# Introduction to Probabilistic Deep Learning and Generative modeling

CSE 849 Deep Learning Spring 2025

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# Supervised vs Unsupervised Learning

Supervised Learning Unsupervised 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.

Data: x

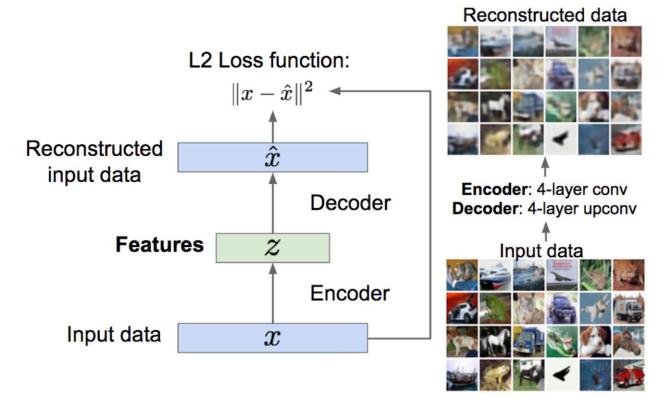
Just data, no labels!

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

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

# Supervised vs Unsupervised Learning

Feature Learning (e.g. autoencoders)



**Unsupervised Learning** 

Data: x

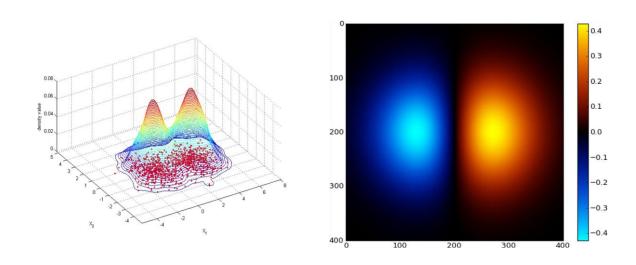
Just data, no labels!

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

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

# Supervised vs Unsupervised Learning

#### **Density Estimation**



#### **Unsupervised Learning**

Data: x

Just data, no labels!

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

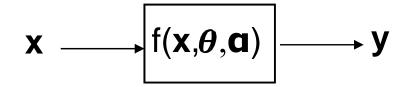
**Examples**: Clustering, dimensionality reduction, feature learning, density estimation, etc.

# Introduction to Probabilistic Machine Learning

- Deterministic machine learning
- Probabilistic machine learning
- Bayesian machine learning

\*By saying machine learning, the techniques include but not limited to deep learning

# Deterministic Machine Learning



- $\mathbf{x} \ni X$ -input,  $\mathbf{y} \ni Y$ -output
- f() the mapping function that maps input to output
- $\theta \ni \Theta$  and  $\alpha \ni A$  are the parameters and hyper-parameters of the mapping function
- The goal is to learn the mapping function parameter  $\theta$  and tune the hyper-parameter  $\alpha$  to map input  $\mathbf{x}$  to output  $\mathbf{y}$
- After training, an optimal set of parameters Θ\* are obtained

#### **Issues**:

- It cannot effectively capture the uncertainties in input data (X), in the model parameters (Θ), and in the output (y). Hence, it cannot quantify the output confidence.
- Its prediction is based on point estimation of the parameters (⊕\*) only and it hence tends to overfit.

# Probabilistic Machine Learning

Probabilistic machine learning constructs the probability distribution of input and output  $P_{\Theta}(x, y)$ , where  $\Theta \ni Q$ ,  $X \ni X$  and  $Y \ni Y$  and use  $P_{\Theta}$  to perform the prediction.

- Generative approach  $-p(X,Y|\Theta)$ 

Learn the parameters  $\Theta^*$  that characterizes the joint probability of X and Y, and performs the classification/regression using

$$Y^*$$
=argmax $_Y$  p( $Y|X$ ,  $\Theta^*$ )

Or only  $p(X | \Theta)$  if no labels, i.e., Y

Discriminative approach – p(Y|X, O)

Learn the parameters  $\Theta^*$  that characterizes the conditional joint probability of Y given X, and performs the classification/regression using

$$Y^*$$
=argmax $_Y$  p( $Y|X$ ,  $\Theta^*$ )

-  $\Theta$  are parameters that characterize the probability distributions, and it is learnt through a training process.

# Probabilistic Machine Learning

#### -- Pros and Cons

#### Pros:

- Capable of capturing the input and output data uncertainties
- Can quantify the output confidence and predict output accuracy

#### Cons:

- Computationally more expensive during both training and prediction; more difficult to train the probabilistic loss function
- Still require a training process to learn the parameters
- Prediction is still based on point-estimation
- Cannot quantify the model uncertainty, i.e., that of  $\Theta$ .

# Bayesian Machine Learning

Bayesian Machine models the posterior distribution of the model parameters  $\Theta$ ,  $P(\Theta|\mathbf{D}, \mathbf{a})$ , where **D** are the training data and **a** are the hyper-parameters that specify the prior probability of  $\Theta$ ,  $p(\Theta \mid \mathbf{a})$ .

Given an input **X**, prediction of output **Y** can be done through empirical or full Bayesian inference

Empirical inference

$$\mathbf{Y}^* = \underset{\mathbf{Y}}{\arg\max} \ p(\mathbf{Y} \,|\, \mathbf{X}, \mathbf{D}, \pmb{\alpha}^*) = \underset{\mathbf{Y}}{\arg\max} \int_{\mathbf{\Theta}} p(\mathbf{Y} \,|\, \mathbf{X}, \mathbf{\Theta}) \, p(\mathbf{\Theta} \,|\, \mathbf{D}, \pmb{\alpha}^*) d\mathbf{\Theta}$$
 – Full Bayesian inference

$$\mathbf{Y}^* = \underset{\mathbf{Y}}{\operatorname{argmax}} \ p(\mathbf{Y} \mid \mathbf{X}, \mathbf{D}) = \underset{\mathbf{Y}}{\operatorname{argmax}} \iint_{\mathbf{\Theta} \ \alpha} p(\mathbf{Y} \mid \mathbf{X}, \mathbf{\Theta}) \ p(\mathbf{\Theta} \mid \mathbf{D}, \boldsymbol{\alpha}) \ p(\boldsymbol{\alpha} \mid \mathbf{D}) d\mathbf{\Theta} d\boldsymbol{\alpha}$$

# Bayesian Machine Learning (cont'd)

- Compared to probabilistic machine learning, Bayesian learning has the following advantages:
- Bayesian inference does not need learn parameters Θ
- Instead of performing point-based prediction, Bayesian inference performs output prediction using all parameters through parameter integration, hence avoiding the overfitting problem.
- Bayesian inference produces not only outputs but also generates their distribution, based on which we can derive both data and model uncertainties.
- Bayesian learning has the following disadvantages:
- It needs either manually specify or learn the hyper-parameters. Manual specification of the hyper-parameters is inaccurate, while automatic hyper-parameter learning is computationally complex.
- Bayesian inference requires integration over all parameters as well as the hyper-parameters, which is computationally intractable and cannot scale up well for a large number of parameters.
- Approximated and inaccurate solutions are often used to approximate the parameter integration, hence leading to non-optimal /inaccurate solutions.

# Introduction to Probabilistic Machine Learning

- Deterministic machine learning
- Probabilistic machine learning
  - Generative
  - Discriminative
- Bayesian machine learning

#### **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

<sup>\*</sup>assume no label Y

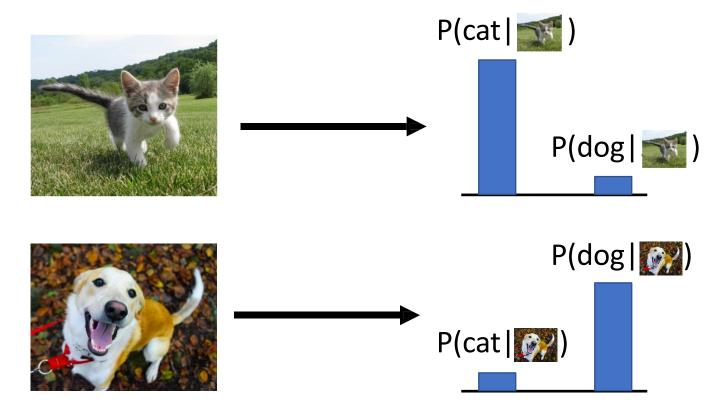
#### **Discriminative Model:**

Learn a probability distribution p(y|x)

#### **Generative Model:**

Learn a probability distribution p(x)

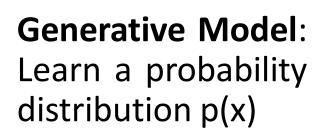
**Conditional Generative Model:** Learn p(x|y)



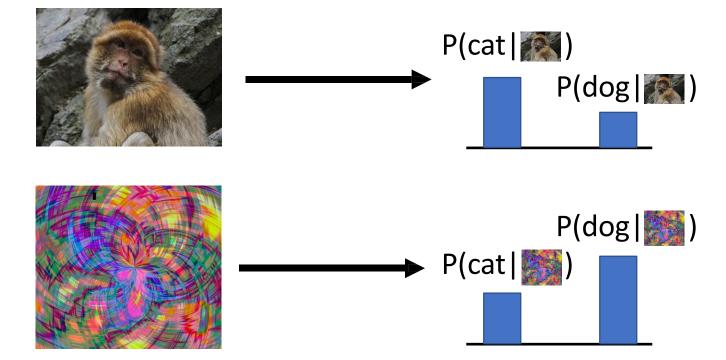
Discriminative model: estimate the distribution over the possible labels y.

But no probabilistic relationships between **images** x

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



**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

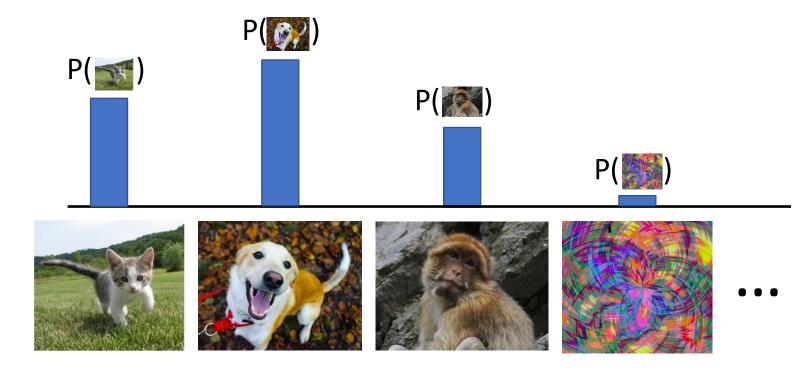
#### **Discriminative Model:**

Learn a probability distribution p(y|x)

#### **Generative Model:**

Learn a probability distribution p(x)

# **Conditional Generative Model:** Learn p(x|y)



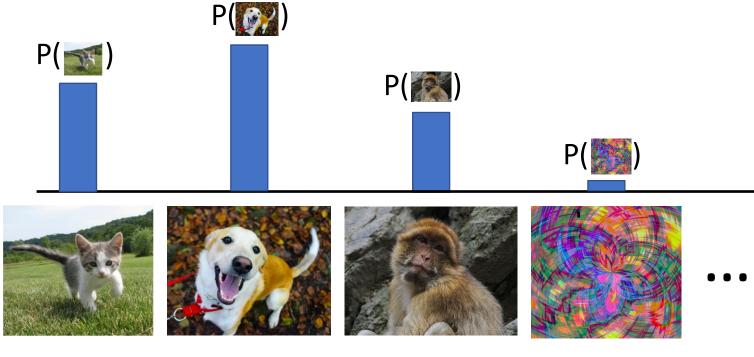
Generative model: estimate a distribution over all images. All possible images compete with each other for probability mass

#### **Discriminative Model:**

Learn a probability distribution p(y|x)

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

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



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

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

#### **Discriminative Model:**

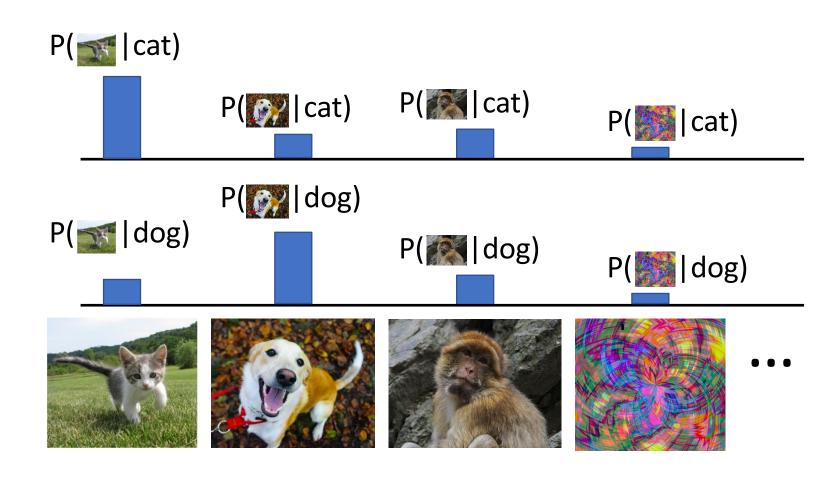
Learn a probability distribution p(y|x)

#### **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 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:

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

Conditional
Generative Model

Prior over labels

Conditional
Conditiona

We can build a conditional generative model from other components

## What can we do with a generative model?

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

Assign labels to dataFeature learning (with labels)

• **Generative Model**: Learn a probability distribution p(x)

Feature learning (without labels)
Sample to **generate** new data

**Detect outliers** 

Conditional Generative
 Model: Learn p(x|y)

Assign labels, while rejecting outliers! Generate new data conditioned on input labels

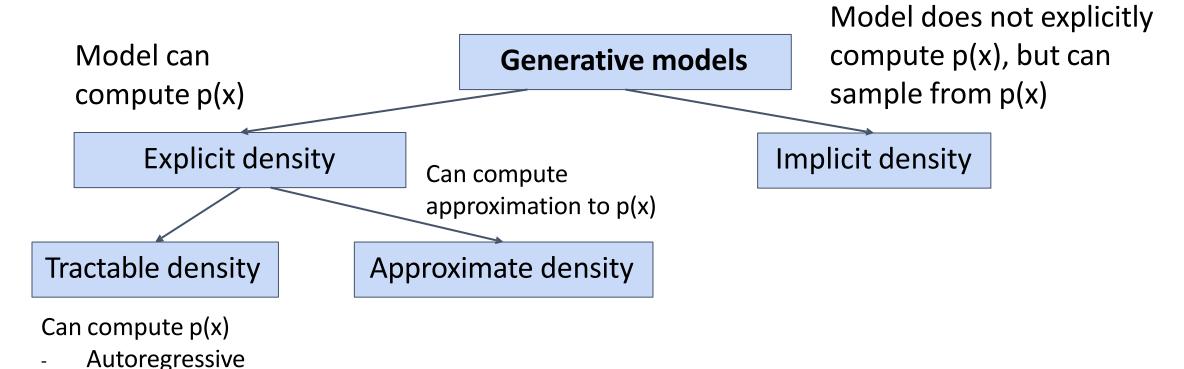
**Generative models** 

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

Explicit density

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

Normalizing flows



Model does not explicitly Model can compute p(x), but can **Generative models** sample from p(x)compute p(x)**Explicit density** Implicit density Can compute approximation to p(x)Tractable density Approximate density Variational Autoencoder Can compute p(x)Autoregressive Energy-based models Normalizing flows Diffusion models

Model can **Generative models** compute p(x)**Explicit density** Can compute approximation to p(x)Approximate density Tractable density Variational Autoencoder Can compute p(x)Autoregressive Energy-based models Normalizing flows Diffusion models

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

Implicit density

Generative Adversarial Networks (GANs)

Model does not explicitly Model can compute p(x), but can **Generative models** sample from p(x)compute p(x)**Explicit density** Implicit density Can compute approximation to p(x)Generative Adversarial Networks (GANs) Tractable density Approximate density Variational Autoencoder Can compute p(x)Autoregressive Energy-based models Normalizing flows Diffusion models We will talk about these three models

# Variational <u>Autoencoders</u>

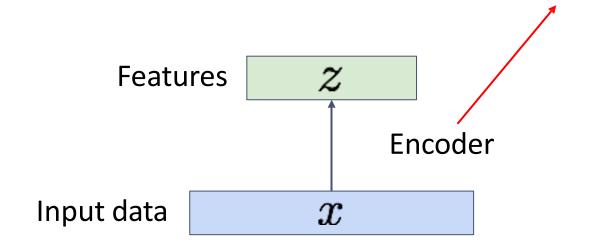
Unsupervised method for learning feature vectors from raw data x, without any labels

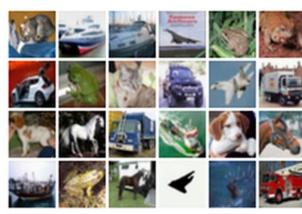
Features should extract useful information (maybe object identities, properties, scene type, etc) that we can use for downstream tasks

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

Later: Deep, fully-connected

Later: ReLU CNN





**Input Data** 

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

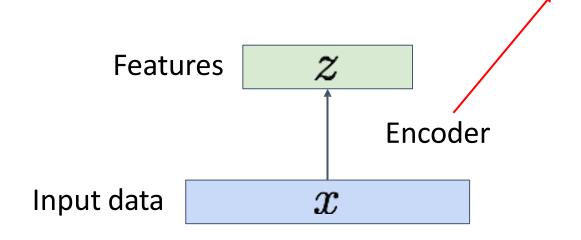
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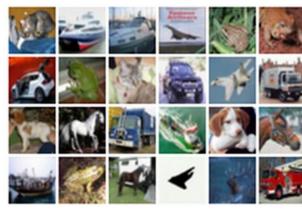
But we can't observe features!

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

Later: Deep, fully-connected

Later: ReLU CNN



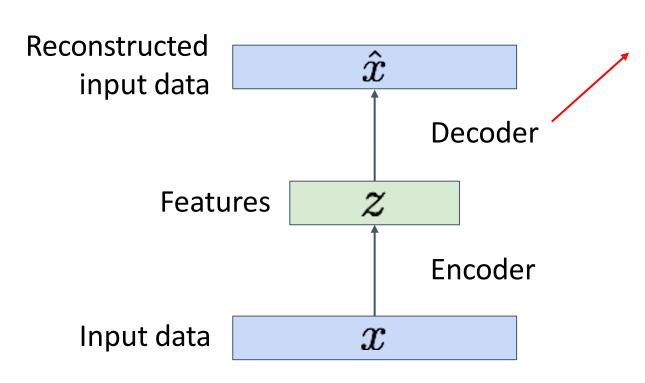


Input Data

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

**Idea**: Use the features to <u>reconstruct</u> the input data with a **decoder** 

"Autoencoding" = encoding itself

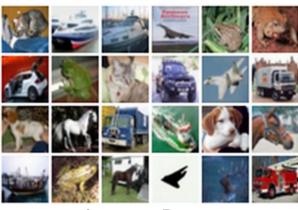


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nonlinearity (sigmoid)

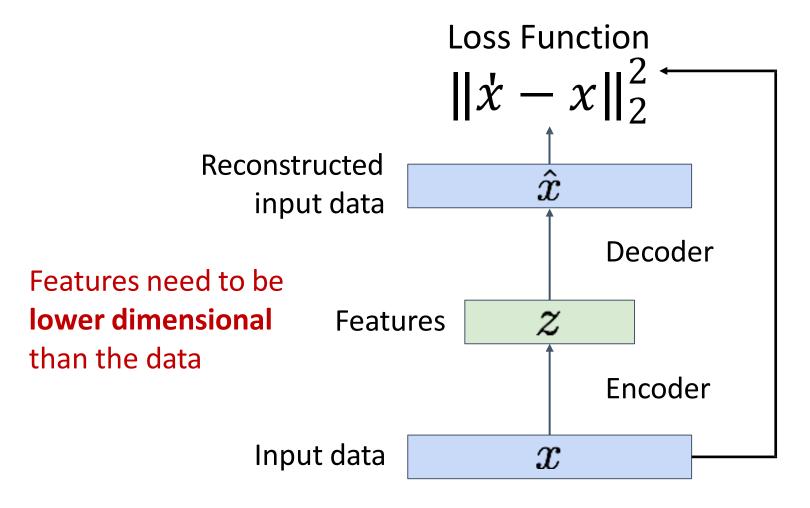
**Later**: Deep, fully-connected

Later: ReLU CNN (upconv)



Input Data

Loss: L2 distance between input and reconstructed data.

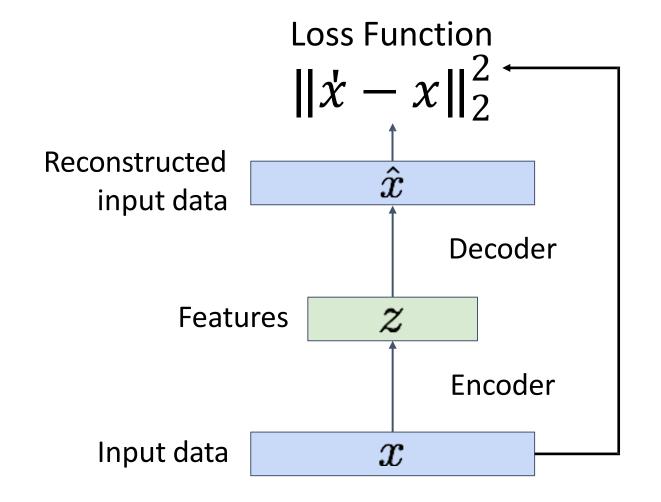


Does not use any labels
Just raw data

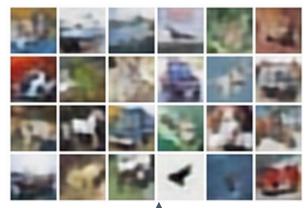


**Input Data** 

**Loss**: L2 distance between input and reconstructed data.



#### Reconstructed data



Decoder:

4 tconv layers

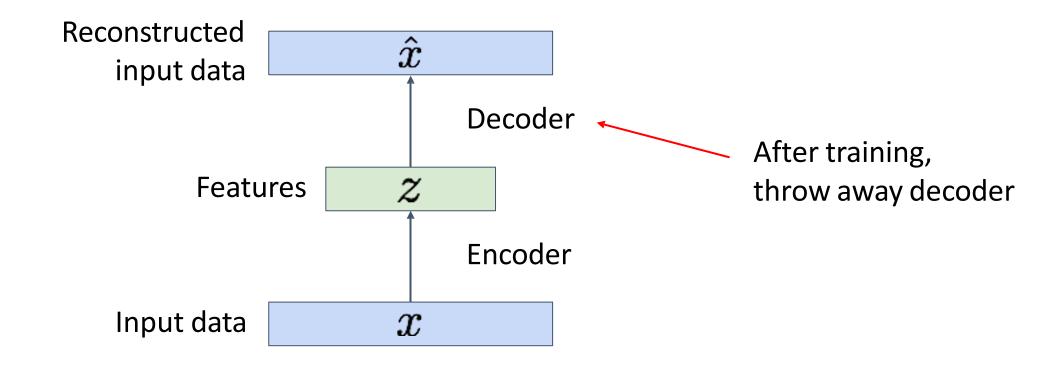
Encoder:

4 conv layers

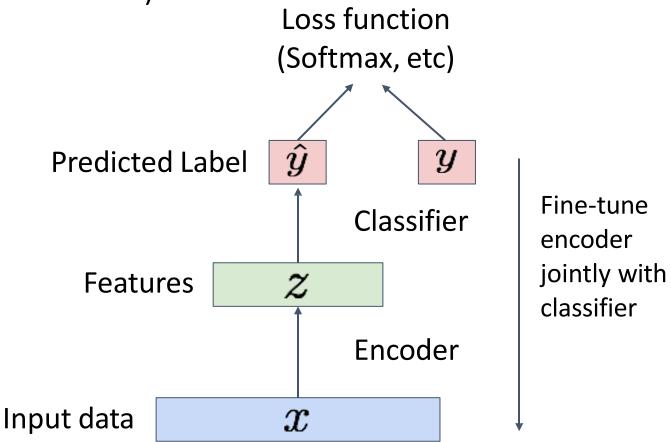


**Input Data** 

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

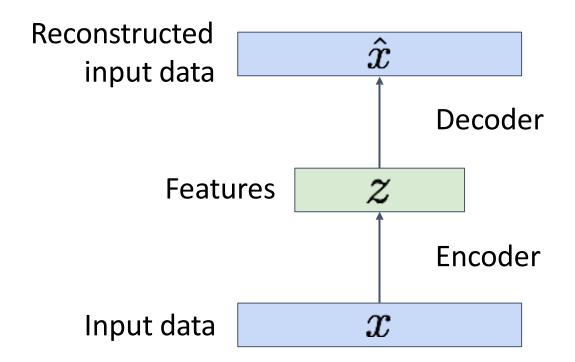


- After training, throw away decoder and use encoder for a downstream task
- Encoder can be used to initialize a supervised model
- Train for final task (sometimes with small data)



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



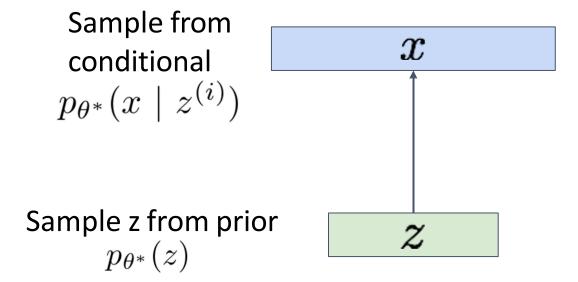
# Variational Autoencoders

### Variational Autoencoders

Probabilistic spin on autoencoders:

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

After training, sample new data like this:



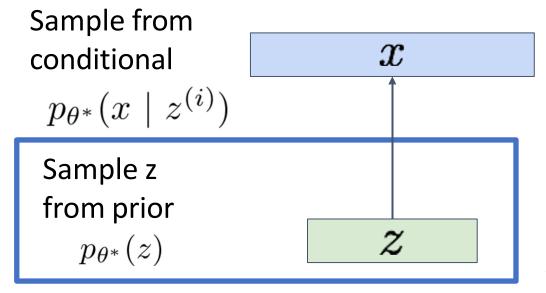
Assume training data  $\left\{x^{(i)}\right\}_{i=1}^{N}$  is generated from unobserved (latent) representation **z** 

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

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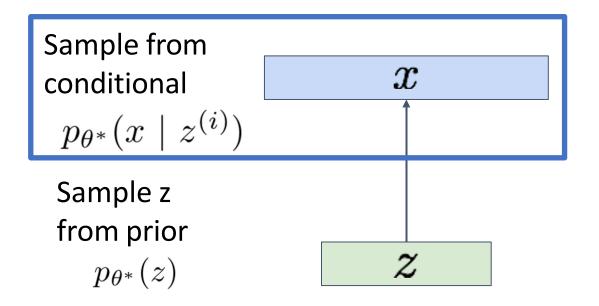
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Assume simple prior p(z), e.g. Gaussian

Probabilistic spin on autoencoders:

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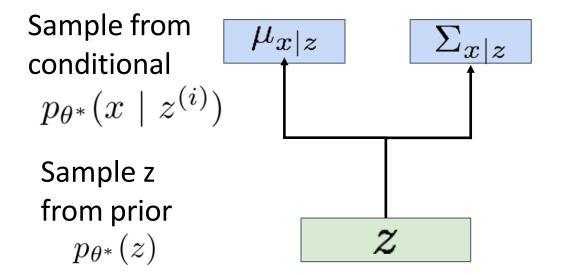
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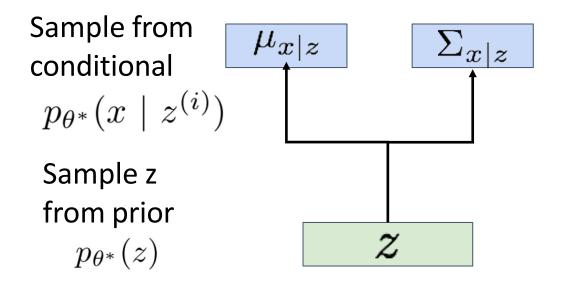
**Intuition: x** is an image, **z** is latent factors used to generate **x**: attributes, orientation, etc.

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



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

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



How to train this model?

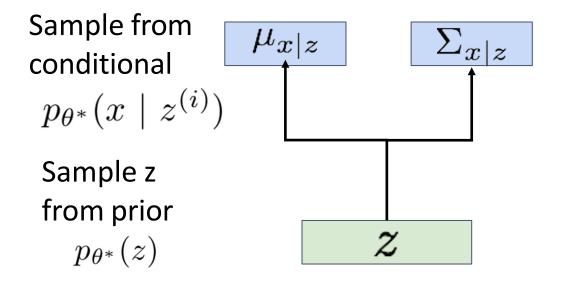
Basic idea: maximize likelihood of data

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

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

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

can compute this with decoder network



How to train this model?

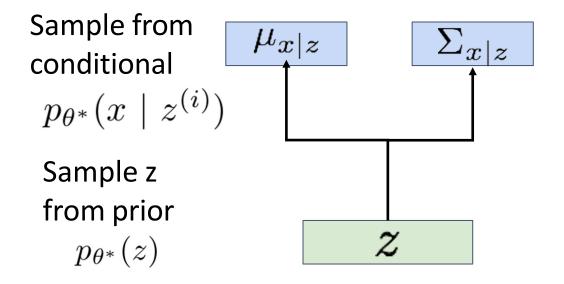
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we assumed Gaussian prior for z



How to train this model?

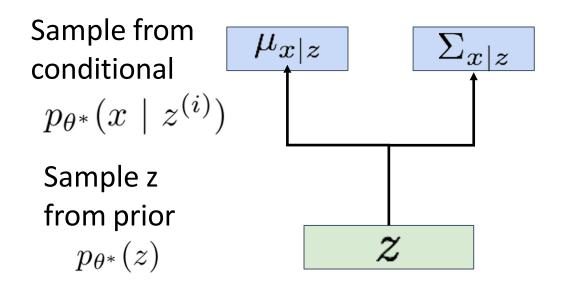
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Problem: Impossible to integrate over all z!

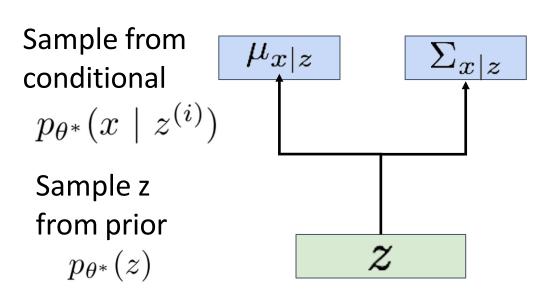


How to train this model?

Basic idea: maximize likelihood of data

Another idea: Try Bayes' Rule:

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



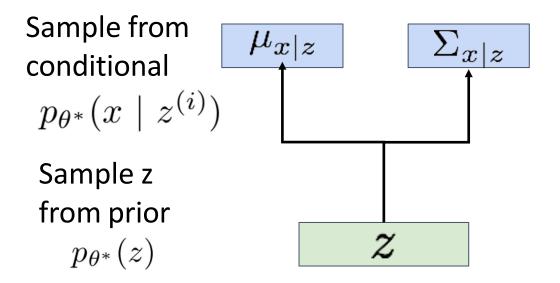
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decoder network



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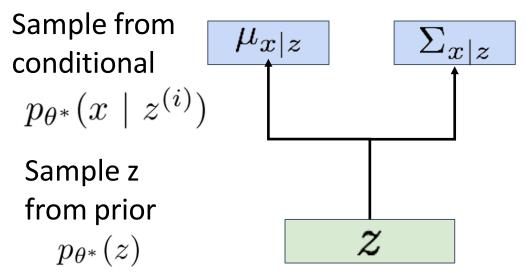
Another idea: Try Bayes' Rule:

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**Problem**: No way to compute this!

**Solution:** Train another network (encoder) that learns

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



How to train this model?

Basic idea: maximize likelihood of data

Another idea: Try Bayes' Rule:

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

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

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

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

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

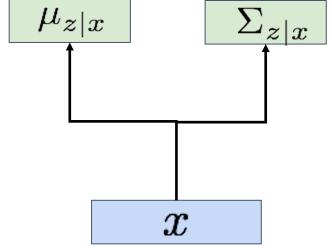
$$p_{\theta}(x \mid z) = N(\mu_{x\mid z}, \Sigma_{x\mid z})$$

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

then we can approximate

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

 $\mu_{x|z}$ 



**Idea**: Jointly train both encoder and decoder

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

Bayes' Rule

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

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

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

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

Split up using rules for logarithms

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

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

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

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

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

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

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

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

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

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

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Data reconstruction

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

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

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

KL divergence between prior, and samples from the encoder network

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

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

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

KL divergence between encoder and posterior of decoder

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

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

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

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

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

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

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

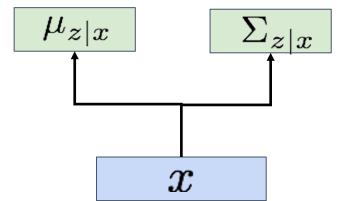
$$\log p_{\theta}(x) \ge E_{z \sim q_{\phi}(z|x)}[\log p_{\theta}(x|z)] - D_{KL}\left(q_{\phi}(z|x), p(z)\right)$$

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

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

**Encoder Network** 

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



**Decoder Network** 

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

$$\mu_{x\mid z} \qquad \Sigma_{x\mid z}$$

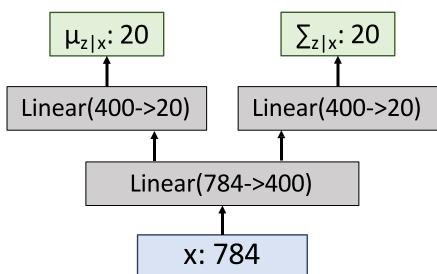
# Example: Fully-Connected VAE

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**

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

