Deep Convolutional Inverse Graphics Networks”, NeurIPS 2014

Variational Autoencoder: Summary

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, e.g., Gaussian Mixture Models (GMMs)
- Incorporating structure in latent variables, e.g., Categorical Distributions

Next Time:
Generative Models, part 2

More Variational Autoencoders,
Generative Adversarial Networks