

Outline

- Generative Models Basics
- Autoregressive Models
- **Autoencoder and Variational Autoencoder**
- Generative Adversarial Network
- Diffusion Models

So far...

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

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

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

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

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

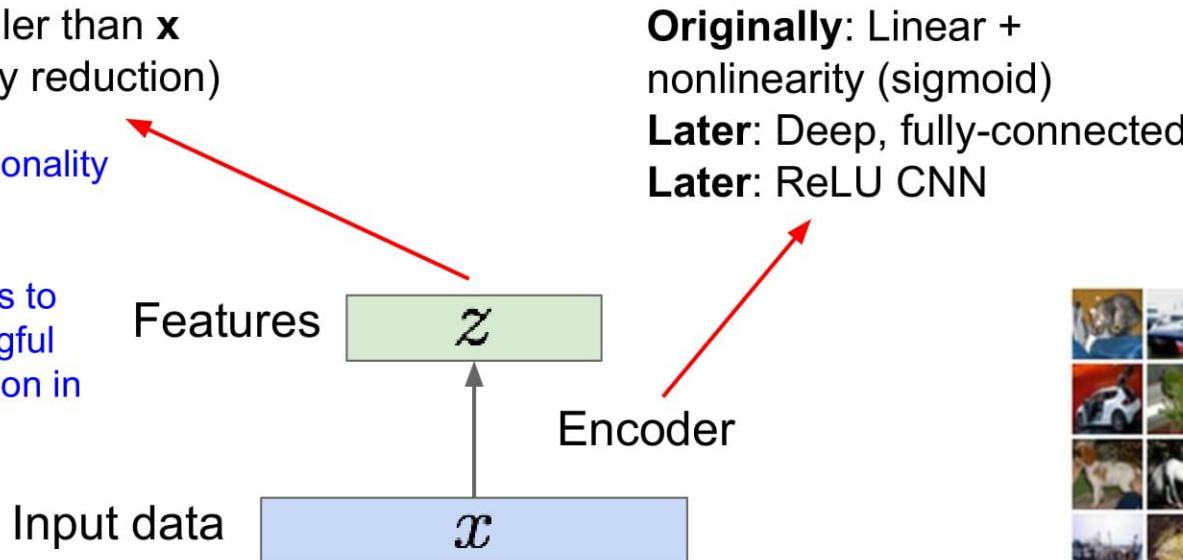
Some background first: Autoencoders

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

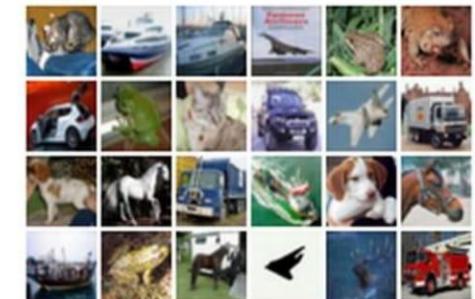
z usually smaller than x
(dimensionality reduction)

Q: Why dimensionality reduction?

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



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

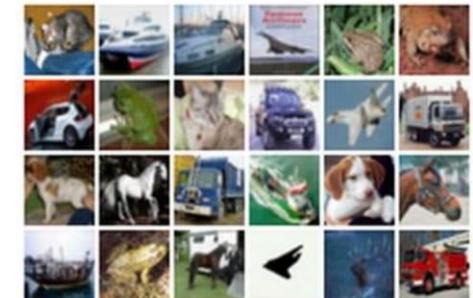
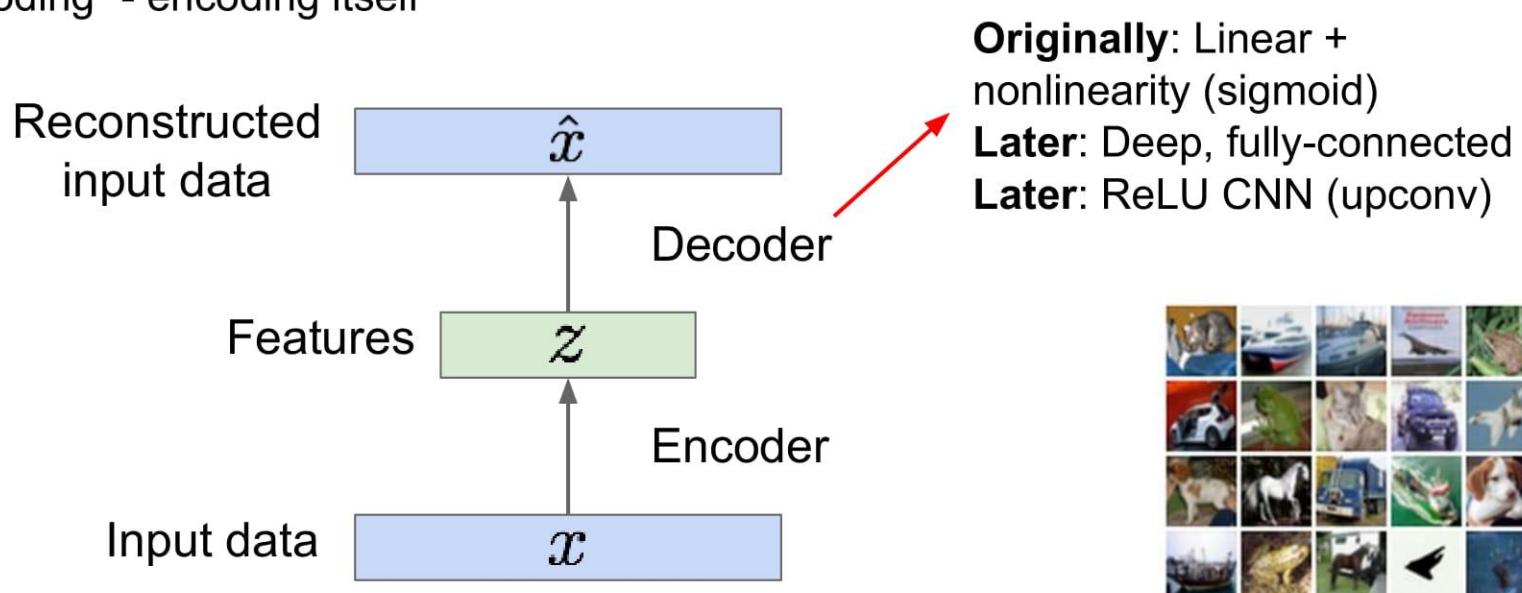


Some background first: Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data

“Autoencoding” - encoding itself

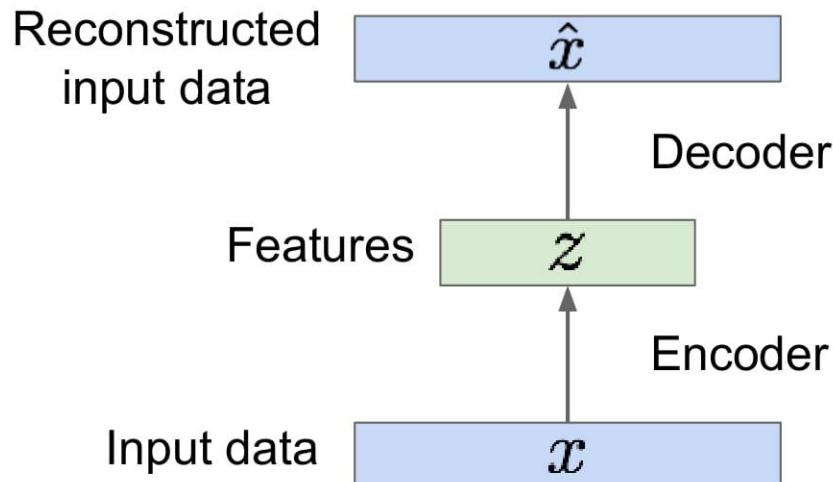


Some background first: Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data

“Autoencoding” - encoding itself



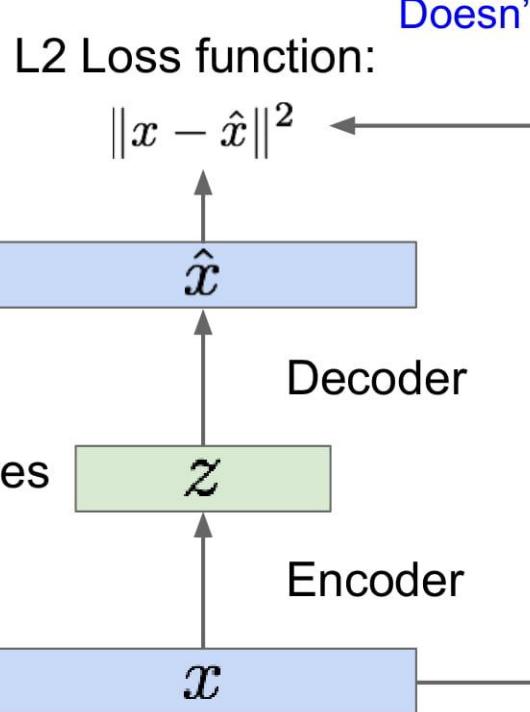
Some background first: Autoencoders

Train such that features
can be used to
reconstruct original data

Reconstructed
input data

Features

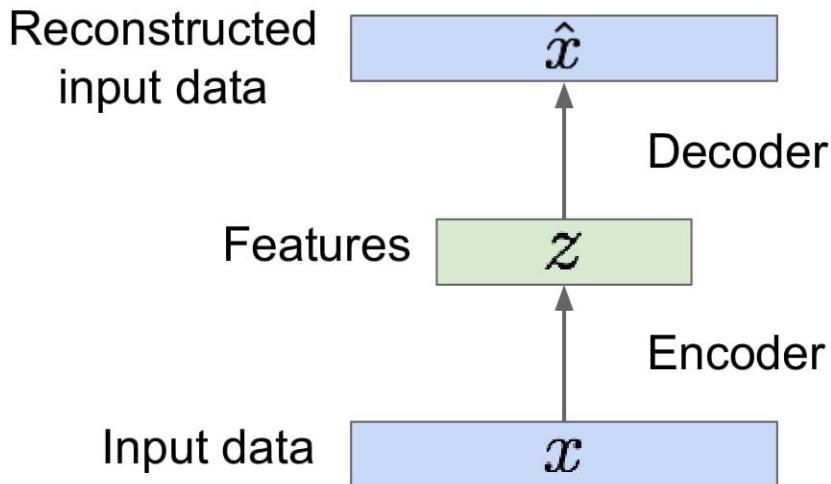
Input data



Doesn't use labels!



Some background first: Autoencoders



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

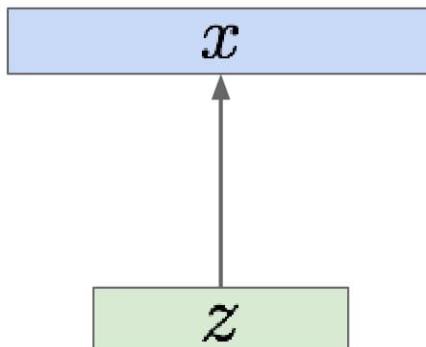
Features capture factors of variation in training data. Can we generate new images from an autoencoder?

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



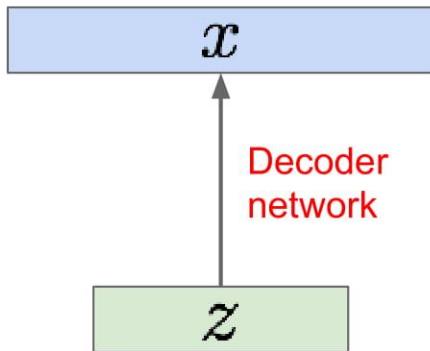
Intuition (remember from autoencoders!):
 x is an image, z is latent factors used to generate x : attributes, orientation, etc.

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

Variational Autoencoders

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

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.

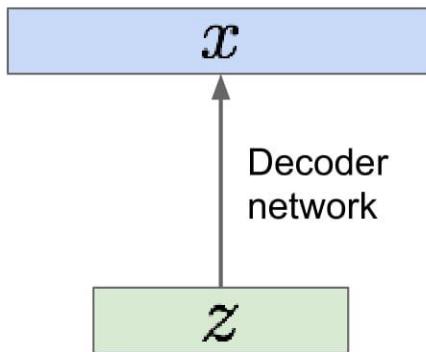
Conditional $p(x|z)$ is complex (generates
image) => represent with neural network

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

Variational Autoencoders

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

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



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

How to train the model?

Learn model parameters to maximize likelihood of training data

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

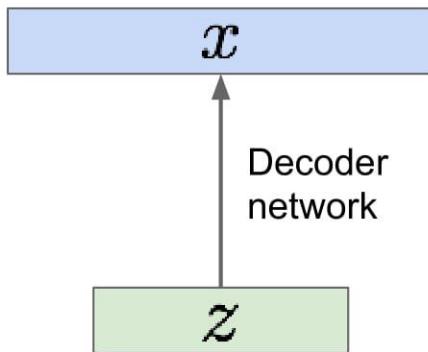
Now with latent z

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

Variational Autoencoders

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

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



We want to estimate 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: $p_{\theta}(x) = \int p_{\theta}(z)p_{\theta}(x|z)dz$

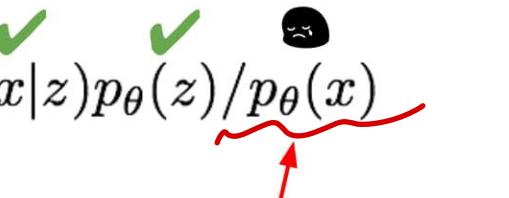
The diagram shows a black silhouette of a person's head at the top left. A red curved arrow originates from the head and points to a red wavy bracket that encloses the term $p_{\theta}(x|z)$. Inside this bracket, the text "Intractible to compute $p(x|z)$ for every z !" is written in red. Above the bracket, there are two green checkmarks. To the right of the bracket, the word "gaussian" is written in blue. A blue curved arrow originates from the right side of the bracket and points to the word "gaussian". Above the entire equation, the text "decoder NN, defined" is written in blue.

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

Variational Autoencoders: Intractability

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

Posterior density also intractable: $p_{\theta}(z|x) = p_{\theta}(x|z)p_{\theta}(z)/p_{\theta}(x)$



Intractable data likelihood

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

Variational Autoencoders: Intractability

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

Posterior density also intractable: $p_{\theta}(z|x) = p_{\theta}(x|z)p_{\theta}(z)/p_{\theta}(x)$

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

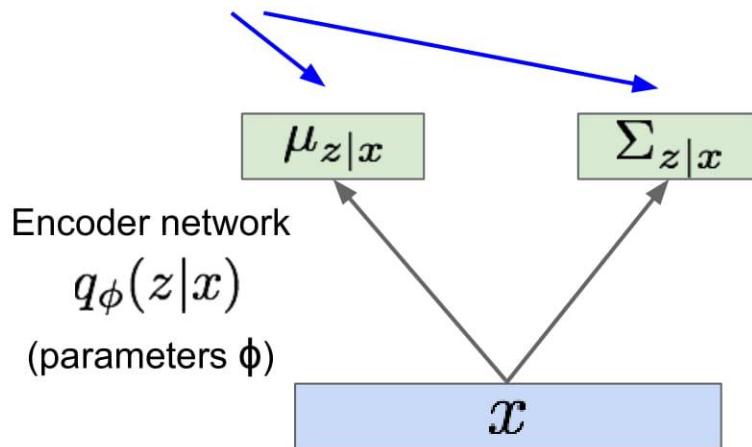
Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

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

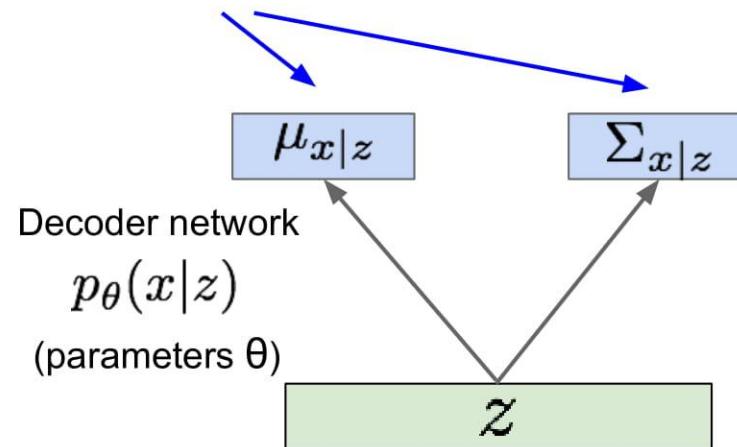
Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic

Mean and (diagonal) covariance of $z | x$



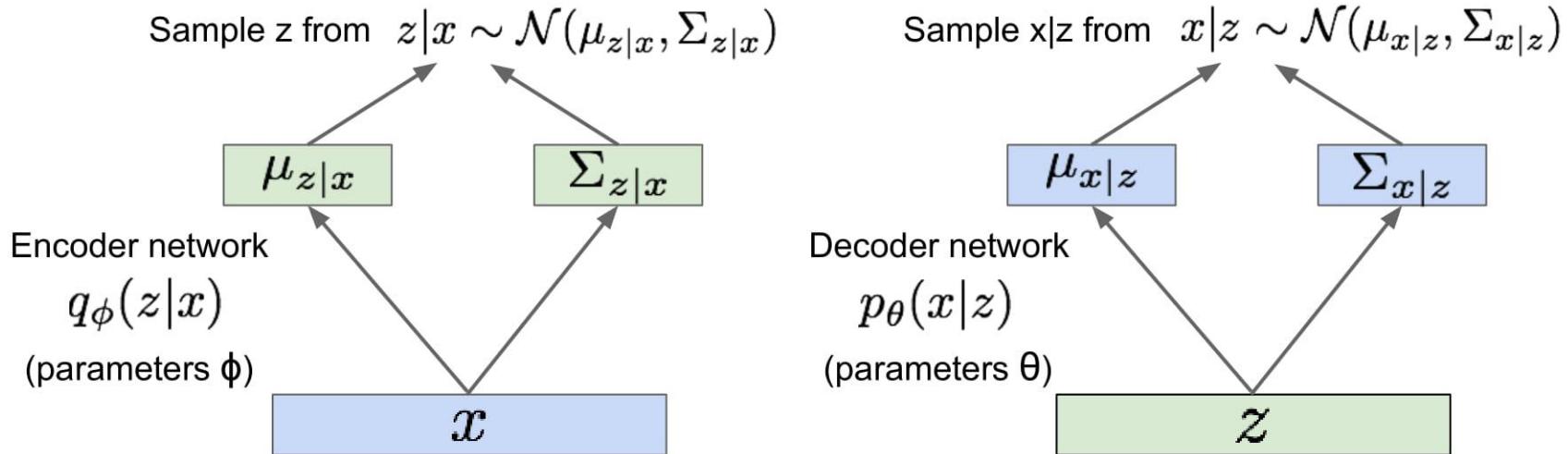
Mean and (diagonal) covariance of $x | z$



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

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



Encoder and decoder networks also called
“recognition”/“inference” and “generation” networks

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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


Taking expectation wrt. z
(using encoder network) will
come in handy later

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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



The expectation wrt. z (using encoder network) let us write nice KL terms

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

↑
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 .

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\begin{aligned}\log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})} [\log p_\theta(x^{(i)})] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \right] \quad (\text{Bayes' Rule}) \\ &= \mathbf{E}_z \left[\log \frac{p_\theta(x^{(i)} | z)p_\theta(z)}{p_\theta(z | x^{(i)})} \frac{q_\phi(z | x^{(i)})}{q_\phi(z | x^{(i)})} \right] \quad (\text{Multiply by constant}) \\ &= \mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z)} \right] + \mathbf{E}_z \left[\log \frac{q_\phi(z | x^{(i)})}{p_\theta(z | x^{(i)})} \right] \quad (\text{Logarithms}) \\ &= \underbrace{\mathbf{E}_z [\log p_\theta(x^{(i)} | z)] - D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z | x^{(i)}) || p_\theta(z | x^{(i)}))}_{\geq 0}\end{aligned}$$

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

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

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

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

Reconstruct
the input data

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

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

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

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

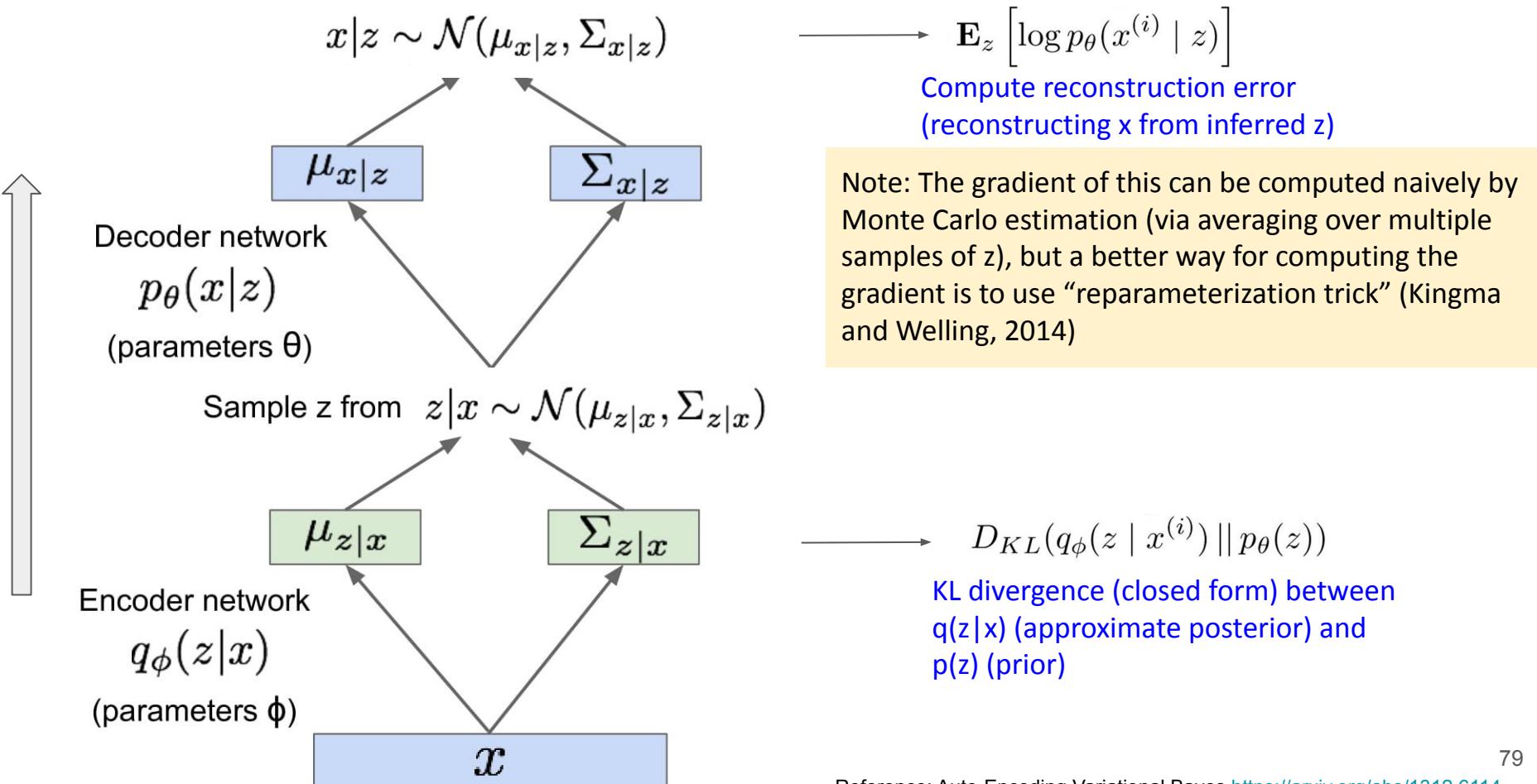
Variational lower bound ("ELBO")

Make approximate posterior distribution close to prior

$$\theta^*, \phi^* = \arg \max_{\theta, \phi} \sum_{i=1}^N \mathcal{L}(x^{(i)}, \theta, \phi)$$

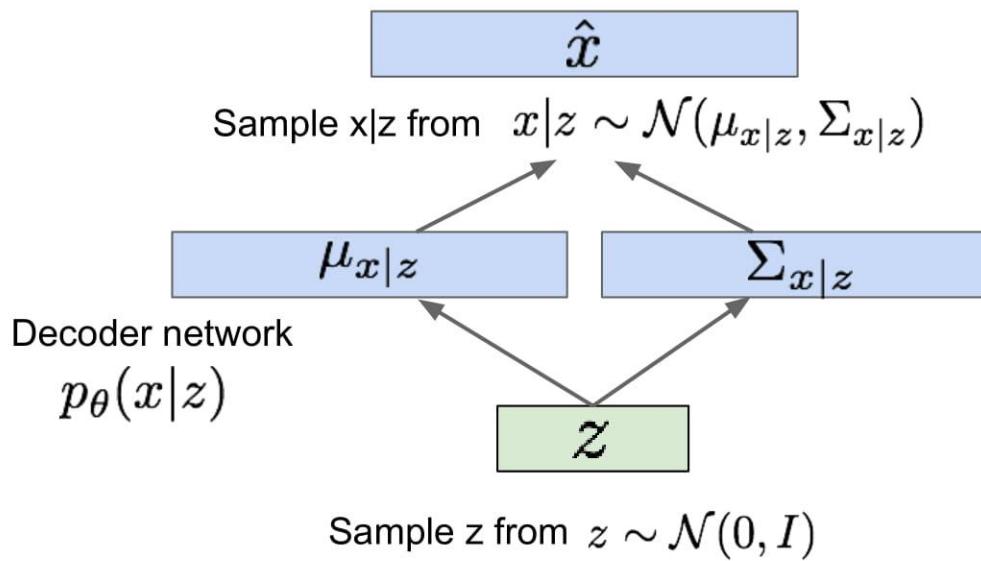
Training: Maximize lower bound

Training objective of VAE: ELBO

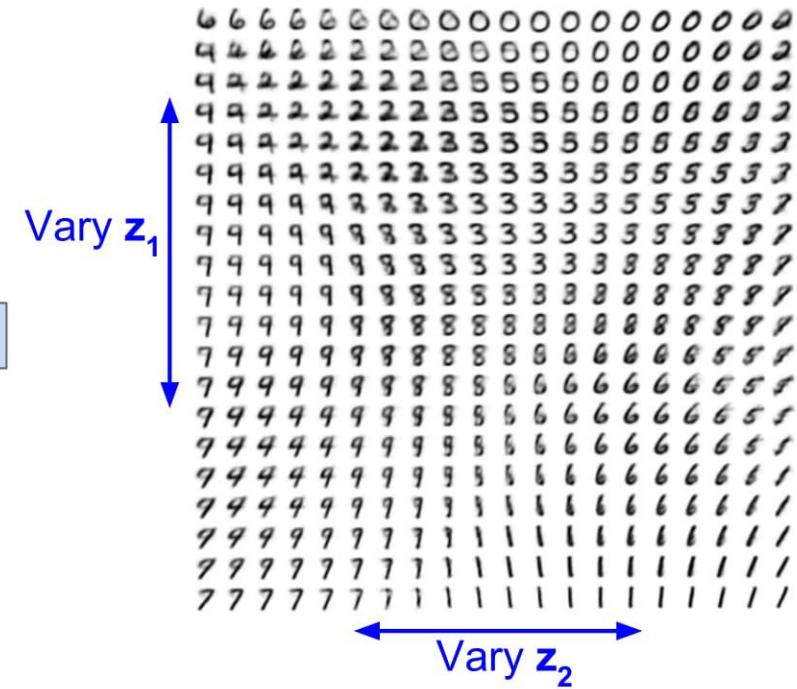


Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Data manifold for 2-d z



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

Variational Autoencoders: Generating Data!

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

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

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

Degree of smile
Vary \mathbf{z}_1



Vary \mathbf{z}_2 Head pose

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

Variational Autoencoder: Summary

Probabilistic spin to traditional autoencoders => allows generating data

Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Allows inference of $q(z|x)$, can be useful feature representation for other tasks

Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Further Extensions:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs)
- Incorporating structure in latent variables, e.g., Categorical Distributions