Generative Models I: FVBN & VAE

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Most slides are based on Fei Fei Li and colleagues lectures, cs231n and some slides from from Bhiksha Raj, 11-785, CMU

Supervised Learning

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

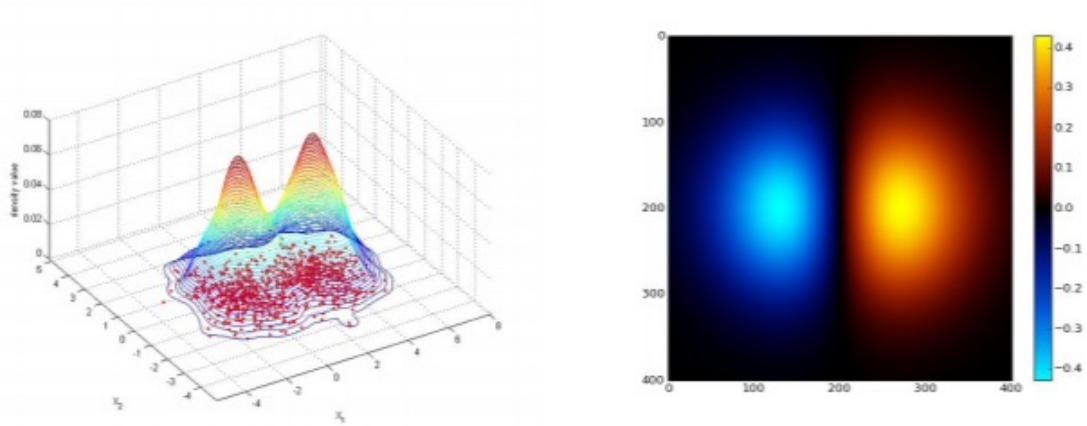
- Goal: Learn a function to map x -> y

- Examples: Classification, regression, object detection, semantic segmentation, image captioning, machine translation, question answering, and etc.

Density Estimation

- Data: x
  - Just data, no labels!
- Goal: Learn some underlying hidden structure of the data
- Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

1-d density estimation



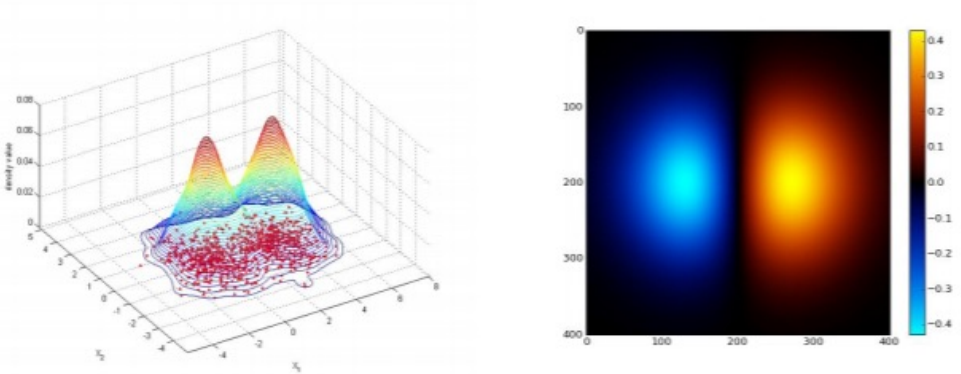
2-d density estimation

Unsupervised Learning: Generative models

Take samples from a distribution and learn the probability distribution underlying them

Figure copyright Ian Goodfellow, 2016. Reproduced with permission.

1-d density estimation



2-d density estimation

2-d density images left and right are CC0 public domain

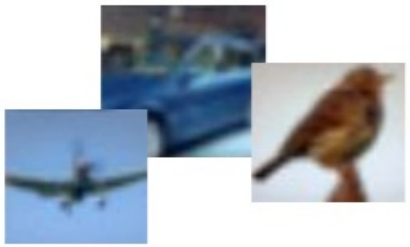
Training data ~ $p_{data}(x)$

Generated samples ~ $p_{model}(x)$

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

Generative Models

Given training data, generate new samples from same distribution



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

Generated samples ~ $p_{model}(x)$

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

- Formulate as density estimation problems:
  - **Explicit density estimation**: explicitly define and solve for $p_{model}(x)$
  - **Implicit density estimation**: learn model that can sample from $p_{model}(x)$ without explicitly defining it.

Generative Models

- Task: Given a dataset of images $\{X_1, X_2, \ldots, X_N\}$ can we learn the distribution of X?

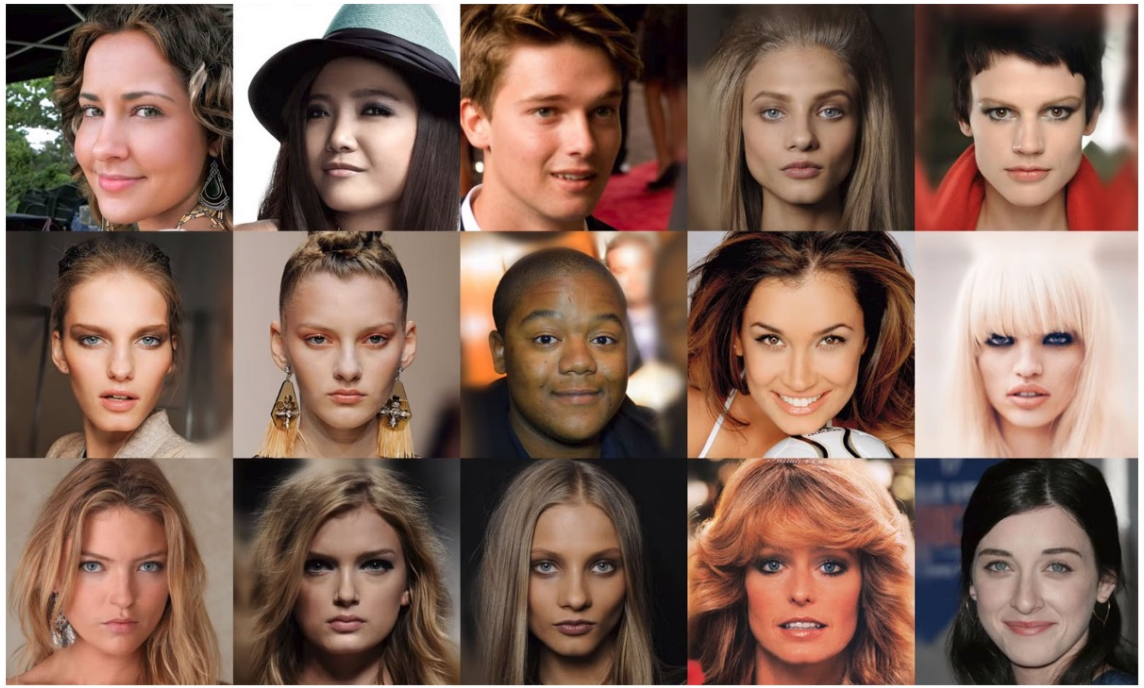
- Given a dataset of training data, generative models find the distribution of data as $P(X)$

- However, we sometimes interested in only sampling from this distribution.
  - Instead of knowing $P(X)$ itself.

Generate samples given training examples

- Given training data, learn to generate samples from the same distribution as these ones.

some training samples



[CelebA dataset]

generated samples

Karras et al., Progressive Growing of GANs for Improved Quality, Stability, and Variation, ICLR 2018.

Generative models

- Most of generative models are based on a latent space

$$P(x) = \int p(x|z)p(z)dz$$

- But, we first introduce Fully visible belief network (FVBN) or autoregressive generative models

$$p(x_1, \dots, x_T) = \prod_{t=1}^{T} P(x_t|x_1, \dots, x_{t-1})$$

Fully visible belief network

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

$$p(x_1, \ldots, x_T) = \prod_{t=1}^{T} P(x_t | x_1, \ldots, x_{t-1})$$

Likelihood of image x

Probability of i'th pixel value given all previous pixels

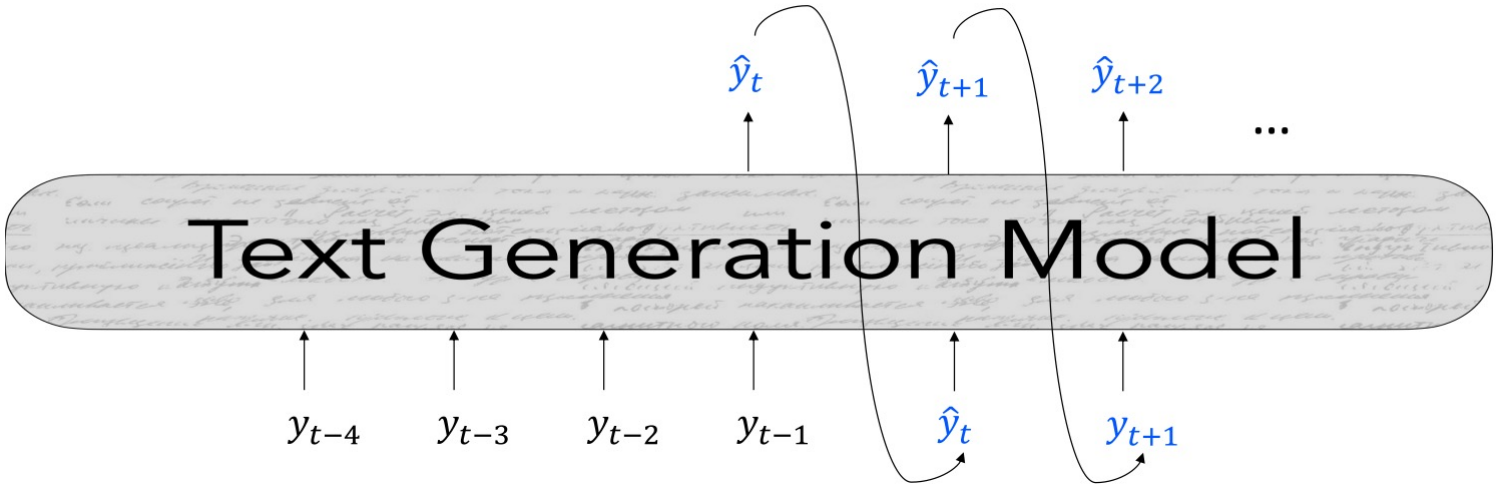
- Then maximize likelihood of training data

To model the above conditional distribution, it used a neural network

It needs ordering of variables

Autoregressive generative models

- Language modeling
  - Sequence of tokens from a finite vocab
  - We learn the distribution $P(w_{t+1}|w_1, \dots, w_t)$ by an RNN



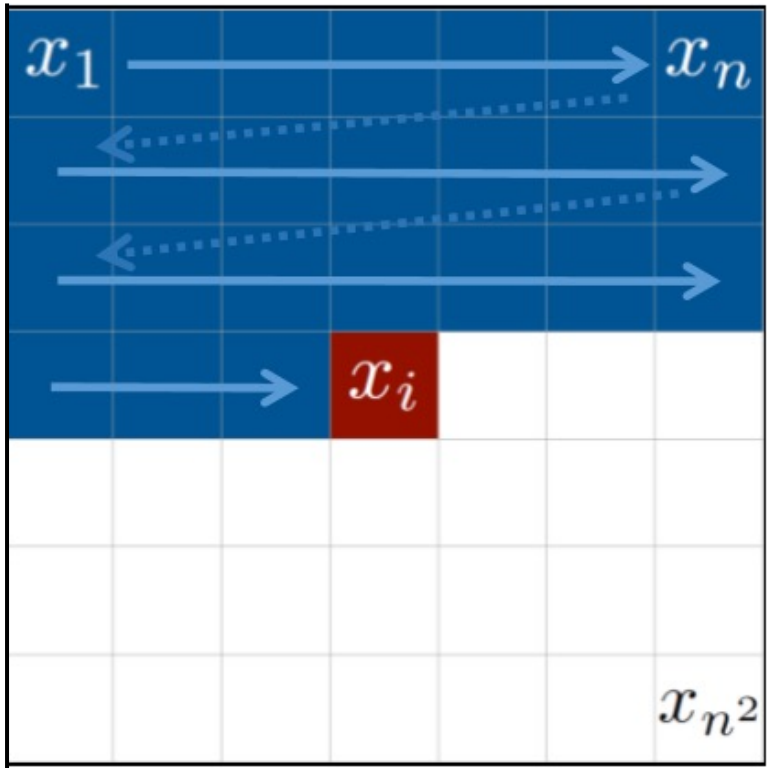
- PixelRNN and PixelCNN

Intuition

$$p(\mathbf{x}) = p(x_1, x_2, ..., x_{n^2})$$

Chain rule:

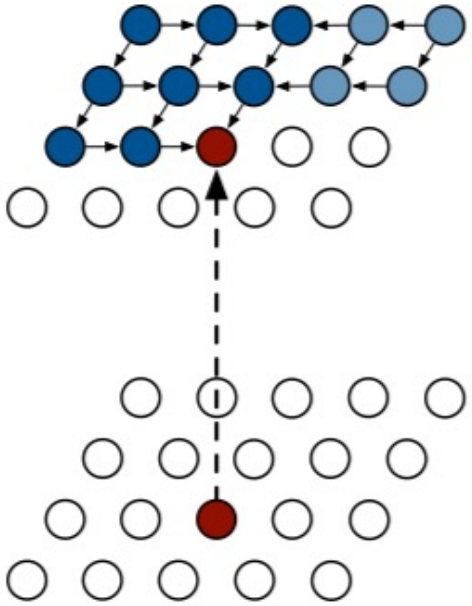
$$p(\mathbf{x}) = \prod_{i=1}^{n^2} p(x_i | x_1, ..., x_{i-1})$$



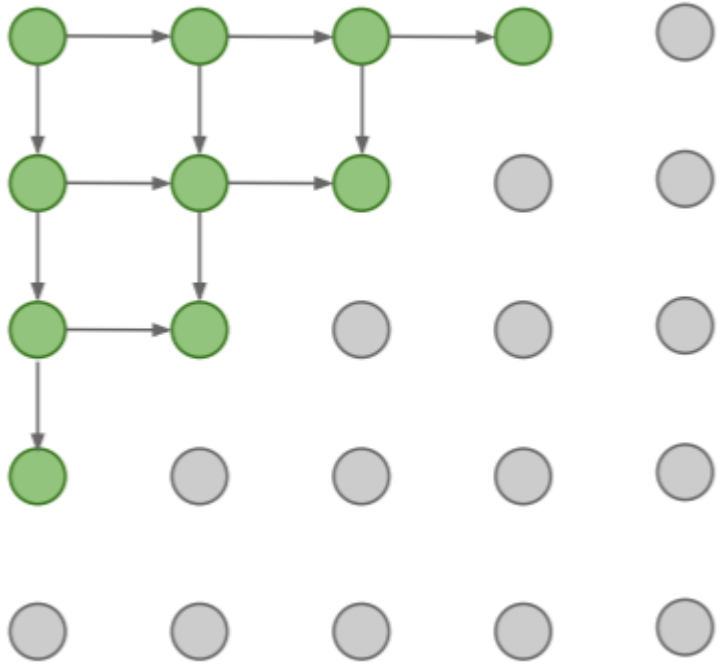
Oord et al., Pixel recurrent neural networks, ICML 2016

PixelRNN

- Generate image pixels starting from corner
- Dependency on previous pixels modeled using an RNN (LSTM)
- Drawback: sequential generation is slow!



Diagonal BiLSTM

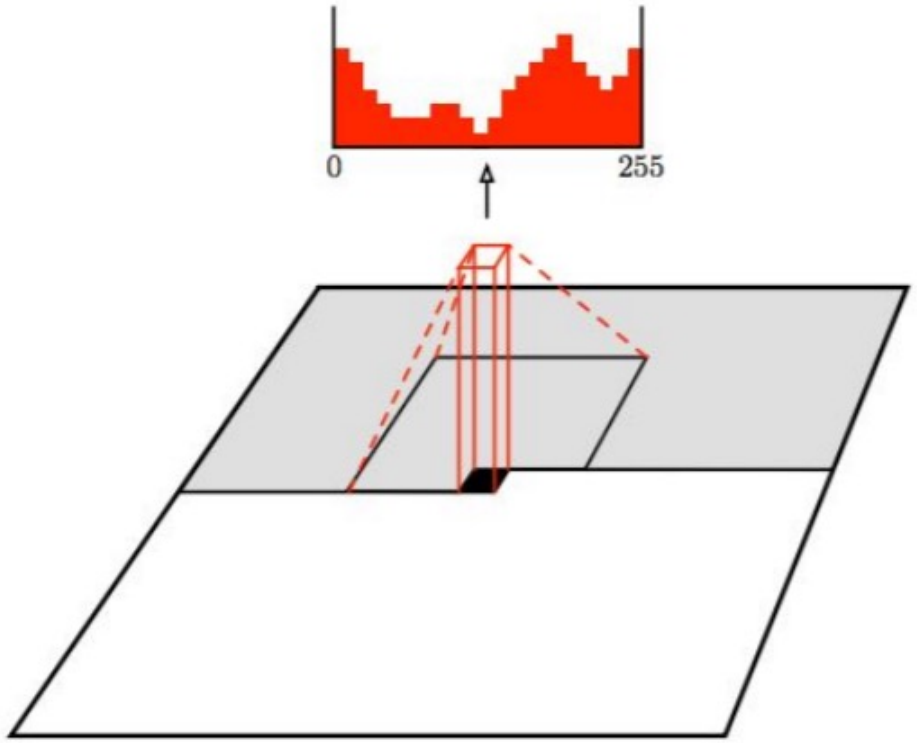


Oord et al., Pixel recurrent neural networks, ICML 2016

PixelCNN

- Still generate image pixels starting from corner
- Dependency on previous pixels now modeled using a CNN over context region

1	1	1	1	1
1	1	1	1	1
1	1	0	0	0
0	0	0	0	0
0	0	0	0	0



Oord et al., Conditional Image Generation with PixelCNN Decoders, 2016

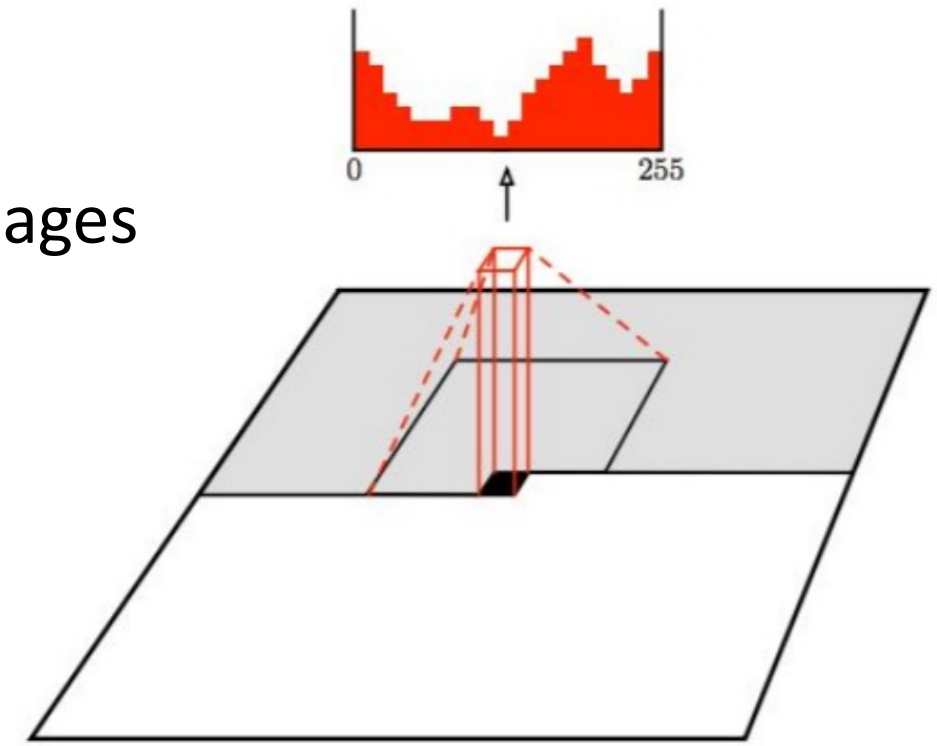
PixelCNN

- 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

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

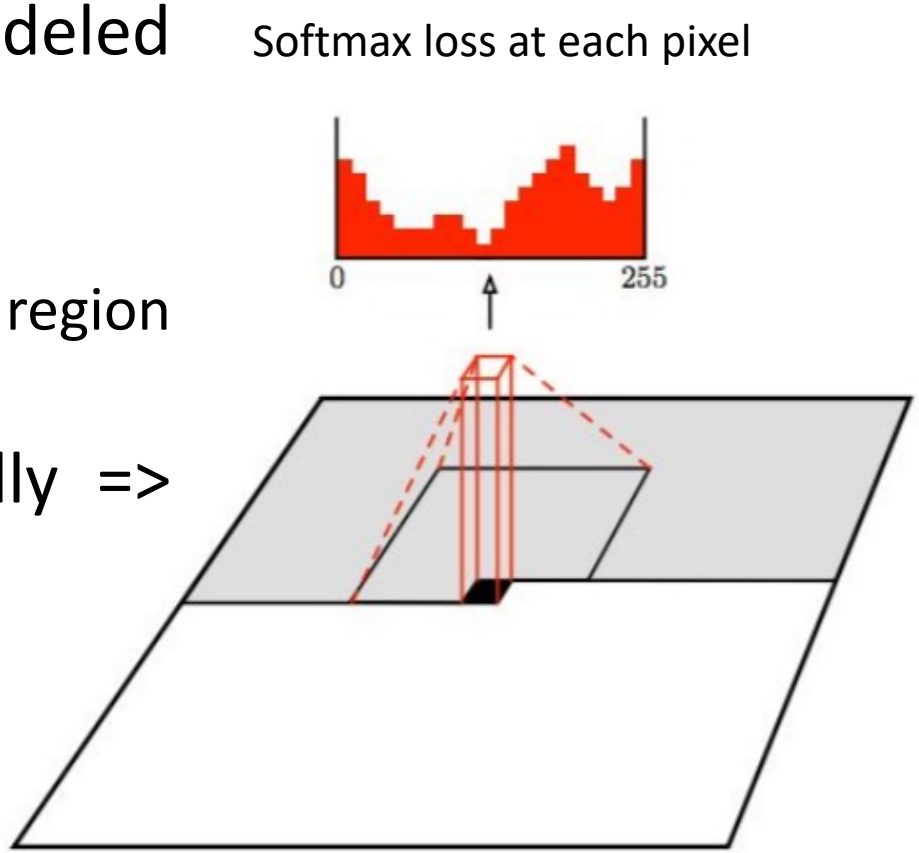
Softmax loss at each pixel



Oord et al., Conditional Image Generation with PixelCNN Decoders, 2016

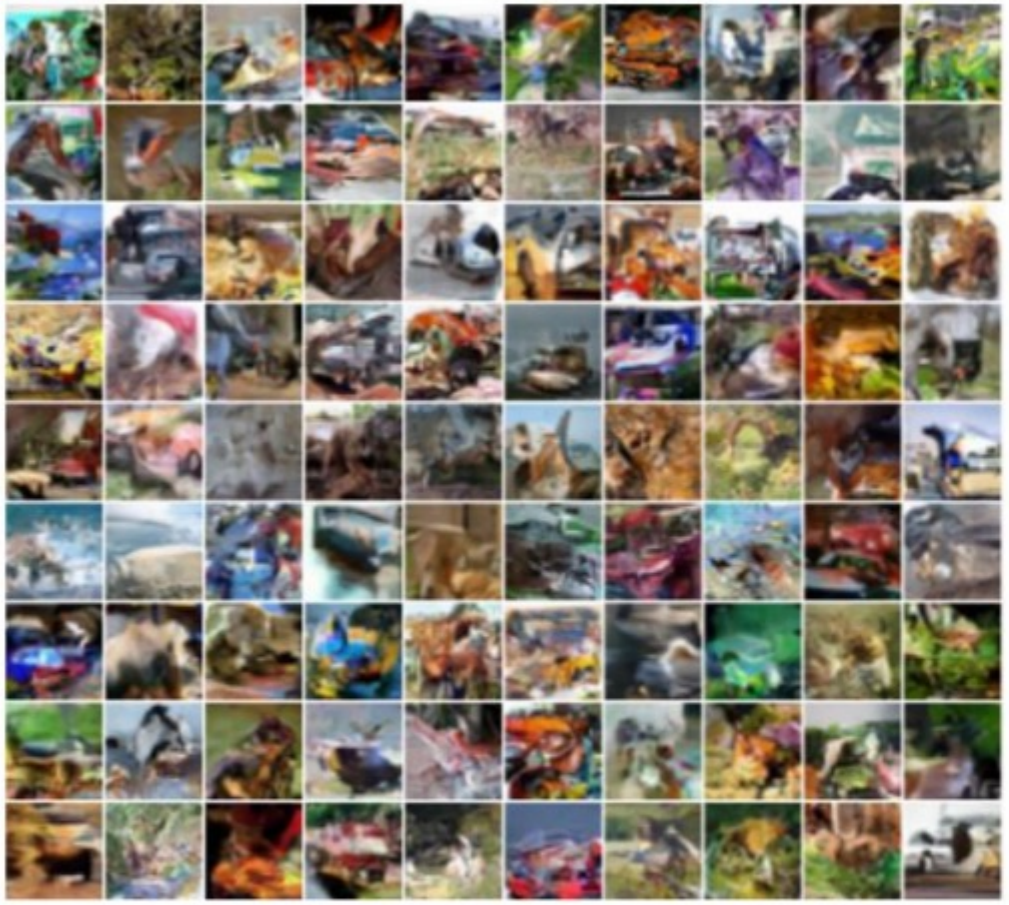
PixelCNN

- Still generate image pixels starting from corner
- Dependency on previous pixels now modeled using a CNN over context region
- Training is faster than PixelRNN
  - can parallelize convolutions since context region values known from training images
- Generation must still proceed sequentially => still slow

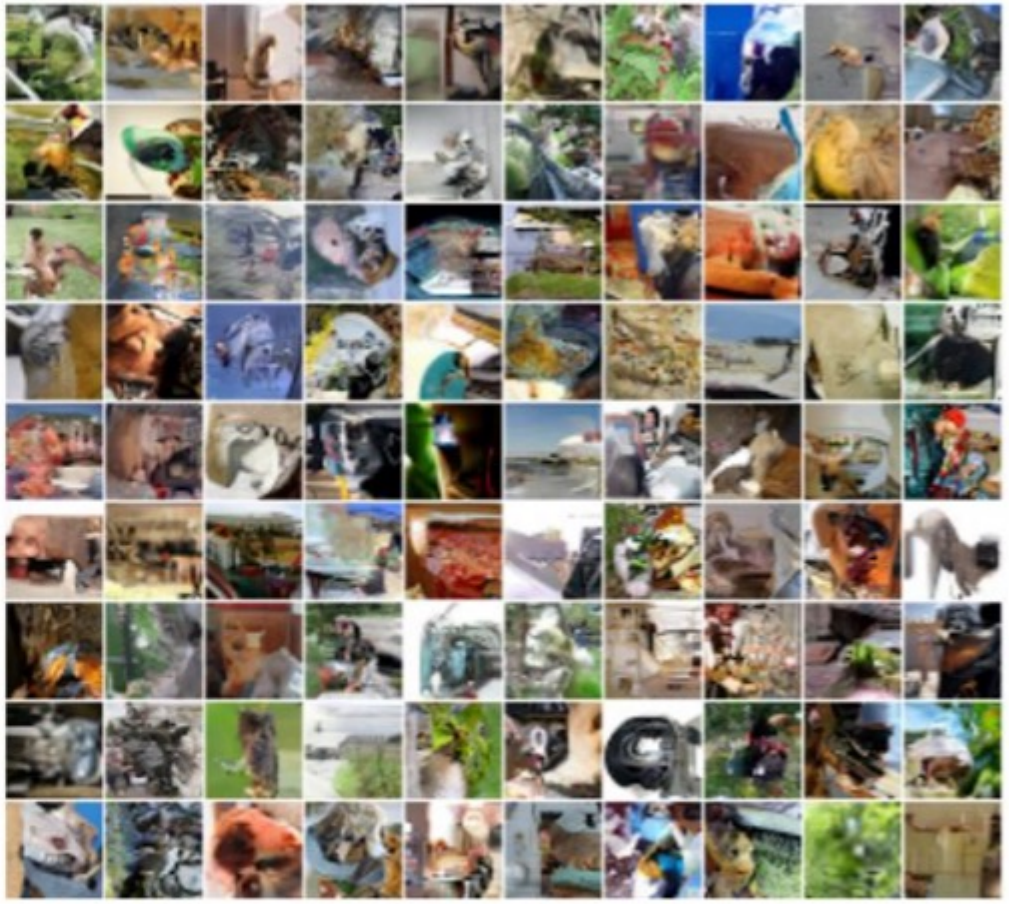


Oord et al., Conditional Image Generation with PixelCNN Decoders, 2016

Generated Samples



32x32 CIFAR-10



32x32 ImageNet

Oord et al., Conditional Image Generation with PixelCNN Decoders, 2016

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

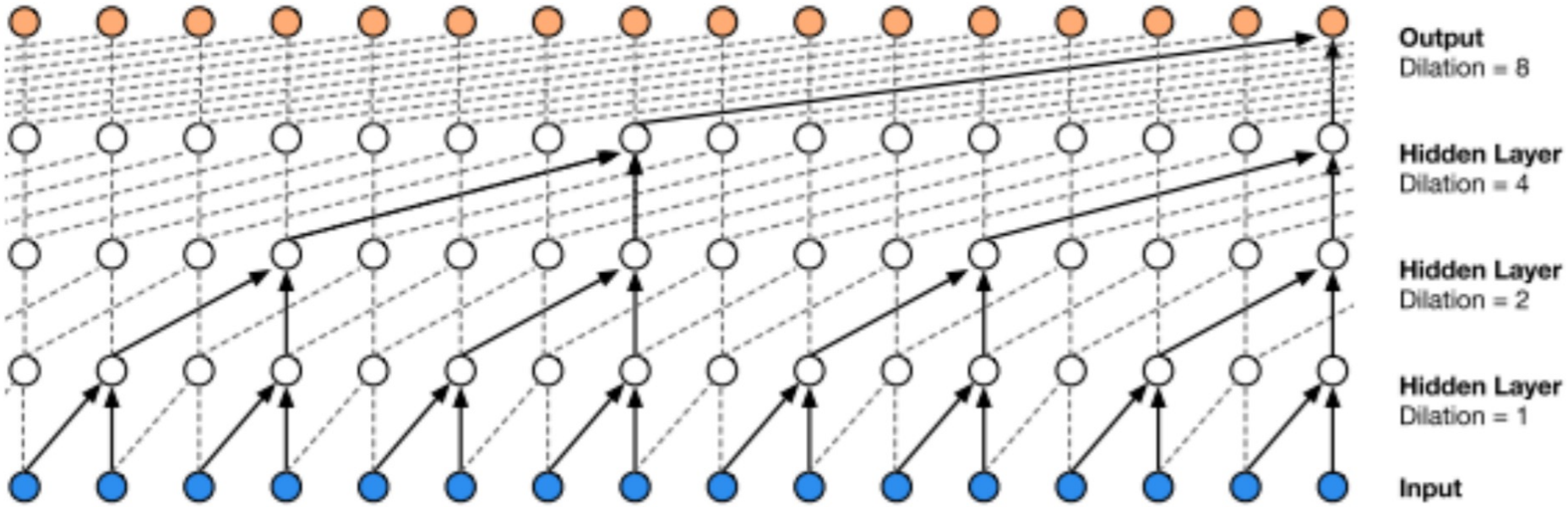
- Gated convolutional layers
- Short-cut connections
- Discretized logistic loss
- Multi-scale
- Training tricks
- Etc…

See

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

WaveNet

- A deep generative model of raw audio waveforms
- Can synthesize audio signals such as speech and music



Oord et al, WaveNet: A Generative Model for Raw Audio, SSW 2016.

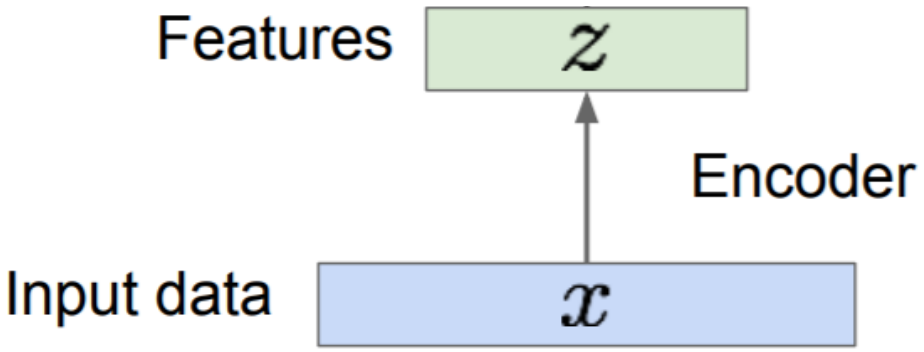
Latent variable models

What is a latent variable?

- Explanatory factors of data

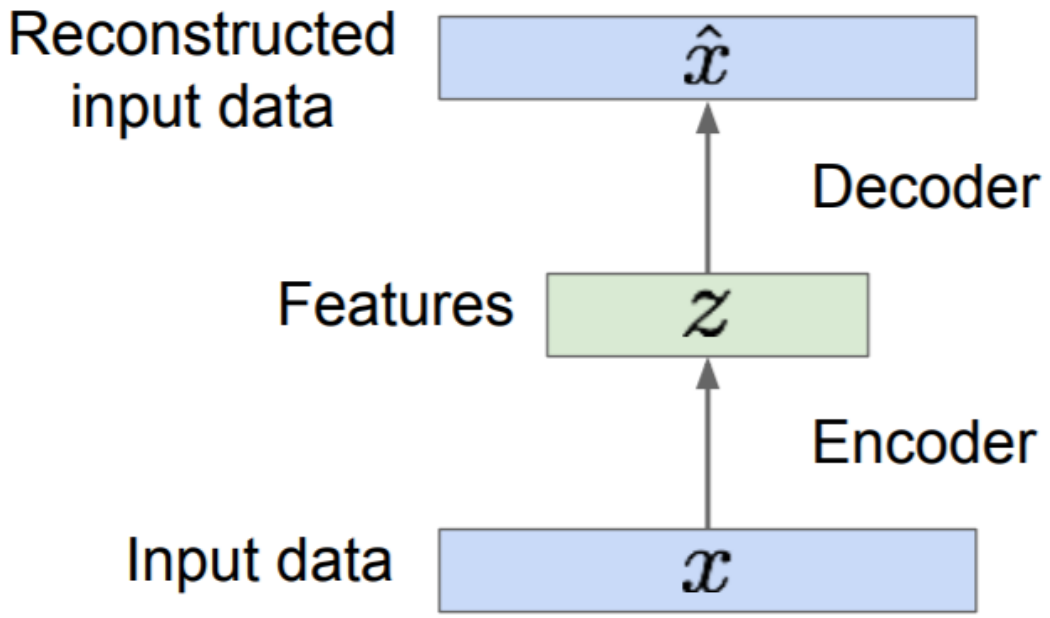
Dimensionality reduction: Autoencoders

- Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data
  - Train such that features can be used to reconstruct original data
    - "Autoencoding" - encoding itself



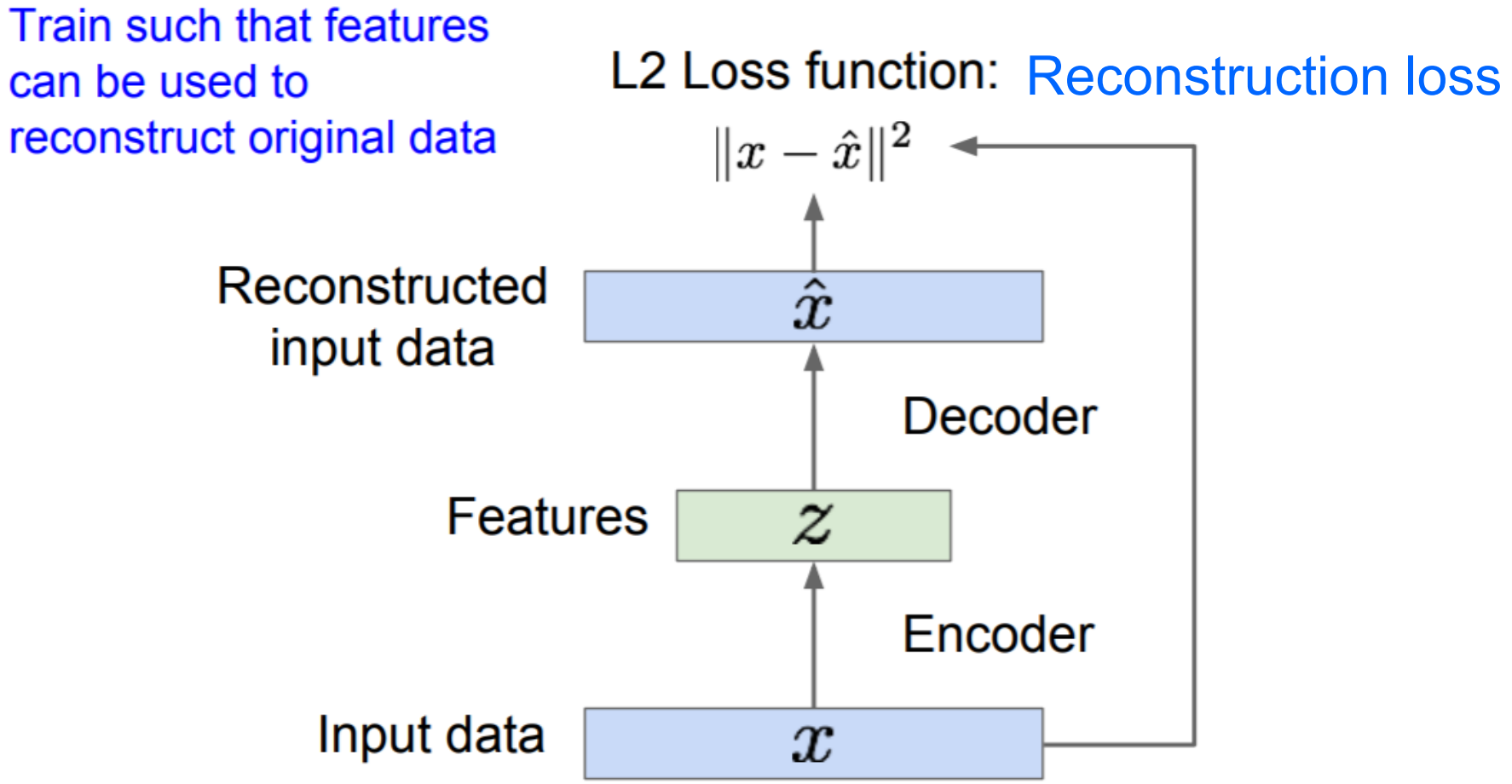
Autoencoders

- Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data
  - Train such that features can be used to reconstruct original data
    - "Autoencoding" - encoding itself



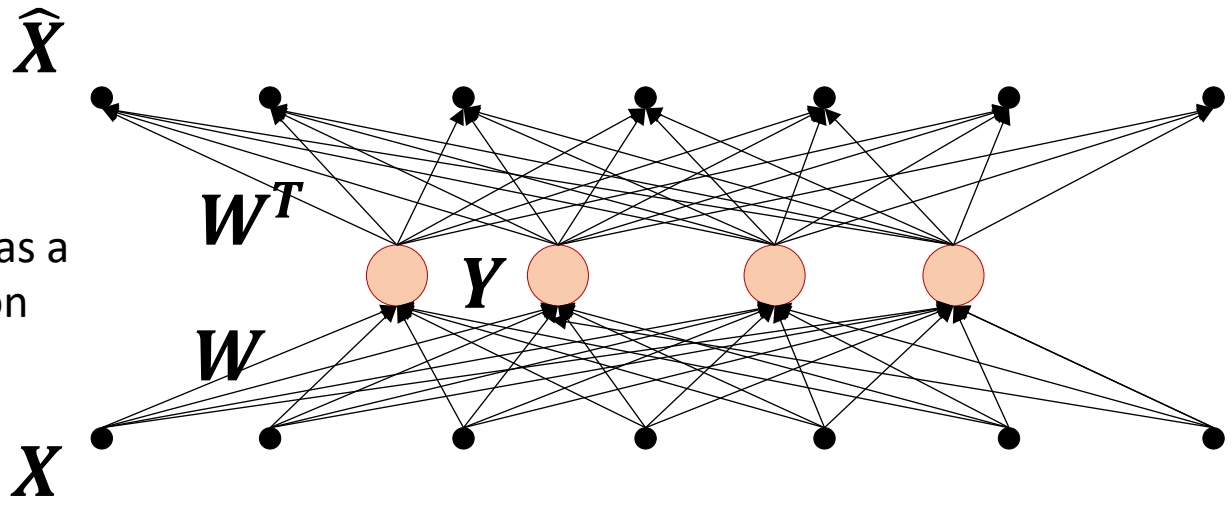
Autoencoders

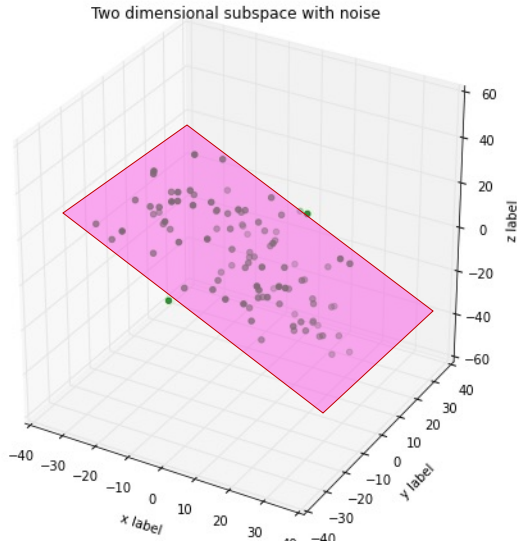
- **Encoder:** The "Analysis" net which computes the hidden representation
- **Decoder:** The "Synthesis" which recomposes the data from the hidden representation



AEs without a non-linearity

hidden layer has a *linear* activation

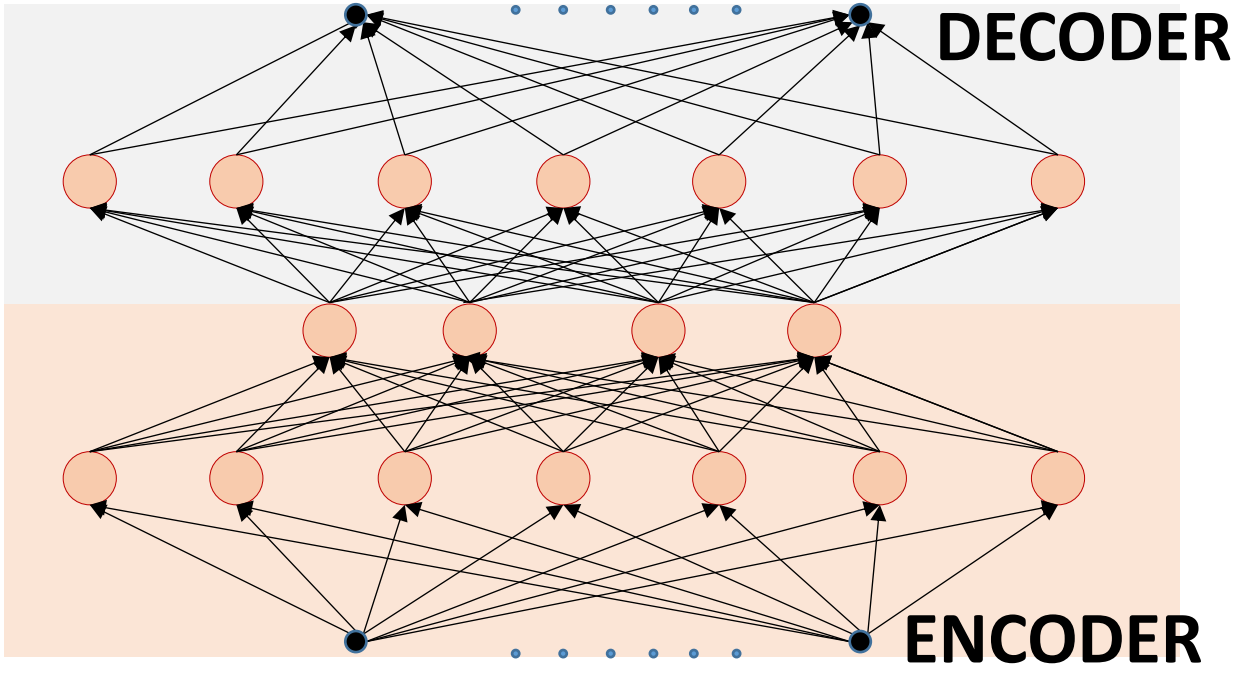


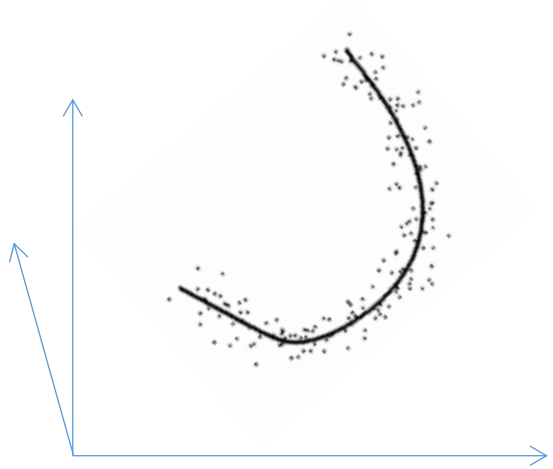


$\mathbf{Y} = \mathbf{WX}$ $\quad \hat{\mathbf{X}} = \mathbf{W}^T\mathbf{Y}$ $\quad E = \|\mathbf{X} - \mathbf{W}^T\mathbf{WX}\|^2$ Find W to minimize Avg[E]

- This is similar to PCA
  - The output of the hidden layer will be in the principal subspace
    - Even if the recomposition weights are different from the “analysis” weights

“Deep” autoencoders

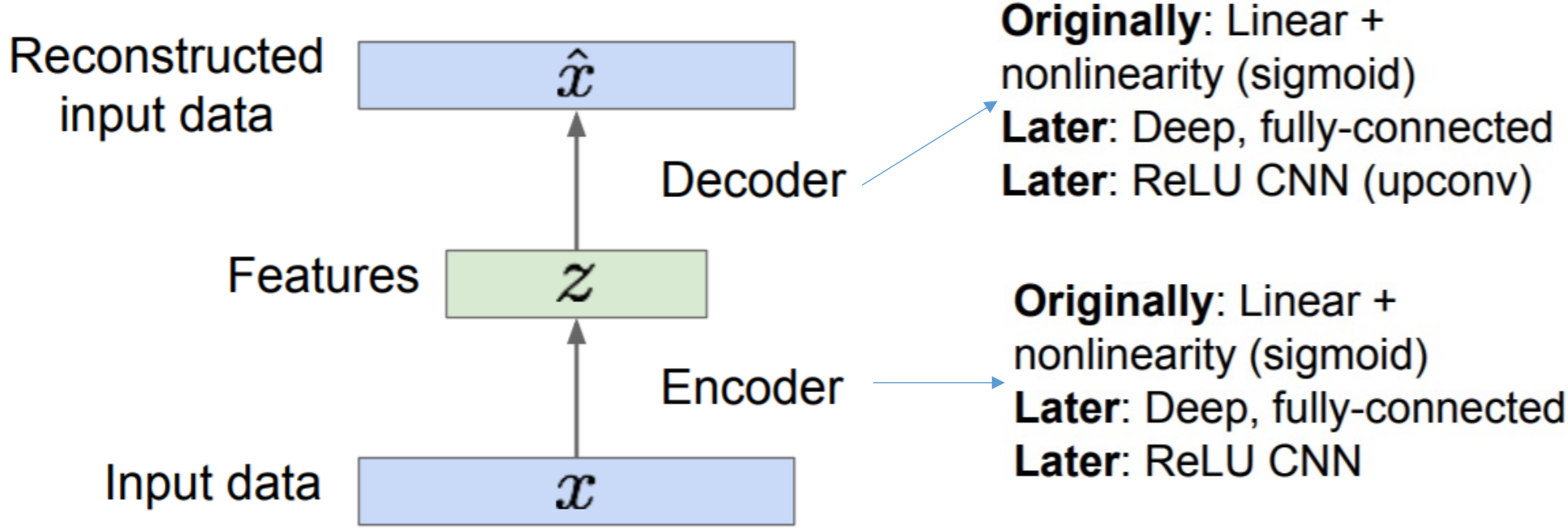




- When the hidden representation is of lower dimensionality than the input, often called a “**bottleneck**” network
  - Nonlinear PCA
  - Learns the manifold for the data
    - If properly trained

Autoencoders

- Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data
  - Train such that features can be used to reconstruct original data
    - "Autoencoding" - encoding itself



Autoencoders

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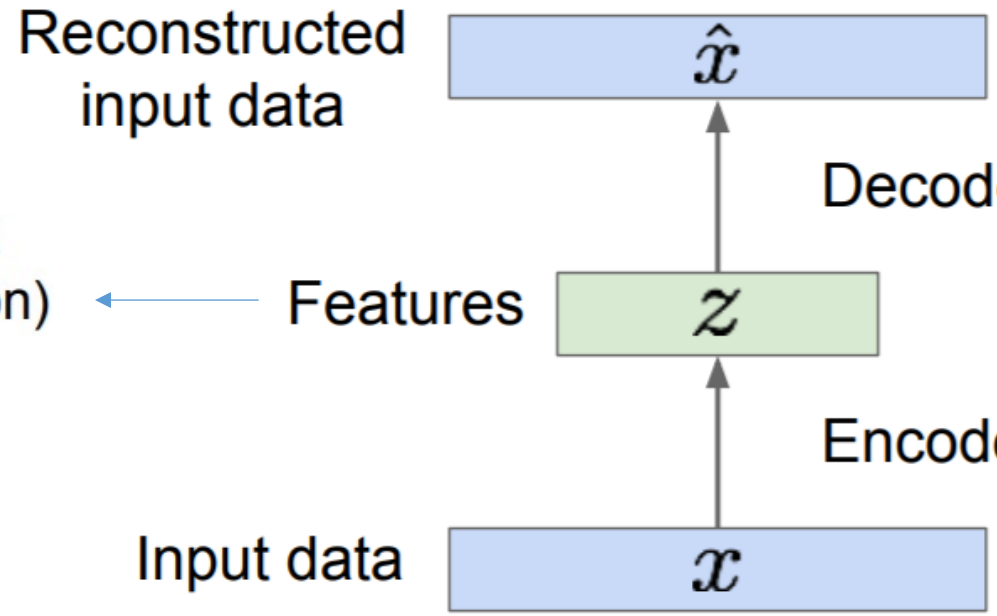


Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN (upconv)

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

Q: Why dimensionality reduction?

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

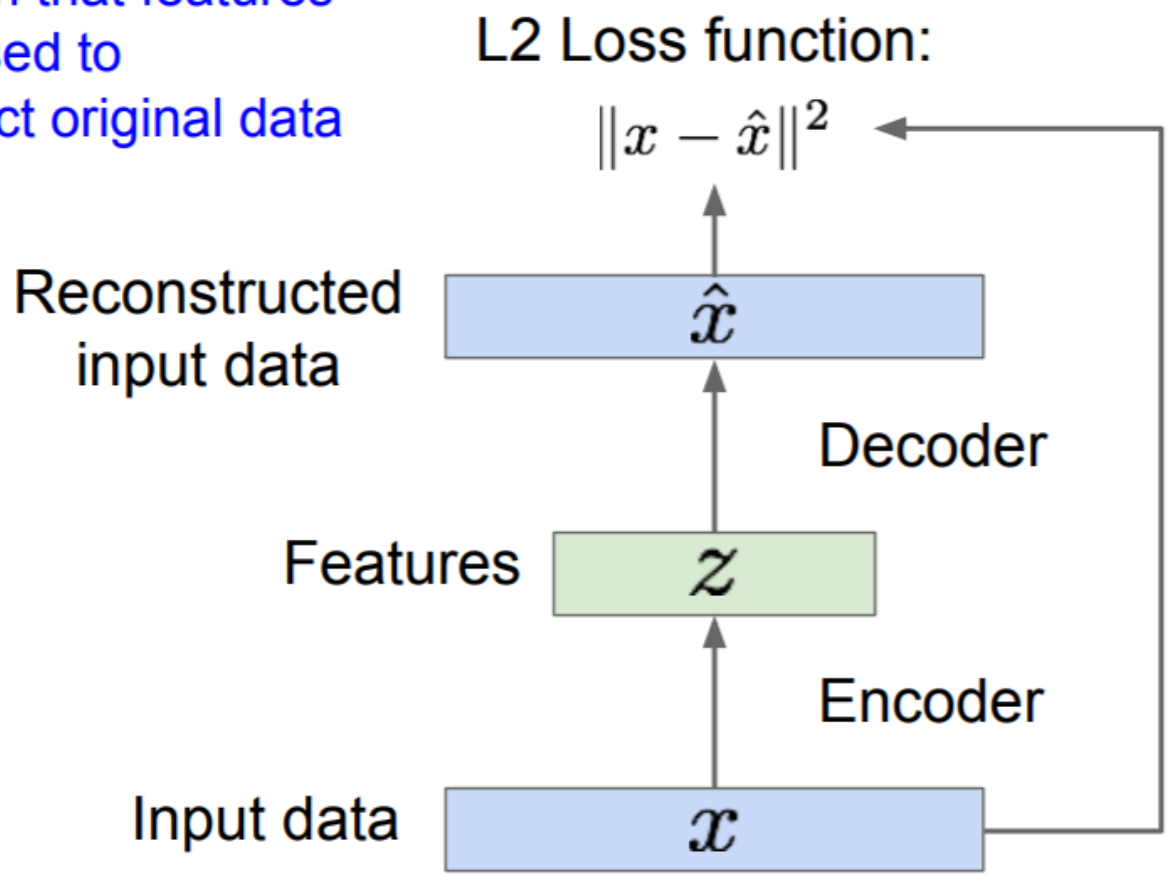
Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN

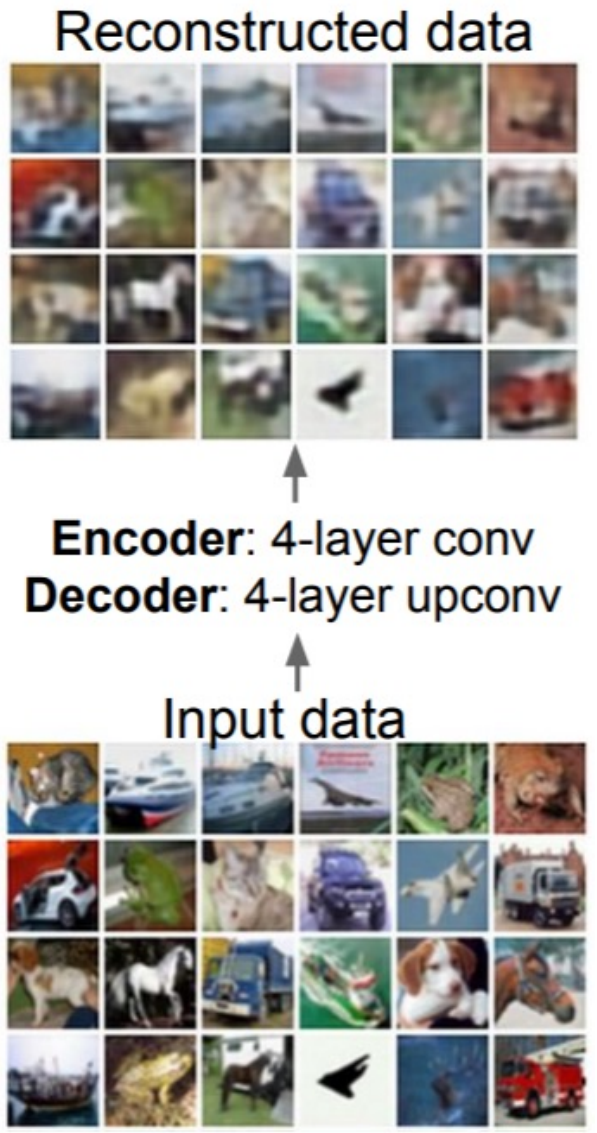
Autoencoders: Pretraining

- Pre-train the encoder with (unlabeled) data

Train such that features can be used to reconstruct original data

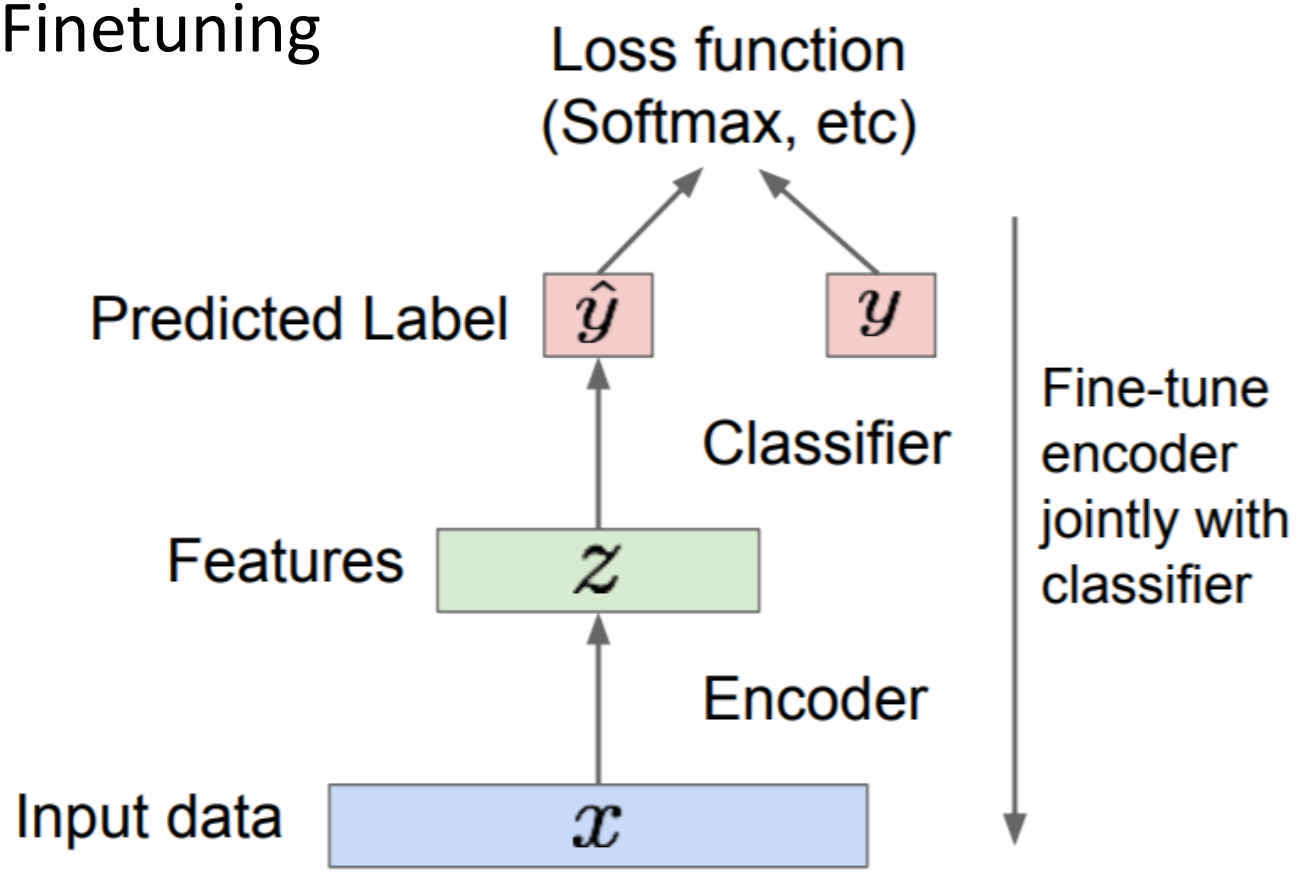
Doesn't use labels!





Autoencoders as pretrained models

- AEs can learn features to initialize a supervised model
- Supervised Finetuning

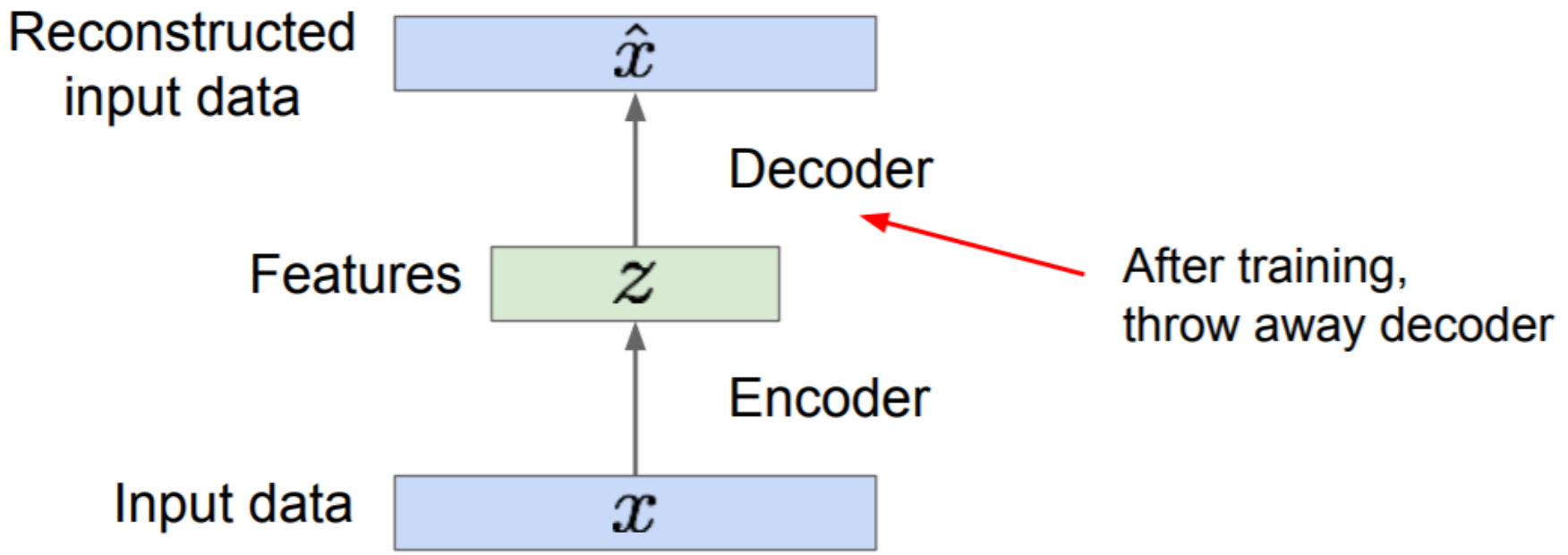


Encoder can be used to initialize a **supervised** model

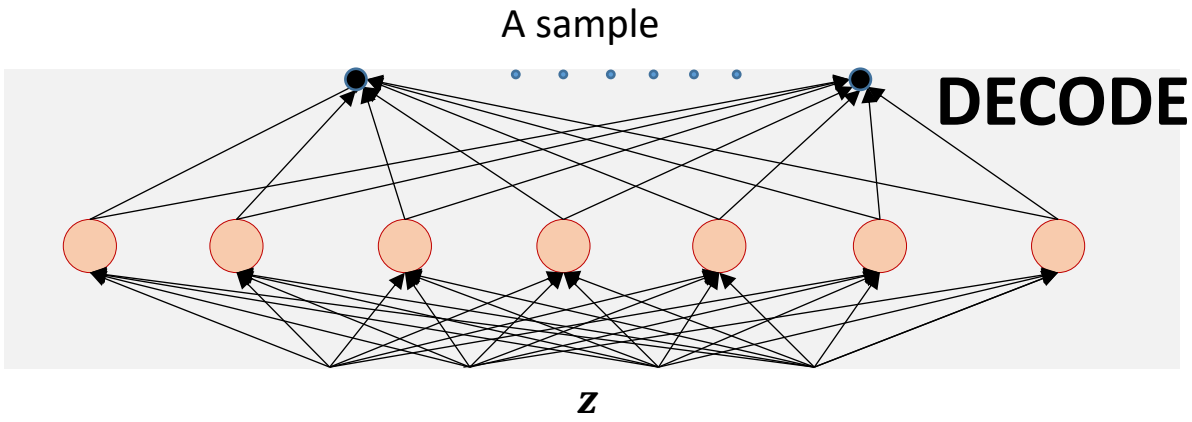
bird plane
dog deer truck

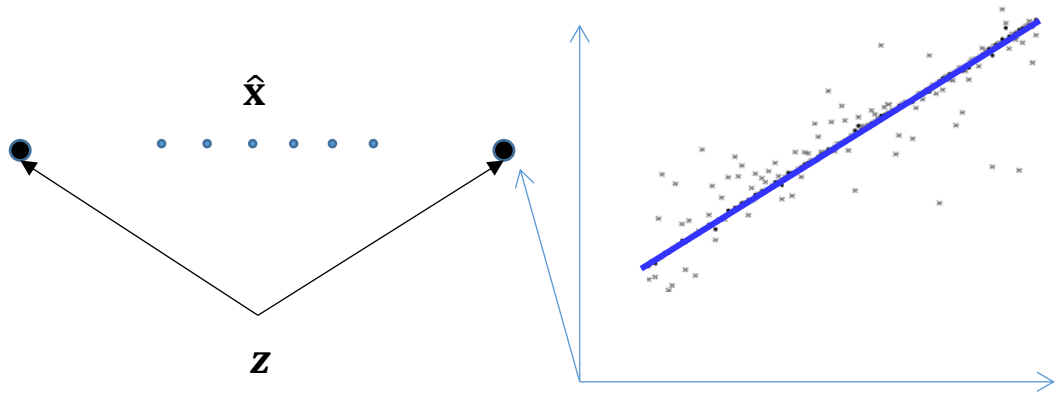
Train for final task (sometimes with small data)

Autoencoders



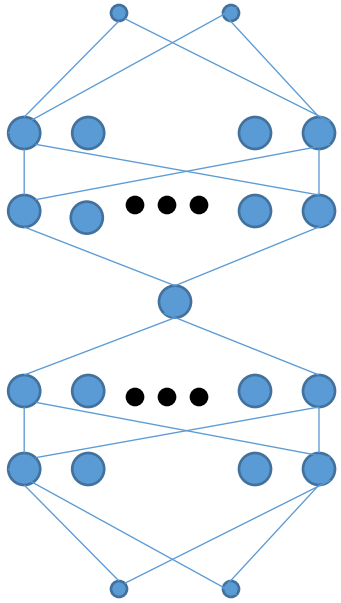
Can the decoder of AE be used for data generation?



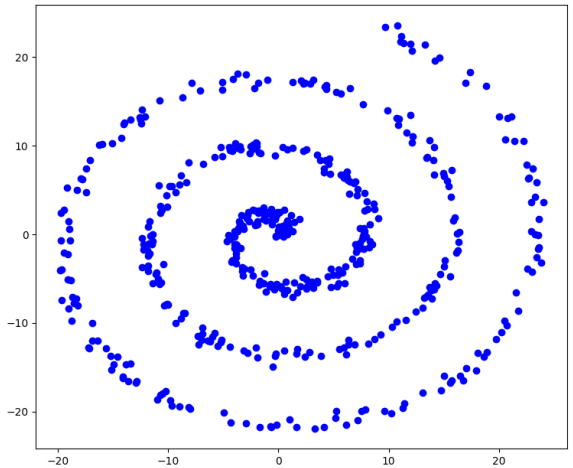


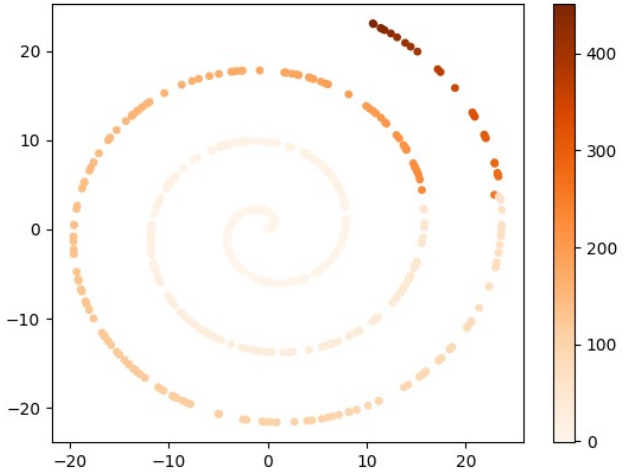
- Varying the hidden value will move along this non-linear manifold
  - Simply varying the hidden representation will result in an output that lies along the major axis
- The decoder can only generate data on the manifold that the training data lie on
- This also makes it an excellent “generator” of the distribution of the training data
  - Any values fed to the (hidden) input to the decoder will produce data similar to the training data

Some examples



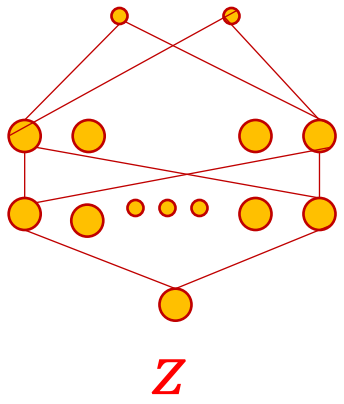
2-D input

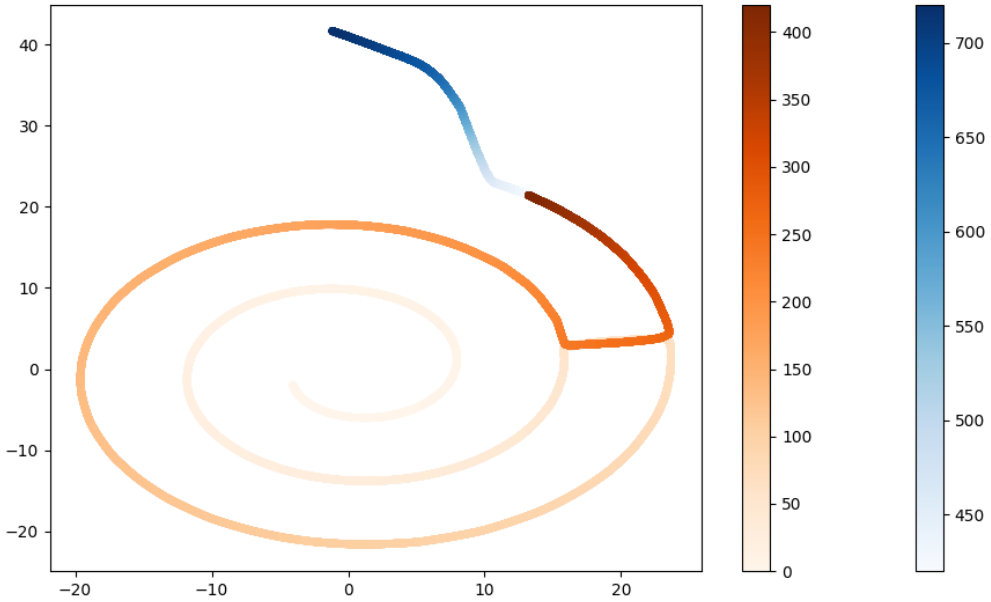




- Encoder and decoder have 2 hidden layers of 100 neurons, but hidden representation has one hidden unit
- Model seems to learn underlying helix structure

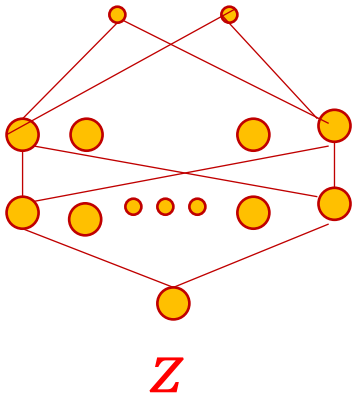
The learned manifold

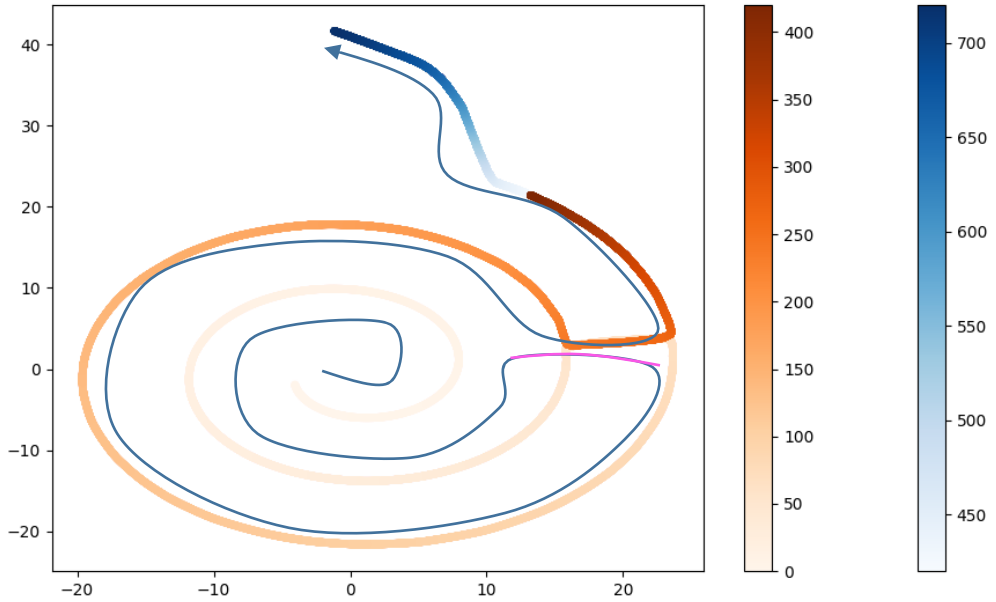




- Not a “clean” function even in range of training points (Red)
  - Color shows value of z
  - z does not vary smoothly along the curve, but bounces back and forth
  - Learns manifold structure (bar) that is not represented in training data
- Does not generalize outside the range of training points (Blue)
  - Extending the range towards the center of the spiral resulted in decoded values outside the page!

The learned manifold





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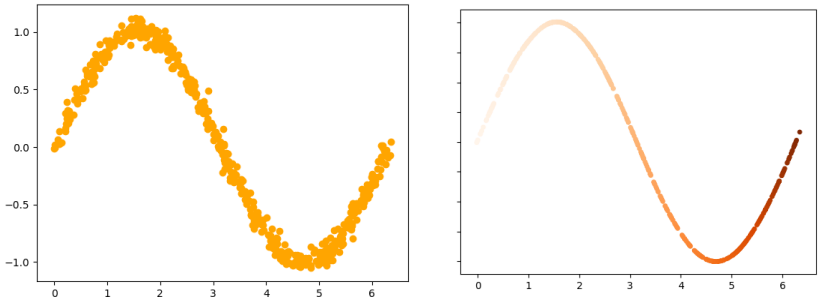
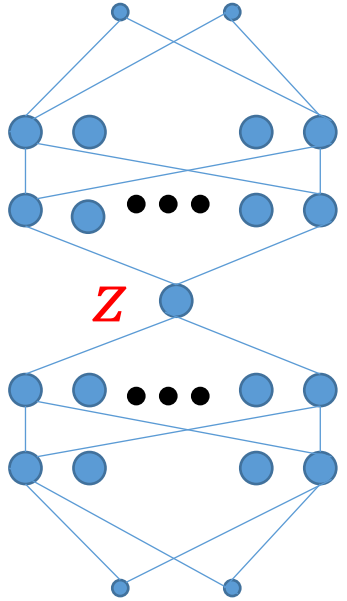
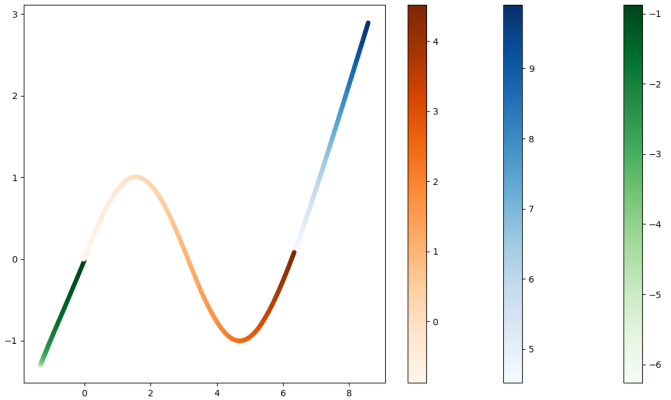
Another example

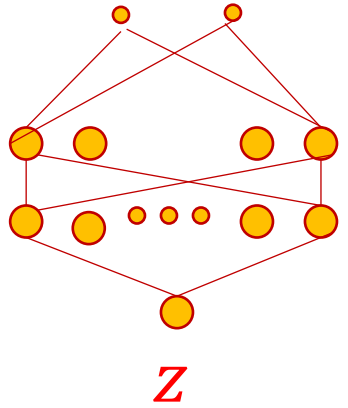
- Learning to reconstruct a sinusoid
  - Input (left): data on a spiral manifold
  - Output (right): Decoded data
- AE seems to "learn" the underlying curved manifold





- The model is specific to the training data.
  - Varying the hidden layer value only generates data along the learned manifold
    - May be poorly learned
  - *Any input* will result in an output along the learned manifold





Latent space

- Neural Networks like Autoencoders can be used for representation generation

- Can auto-encoders find latent space?
  - Bottleneck hidden layer forces to learn a compressed representation
  - Reconstruction loss forces the hidden layer preserve as much as information about the data as possible

- Only generates data along the learned manifold
  - This may be poorly learned
  - Any and every input will result in an output along the learned manifold

Latent space properties

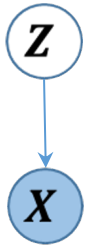
- For the generation purpose, we need the latent space shows the following properties:
  - **Continuity**: Similar point in the latent space will be similar after decoding
  - **Completeness**: Samples of the latent space leads to meaningful content after decoding

This slide has been adapted from Ava Amini & Alex Amini

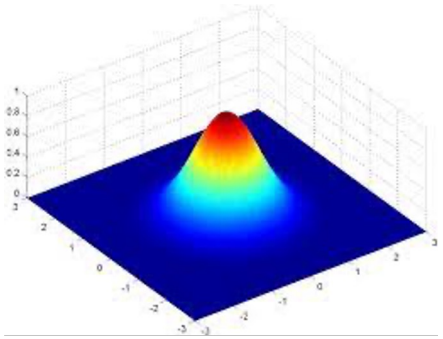
Latent variables

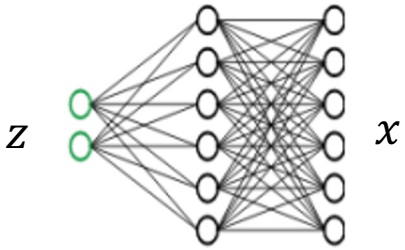
We define a simple distribution on the latent space, i.e., $p(z)$ and a decoder network $p_\theta(x|z)$ to map the latent variable to the data space

$$p(x) = \int p(x|z)p(z)dz$$

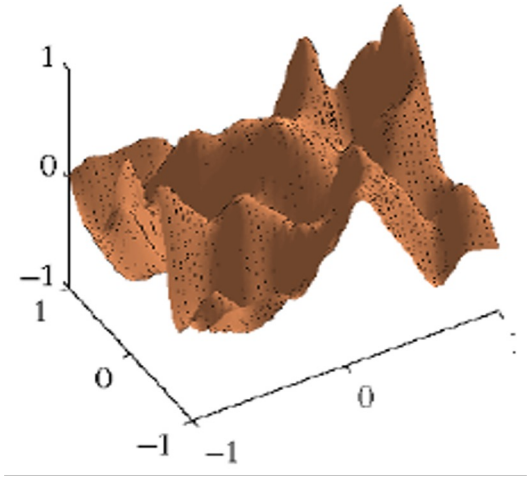


$p(z)$

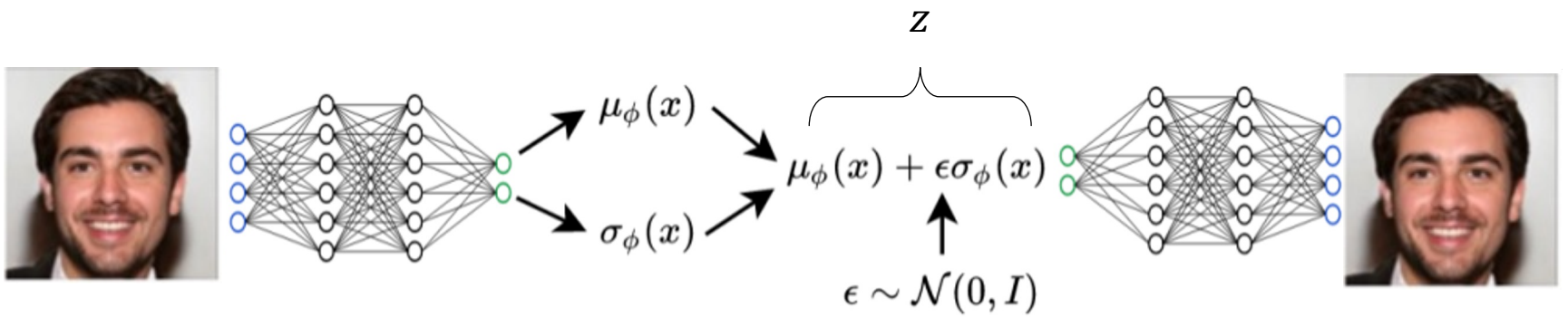




$p(x)$

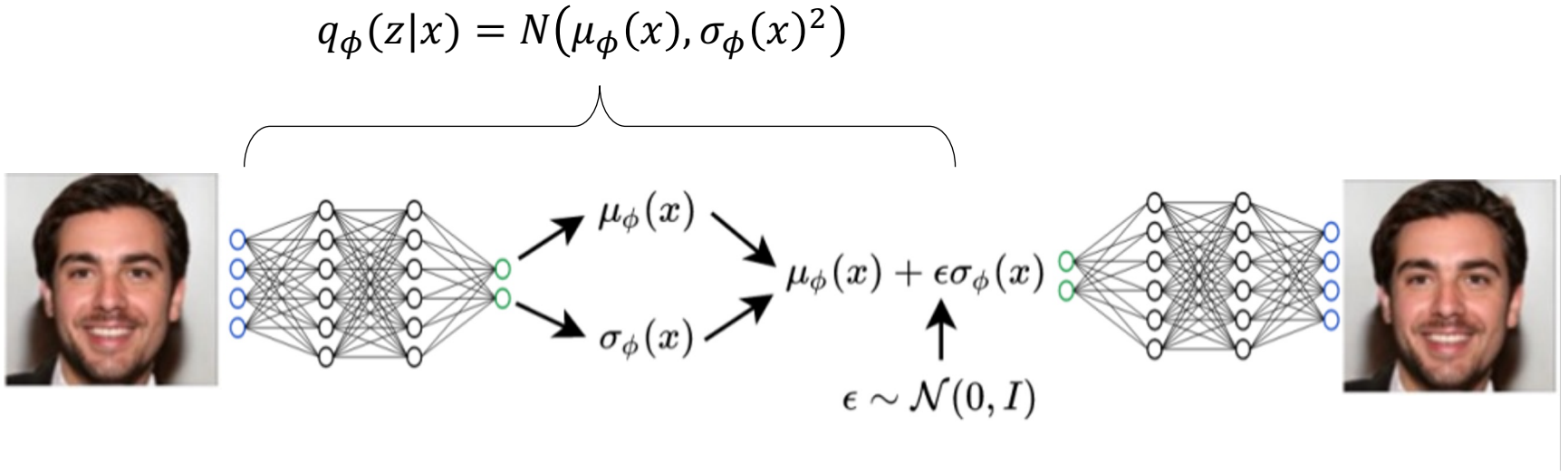


Variational Auto Encoder (VAE)



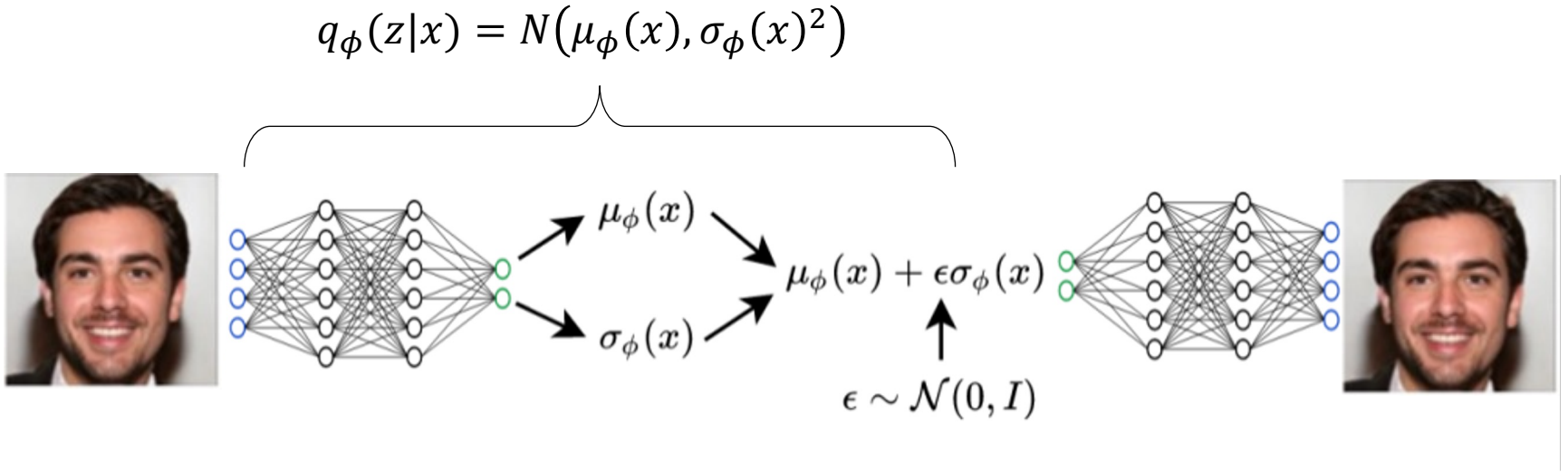
VAE loss: $\mathcal{L}(x; \theta, \phi)$ = reconstruction loss + regularization term

Variational Auto Encoder (VAE)



VAE loss: $\mathcal{L}(x; \theta, \phi)$ = reconstruction loss + regularization term

Variational Auto Encoder (VAE)



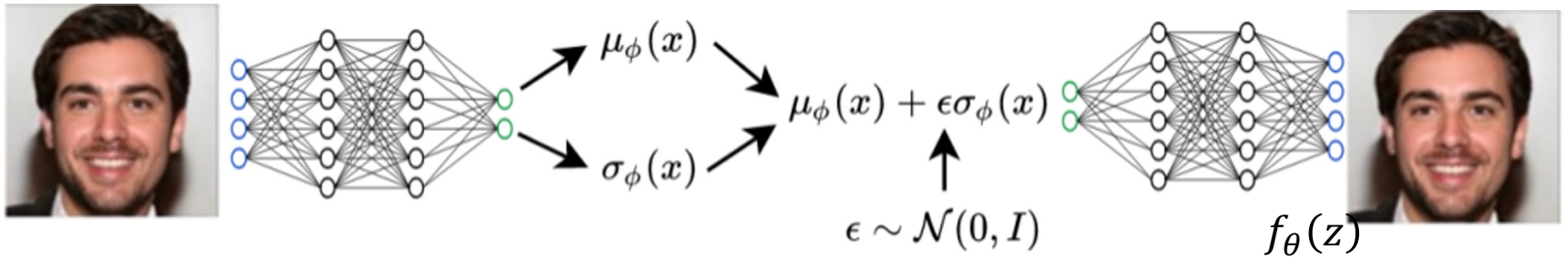
VAE loss: $\mathcal{L}(x, \theta, \phi) =$ reconstruction loss + regularization term

$\left\|x^{(i)} - \hat{x}^{(i)}\right\|^2$ $\quad$ $KL\left(q_\phi\left(z|x^{(i)}\right)||p(z)\right)$

Fixed prior on the latent distribution

Variational Auto Encoder (VAE)

$q_\phi(z|x) = N(\mu_\phi(x), \sigma_\phi(x)^2)$ $p_\theta(x|z) = N(f_\theta(z), \sigma^2 I)$



VAE loss: $\mathcal{L}(x, \theta, \phi) =$ reconstruction loss + regularization term

$\|x^{(i)} - \hat{x}^{(i)}\|^2$ $KL(q_\phi(z|x^{(i)})||N(0, I))$

$f_\theta(z) = f_\theta\left(\mu_\phi(x^{(i)}) + \epsilon\sigma_\phi(x^{(i)})\right)$

Common choice of prior on the latent distribution

KL between two Gaussians

- KL between two Gaussians can be easily computed in a closed form

- KL between $q_\phi(z|x)$ and $N(0, I)$:

$$D_{KL}\left(q_\phi(z|x)||N(0,I)\right) = -\frac{1}{2}\sum_{j=1}^{k}(\sigma_j + \mu_j^2 - \log\sigma_j - 1)$$

Variational Auto Encoder (VAE): Prior distribution

- Encourage encodings to be evenly distributed around the center of the latent space
- Penalize the network when it tries to memorize data

What does the VAE actually do

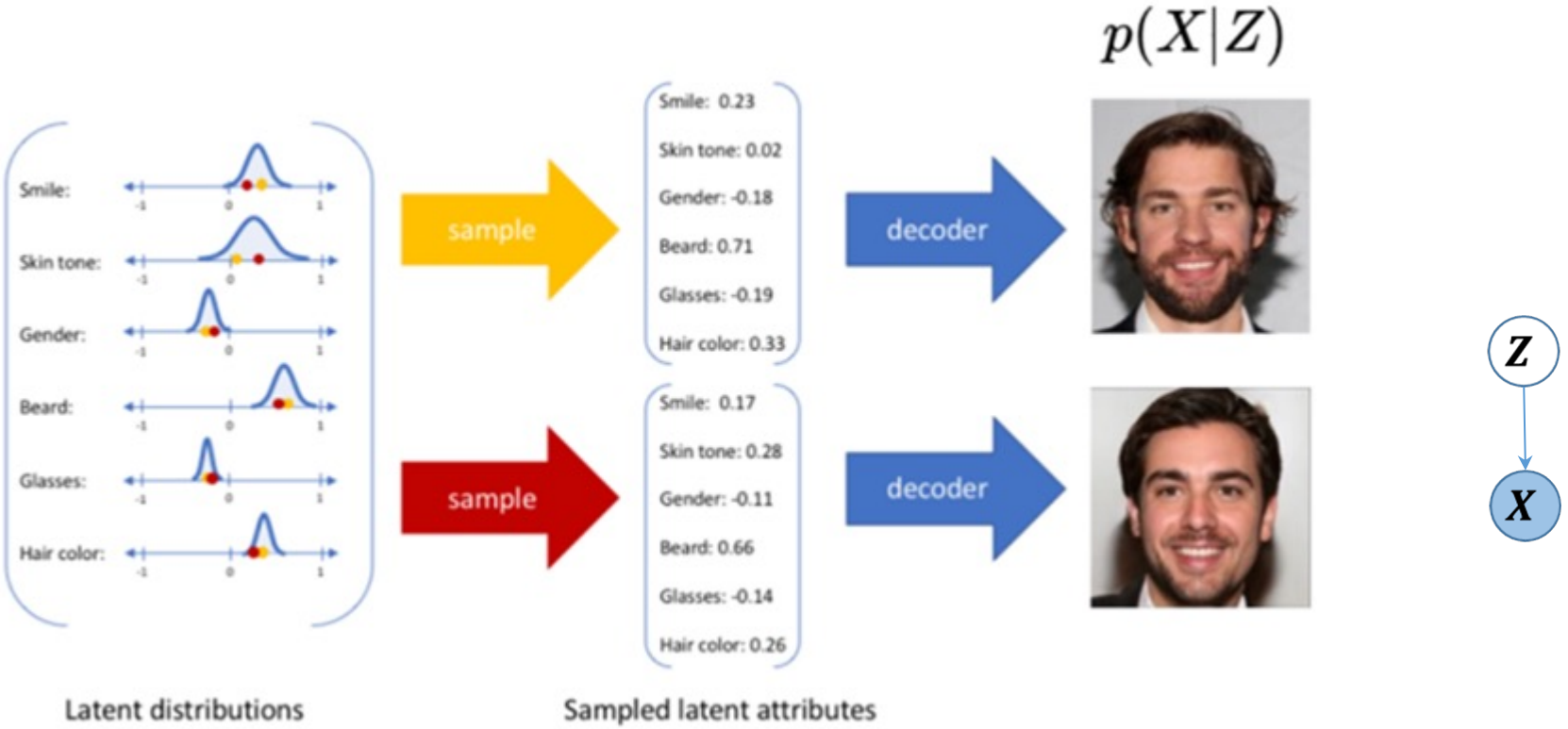
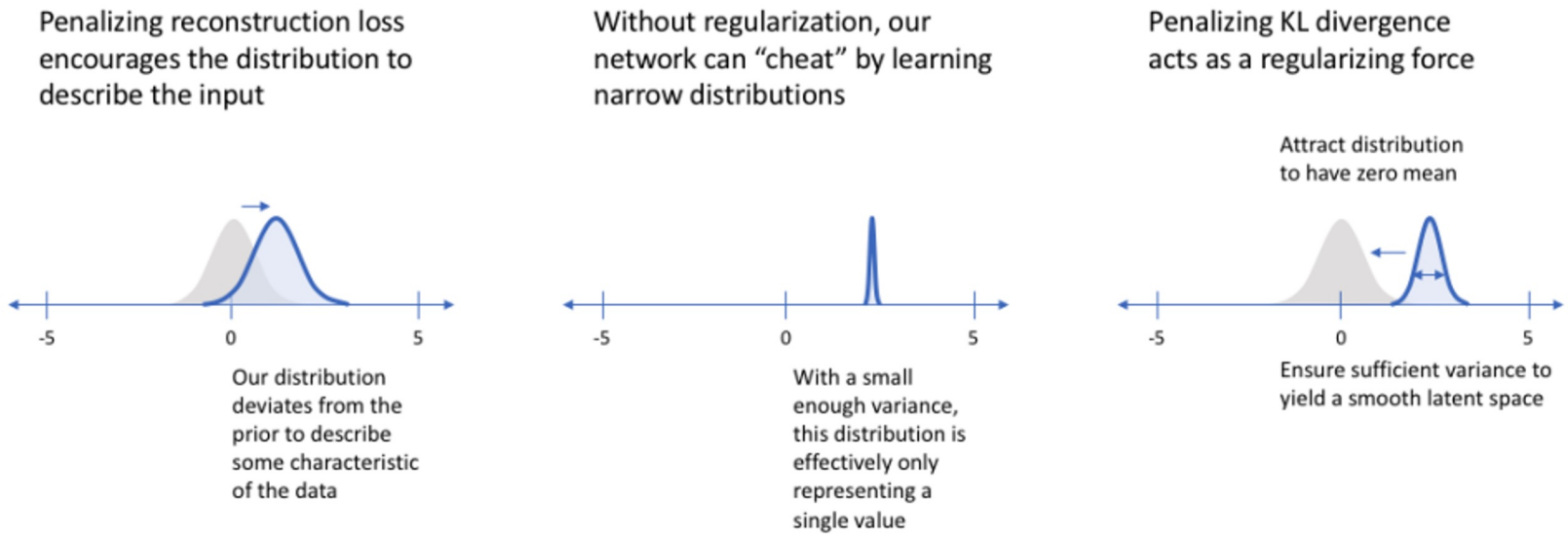


Image credit: Jeremy Jordan's blog post.

What does the VAE actually do



The VAE objectives arranges data on a compact manifold (we can sample from) in a continuous smooth way.

Image credit: Jeremy Jordan's blog post

Theory of VAE

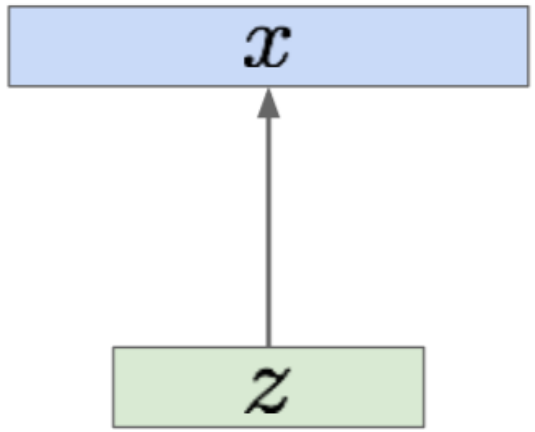
Variational Autoencoders

- 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 underlying unobserved (latent) representation **z**

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

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



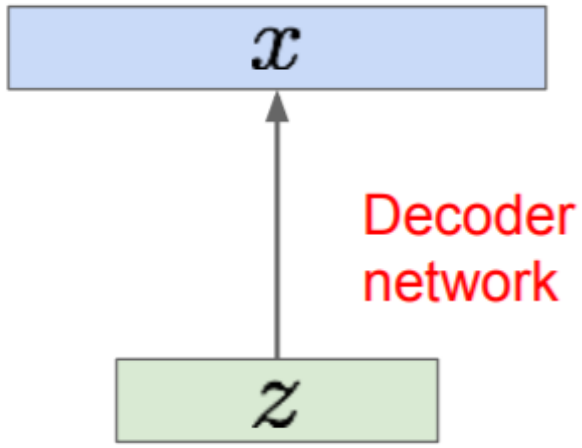
Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

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



We want to estimate the true parameters θ^* of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian.

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

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

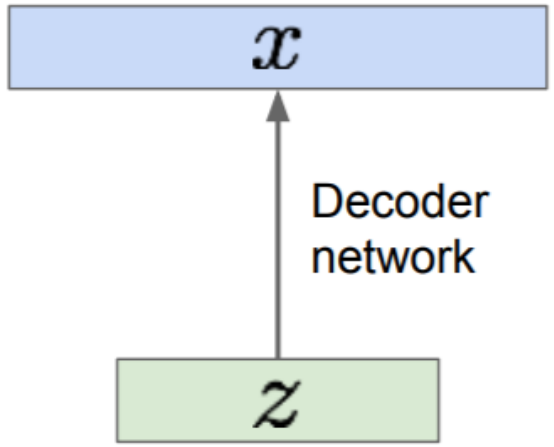
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

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



We want to optimize the true parameters θ^* of this generative model

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

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

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

Variational Inference

$$\log p_{\boldsymbol{\theta}}(x) = \log \sum_z p_{\boldsymbol{\theta}}(x, z)$$

$$= \log \sum_z q(z) \frac{p_{\boldsymbol{\theta}}(x, z)}{q(z)}$$

$$\geq \sum_z q(z) \log \frac{p_{\boldsymbol{\theta}}(x, z)}{q(z)} \qquad \text{Jensen Inequality}$$

$$= \sum_z q(z) \log \frac{p_{\boldsymbol{\theta}}(x|z) p_{\boldsymbol{\theta}}(z)}{q(z)} = \boxed{E_{q(z)}[\log p_{\boldsymbol{\theta}}(x|z)] - KL(q(z)||p_\theta(z))}$$

$\mathcal{L}_q(x, \theta)$ **Evidence Lower Bound (ELBO)**

When is the ELBO gap minimized?

- We want to maximize the log-likelihood
- What is the gap between ELBO and likelihood?

$$\log p_\theta(x) = \mathcal{L}_q(x, \theta) + KL(q(z)||p_\theta(z|x))$$

- To minimize the ELBO gap, we need $q(z) = p_\theta(z|x)$

- However $p_\theta(z|x)$ is intractable

Lower bound for log likelihood

$$\log p(x) = E_{z\sim q(z|x)}[\log p(x)] \qquad (p(x) \text{ does not depend on z})$$

$$= E_{z\sim q(z|x)}\left[\log \frac{p(x|z)p(z)}{p(z|x)}\right] \qquad \text{(Bayes' rule)}$$

$$= E_{z\sim q(z|x)}\left[\log \left(\frac{p(x|z)p(z)}{p(z|x)} \times \frac{q(z|x)}{q(z|x)}\right)\right] \qquad \text{(Multiply by constant)}$$

$$= E_{z\sim q(z|x)}[\log p(x|z)] - E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z)}\right)\right] + E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z|x)}\right)\right]$$

$$= E_{z\sim q(z|x)}[\log p(x|z)] - D_{KL}\big(q(z|x)||p(z)\big) + D_{KL}\big(q(z|x)||p(z|x)\big)$$

Lower bound for log likelihood

$$\log p(x) = E_{z\sim q(z|x)}[\log p(x)]$$ ($p(x)$ does not depend on z)

$$= E_{z\sim q(z|x)}\left[\log \frac{p(x|z)p(z)}{p(z|x)}\right]$$ (Bayes' rule)

$$= E_{z\sim q(z|x)}\left[\log \left(\frac{p(x|z)p(z)}{p(z|x)} \times \frac{q(z|x)}{q(z|x)}\right)\right]$$ (Multiply by constant)

$$= E_{z\sim q(z|x)}[\log p(x|z)] - E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z)}\right)\right] + E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z|x)}\right)\right]$$

$$= E_{z\sim q(z|x)}[\log p(x|z)] - D_{KL}\big(q(z|x)||p(z)\big) + D_{KL}\big(q(z|x)||p(z|x)\big)$$

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling. (Sampling differentiable through reparam. trick, see paper.)

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

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

Lower bound for log likelihood

$$\log p(x) = E_{z\sim q(z|x)}[\log p(x)] \qquad (p(x) \text{ does not depend on z})$$

$$= E_{z\sim q(z|x)}\left[\log \frac{p(x|z)p(z)}{p(z|x)}\right] \qquad \text{(Bayes' rule)}$$

$$= E_{z\sim q(z|x)}\left[\log \left(\frac{p(x|z)p(z)}{p(z|x)} \times \frac{q(z|x)}{q(z|x)}\right)\right] \qquad \text{(Multiply by constant)}$$

$$= E_{z\sim q(z|x)}[\log p(x|z)] - E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z)}\right)\right] + E_{z\sim q(z|x)}\left[\log \left(\frac{q(z|x)}{p(z|x)}\right)\right]$$

$$= E_{z\sim q(z|x)}[\log p(x|z)] - D_{KL}\big(q(z|x)||p(z)\big) + D_{KL}\big(q(z|x)||p(z|x)\big)$$

Tractable lower bound which we can take gradient of and optimize!

≥ 0

Lower bound for log likelihood

$$\log p_\theta(x) = E_{z\sim q_\phi(z|x)}[\log p_\theta(x)] \qquad (p(x) \text{ does not depend on z})$$

$$= E_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x|z)p_\theta(z)}{p_\theta(z|x)}\right] \qquad \text{(Bayes' rule)}$$

$$= E_{z\sim q_\phi(z|x)}\left[\log \left(\frac{p_\theta(x|z)p_\theta(z)}{p_\theta(z|x)} \times \frac{q_\phi(z|x)}{q_\phi(z|x)}\right)\right] \qquad \text{(Multiply by constant)}$$

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

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

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

≥ 0

Lower bound for log likelihood

$$\log p_\theta(x) = E_{z\sim q_\phi(z|x)}[\log p_\theta(x)] \qquad (p(x) \text{ does not depend on z})$$

$$= E_{z\sim q_\phi(z|x)}\left[\log \frac{p_\theta(x|z)p_\theta(z)}{p_\theta(z|x)}\right] \qquad \text{(Bayes' rule)}$$

$$= E_{z\sim q_\phi(z|x)}\left[\log \left(\frac{p_\theta(x|z)p_\theta(z)}{p_\theta(z|x)} \times \frac{q_\phi(z|x)}{q_\phi(z|x)}\right)\right] \qquad \text{(Multiply by constant)}$$

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

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

$\mathcal{L}(x,\theta,\phi)$ $\qquad\qquad$ ≥ 0

$$\log p_\theta(x) \geq \mathcal{L}(x,\theta,\phi)$$

Evidence Lower Bound (ELBO)

Training: Maximize lower bound

$$\theta^*, \phi^* = \underset{\theta,\phi}{\text{argmax}} \sum_{i=1}^{n} \mathcal{L}(x^{(i)},\theta,\phi)$$

Why is posterior intractable?

- For many models with latent variables $q(z) = p_\theta(Z|X)$ is intractable

$$p_\theta(Z|X) = \frac{p_\theta(Z)p_\theta(X|Z)}{p_\theta(X)}$$

- Since we need integral over z that is intractable

$$p_\theta(X) = \int p_\theta(X|Z)p_\theta(Z)dZ$$

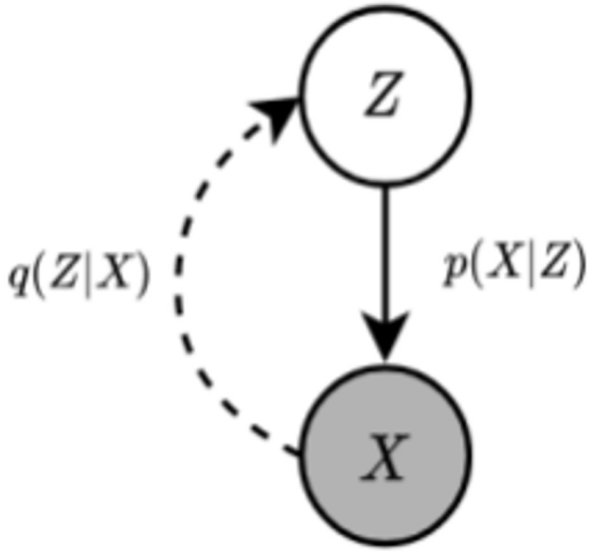
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

General solution

- Introduce inference distribution $q_\phi(Z|X)$
- To minimize the ELBO gap we choose $q(Z) = q_\phi(Z|X)$.

Solution: In addition to decoder network modeling $p_\theta(x|z)$, define additional encoder network $q_\phi(z|x)$ that approximates $p_\theta(z|x)$

Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize



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

ELBO using the decoder network

- The ELBO consists of two terms: reconstruction and a KL regularization:

$$\mathcal{L}_{\phi,\boldsymbol{\theta}}(X) = \underbrace{\mathbb{E}_{q_\phi(Z|X)}[p_{\boldsymbol{\theta}}(X|Z)]}_{\text{Reconstruction}} - \underbrace{KL\big(q_\phi(Z|X)||P(Z)\big)}_{\text{Regularization}}$$

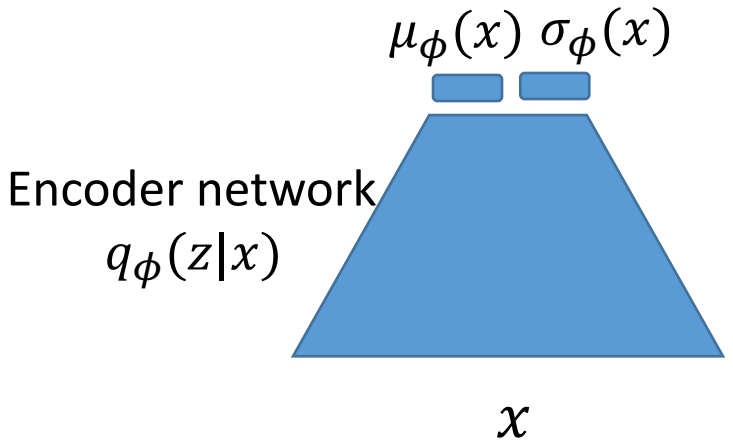
- $q_\phi(Z|X)$: multivariate normal distribution parameterized by a neural network

$$q_\phi(Z|X) = N\big(Z|\mu_\phi(X), \sigma_\phi(X)\big)$$

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

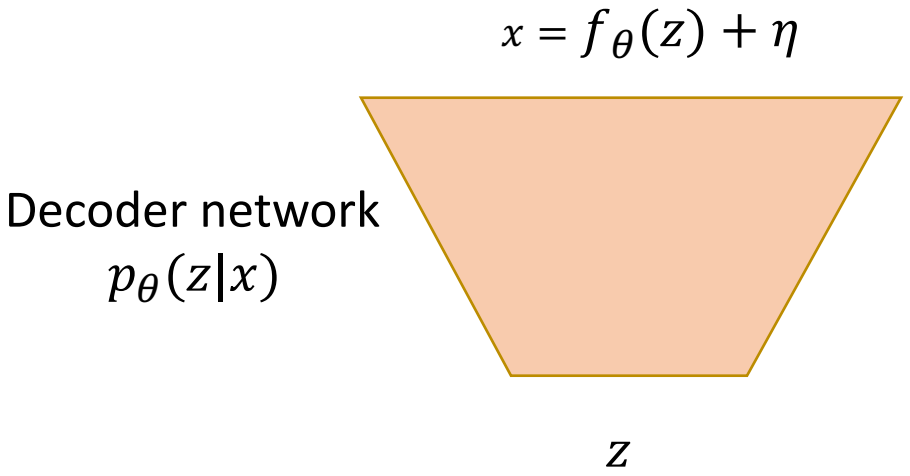
Encoder network

- Model $q_\phi(z|x)$ with a neural network (called encoder network)
- Assume $q_\phi(z|x)$ to be Gaussian
- Neural network outputs the mean vector $\mu_\phi(x)$ and standard deviation vector $\sigma_\phi(x)$
- Called recognition/inference network



Decoder network

- Model $p_\theta(x|z)$ with a neural network (called decoder network)
  - let $f_\theta(z)$ be the network output.
  - Assume $p_\theta(x|z)$ to be i.i.d. Gaussian, e.g.,
    - $x = f_\theta(z) + \eta$, where $\eta \sim N(0, \sigma^2 I)$
- Called also generation network

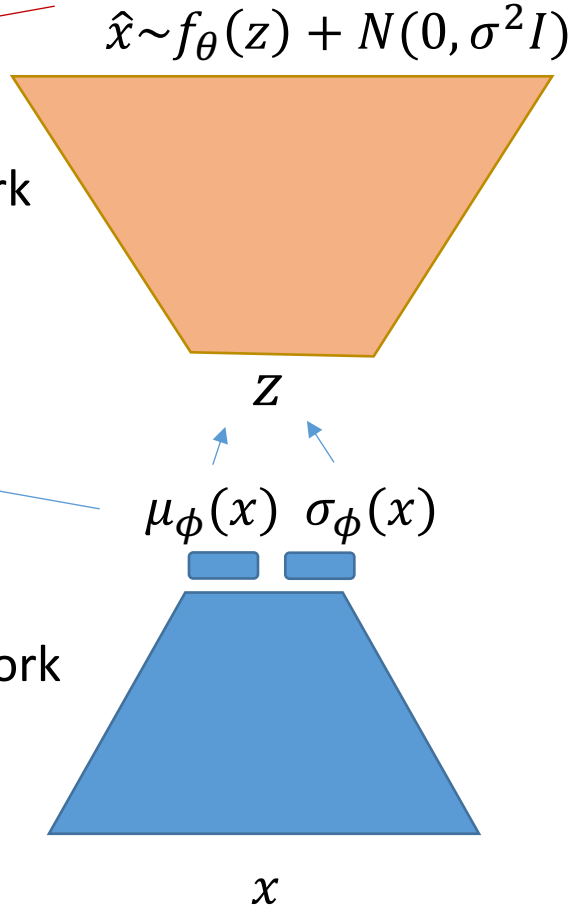


Variational Autoencoders

Maximize likelihood of original input given z or f(z)

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

Make approximate posterior distribution close to the prior



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

Variational Autoencoders

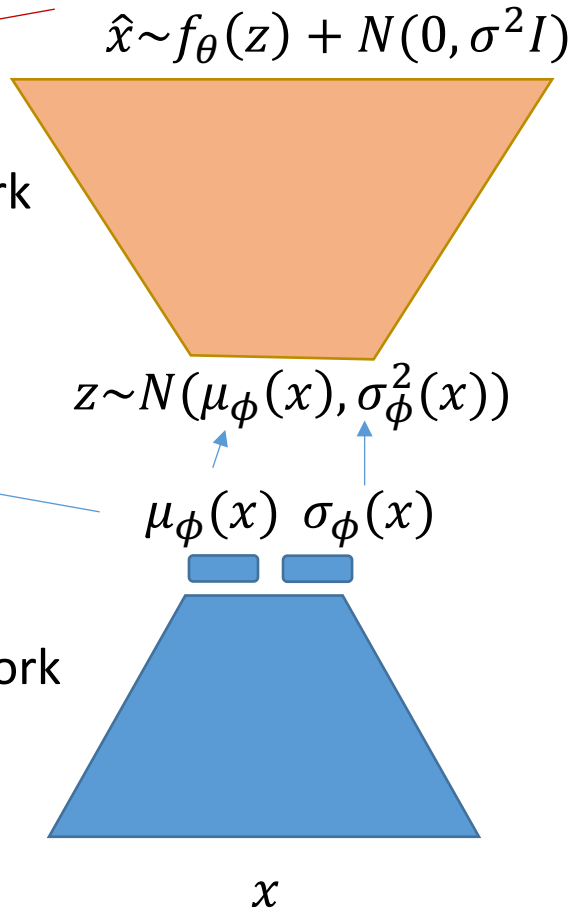
- Putting altogether=maximizing likelihood lower bound

Maximize likelihood of original input given z or f(z)

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

Make approximate posterior distribution close to the prior

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



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

Cost function

If we consider:

$$p_\theta(x|z) = N(f_\theta(z), \sigma^2 I)$$

$$p_\theta(x|z) = \frac{1}{\left(\sqrt{2\pi}\sigma\right)^D} e^{-\frac{1}{2\sigma^2}\|x - f_\theta(z)\|^2}$$

We have:

$$\log p_\theta(x|z) = C - \frac{1}{2\sigma^2}\|x - f_\theta(z)\|^2$$

- Putting it all together (given a (x, z) pair where $z \sim q_\phi(z|x)$):

$$L = \frac{1}{2\sigma^2}\|x - f_\theta(z)\|^2 + D_{KL}[q_\phi(z|x)||p(z)]$$

Corresponding to $E_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]$ term since $z \sim q_\phi(z|x)$ in the training data

$p(z) = N(0, I)$

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

Maximizing ELBO

- Maximizing ELBO composed of:
  - Reconstruction cost: The expected log-likelihood measures how well samples from q(z|x) are able to explain the data x.
  - Penalty: Ensures that the explanation of the data q(z|x) doesn't deviate too far from your beliefs p(z).
- When approximate posterior distribution q(z|x) is the best match to true posterior p(z|x) this lower bound gets tight

$$\underset{\theta,\phi}{\operatorname{argmax}} \sum_{i=1}^{n} \mathcal{L}(x^{(i)}, \theta, \phi)$$

$$= \sum_{i=1}^{n} E_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta\left(x^{(i)}|z\right)\right] - \sum_{i=1}^{n} D_{KL}\left(q_\phi\left(z|x^{(i)}\right)||p_\theta(z)\right)$$

Reconstruct the input

Make the posterior close to prior

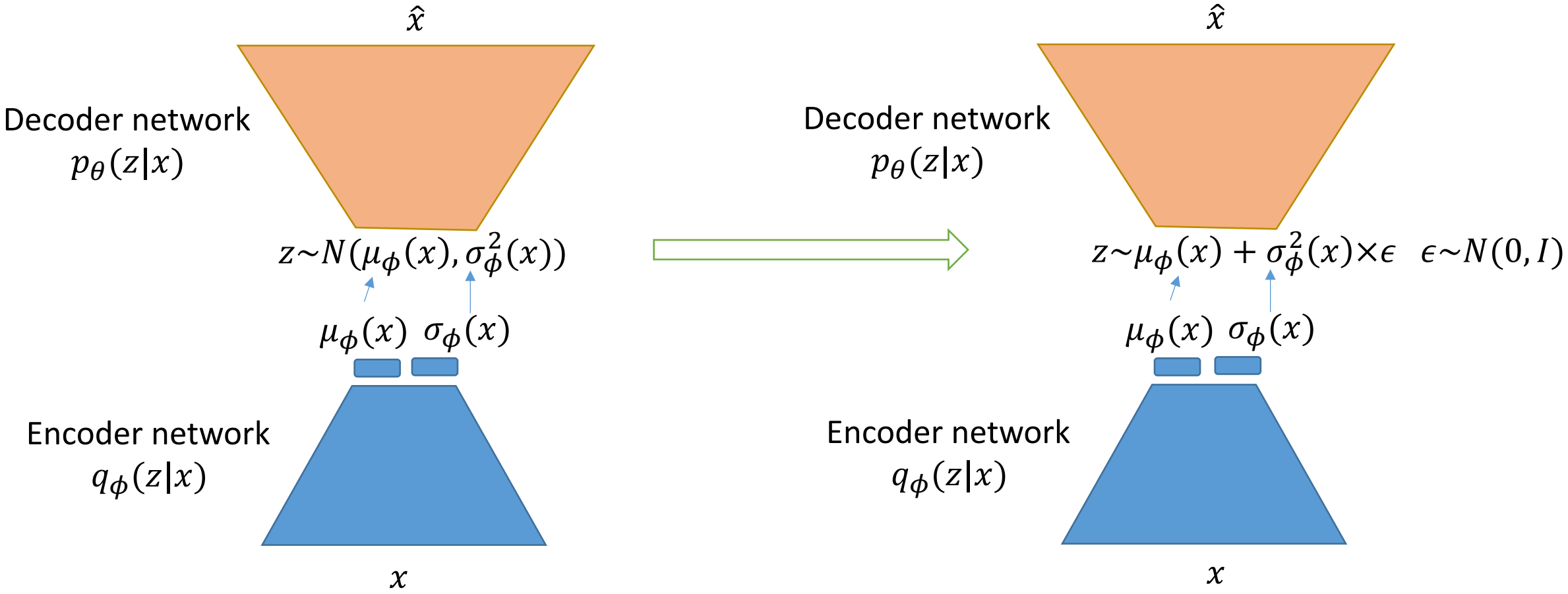
Optimizing the ELBO

Need to compute

$$\nabla_{\phi,\theta}\mathbb{E}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] \approx \nabla_{\phi,\theta}\hat{\mathbb{E}}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]$$

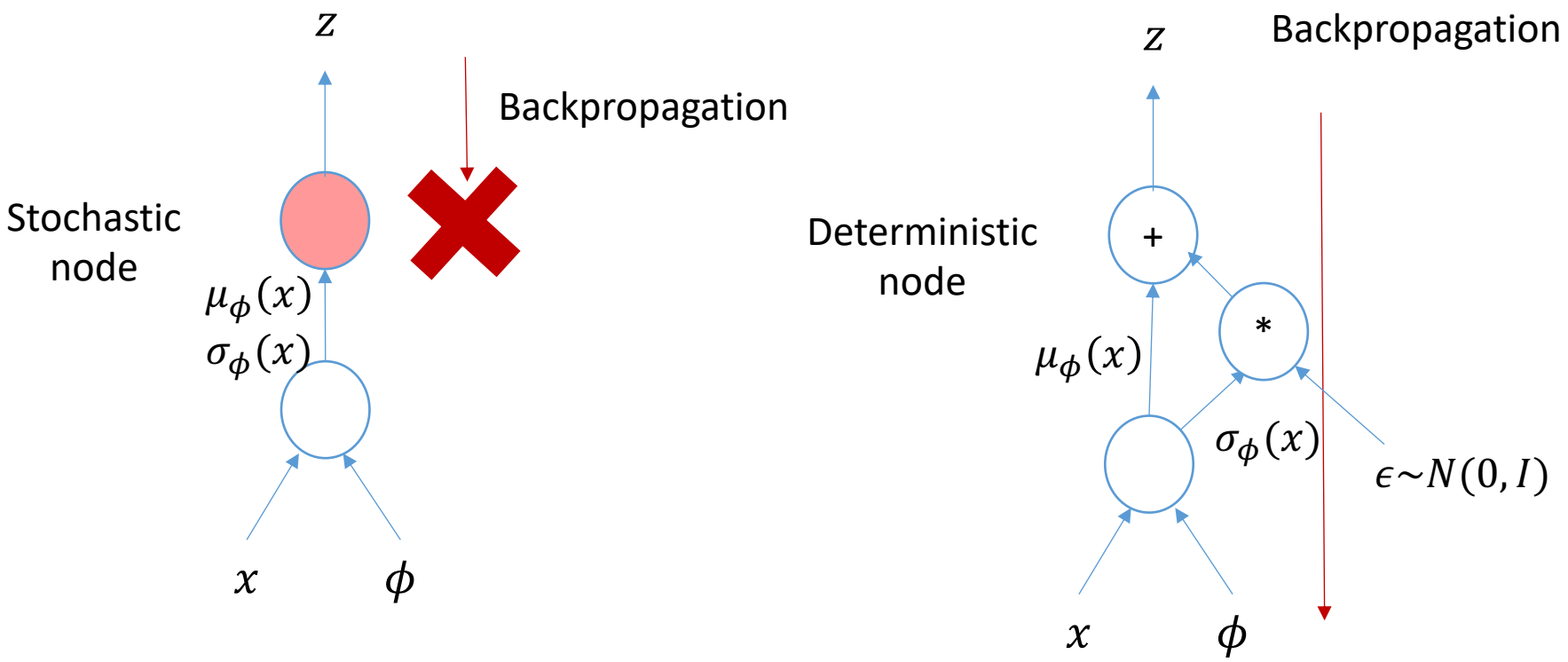
This slide has been adapted from Chelsea Finn, CS330

Reparameterizing the sampling layer



Reparameterization trick

Reparameterizing the sampling layer



Optimizing the ELBO

Need to compute

$$\nabla_{\phi,\theta}\mathbb{E}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] \approx \nabla_{\phi,\theta}\hat{\mathbb{E}}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]$$

Reparameterization Trick:

$$\tilde{z} = \mu_\phi(x) + \epsilon\sigma_\phi(x), \text{ where } \epsilon \sim \mathcal{N}(0, I)$$

This slide has been adapted from Chelsea Finn, CS330

Optimizing the ELBO

Need to compute

$$\nabla_{\phi,\theta}\mathbb{E}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] \approx \nabla_{\phi,\theta}\hat{\mathbb{E}}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)]$$

Reparameterization Trick:

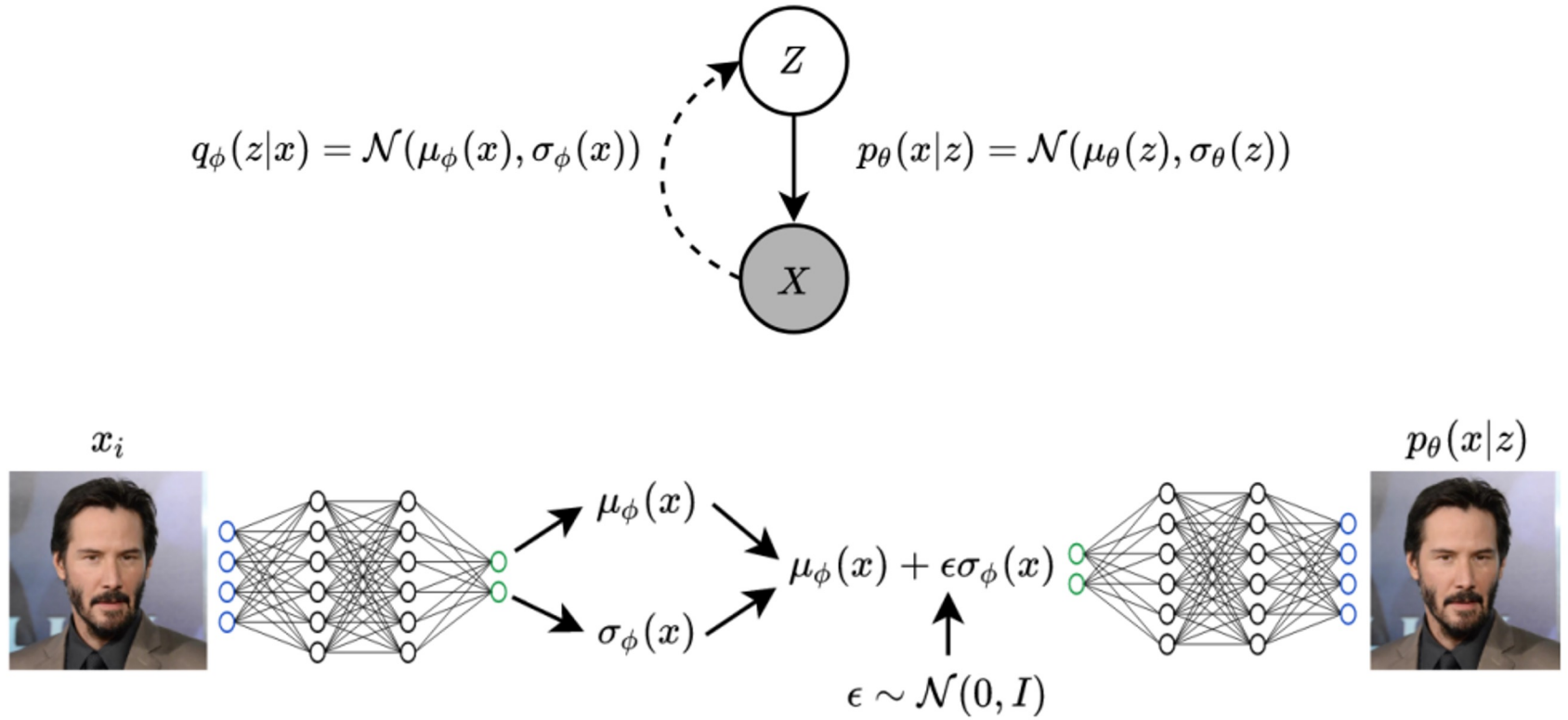
$$\tilde{z} = \mu_\phi(x) + \epsilon\sigma_\phi(x), \text{ where } \epsilon \sim \mathcal{N}(0, I)$$

$$\nabla_{\phi,\theta}\mathbb{E}_{z\sim q_\phi(z|x)}[\log p_\theta(x|z)] \approx \nabla_{\phi,\theta}\frac{1}{M}\sum_{j=1}^{M}\log p_\theta(x|\underbrace{\mu_\phi(x) + \epsilon^{(j)}\sigma_\phi(x)}_{\tilde{z}^{(j)}\sim\mathcal{N}(\mu_\phi(x),\sigma_\phi(x))})$$

In practice usually $M = 1$.

This slide has been adapted from Chelsea Finn, CS330

Variational Auto Encoder (VAE)

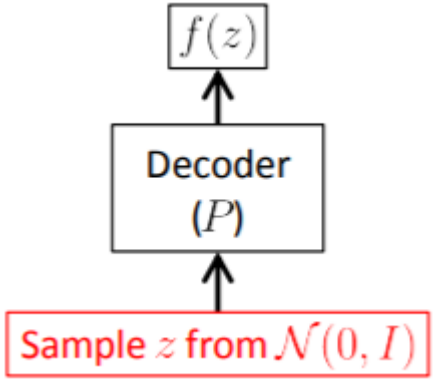


$$\max_{\phi,\theta} \frac{1}{N} \sum_{i=1}^{N} \log p_\theta(x_i|\mu_\phi(x) + \epsilon\sigma_\phi(x)) - \mathbb{D}_{KL}[\mathcal{N}(\mu_\phi(x_i), \sigma_\phi(x_i))||\mathcal{N}(0, I)]$$

This slide has been adapted from Chelsea Finn, CS330

Generate Image: At Test Time

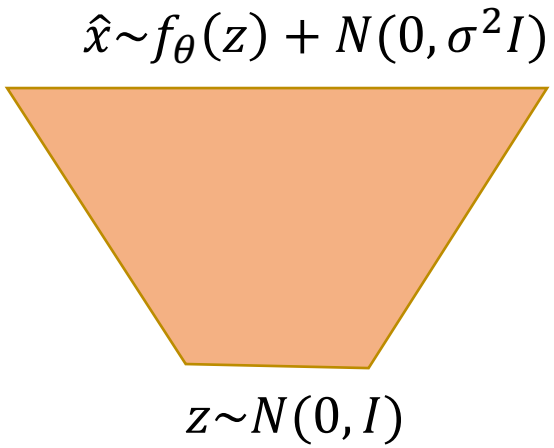
- Remove the Encoder
- Sample z ~ N(0,I) and pass it through the Decoder.
- No good quantitative metric, relies on visual inspection

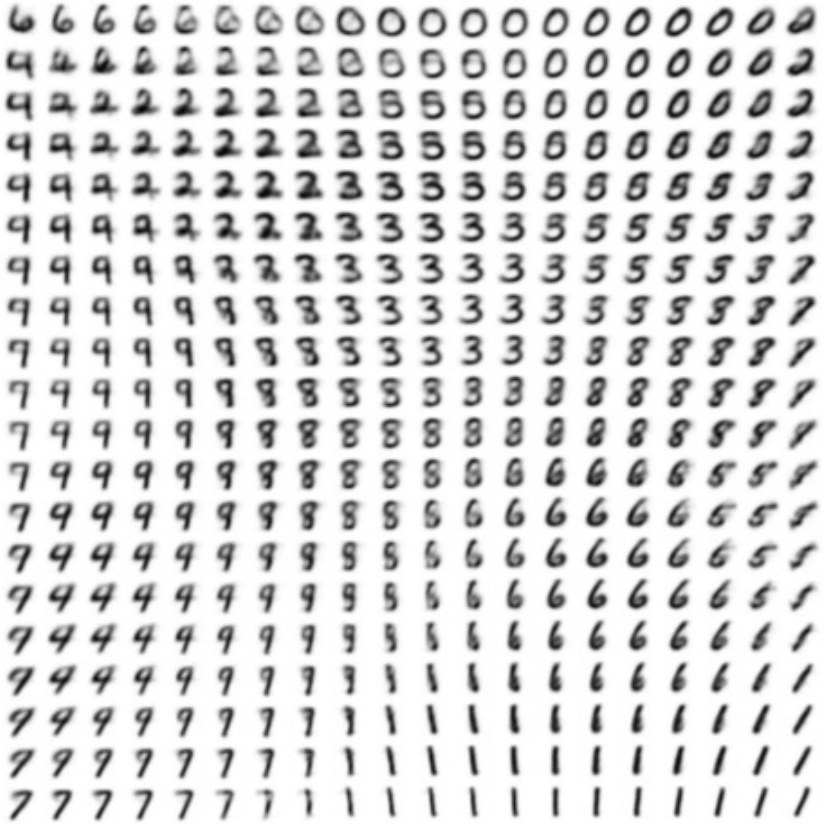


Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

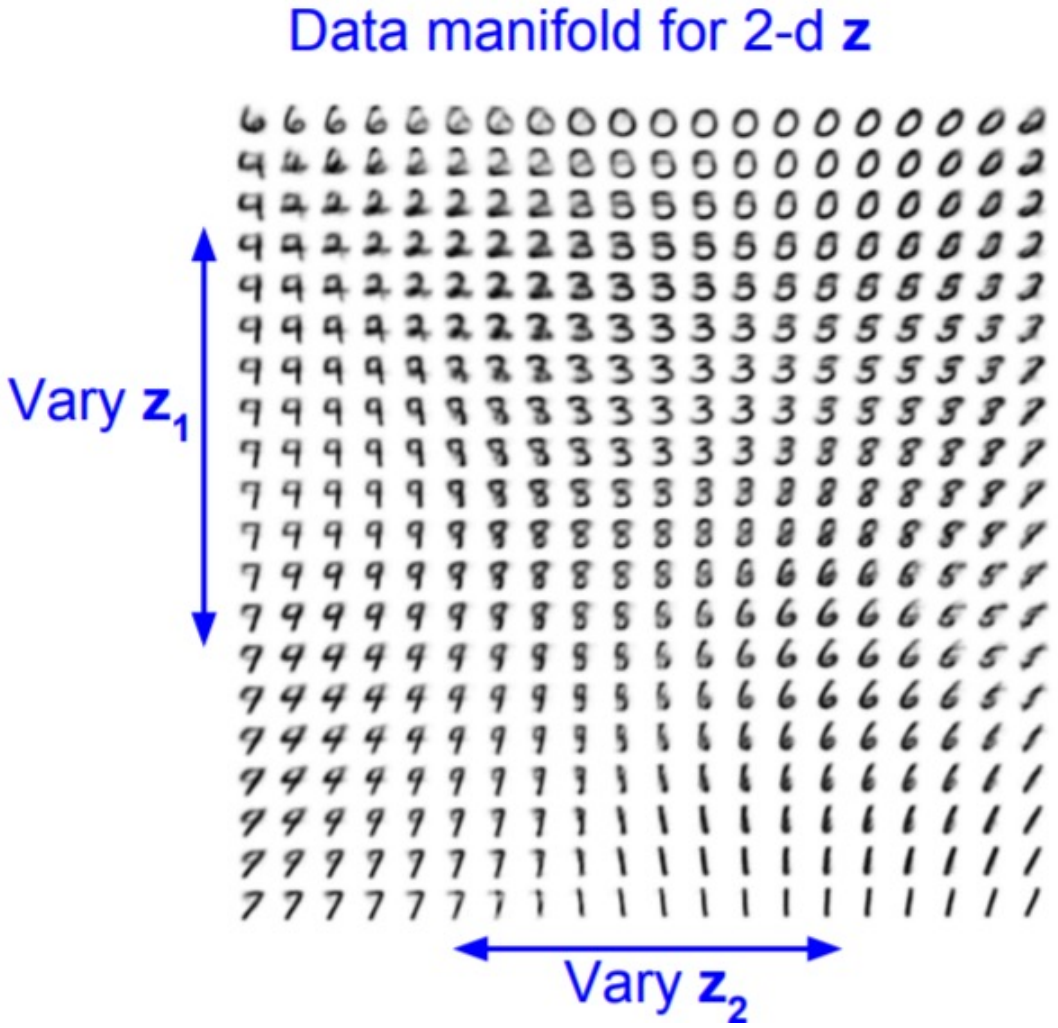
- Sample from the prior and use the decoder to generate an image





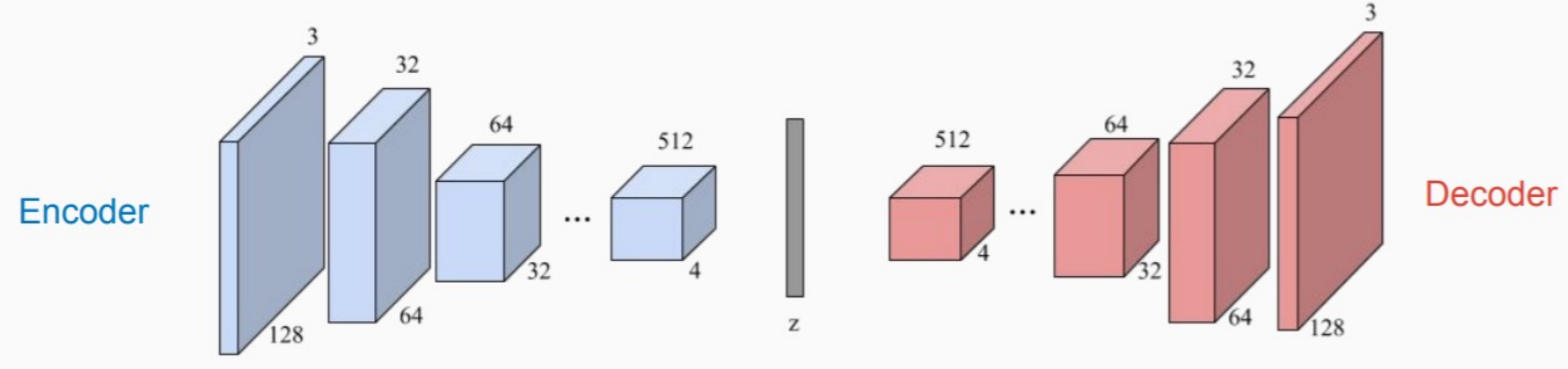
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!



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

Common VAE Architecture for Image Generation



Variational Autoencoders: Generating Data!

32x32 CIFAR-10

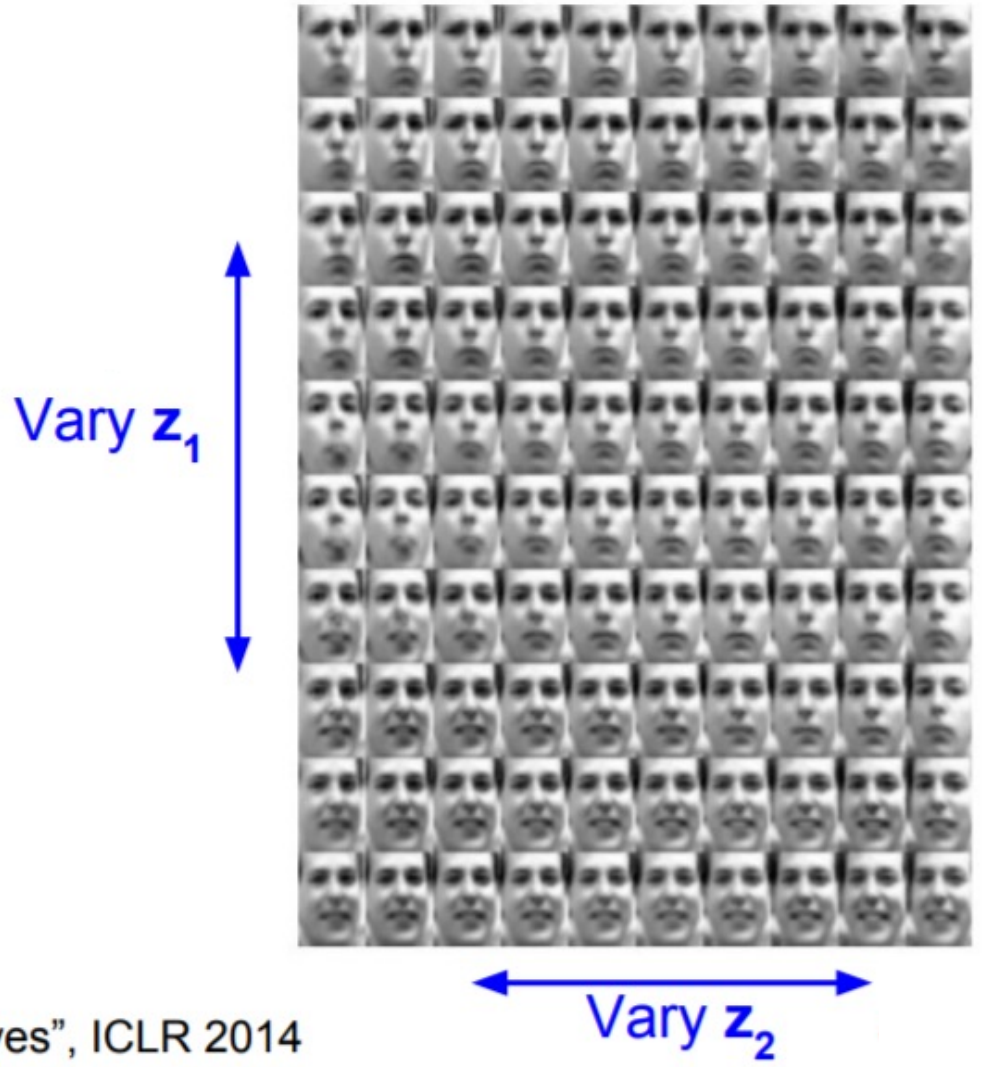
Labeled Faces in the Wild

VAE: Factors of variations

- When different dimensions of latent space encode different interpretable latent variables, it is pleasant

- Latent perturbation: slowly change a latent variable while keeping fixed others

Variational Autoencoders: Generating Data!

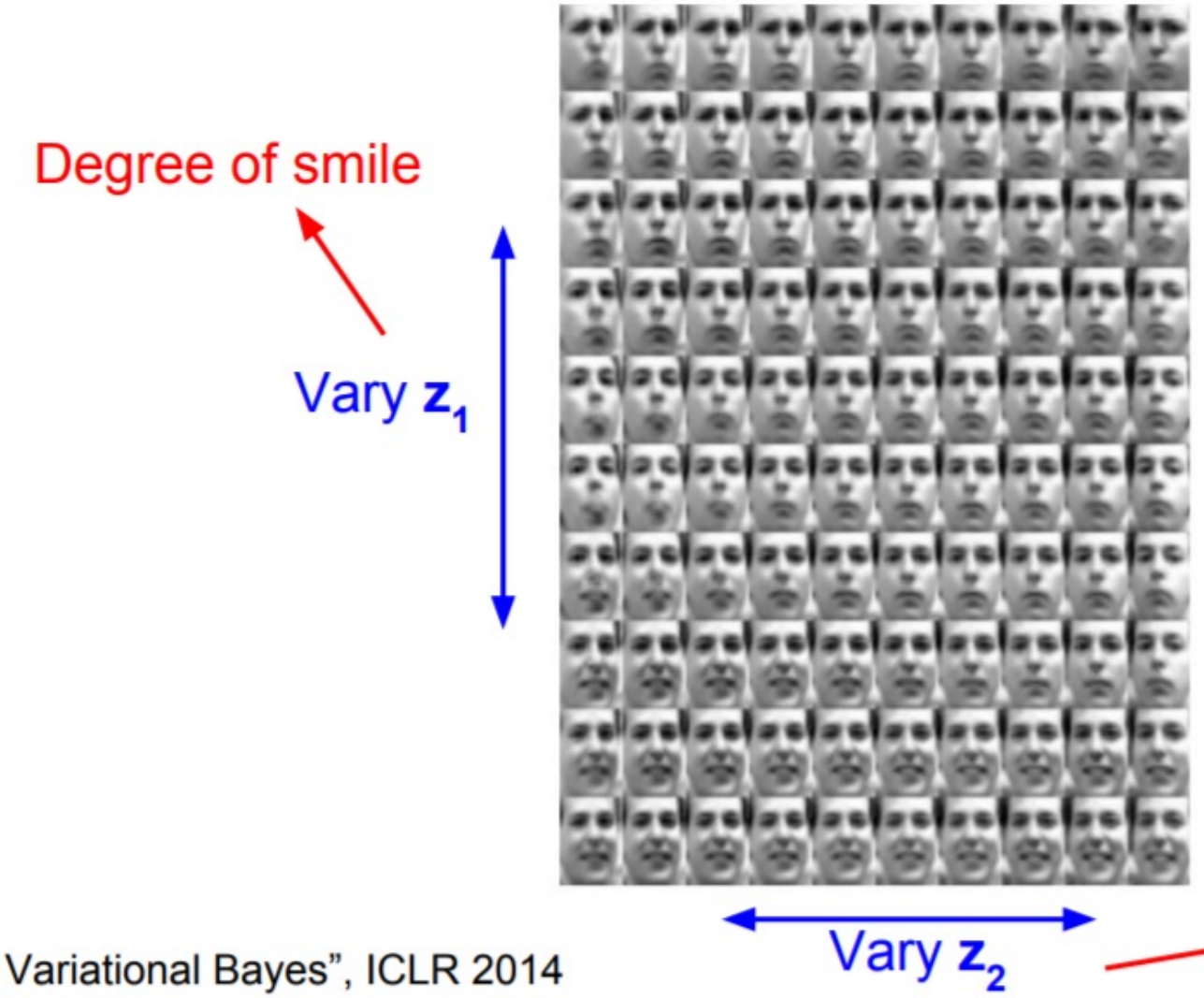


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

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

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



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

Disentanglement

- Disentanglement: Ideally, we want independent latent variables
- Enforce the diagonal prior on the latent variables to encourage independence

Beta-VAE

- Beta-VAE loss: $\beta > 1$

$$\sum_{i=1}^{n} E_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta\left(x^{(i)}|z\right)\right] - \beta \sum_{i=1}^{n} D_{KL}\left(q_\phi\left(z|x^{(i)}\right)||p_\theta(z)\right)$$

Higgins et al., ICLR 2017

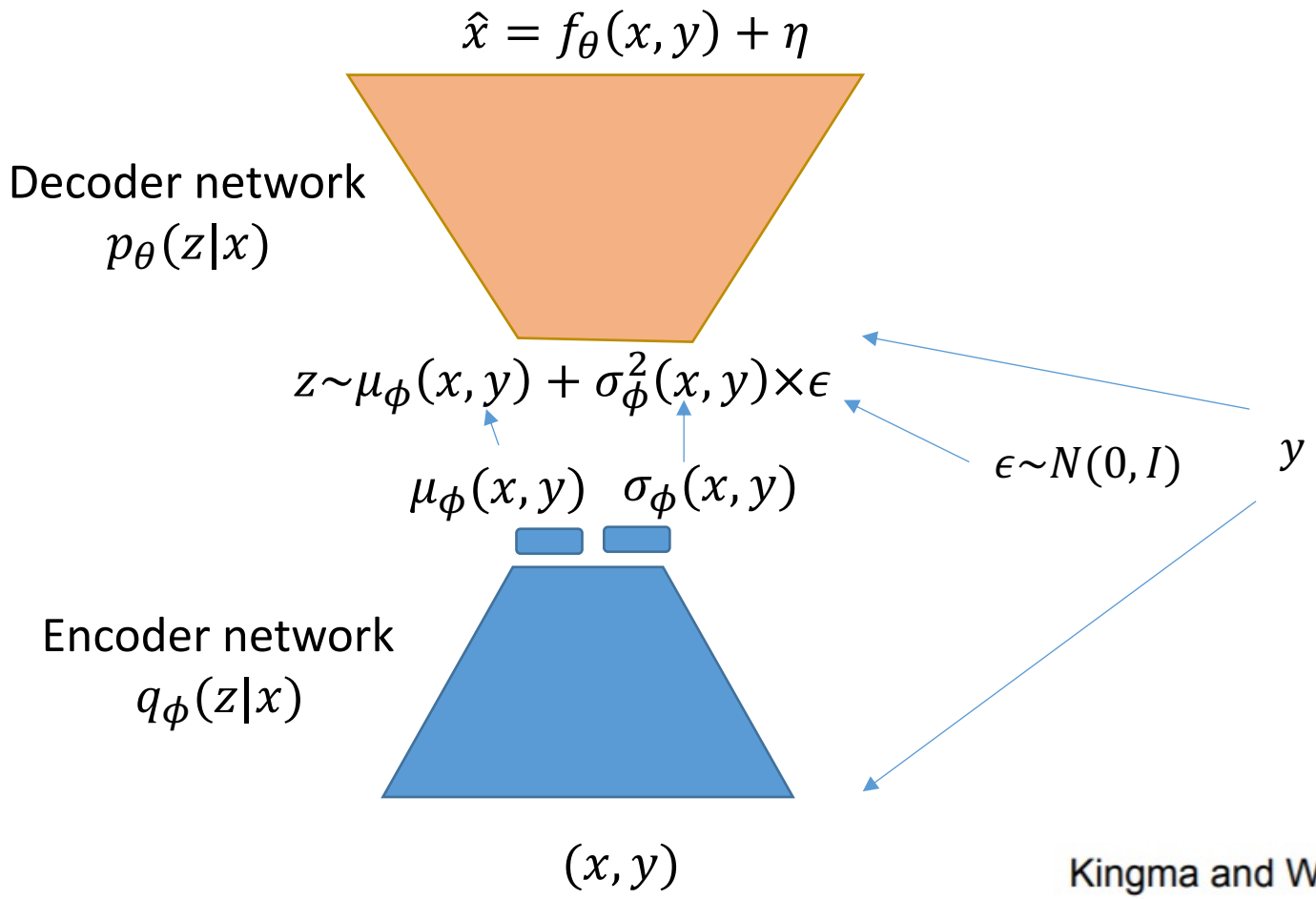
Beta-VAE

- β=250

Higgins et al., ICLR 2017

Conditional VAE (CVAE)

- Replace all p(x|z) with p(x|z,y)
- Replace all q(z|x) with q(z|x,y).



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

CVAE

Go through the same KL divergence procedure, to get the same lower bound.

Lower bound of log conditional likelihood:

$$\log p(x|y) - D_{KL}\big(q(z|y,x)||p(z|y,x)\big)$$
$$= E_{z\sim q(z|x,y)}[\log p(x|y,z)] - D_{KL}\big(q(z|y,x)||p(z)\big)$$

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

Variational Autoencoders

- Probabilistic spin to traditional autoencoders => allows generating data
- Defines an intractable density => derive and optimize a (variational) lower bound
- Pros:
  - Principled approach to generative models
  - Allows inference of q(z|x), can be useful feature representation for other tasks
- Cons:
  - Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
  - Samples blurrier and lower quality compared to state-of-the-art (GANs and diffusion models)
- Active areas of research:
  - More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian
  - Incorporating structure in latent variables

Explicit Generative Models: So far

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

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

VAEs define intractable density function with latent **z**:

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

Cannot optimize directly, derive and optimize lower bound on likelihood instead