CS 4644-DL / 7643-A: LECTURE 17
DANFEI XU

Generative Models:

PixelCNN / PixelRNN

Variational AutoEncoders (VAEs)

Administrative

- We'll come back to 3D Vision after this …
- Milestone Report is due EOD 11/4 NO GRACE PERIOD
- HW3 due EOD 10/22 (grace period ends EOD 10/24)
- HW4 release 10/22, due 11/12

Supervised Learning

- Train Input: $\{X, Y\}$
- Learning output: $f : X \rightarrow Y$, e.g. $P(y|x)$

Unsupervised Learning

- Input: $\{X\}$
- Learning output: $P(x)$
- Example: Clustering, density estimation, etc.

Reinforcement Learning

- Supervision in form of **reward**
- No supervision on what action to take

Very often combined, sometimes within the same model!

Supervised Learning

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Reinforcement Learning

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Very often combined, sometimes within the same model!

What if all we have are data without label?

We have lots of *raw* data (e.g., Internet)!

Can we still learn useful things without labels?

Generative Models

Supervised vs Unsupervised Learning

Supervised Learning

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

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

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

Supervised vs Unsupervised Learning

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.

→ Cat

Classification

Supervised vs Unsupervised Learning

Supervised Learning

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x is data, y is label

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

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

A cat sitting on a suitcase on the floor

Image captioning

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.

DOG, DOG, CAT

Object Detection

Supervised vs Unsupervised Learning

Supervised Learning

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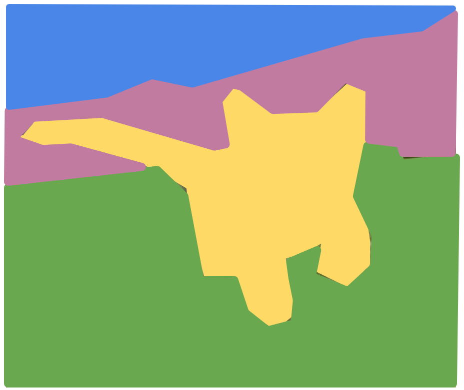
Goal: Learn a *function* to map x -> y

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



GRASS, CAT, TREE, SKY

Semantic Segmentation

Supervised vs Unsupervised Learning

Unsupervised Learning

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

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

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

Supervised vs Unsupervised Learning

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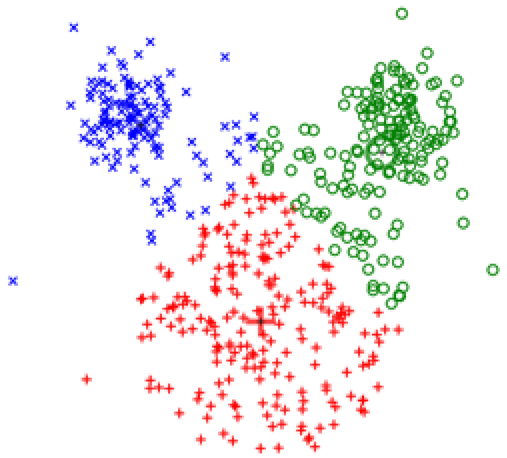


K-means clustering

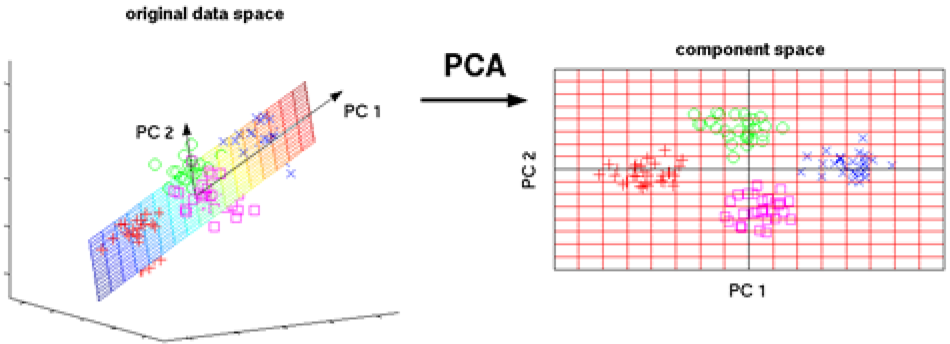
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



3-d → 2-d

Principal Component Analysis
(Dimensionality reduction)

Supervised vs Unsupervised Learning

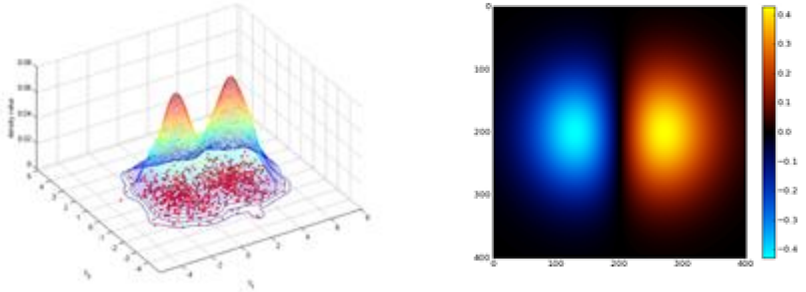
Unsupervised Learning

Data: x
Just data, no labels!

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

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

1-d density estimation



2-d density estimation

Modeling p(x)

Supervised vs Unsupervised Learning

Supervised Learning

Data: (x, y)
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Goal: Learn a *function* to map x -> y

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

Unsupervised Learning

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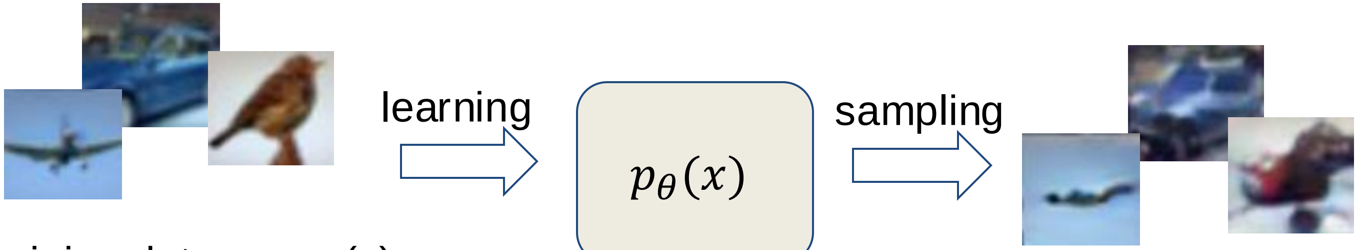
Generative Modeling

Given training data, generate new samples from same distribution



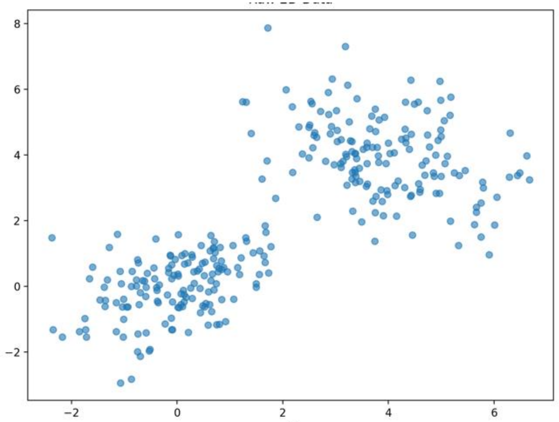
Training data ~ $p_{data}(x)$

Objectives:

1. Learn $p_\theta(x)$ that approximates an unknown $p_{\text{data}}(x)$
2. Sampling new x from $p_{model}(x)$

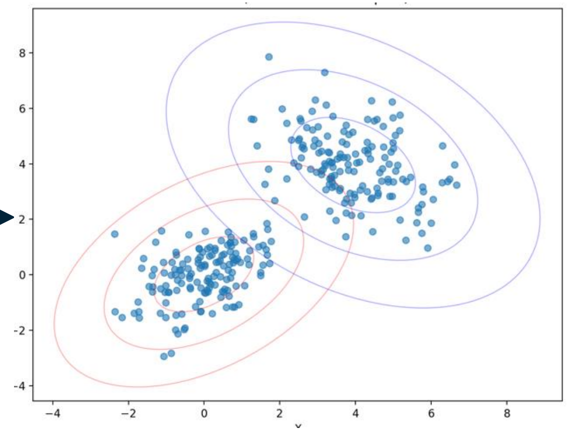
Generative Modeling

Gaussian Mixture Model (GMM) as a generative model



Training Data from $p_{\mathrm{data}}(x)$

Learn



Learned "generative model" $p_\theta(x)$,
where $p_\theta(x) = \sum_{i=1}^{K} \phi_i N(x|\mu_i, \sigma_i)$

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Generative Modeling

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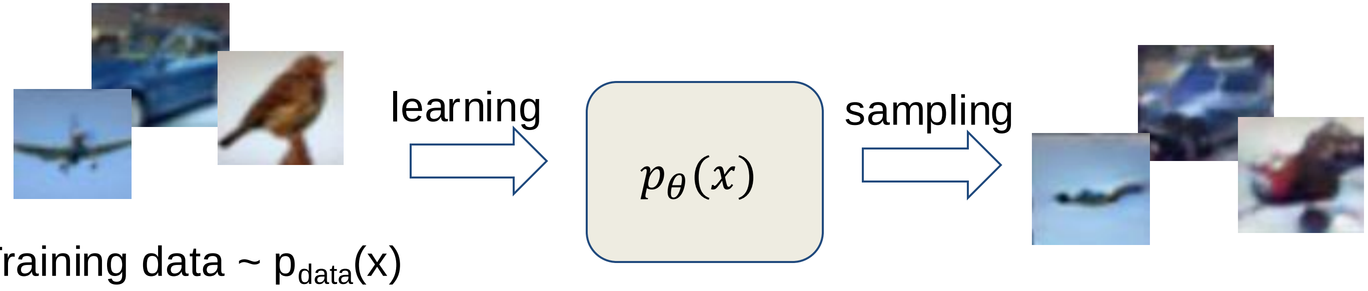


Formulate as density estimation problems**:**

- **Explicit density estimation**: explicitly define and solve for $p_\theta(x)$, e.g., a high-dimensional Gaussian Mixture Model (GMM)
- **Implicit density estimation**: learn model that can sample from $p_\theta(x)$ **without explicitly defining it.**

Deep Generative Models

Given training data, generate new samples from same distribution

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

learning

$p_\theta(x)$

sampling

Use deep neural networks to represent $p_\theta(x)$!

Example: a DNN with GMM output

DNN $\rightarrow$ $\{\phi_i, \mu_i, \sigma_i\}_i^K$

Taxonomy of Generative Models

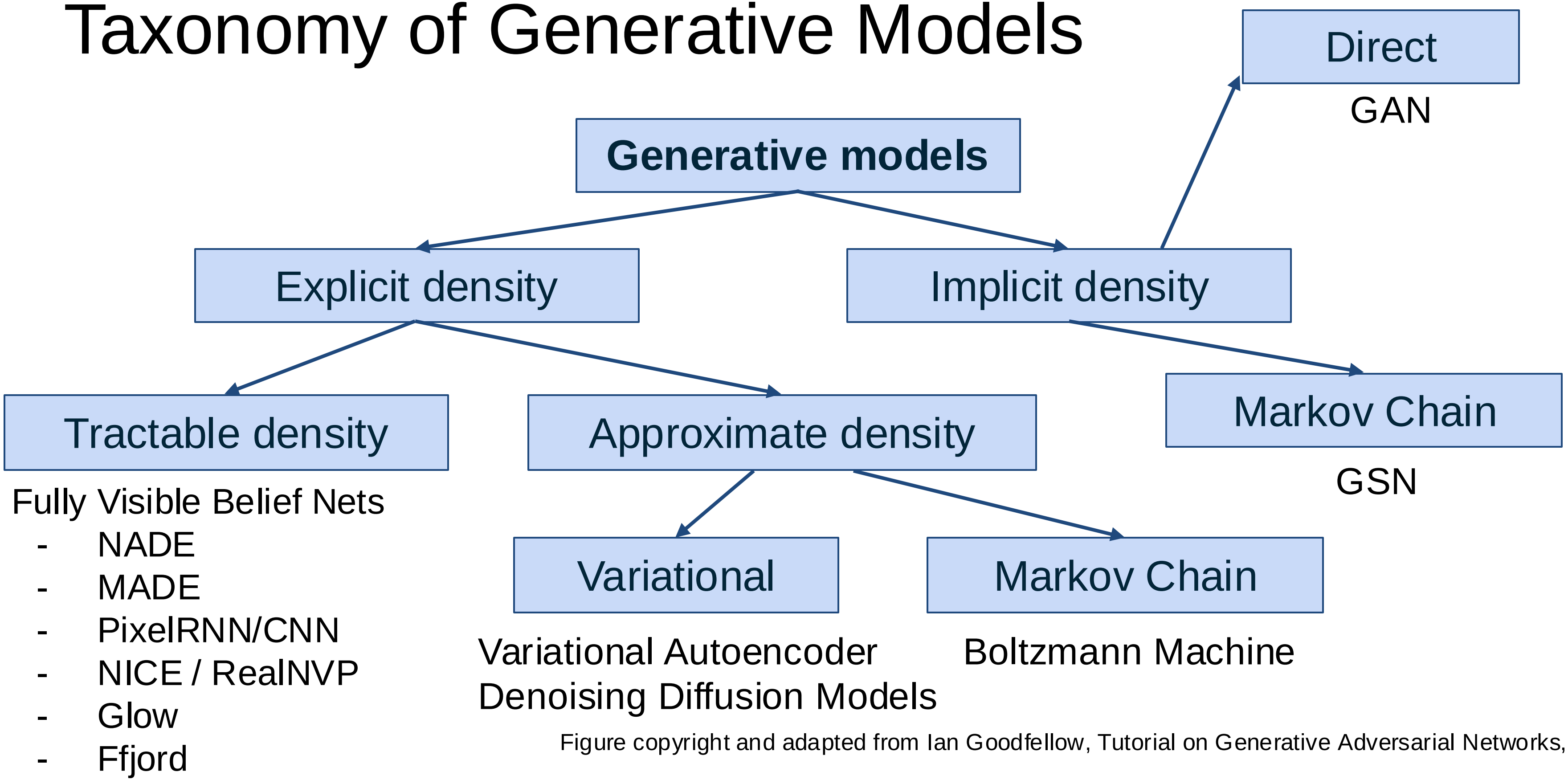


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Taxonomy of Generative Models

Today and the next lecture: discuss 4 most popular types of generative models

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

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

PixelRNN and PixelCNN

(Autoregressive Generative Model)

Fully visible belief network (FVBN)

Explicit density model

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

Likelihood of image x

Joint likelihood of each pixel in the image

Fully visible belief network (FVBN)

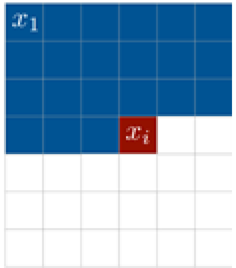
Explicit density model

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

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

Likelihood of image x

Probability of i'th pixel value given all previous pixels



Then maximize likelihood of training data

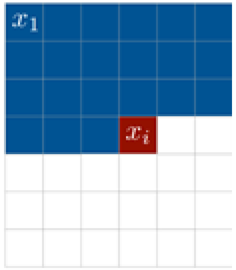
Fully visible belief network (FVBN)

Explicit density model

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

E.g. softmax over 0-255

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



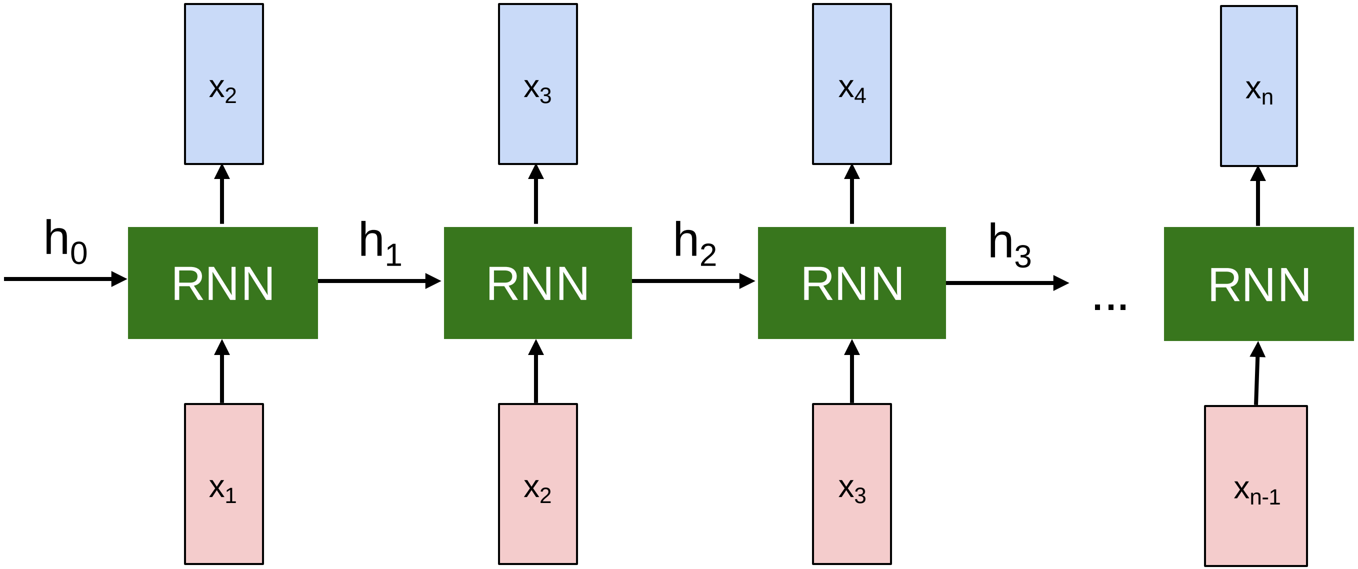
Likelihood of image x

Probability of i'th pixel value given all previous pixels

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

Then maximize likelihood of training data

Recurrent Neural Network

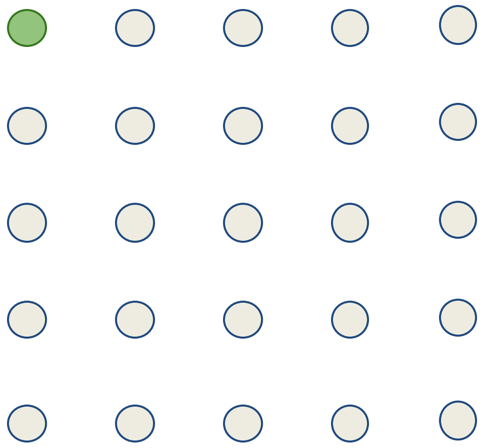


$$p(x_i|x_1, ..., x_{i-1})$$

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

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)



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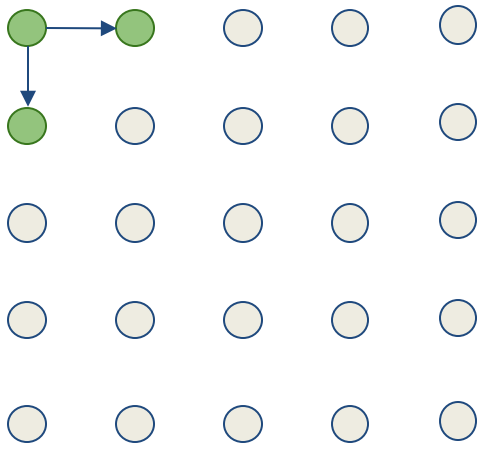

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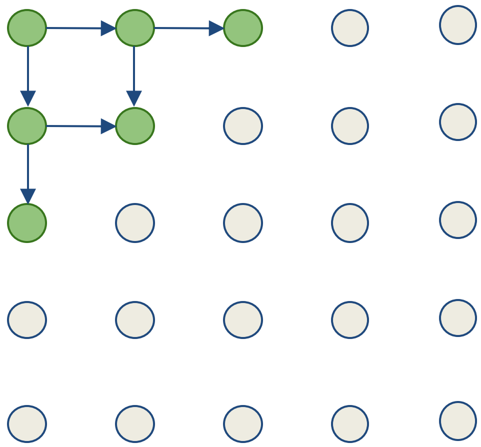
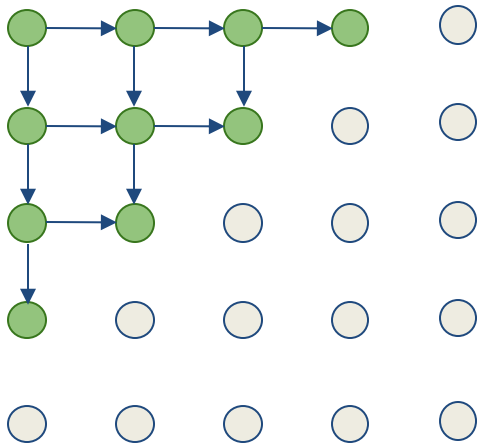


PixelRNN *[van der Oord et al. 2016]*

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

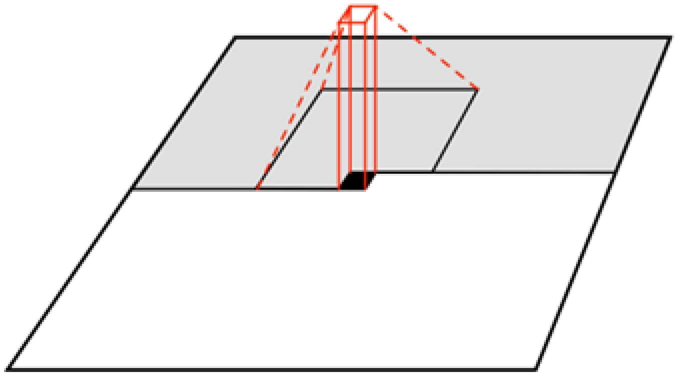
Drawback: sequential generation is slow in both training and inference!



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

Still generate image pixels starting from corner

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



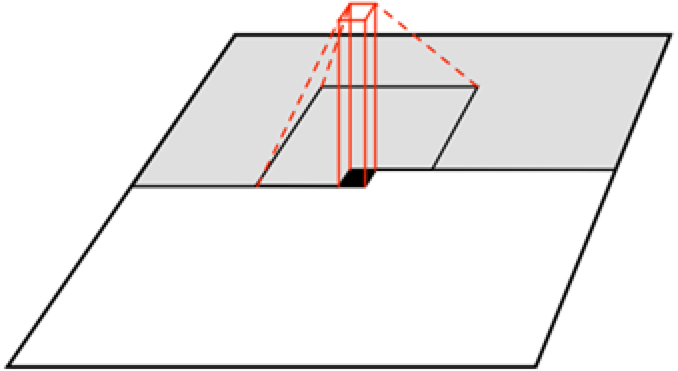
PixelCNN *[van der Oord et al. 2016]*

Still generate image pixels starting from corner

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

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

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



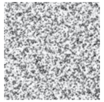
Generation Samples

32x32 CIFAR-10

32x32 ImageNet

PixelRNN and PixelCNN

→ P(x) = 0.12



→ P(x) = 0.00003

Pros:

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

Con:

- Sequential generation => slow

Improving PixelCNN performance

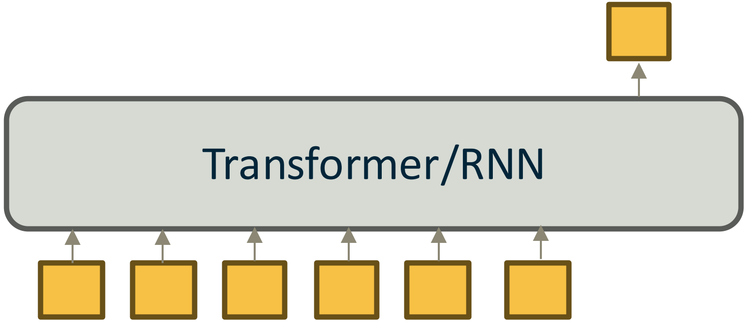
- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See

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

Aside: Why are LLMs "Generative"?

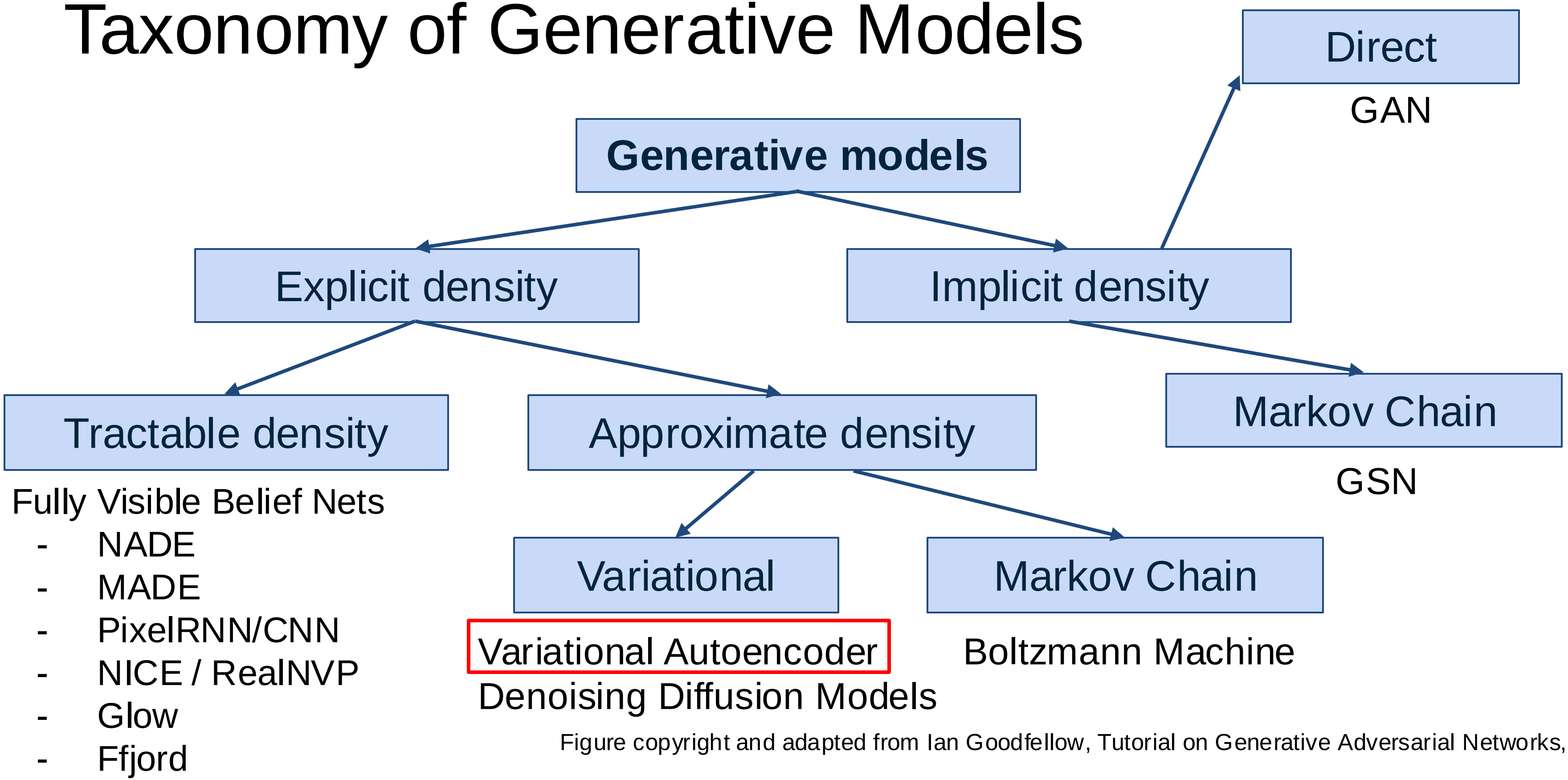
$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$



Language models, especially built on RNN or Transformers with proper causal masking, can be thought of as **autoregressive generative models (predict future based on the past),** similar to PixelRNN and PixelCNN.

Sample an entire sentence by taking sequence of word samples following the probability chain rule decomposition.

Taxonomy of Generative Models



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Variational Autoencoders (VAE)

So far...

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

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

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

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

No dependencies among pixels, can generate all pixels at the same time!
Latent variable z that captures important *factors of variations* in dataset

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Cannot optimize (maximum likelihood estimation) directly, derive and optimize lower bound on likelihood instead

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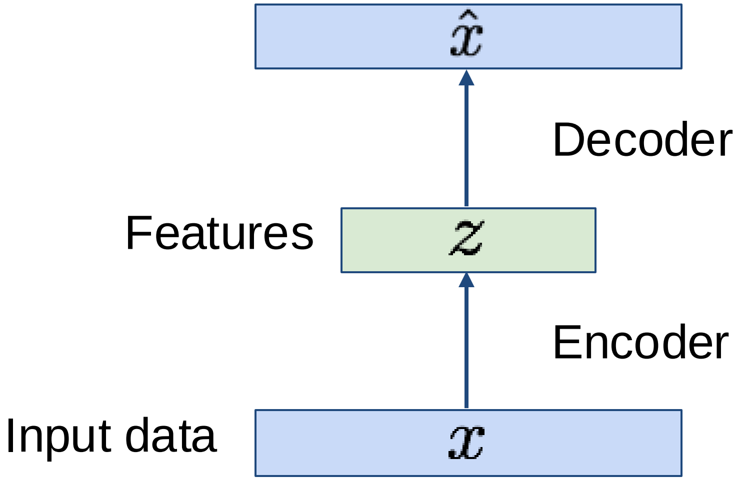
Some background first: Autoencoders

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

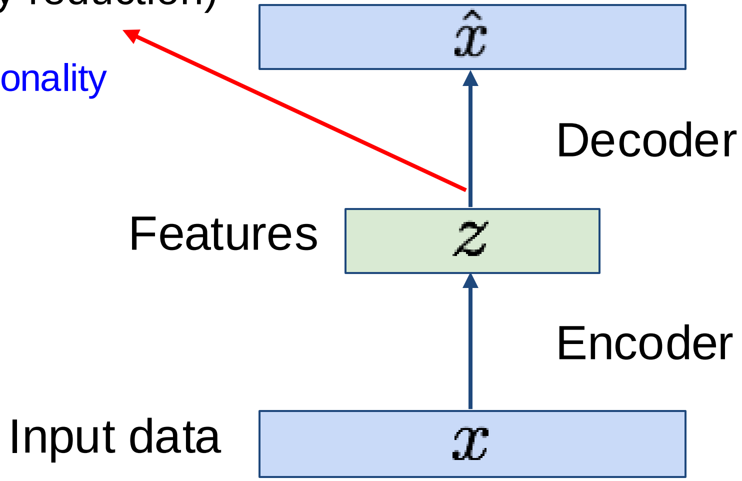


Some background first: Autoencoders

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

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

Q: Why dimensionality reduction?



Some background first: Autoencoders

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

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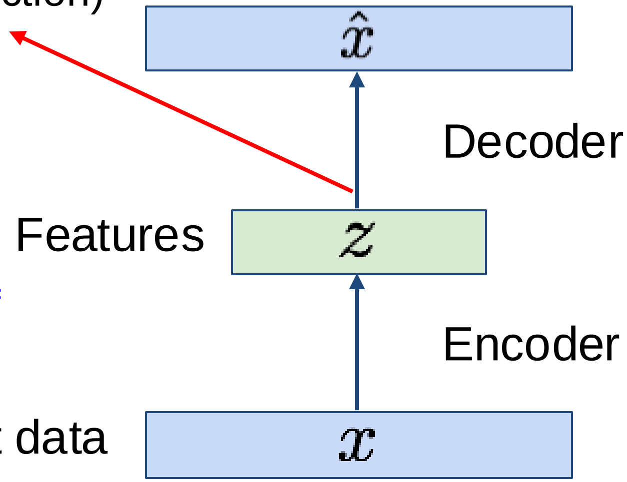
Q: Why dimensionality reduction?

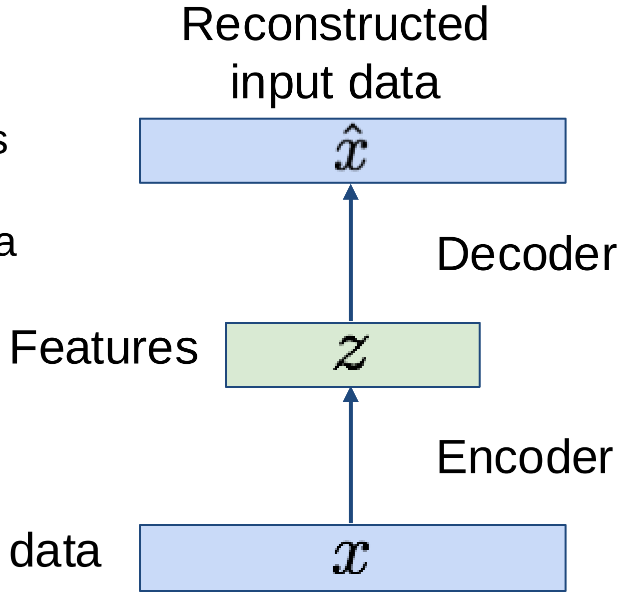
A: Want features to capture the “essence” of the dataset. Think of compression.



Some background first: Autoencoders

How to learn this feature representation?

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



Reconstructed data

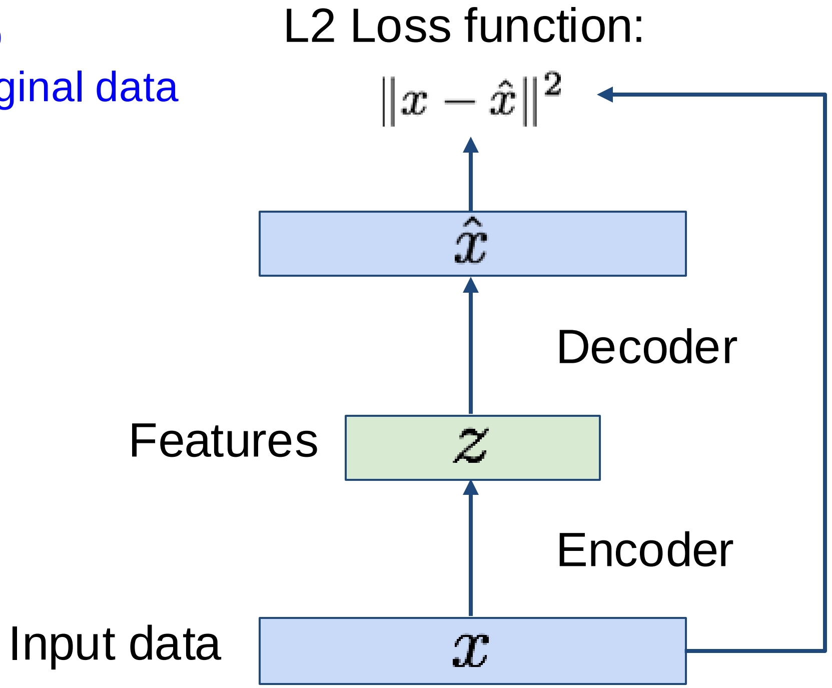
Encoder: 4-layer conv
Decoder: 4-layer upconv

Input data

Some background first: Autoencoders

Train such that features can be used to reconstruct original data

Doesn’t use labels!



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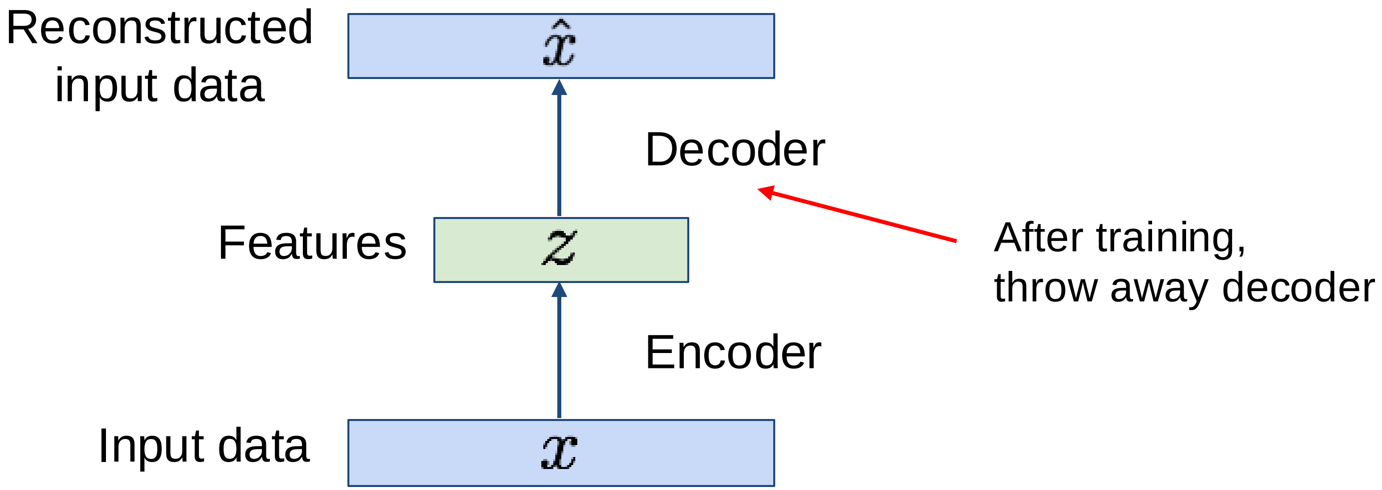
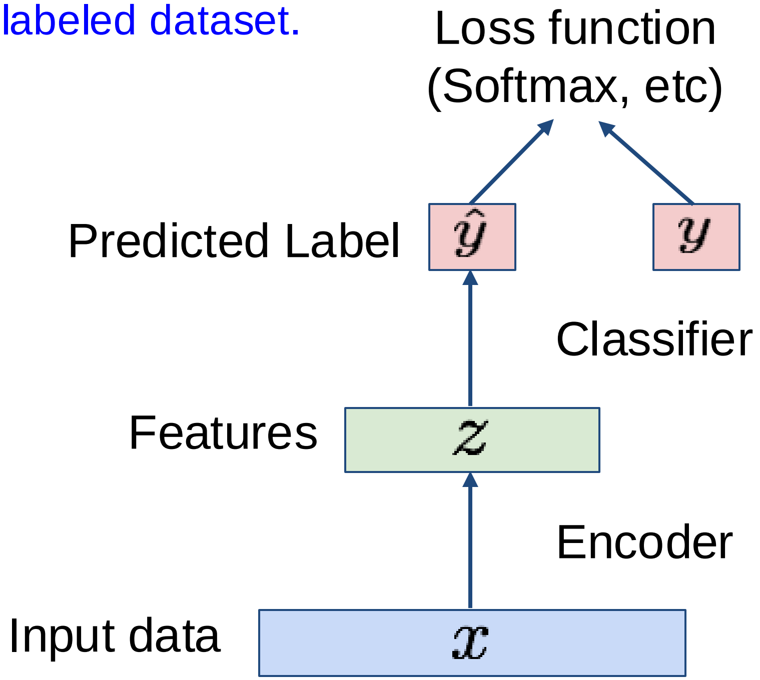


Some background first: Autoencoders

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

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

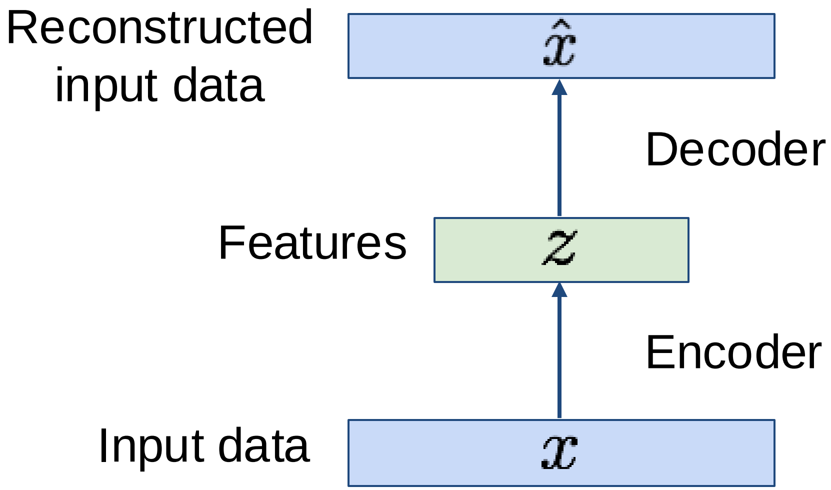


Fine-tune encoder jointly with classifier

bird plane
dog deer truck

Train for final task (sometimes with small data)

Some background first: Autoencoders

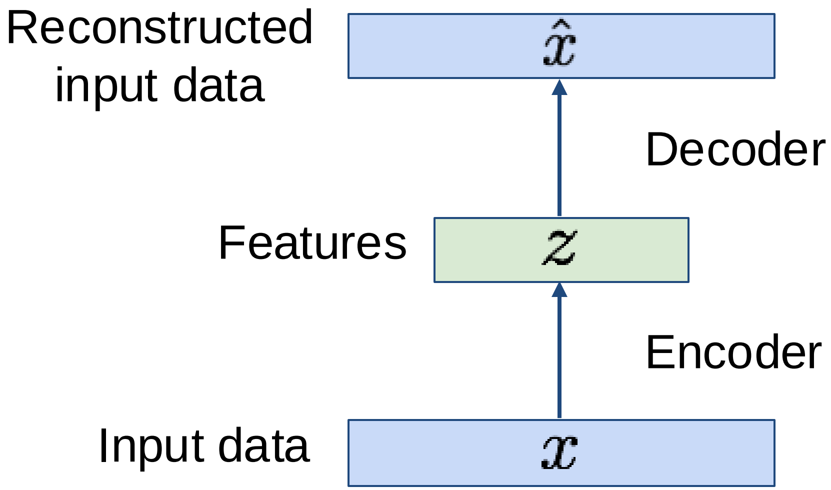


Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data.

Ideally, knowing the space of Z is sufficient to recover the *entire training set* through the decoder.

Some background first: Autoencoders



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

Features capture factors of variation in training data.

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VAE: Model data distribution p(x) through a probabilistic latent space p(z) and a probabilistic decoder p(x|z).

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

Variational Autoencoders

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

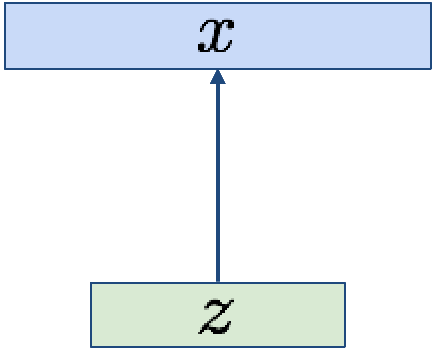
Variational Autoencoders

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

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

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

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



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

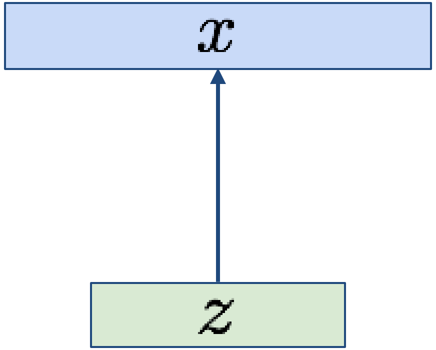
Variational Autoencoders

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

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

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

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



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Variational Autoencoders

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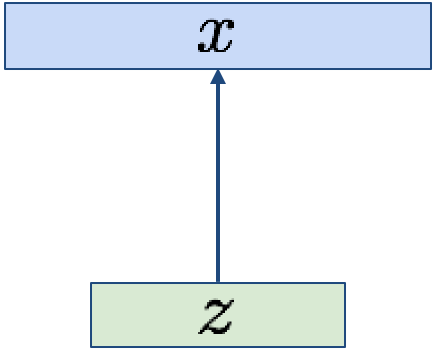

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Goal of Variational Autoencoder:
We want to estimate the true parameters θ^* of this generative model given training data x.

θ^* includes both the decoder neural network parameters and the prior distribution

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

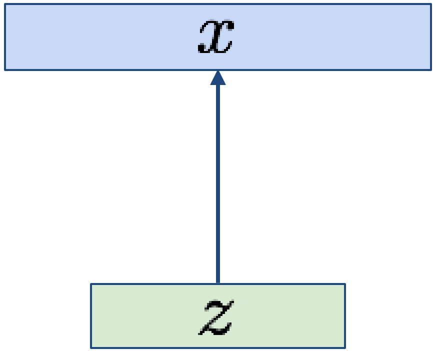
Variational Autoencoders

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

How should we represent this model?

Sample from true conditional

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



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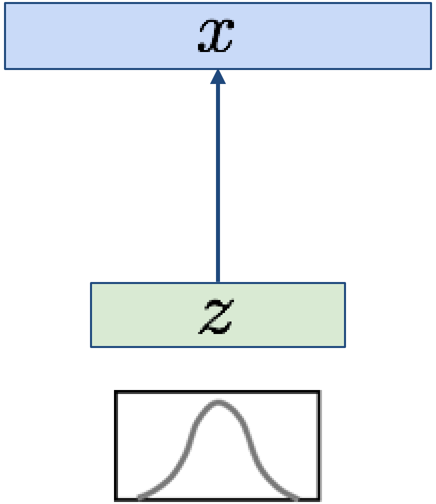


Sample from true prior

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

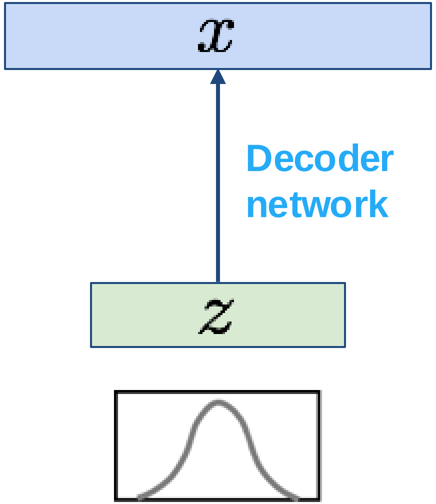
How should we represent this model?

Assume p(z) is *known* and *simple*, e.g. isotropic Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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

Variational Autoencoders

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



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

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

How should we represent this model?

Assume p(z) is *known* and ***simple***, e.g. isotropic Gaussian. Reasonable for latent attributes, e.g. pose, how much smile.

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

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

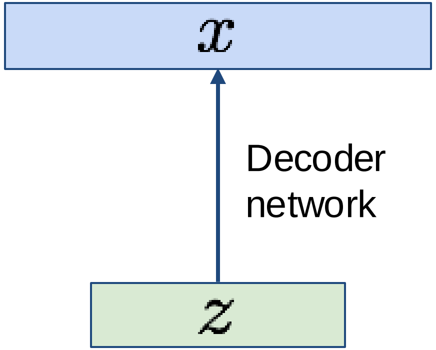
Variational Autoencoders

Sample from
true conditional

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

Sample from
true prior

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



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How to train the model?

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

Variational Autoencoders

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Sample from true prior

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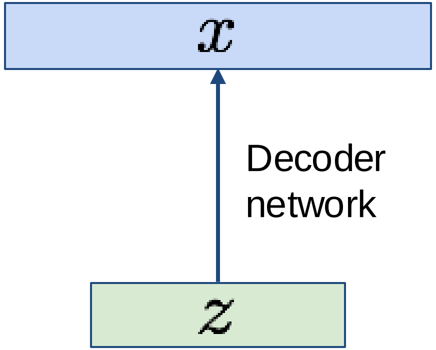


We want to estimate the true parameters θ^* of this generative model given training data x.

How to train the model?

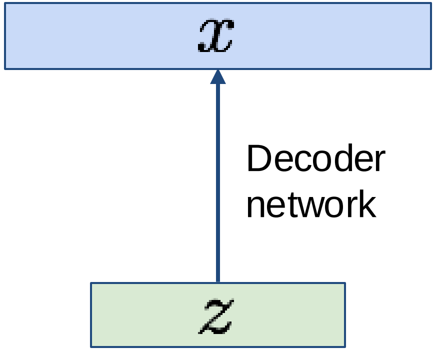
Learn model parameters to maximize likelihood of training data

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

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

Variational Autoencoders

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



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

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

How to train the model?

Learn model parameters to maximize likelihood of training data

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

Q: What is the problem with this?

Intractable!

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

Variational Autoencoders: Intractability

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

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

Variational Autoencoders: Intractability

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

Simple Gaussian prior

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

Variational Autoencoders: Intractability

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

Decoder neural network

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

Variational Autoencoders: Intractability

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

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

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

Variational Autoencoders: Intractability

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

Variational Autoencoders: Intractability

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

Can we do Monte Carlo sampling?

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

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

Variational Autoencoders: Intractability

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

Can we do Monte Carlo sampling?

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

We don't know which z corresponds to a sample (x)! Most z's will be sampled from where p(x|z) is zero.

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

Variational Autoencoders: Intractability

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

Can we do Monte Carlo sampling?

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

Can we estimate posterior density?

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

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

Variational Autoencoders: Intractability

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

Can we do Monte Carlo sampling?

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

Can we estimate posterior density? Not quite, but …

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

Intractable data likelihood

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

Variational Autoencoders: Intractability

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

Can we do Monte Carlo sampling?

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

Can we estimate posterior density? Not quite, but …

$$p_\theta(z|x) = p_\theta(x|z) p_\theta(z) / p_\theta(x)$$

VAE: We can use an approximate posterior $q_\theta(z|x)$ (variational distribution) to form a *tractable lower bound* of the data likelihood p(x).

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

Variational Autoencoders

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

Variational Autoencoders

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

Let's assume we can sample from some approximate posterior for now …

Variational Autoencoders

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

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

Variational Autoencoders

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

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$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

Variational Autoencoders

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

Variational Autoencoders

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

Recall: $D_{KL}(q||p) = \mathbf{E}_q[\log \frac{q}{p}]$

Variational Autoencoders

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

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

Variational Autoencoders

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

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

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad (\text{Multiply by constant})$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad (\text{Logarithms})$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\geq 0}$$

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

ELBO: Evidence Lower Bound

Variational inference: Optimize q(z|x) to approximate log[p(x)] by raising ELBO. Higher ELBO -> lower KL(q(z|x)|p(z|x))

Variational Autoencoders

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

Maximize the likelihood of the sample $x^{(i)}$ (e.g., an image) given a latent prior sample.

Minimize KL -> Make the approximate posterior more like the prior!
Use NN to model the approximate posterior.

Variational Autoencoders

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

Maximize the likelihood of the sample $x^{(i)}$ (e.g., an image) given a latent prior sample. **Can be thought of a decoder model**

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

Variational Autoencoders

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

We want to maximize the data likelihood

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

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

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

Variational Autoencoders

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\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
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&= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)}}
\end{aligned}
$$

We want to maximize the data likelihood

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

Variational Autoencoders

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

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

Decoder: reconstruct the input data

Encoder: make approximate posterior distribution close to prior

Sample z from the learned posterior (encoder) to train the decoder to reconstruct!

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

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

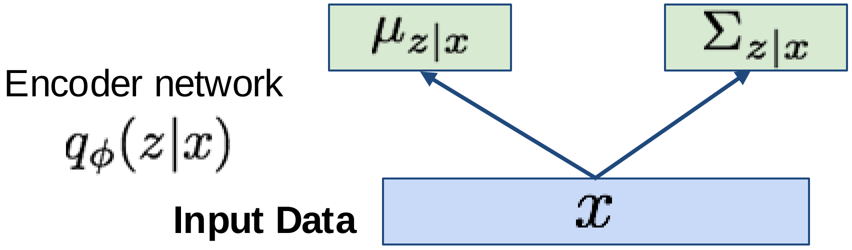
Let's look at computing the KL divergence between the estimated posterior and the prior given some data

Input Data x

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

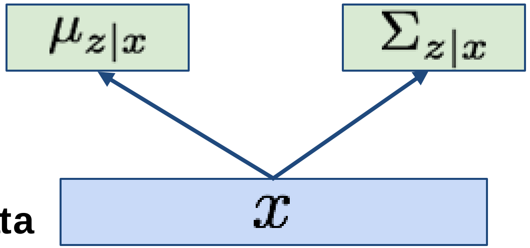
$$D_{KL}(\mathcal{N}(\mu_{z|x}, \Sigma_{z|x}) || \mathcal{N}(0, I))$$

Have analytical solution

Encoder network

$q_\phi(z|x)$

Input Data



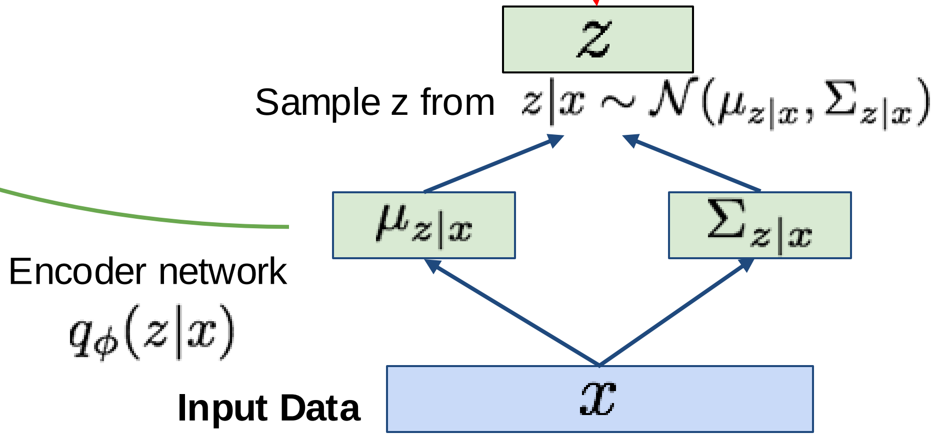
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Not part of the computation graph!

Make approximate posterior distribution close to prior



Variational Autoencoders

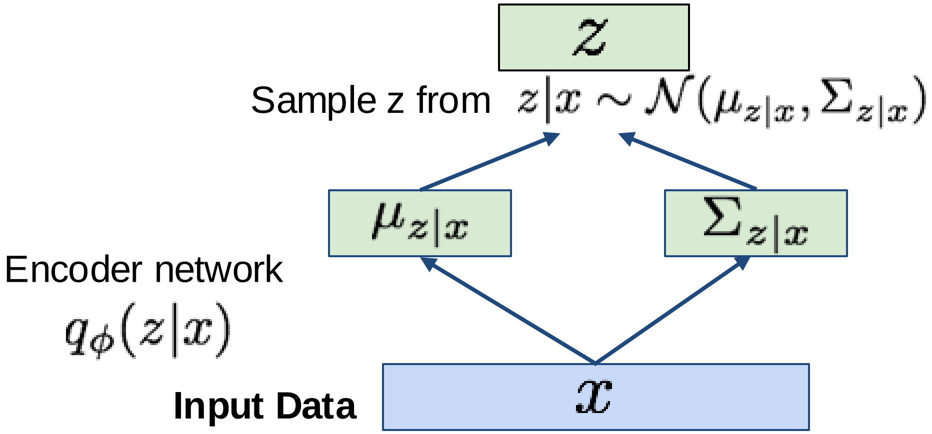
Putting it all together: maximizing the likelihood lower bound

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

Reparameterization trick to make sampling differentiable:

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

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



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

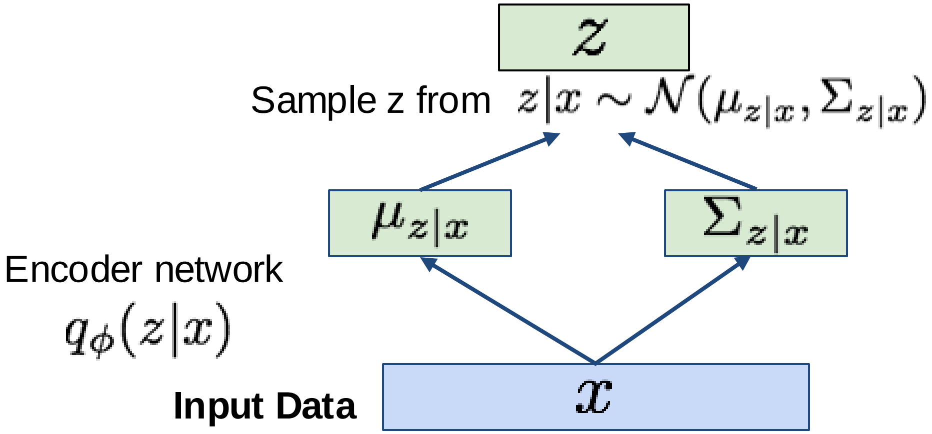
Reparameterization trick to make sampling differentiable:

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

Input to the graph

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

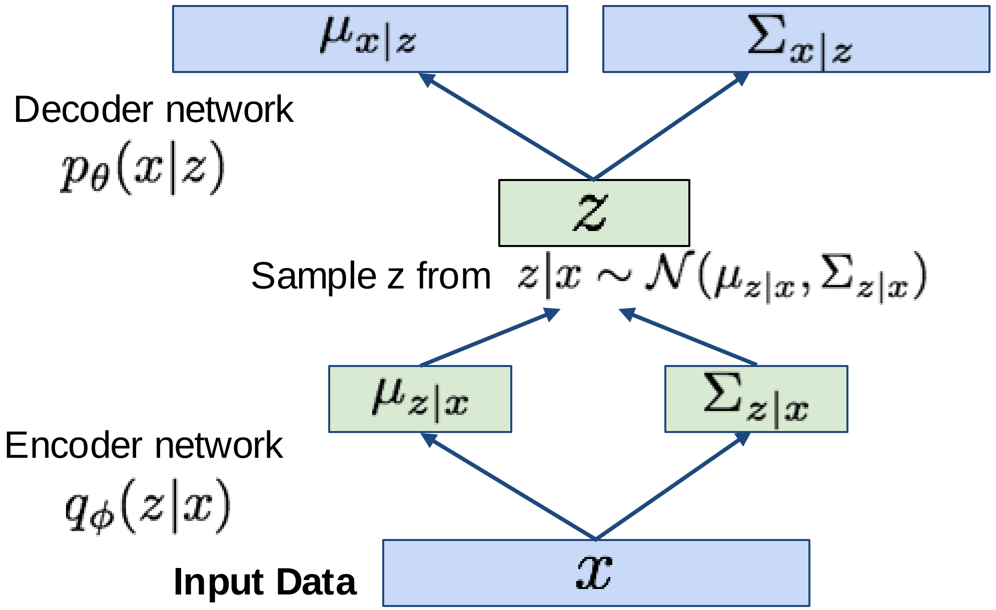
Part of computation graph



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

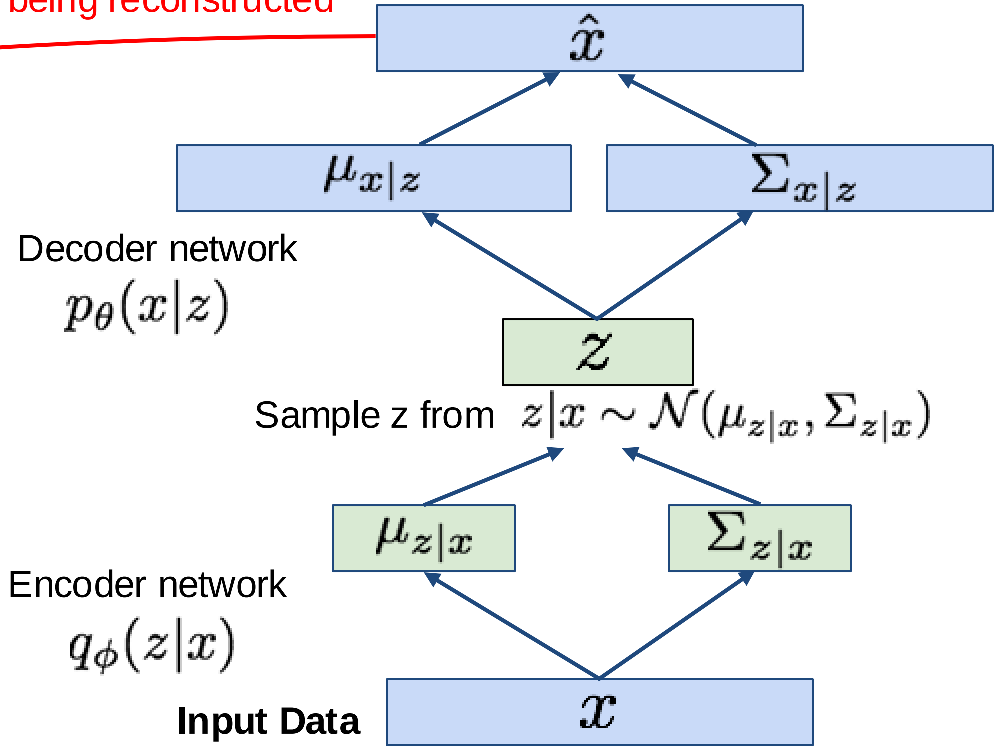


Variational Autoencoders

Maximize likelihood of original input being reconstructed

Putting it all together: maximizing the likelihood lower bound

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

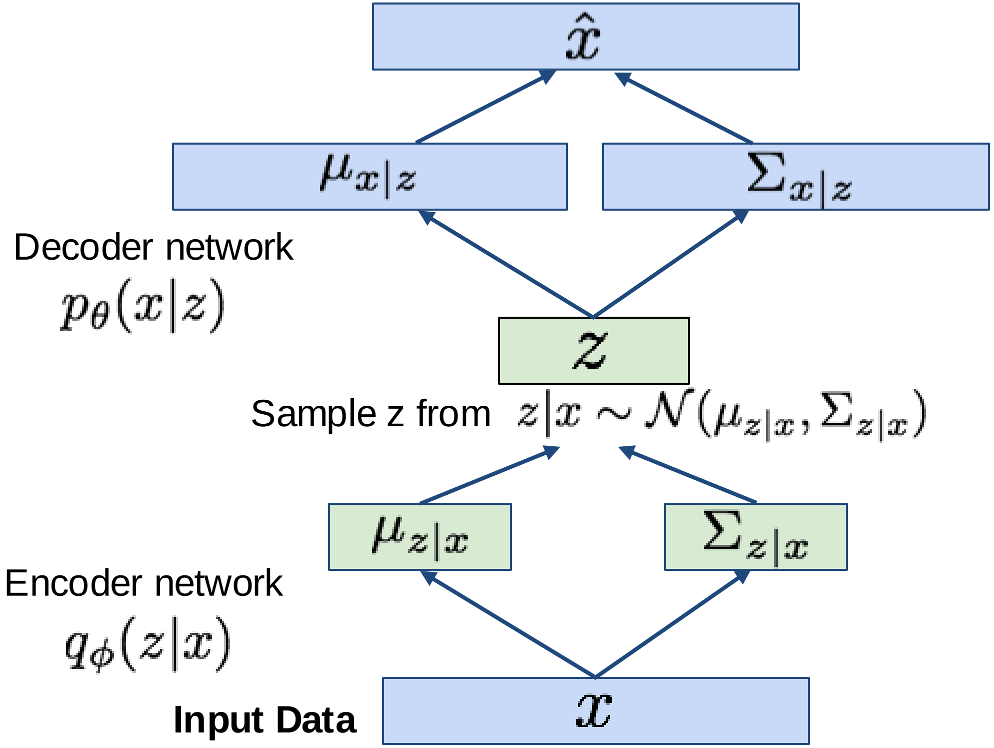


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Hyperparameter to weigh the strength of the prior matching objective

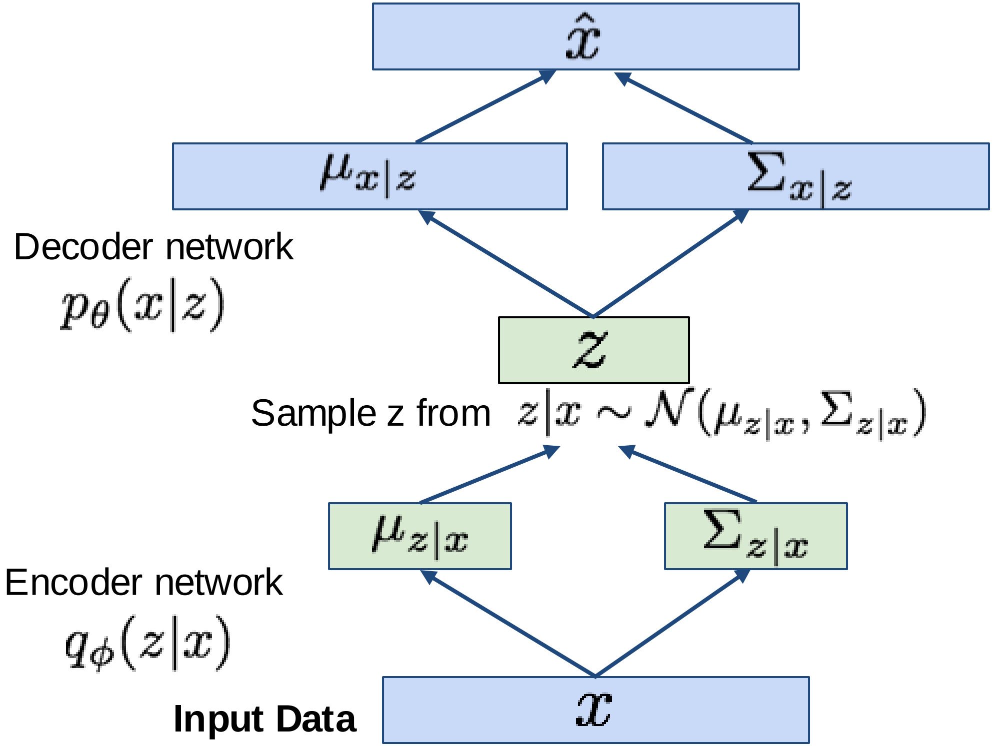


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

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

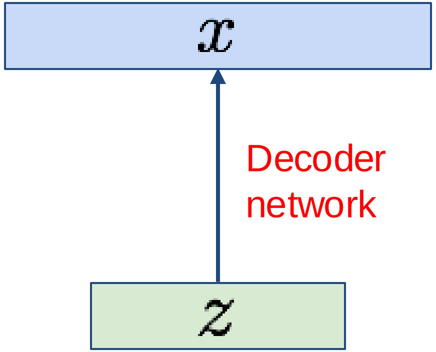


Variational Autoencoders: Generating Data!

Our assumption about data generation process

Sample from true conditional

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



Sample from true prior

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

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

Variational Autoencoders: Generating Data!

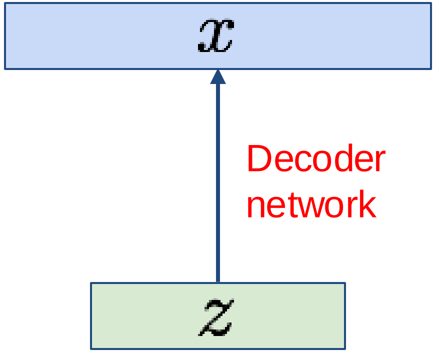
Our assumption about data generation process

Sample from true conditional

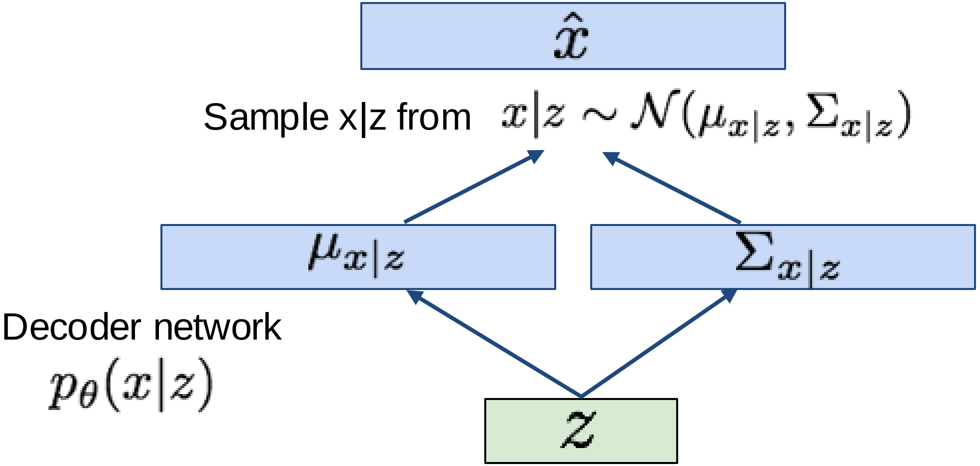
$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

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



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

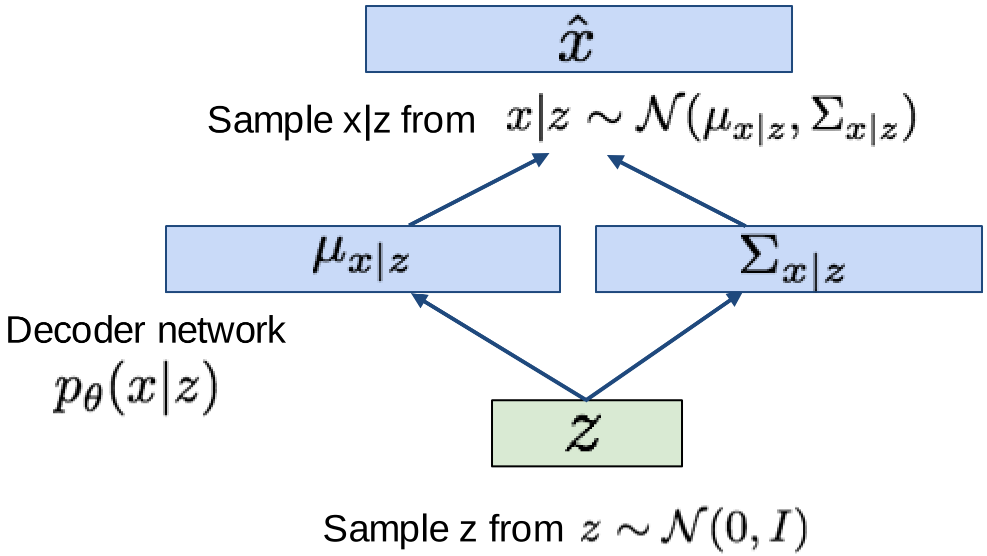


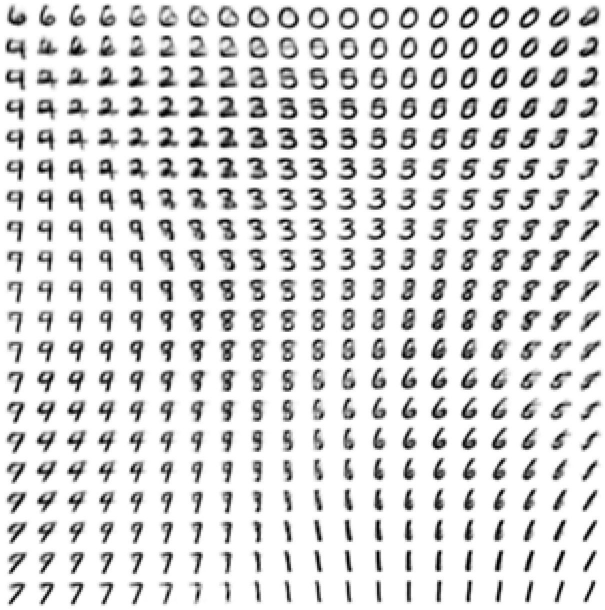
Sample z from $z \sim \mathcal{N}(0, I)$

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

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

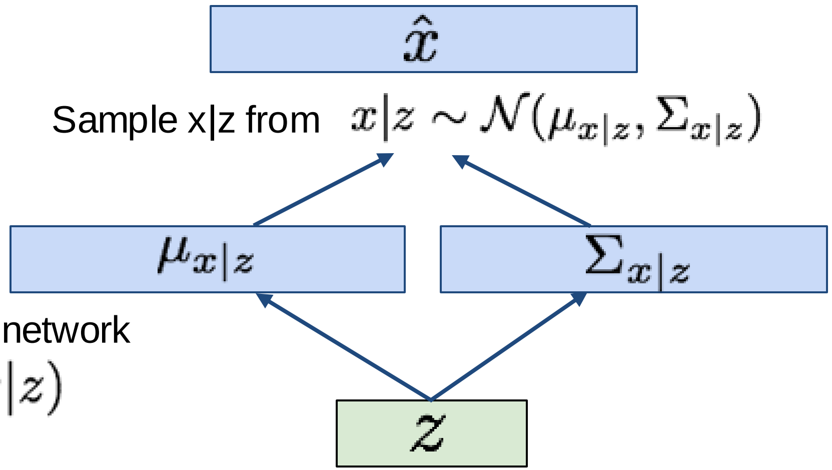




Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

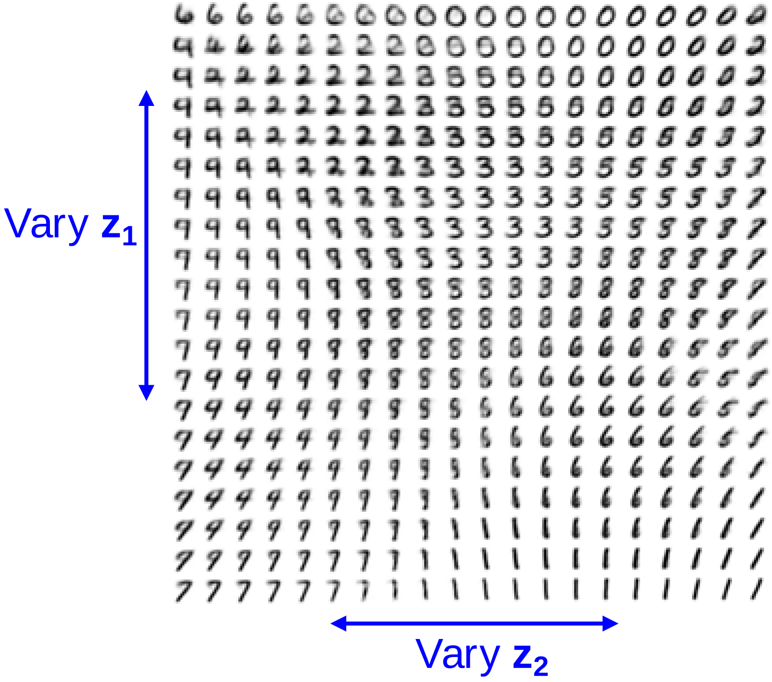


Decoder network
$p_\theta(x|z)$

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

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

Data manifold for 2-d **z**



Variational Autoencoders: Generating Data!

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

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

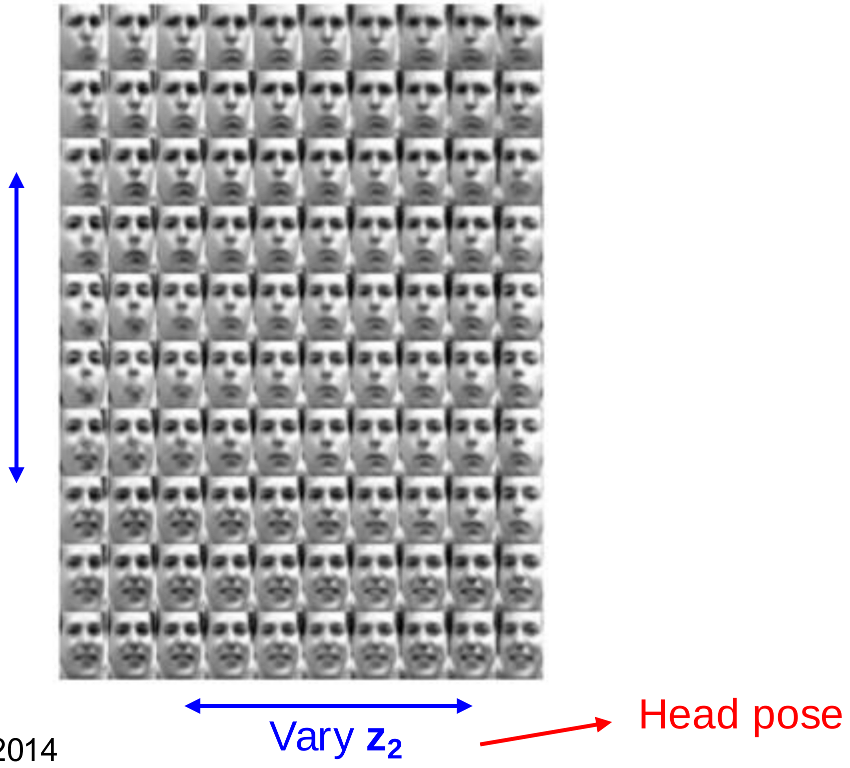
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

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

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

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



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

Variational Autoencoders: Generating Data!

32x32 CIFAR-10

Labeled Faces in the Wild

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Latent space z is interpretable and may be useful for other downstream tasks.

Cons:

- Samples are blurry
- KL weights are hard to tune
- Latent distributions are aggressive representation bottlenecks that may limit the expressiveness of the model.

Can be made more powerful by making VAE hierarchical (multiple layers of latents).
Diffusion model (denoising diffusion) can be thought of a type of hierarchical VAE!

Next Time: Denoising Diffusion