Deep Learning

Lecture 17

Generative Models

Part 1

Supervised vs Unsupervised Learning

Supervised Learning

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

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

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

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

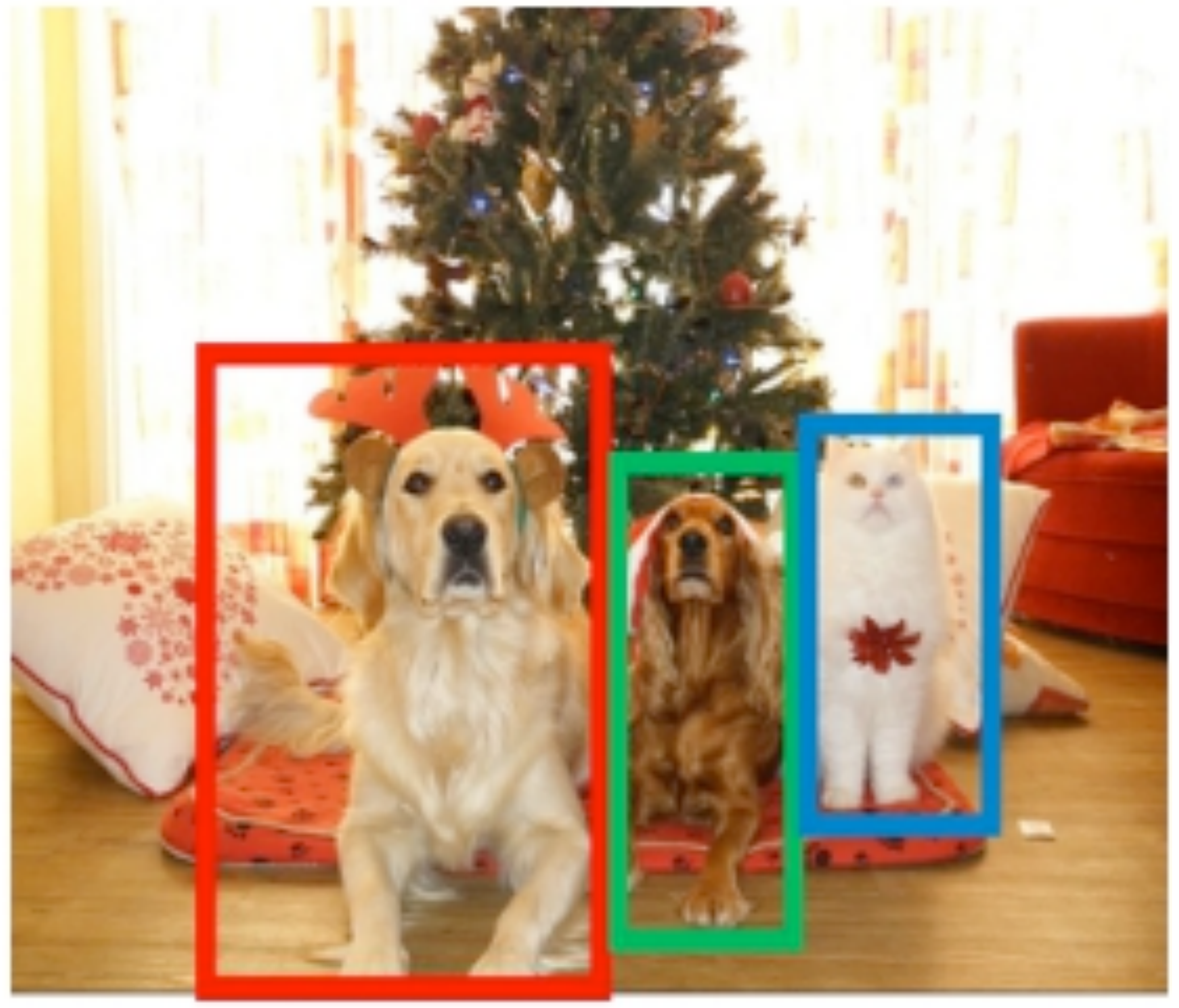
Supervised vs Unsupervised Learning

Supervised Learning

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

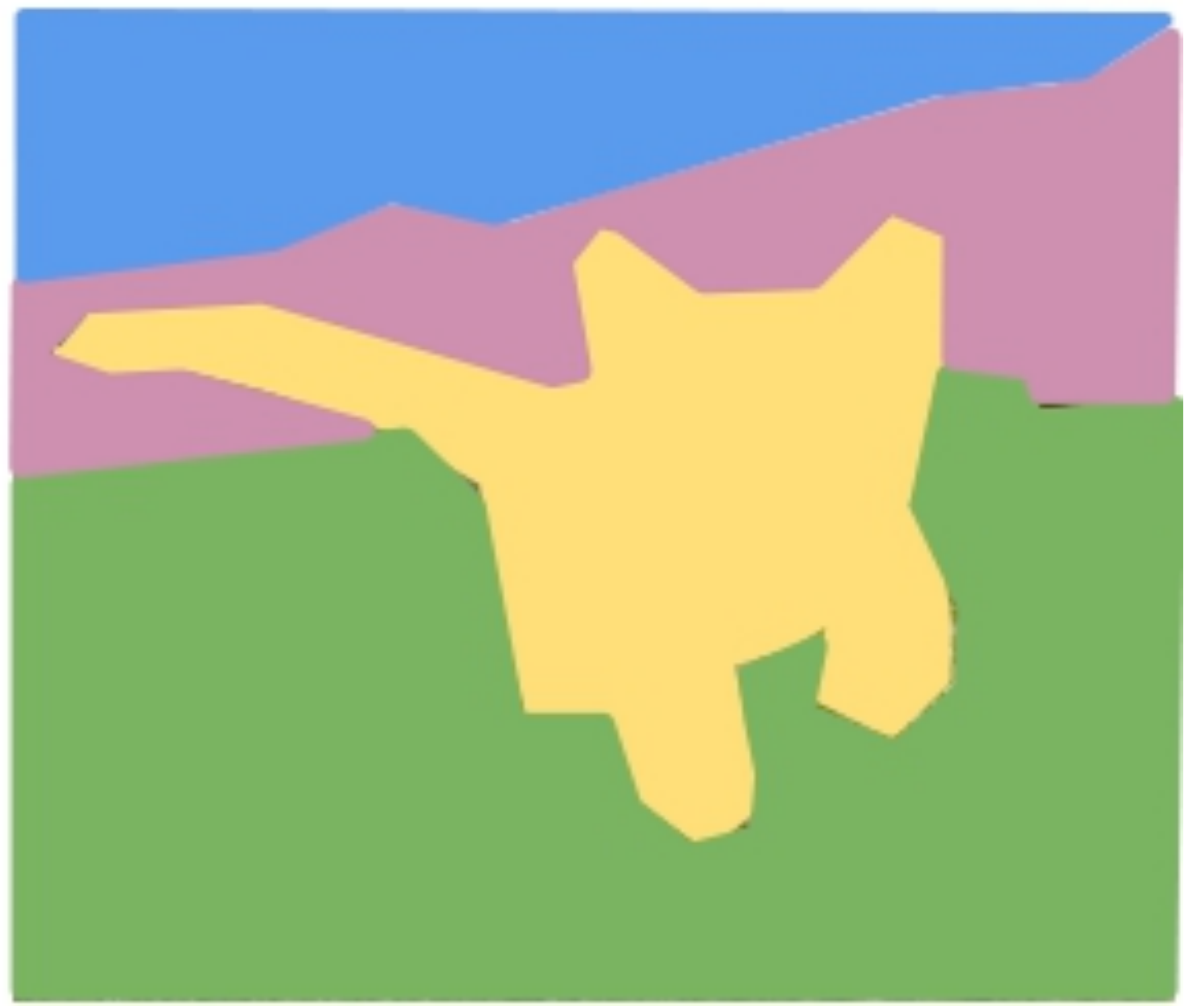
Supervised vs Unsupervised Learning

Supervised Learning

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.



GRASS , CAT , TREE , SKY

Semantic Segmentation

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.

A cat sitting on a suitcase on the floor

Image captioning

Caption generated using neuraltalk2
Image is CC0 Public domain.

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, feature learning, density estimation, etc.

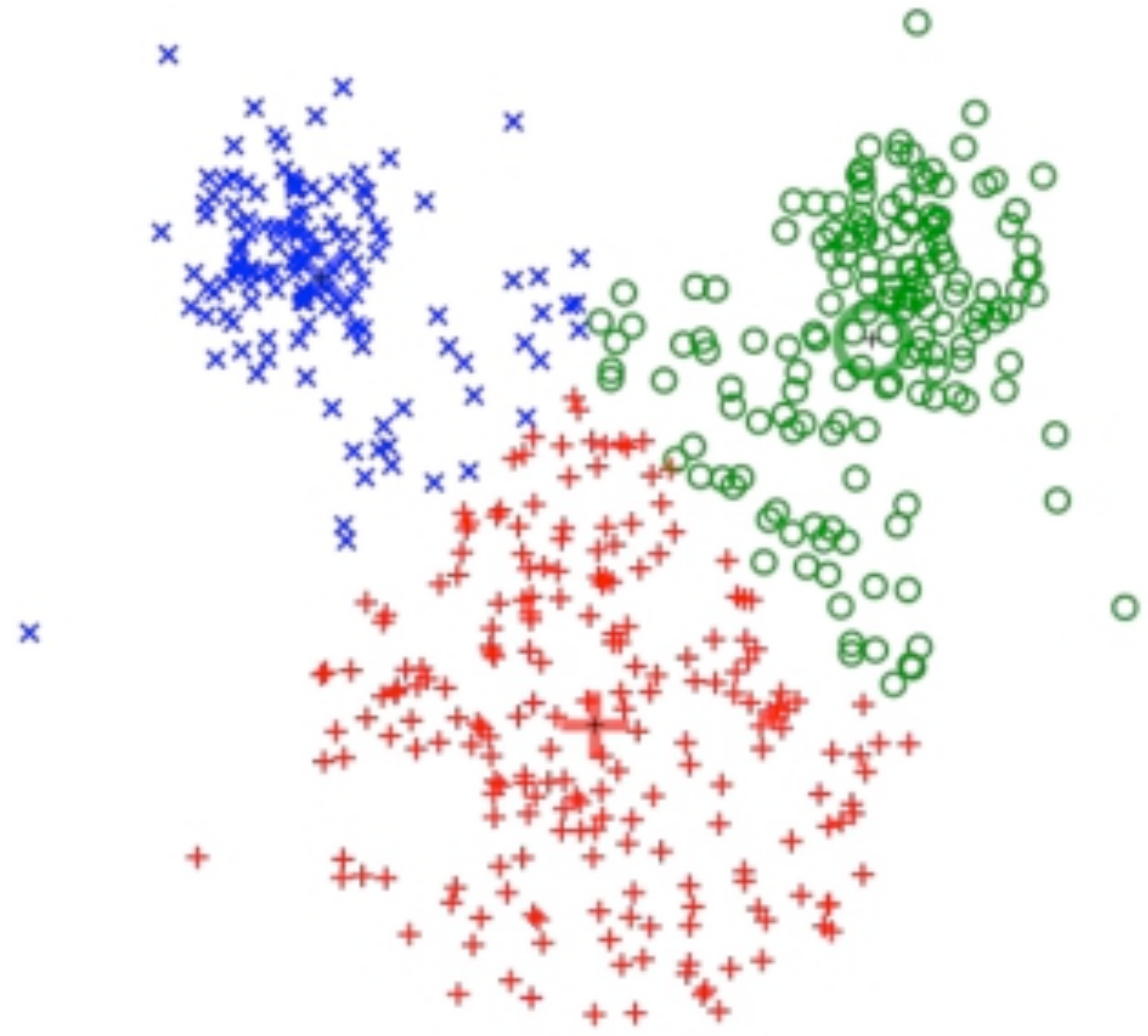
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



K-means clustering

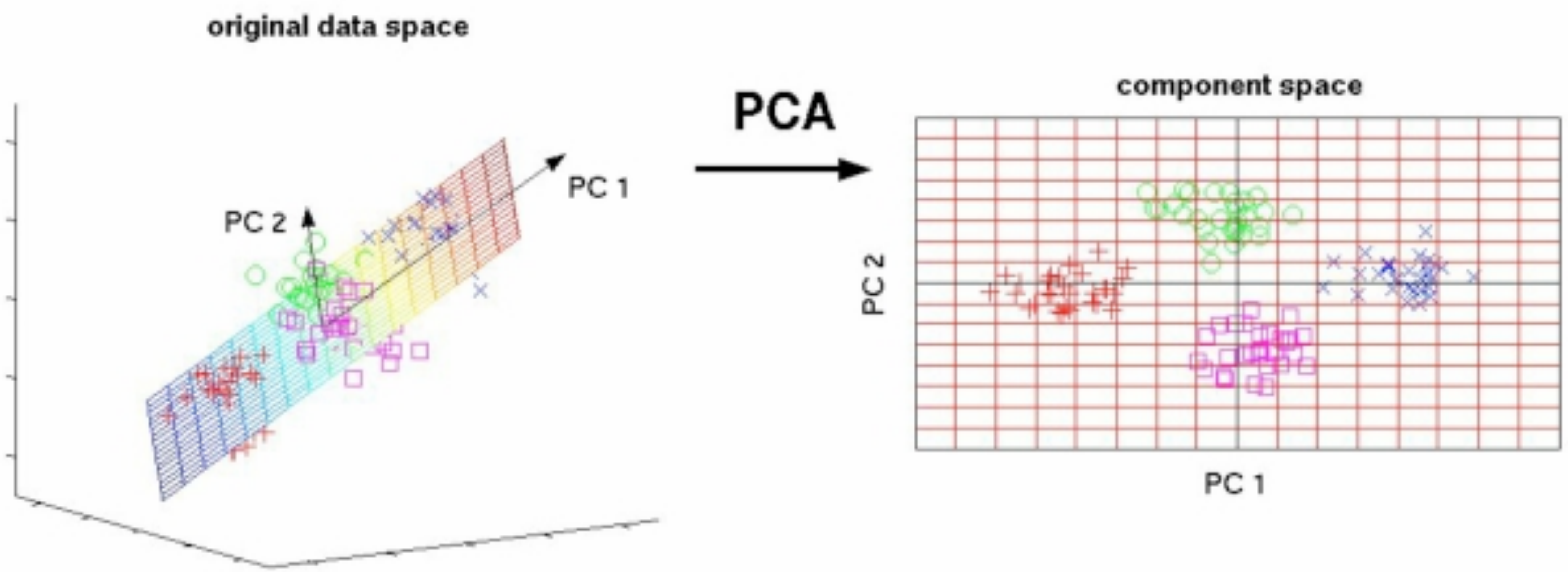
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



3-d → 2-d

Principal Component Analysis
(Dimensionality reduction)

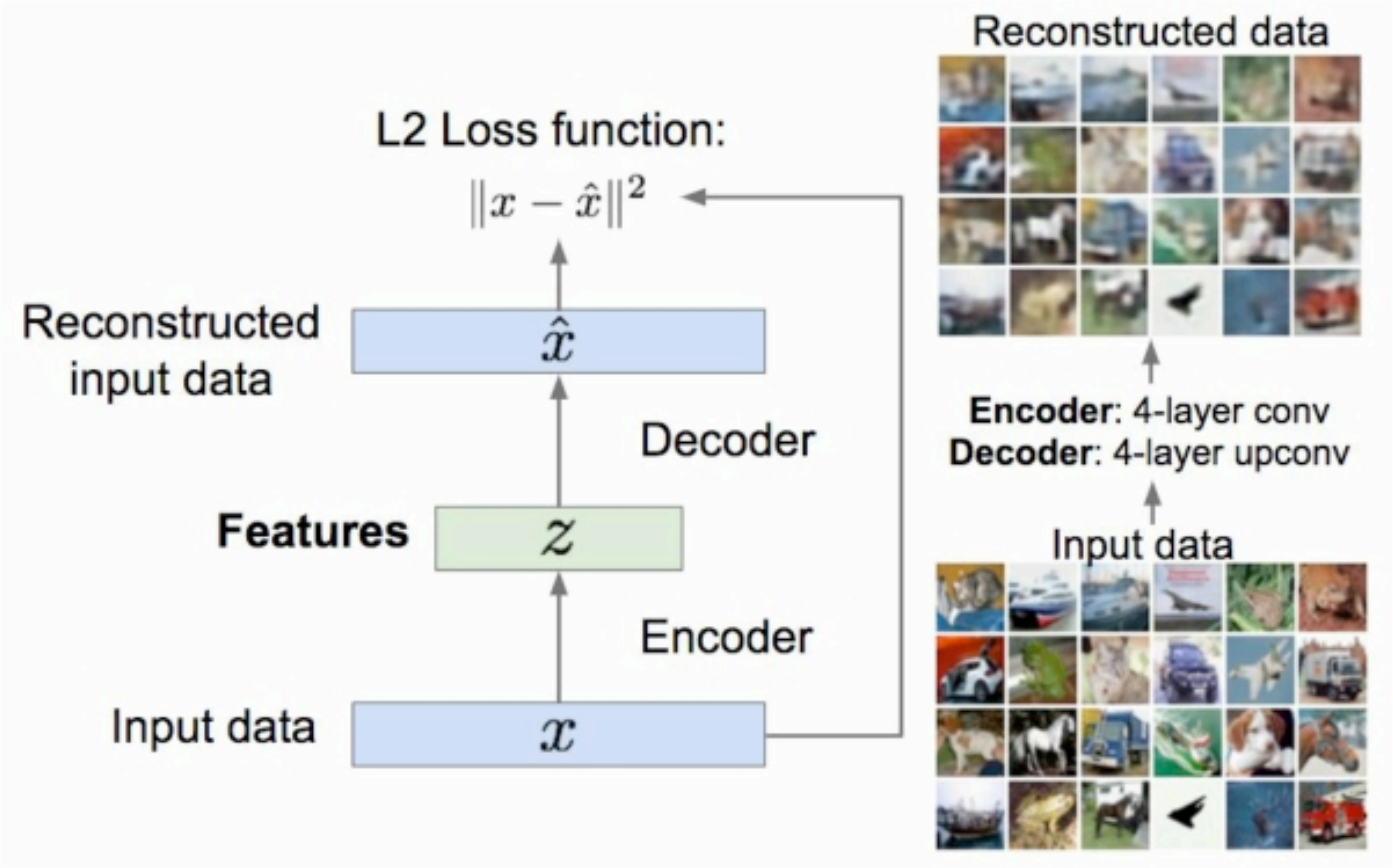
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



Autoencoders
(Feature learning)

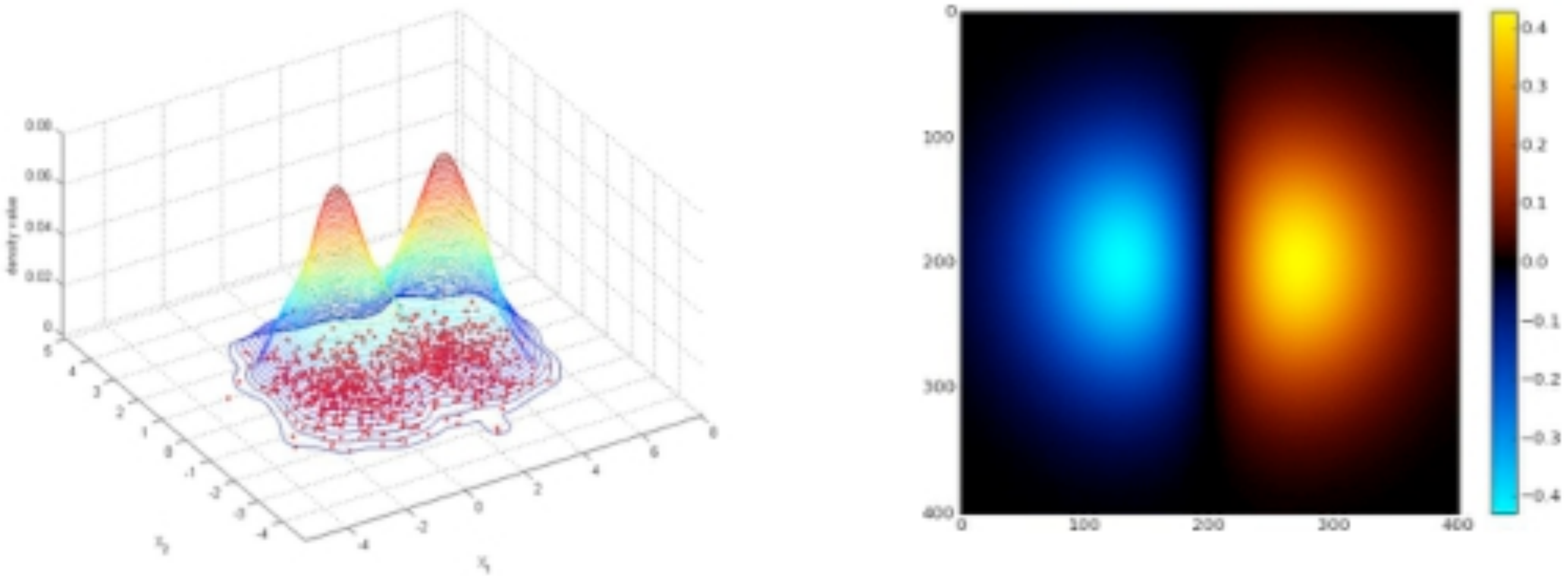
Supervised vs Unsupervised Learning

Unsupervised Learning

Data: x
Just data, no labels!

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

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



2-d density estimation

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.

Unsupervised Learning

Data: x
Just data, no labels!

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

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

Supervised vs Unsupervised Learning

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.

Unsupervised Learning

Training data is cheap

Data: x
Just data, no labels!

Holy grail: Solve unsupervised learning => understand structure of visual world

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

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

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 $p_{data}(x)$

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 $p_{data}(x)$

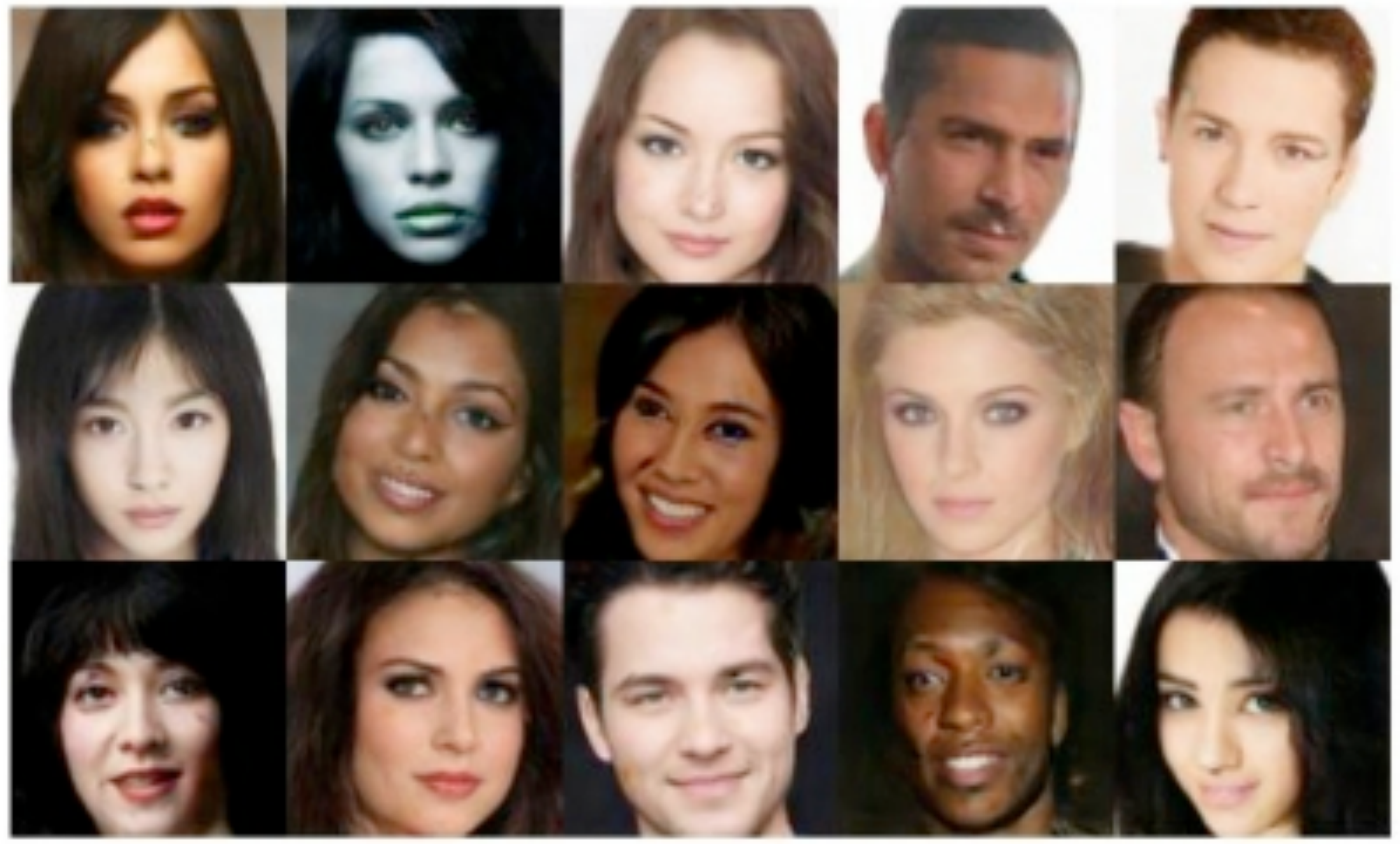
Addresses density estimation, a core problem in unsupervised learning

Several flavors:

- Explicit density estimation: explicitly define and solve for $p_{model}(x)$
- Implicit density estimation: learn model that can sample from $p_{model}(x)$ w/o explicitly defining it

Why Generative Models?

- Realistic samples for artwork, super-resolution, colorization, etc.



- Generative models of time-series data can be used for simulation and planning (reinforcement learning applications!)
- Training generative models can also enable inference of latent representations that can be useful as general features

Taxonomy of Generative Models

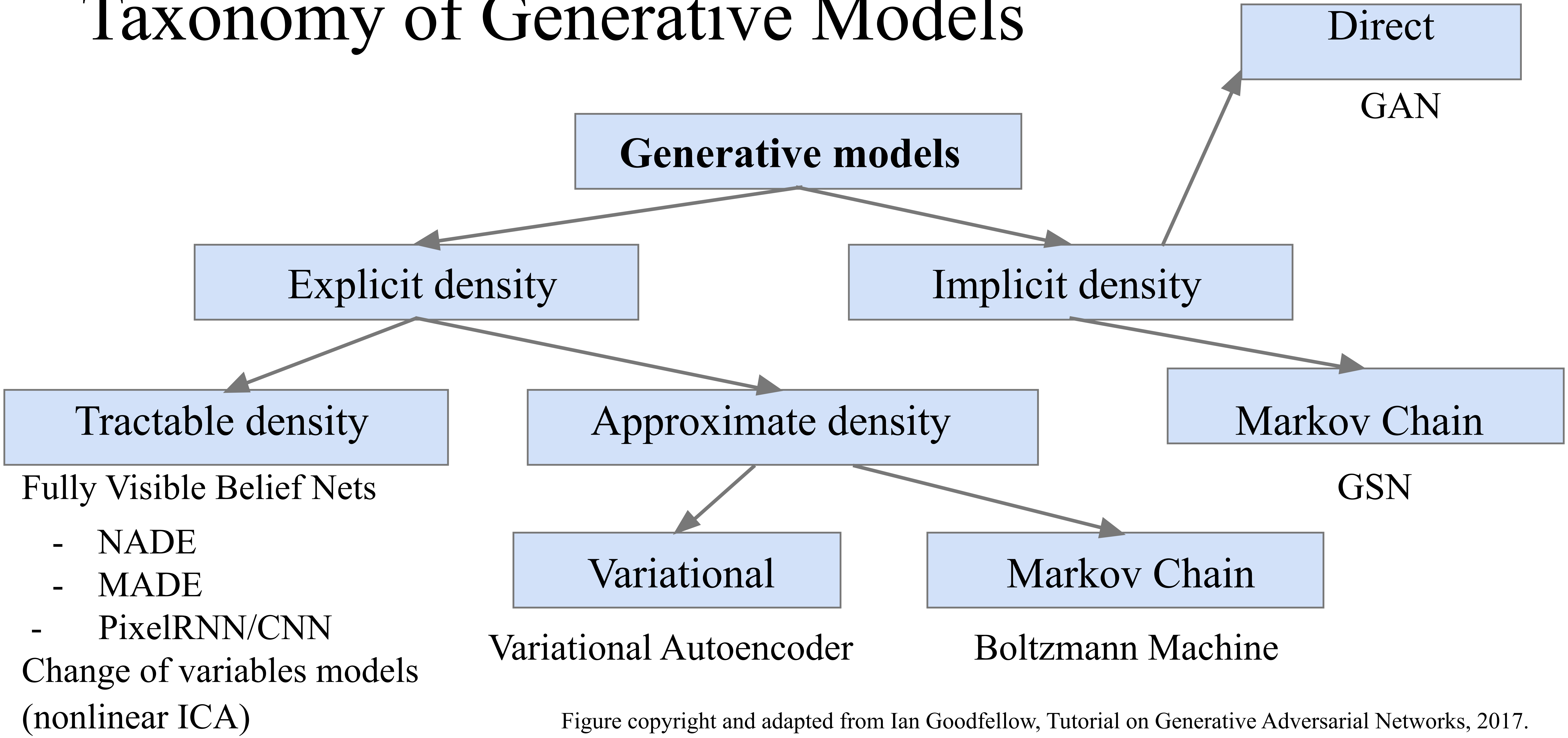


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

Taxonomy of Generative Models

Today: discuss 3 most popular types of generative models today

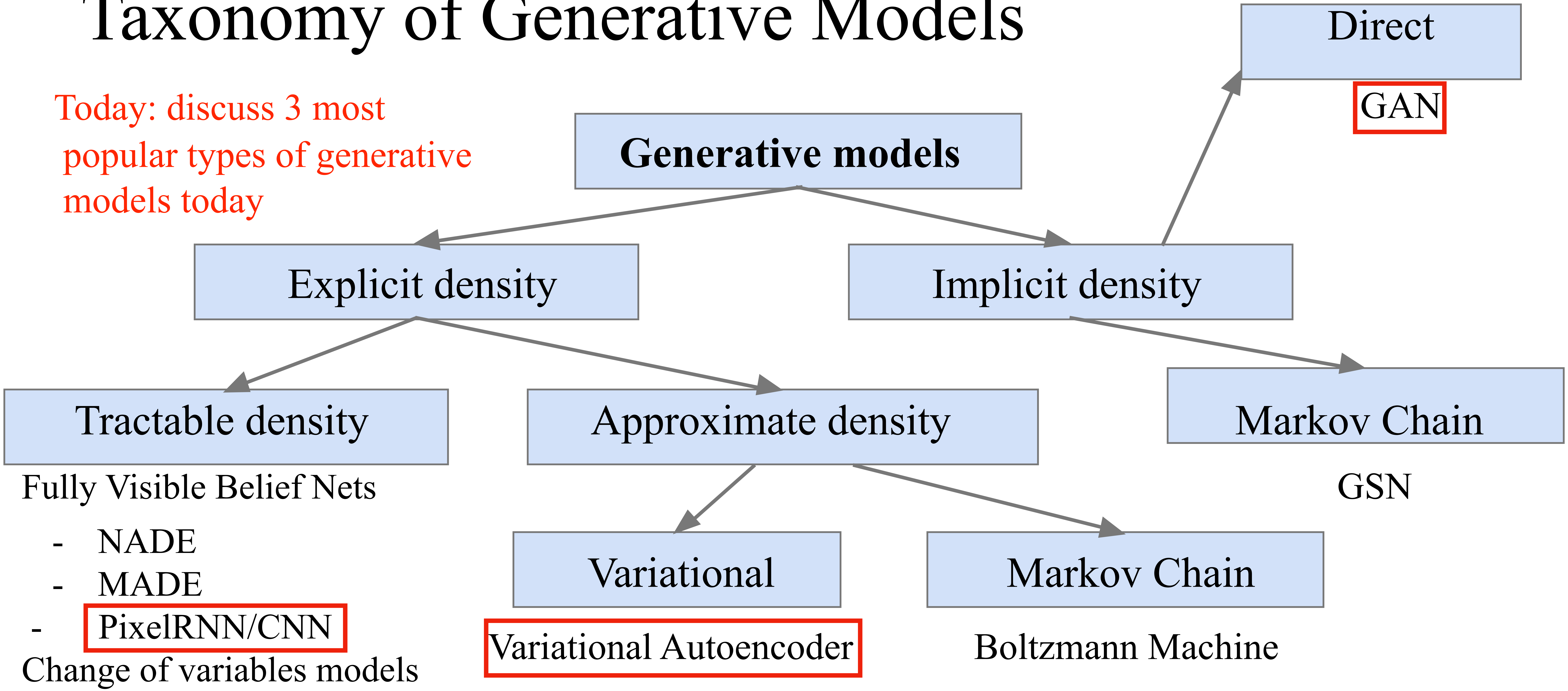


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

PixelRNN and PixelCNN

Fully visible belief network

Explicit density model

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

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

Likelihood of image x

Probability of i’th pixel value given all previous pixels

Then maximize likelihood of training data

Fully visible belief network

Explicit density model

Use 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

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

Then maximize likelihood of training data

Fully visible belief network

Explicit density model

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

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

Likelihood of image x

Probability of i'th pixel value given all previous pixels

Will need to define ordering of "previous pixels"

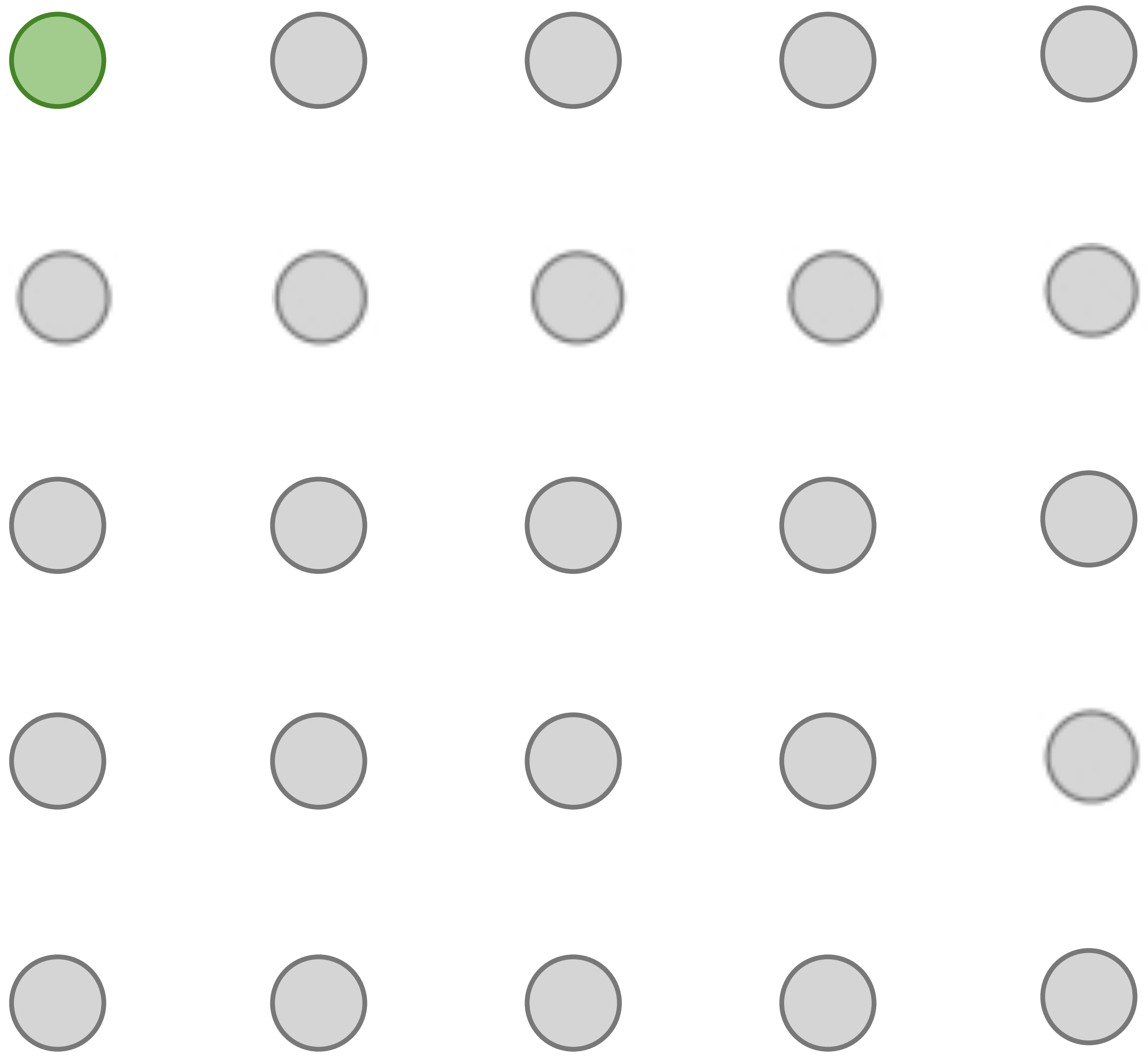
Complex distribution over pixel values => Express using a neural network!

Then maximize likelihood of training data

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

Generate image pixels starting from corner

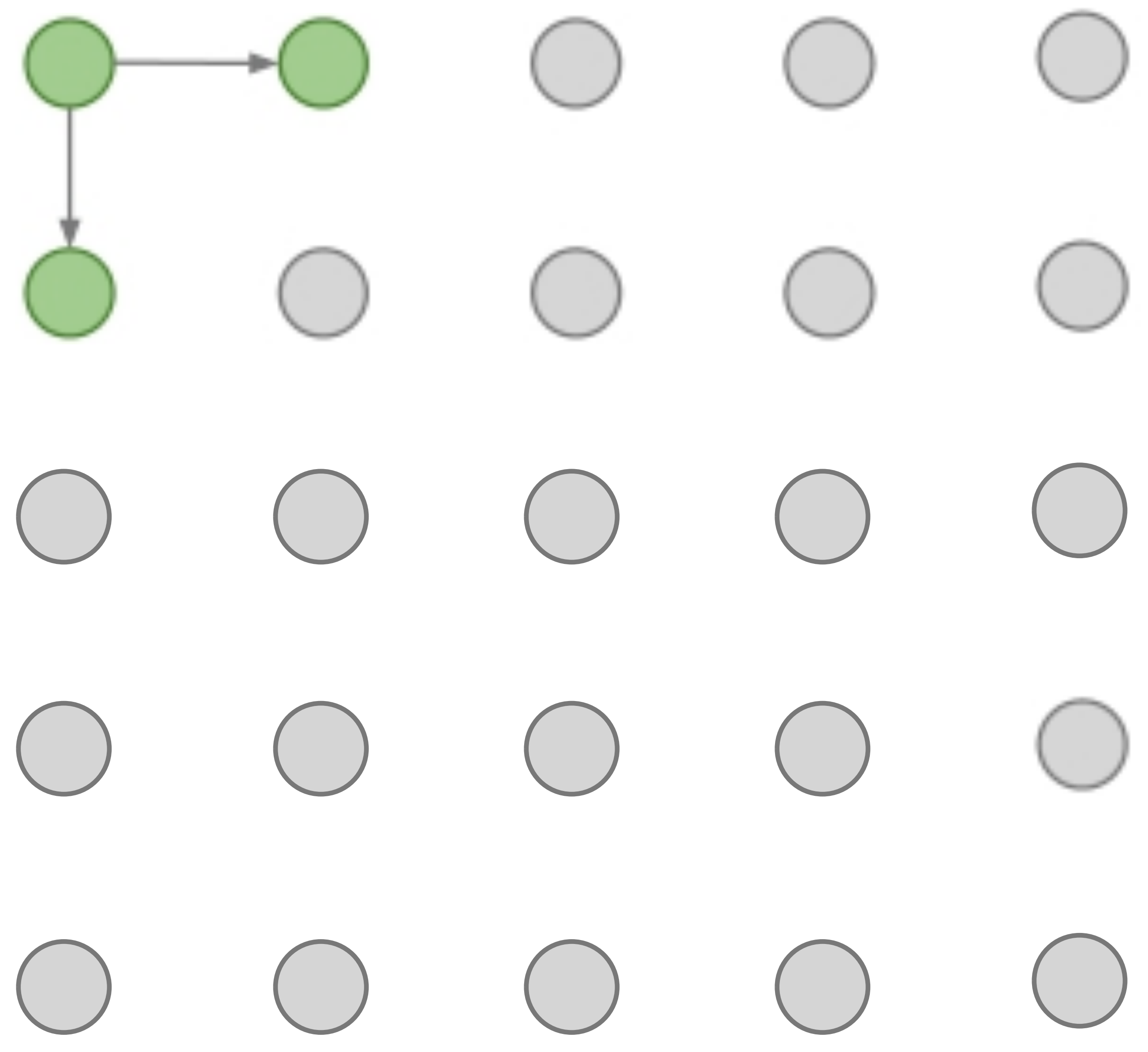
Dependency on previous pixels modeled using an RNN (LSTM)



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

Generate image pixels starting from corner

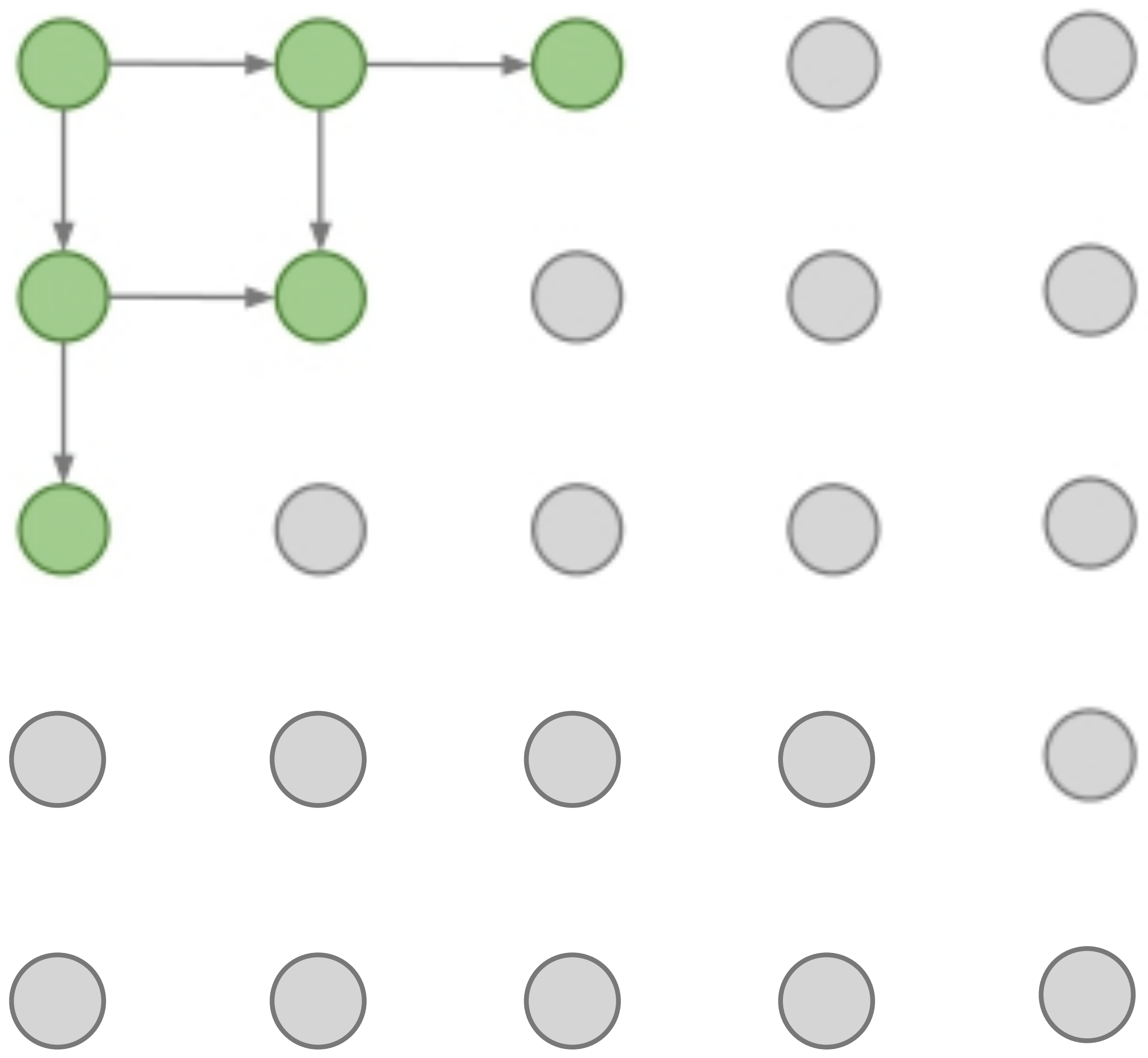
Dependency on previous pixels modeled using an RNN (LSTM)



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

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

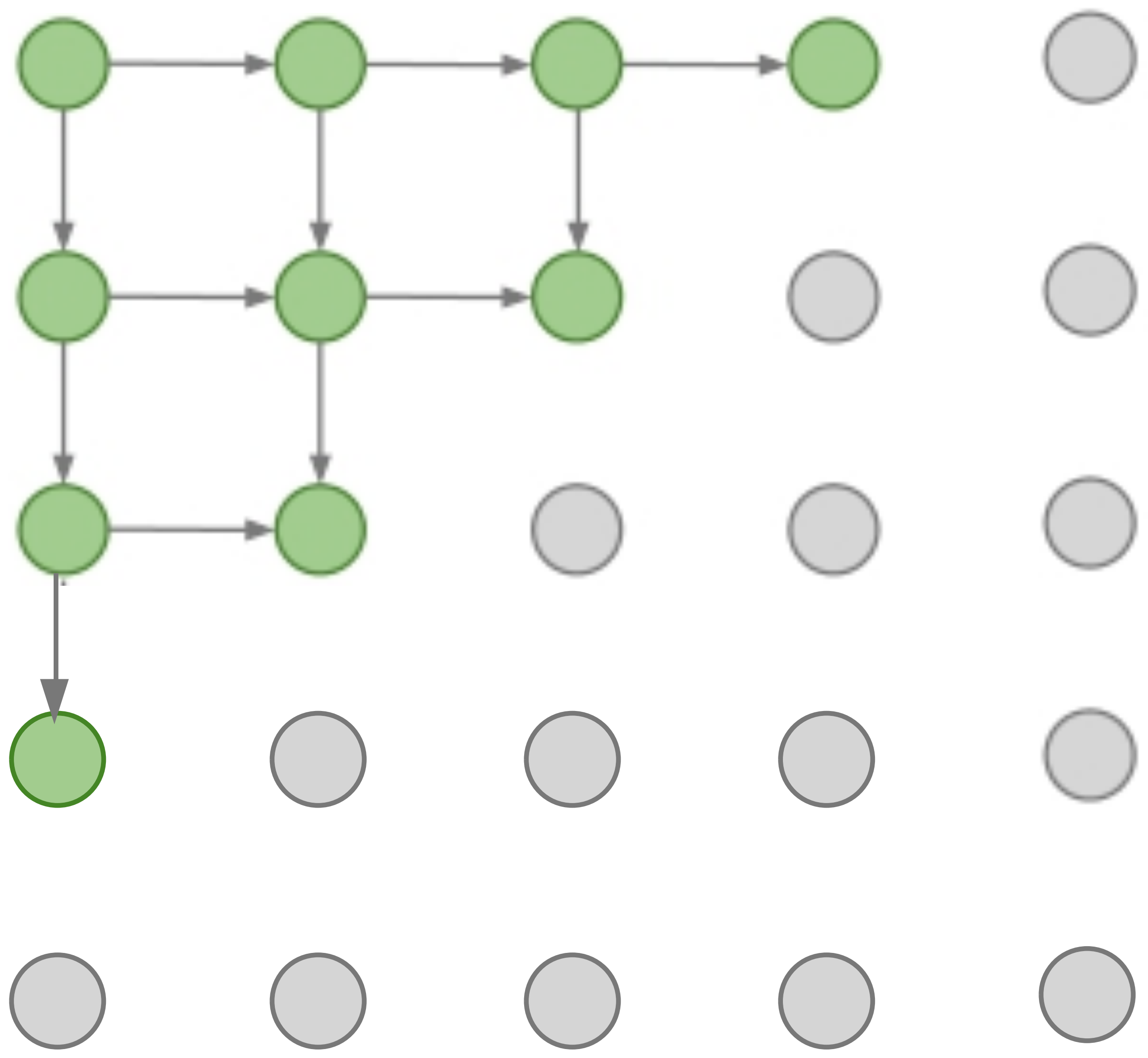


PixelRNN *[van der Oord et al. 2016]*

Generate image pixels starting from corner

Dependency on previous pixels modeled using an RNN (LSTM)

Drawback: sequential generation is slow!



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

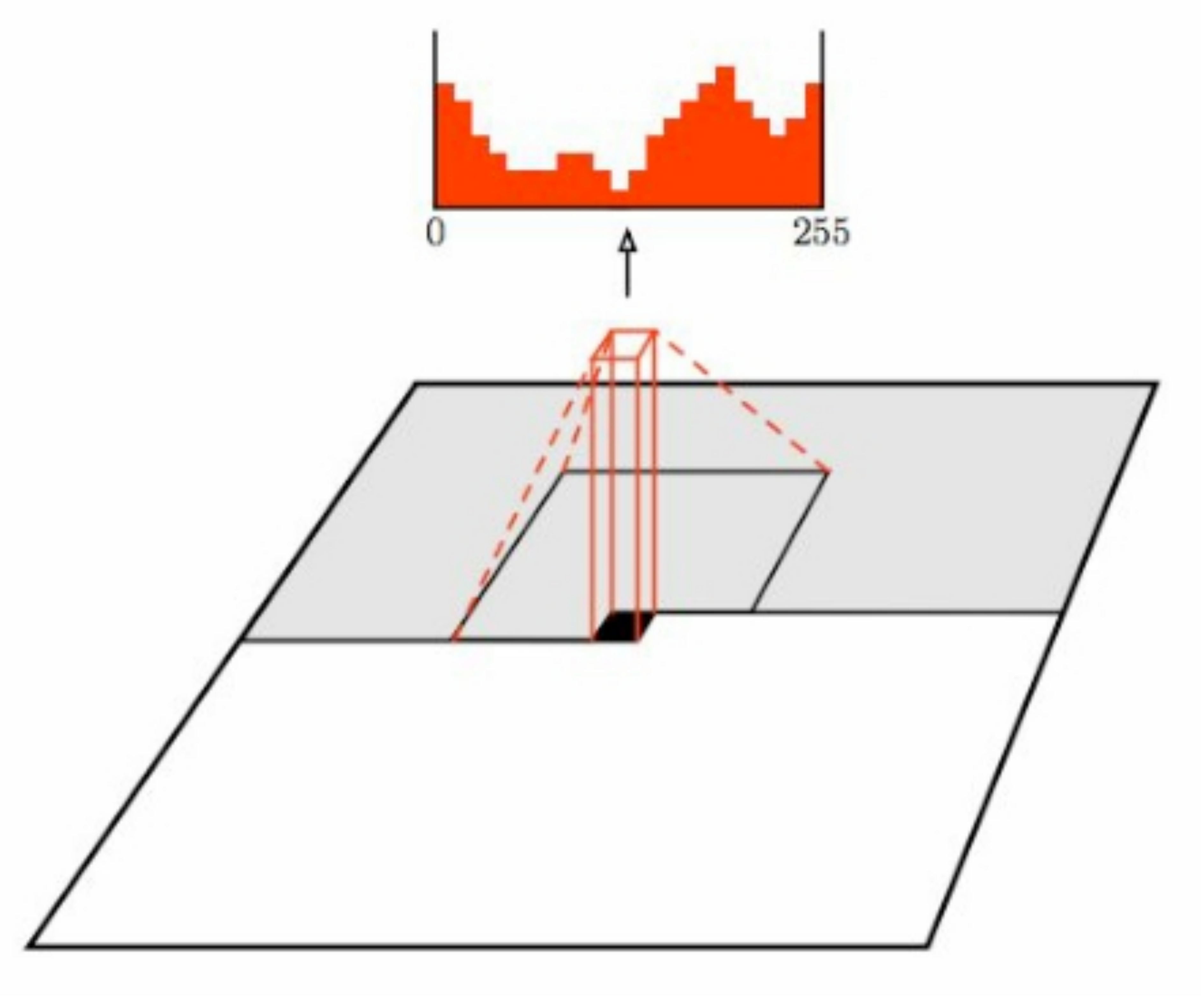


Figure copyright van der Oord et al., 2016. Reproduced with permission.

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

Softmax loss at each pixel

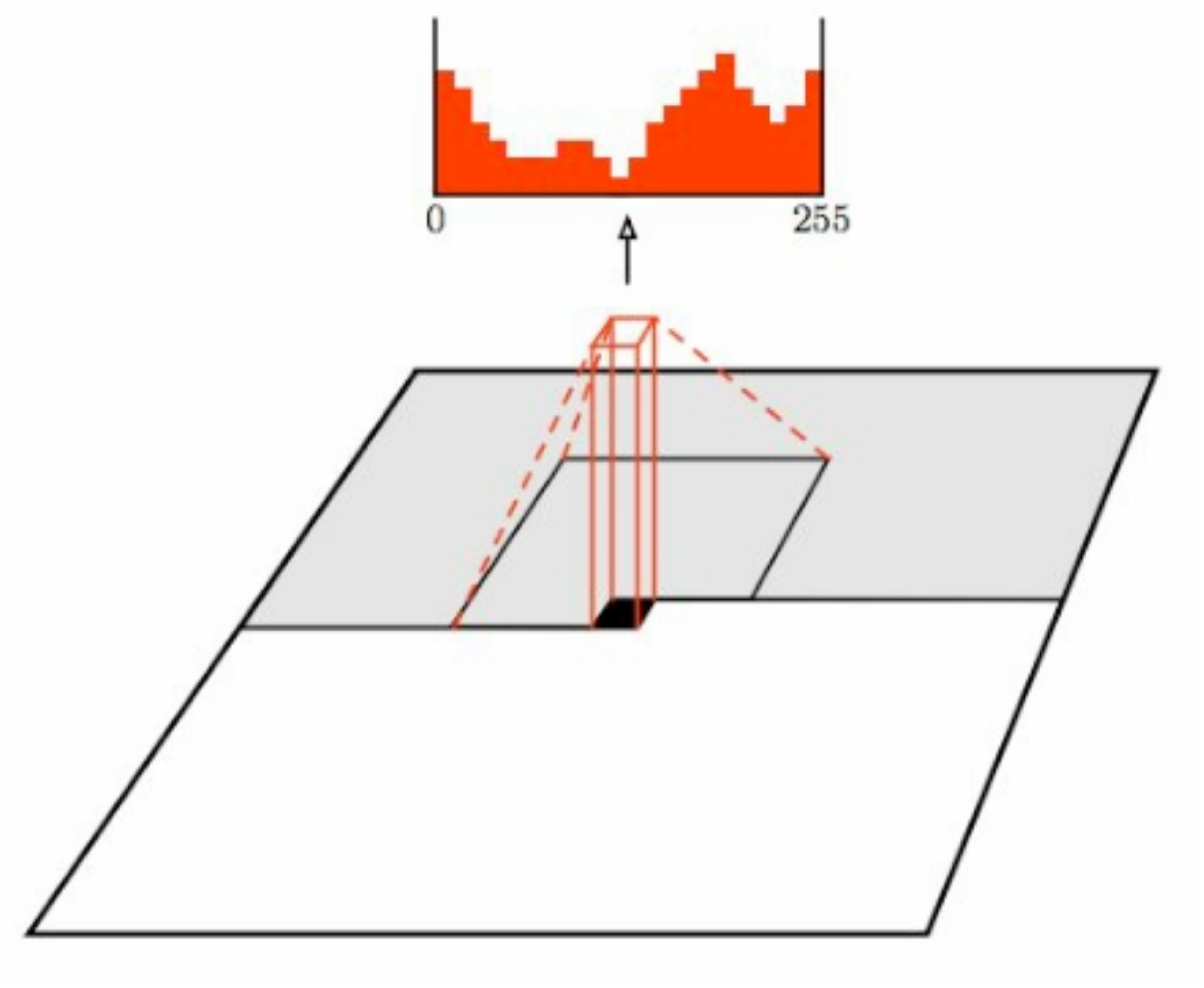


Figure copyright van der Oord et al., 2016. Reproduced with permission.

Still generate image pixels starting from corner

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

Training: maximize likelihood of training images

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

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

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

Generation must still proceed sequentially
=> still slow

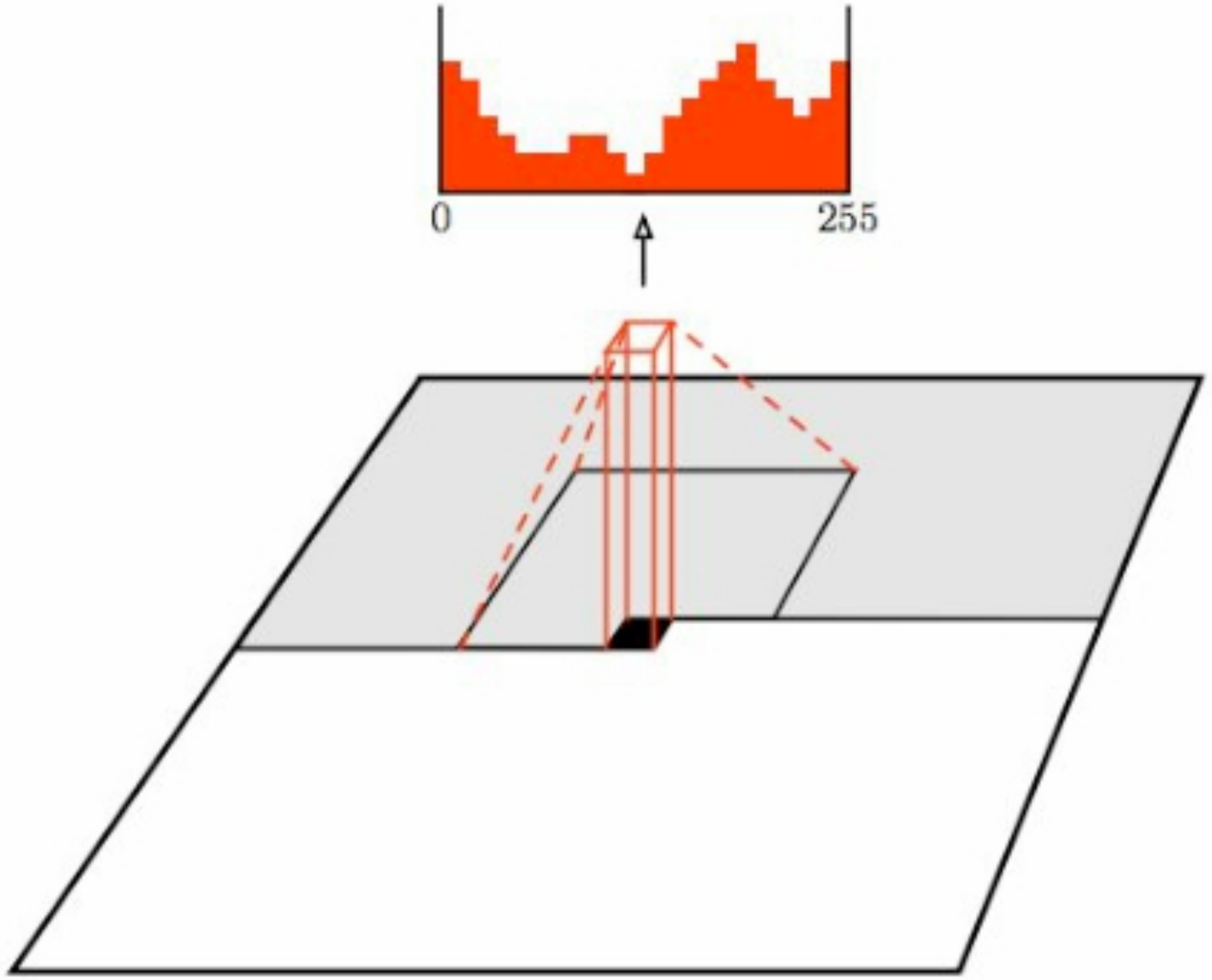
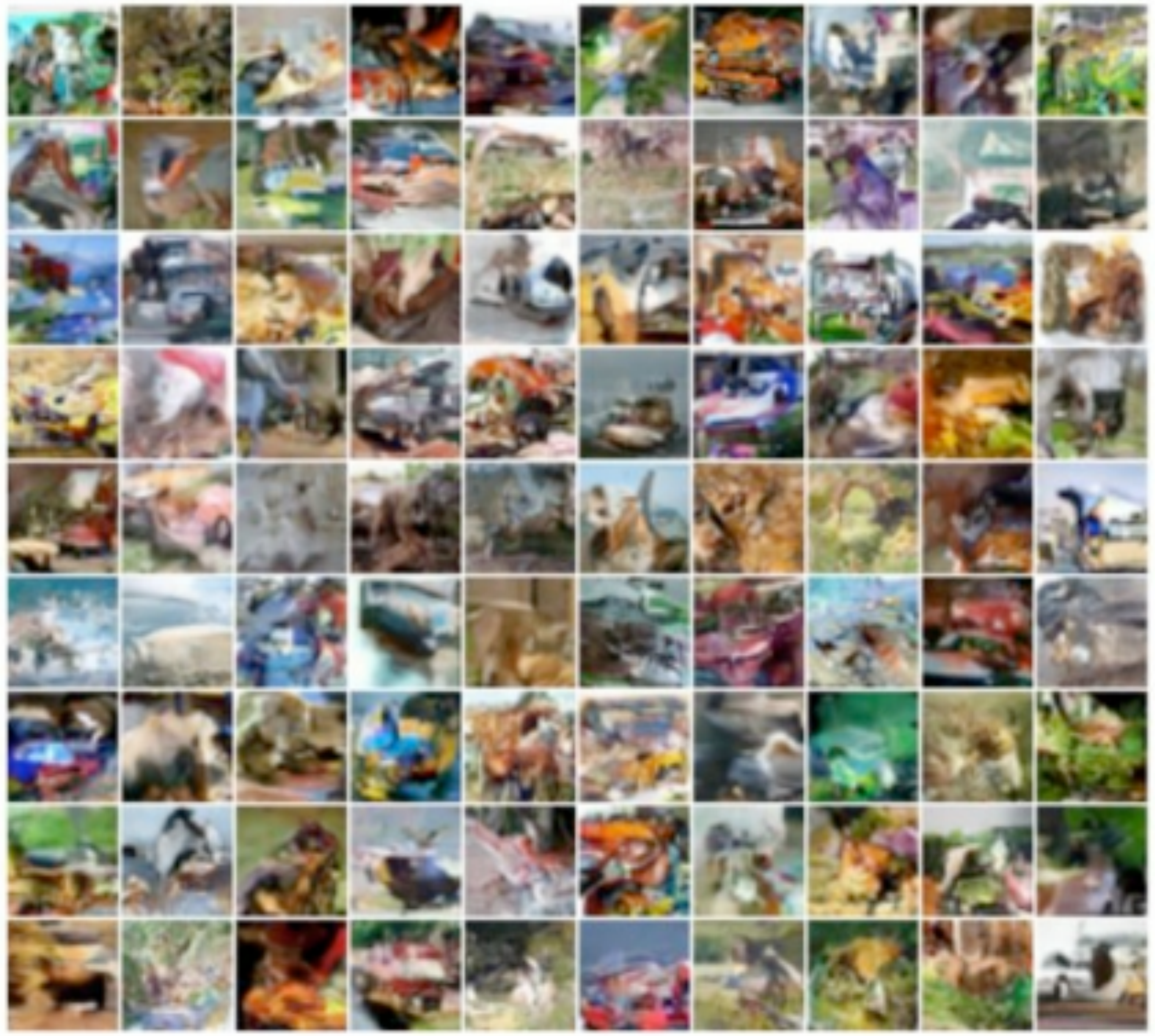
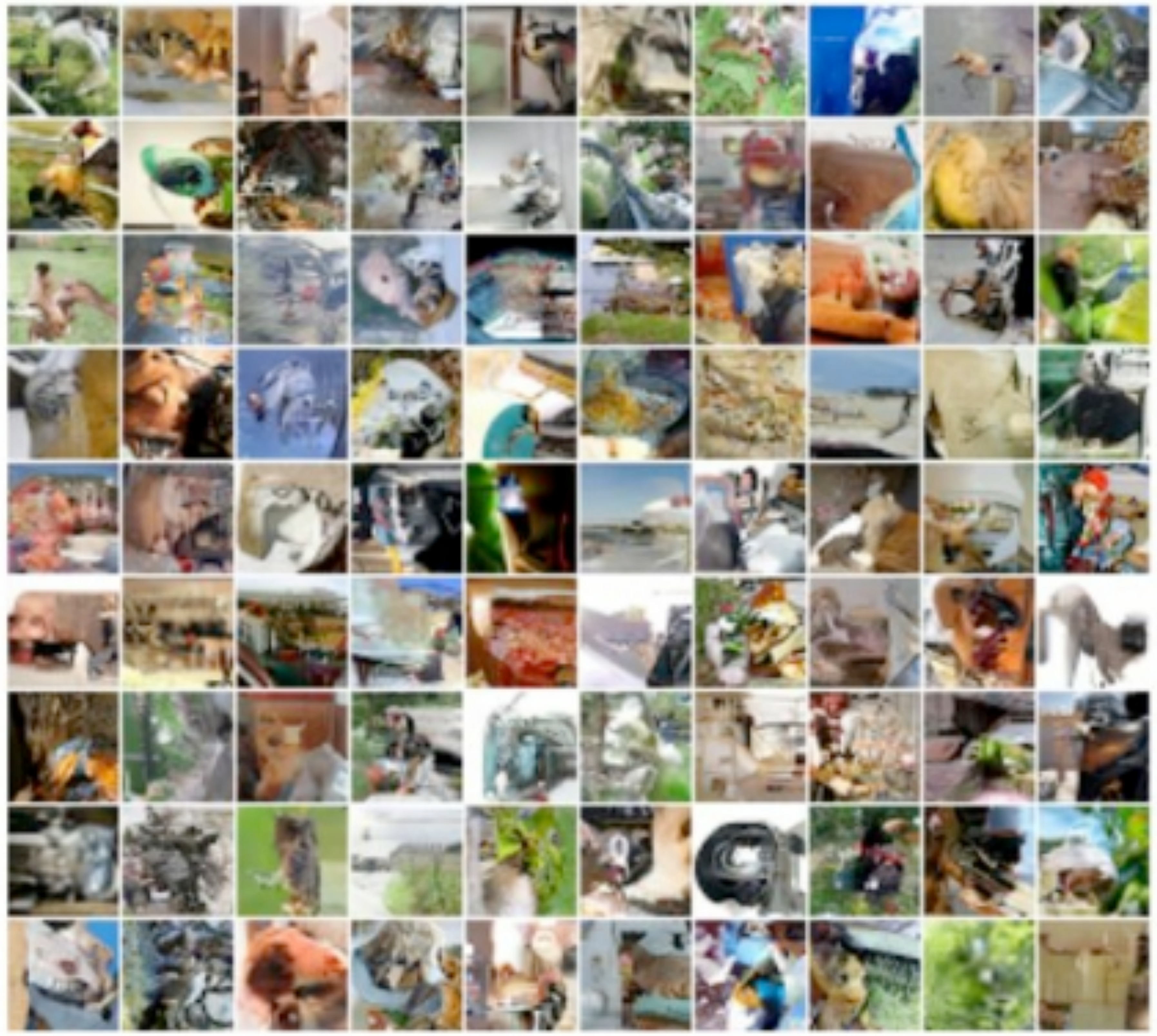


Figure copyright van der Oord et al., 2016. Reproduced with permission.

Generation Samples



32x32 CIFAR-10



32x32 ImageNet

PixelRNN and PixelCNN

Pros:
- Can explicitly compute likelihood p(x)
- Explicit likelihood of training data gives good evaluation metric
- Good samples

Con:
- Sequential generation => slow

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

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

Variational Autoencoders (VAE)

So far...

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

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

So far...

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

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

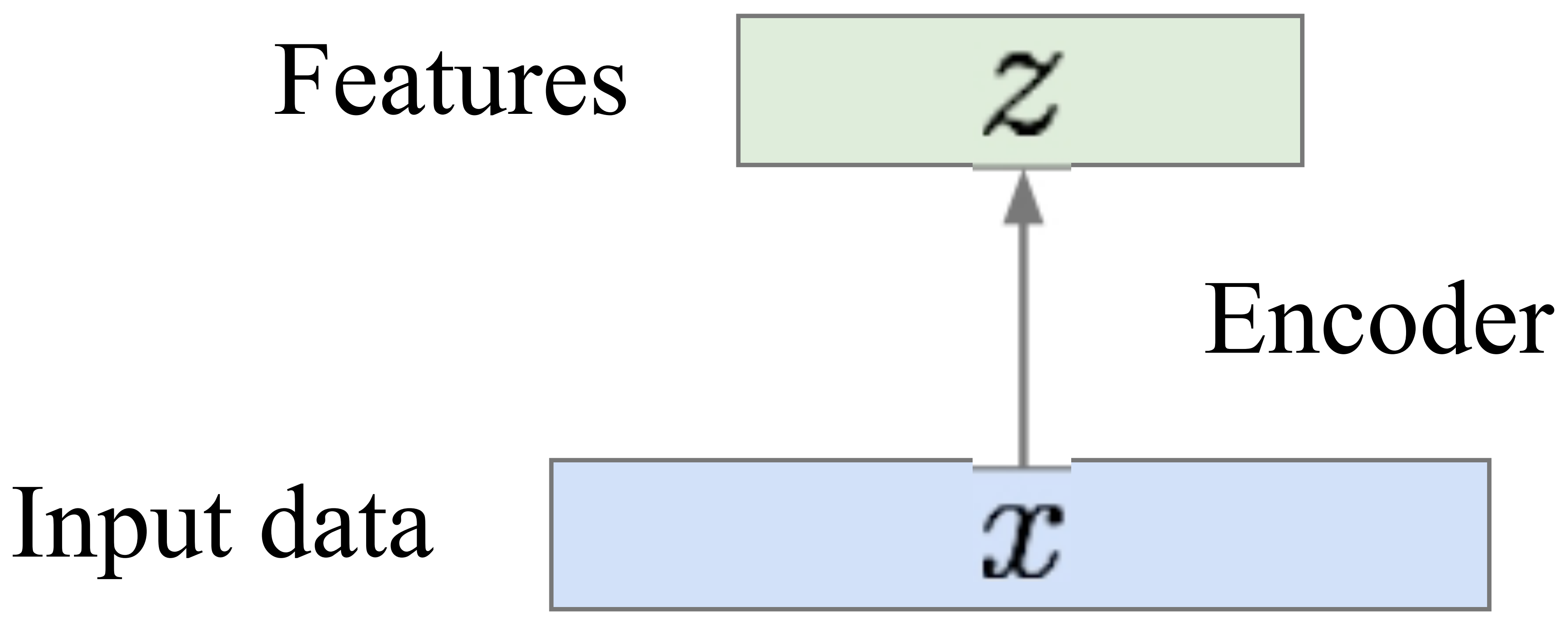
VAEs define intractable density function with latent **z** :

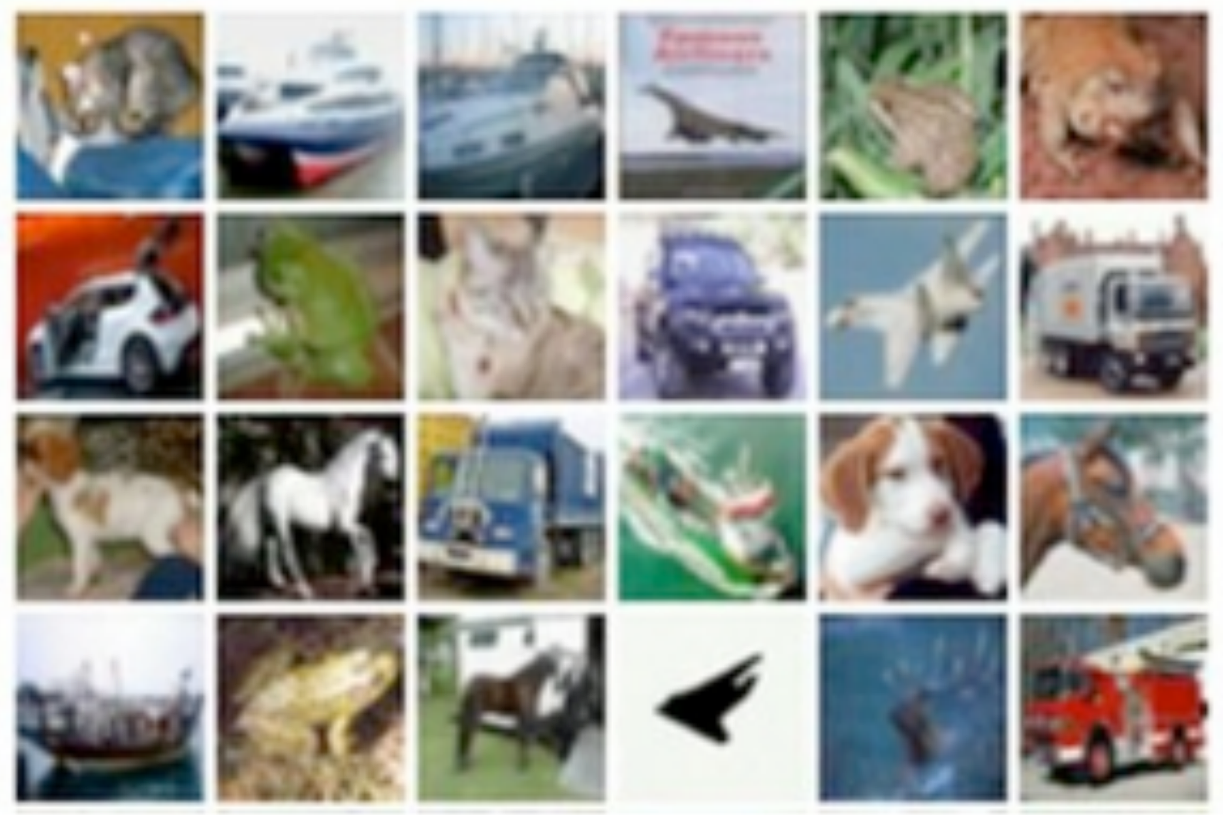
$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

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

Some background first: Autoencoders

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

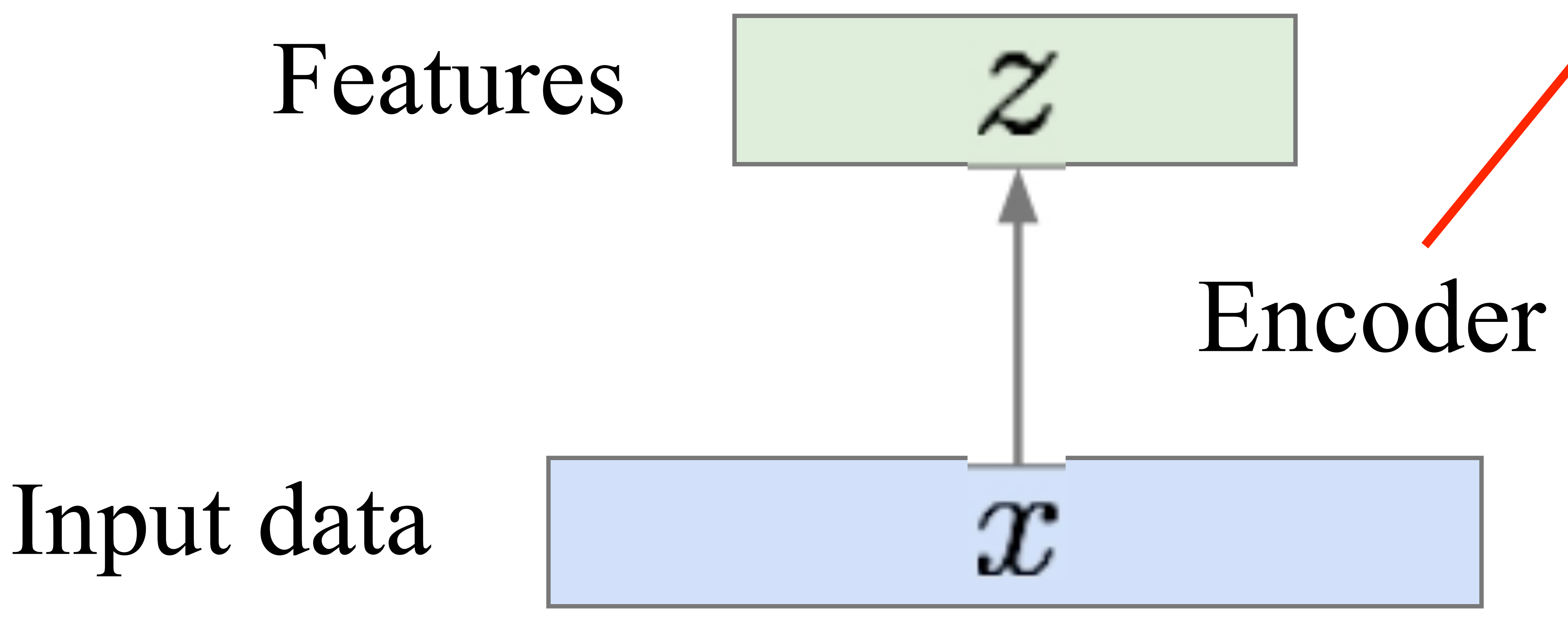


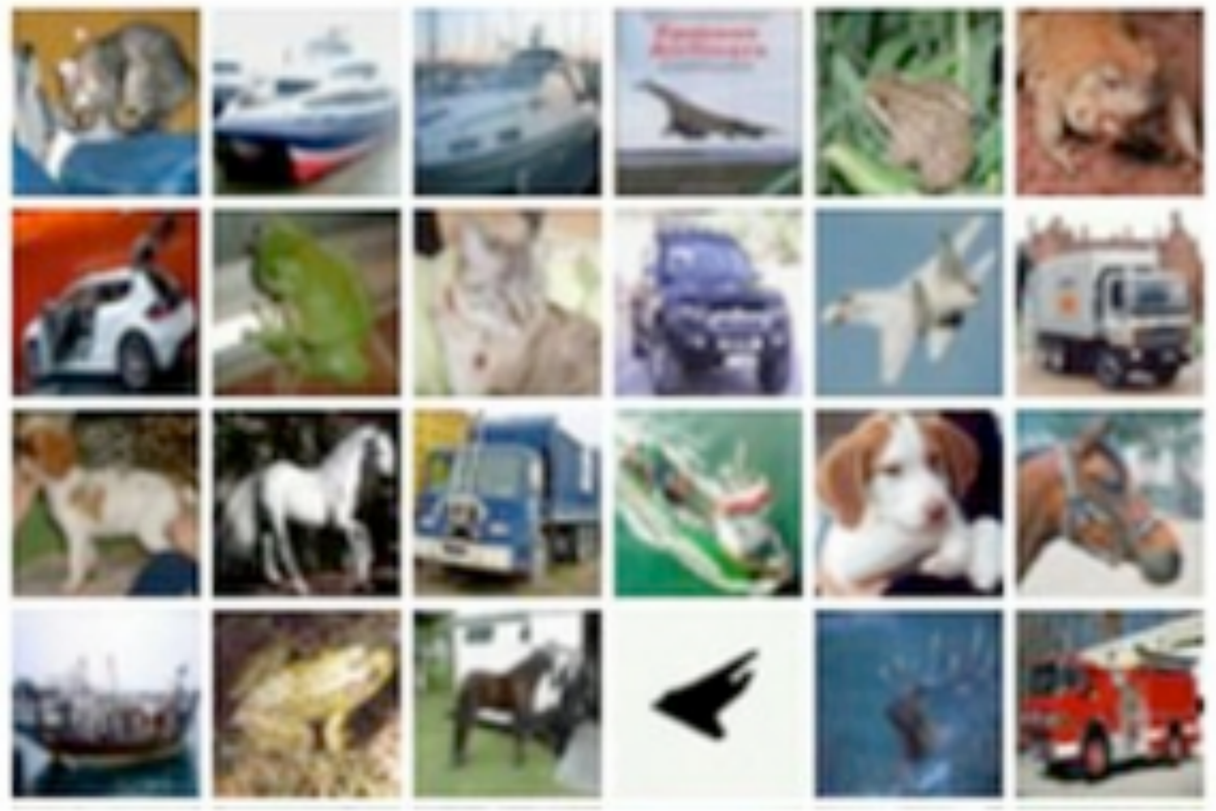


Some background first: Autoencoders

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

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





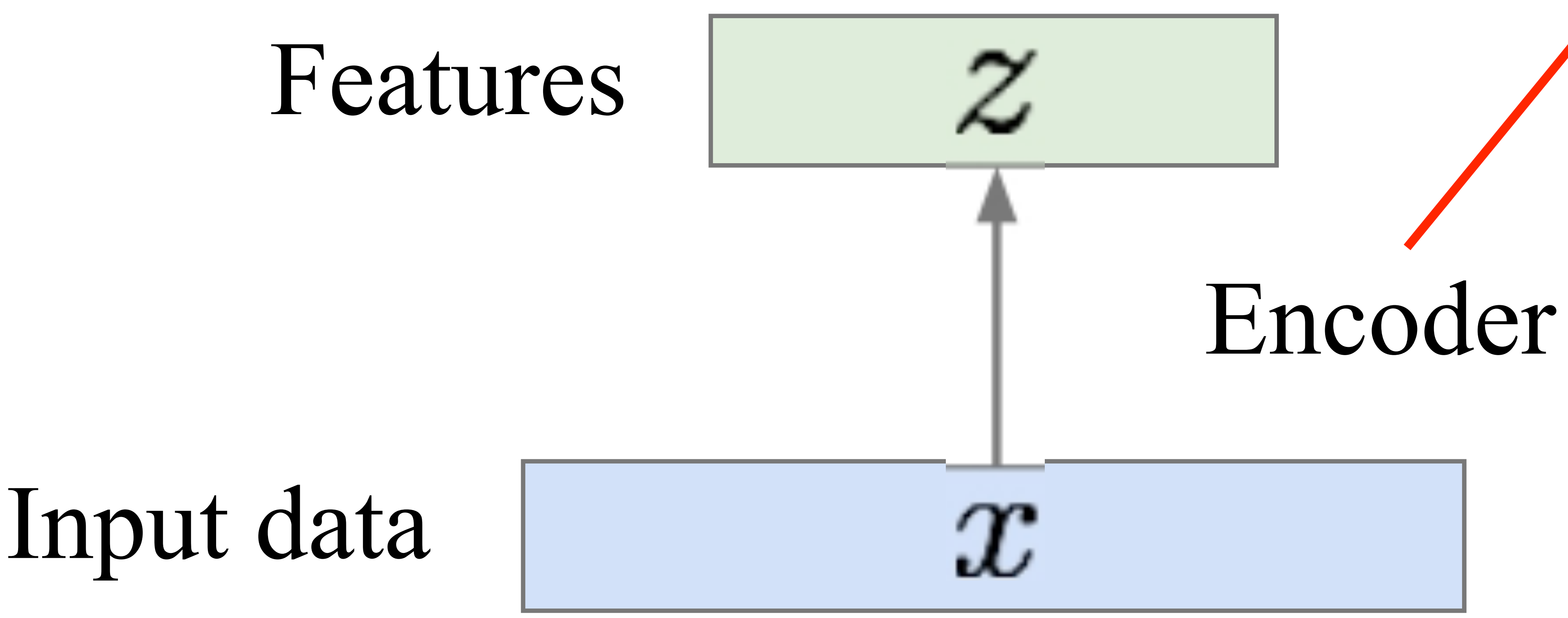
Some background first: Autoencoders

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

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

Q: Why dimensionality reduction?

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



Some background first: Autoencoders

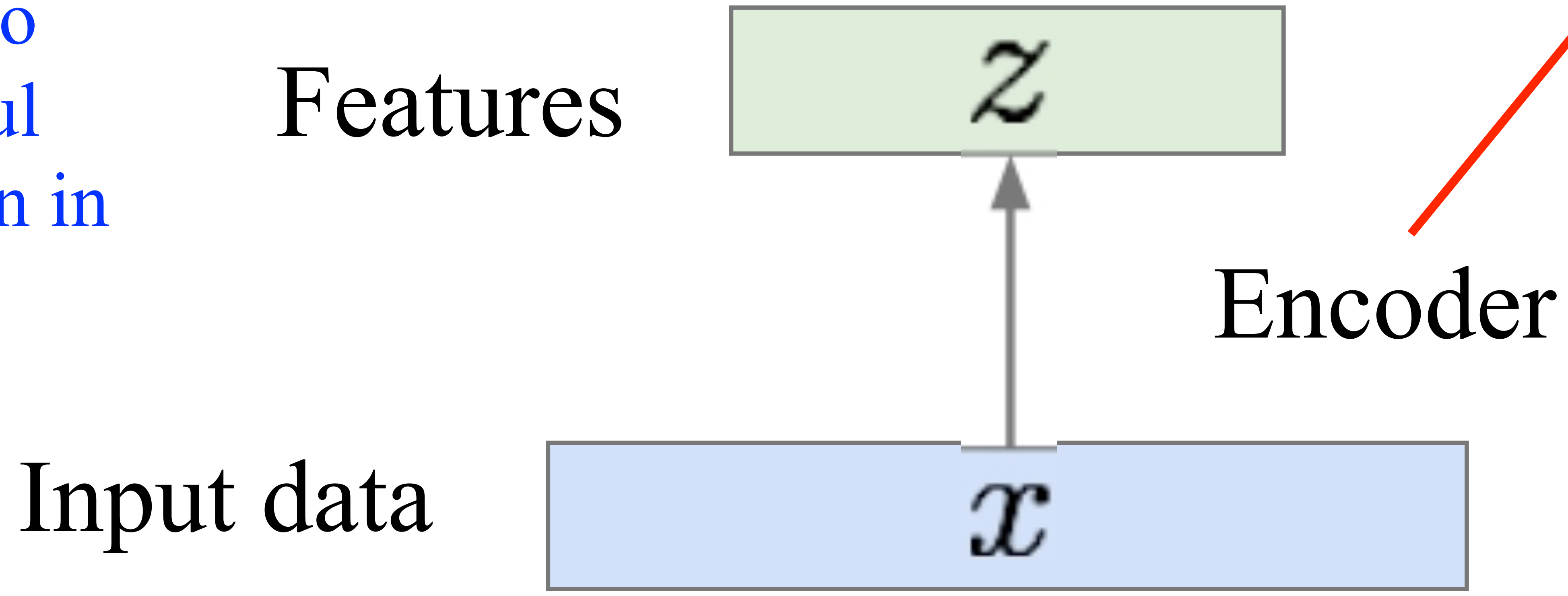
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

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

Q: Why dimensionality reduction?

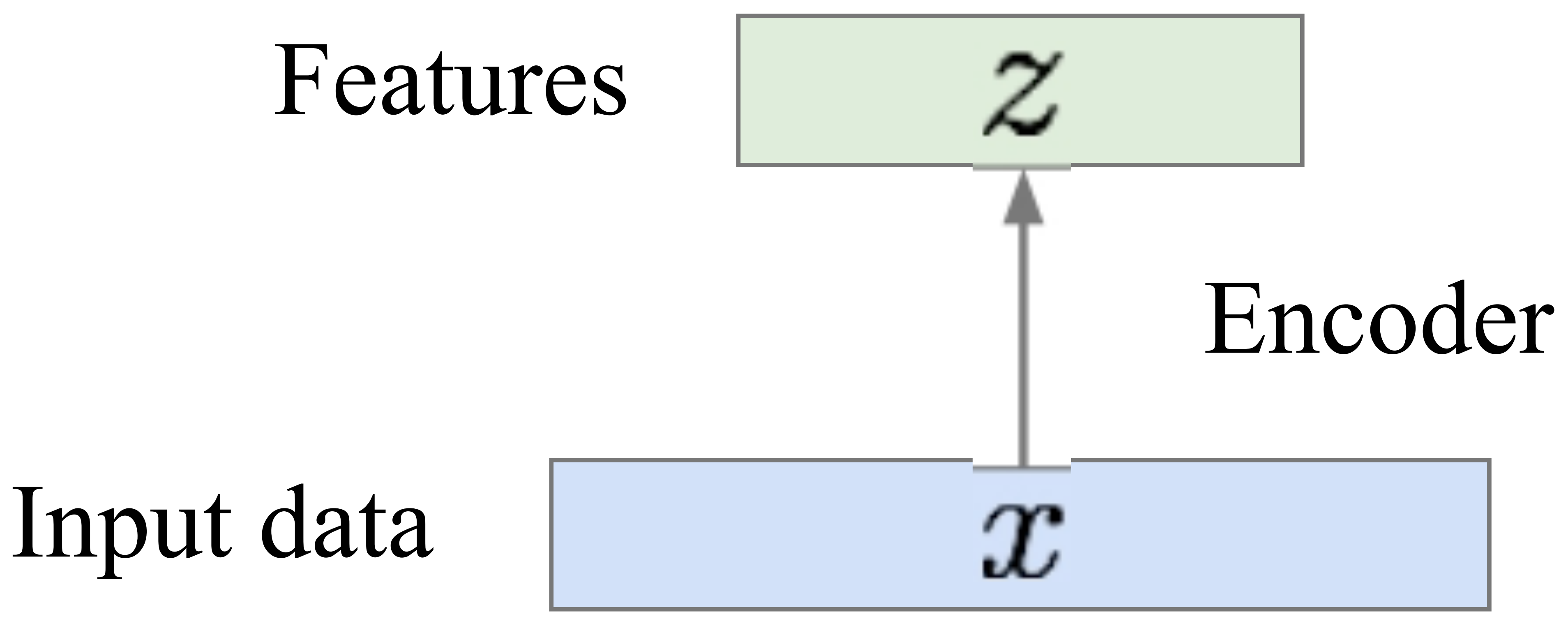
A: Want features to capture meaningful factors of variation in data

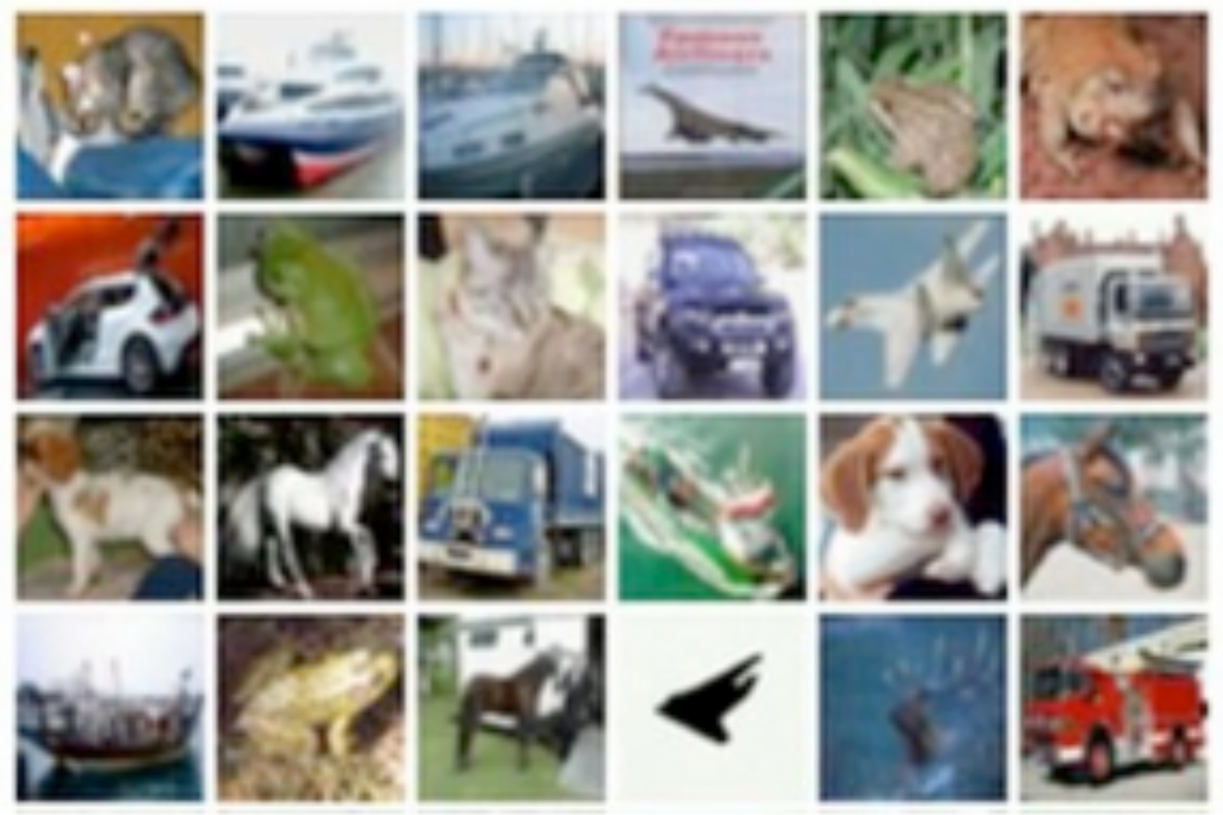
Originally : Linear + nonlinearity (sigmoid)
Later : Deep, fully-connected
Later : ReLU CNN



Some background first: Autoencoders

How to learn this feature representation?





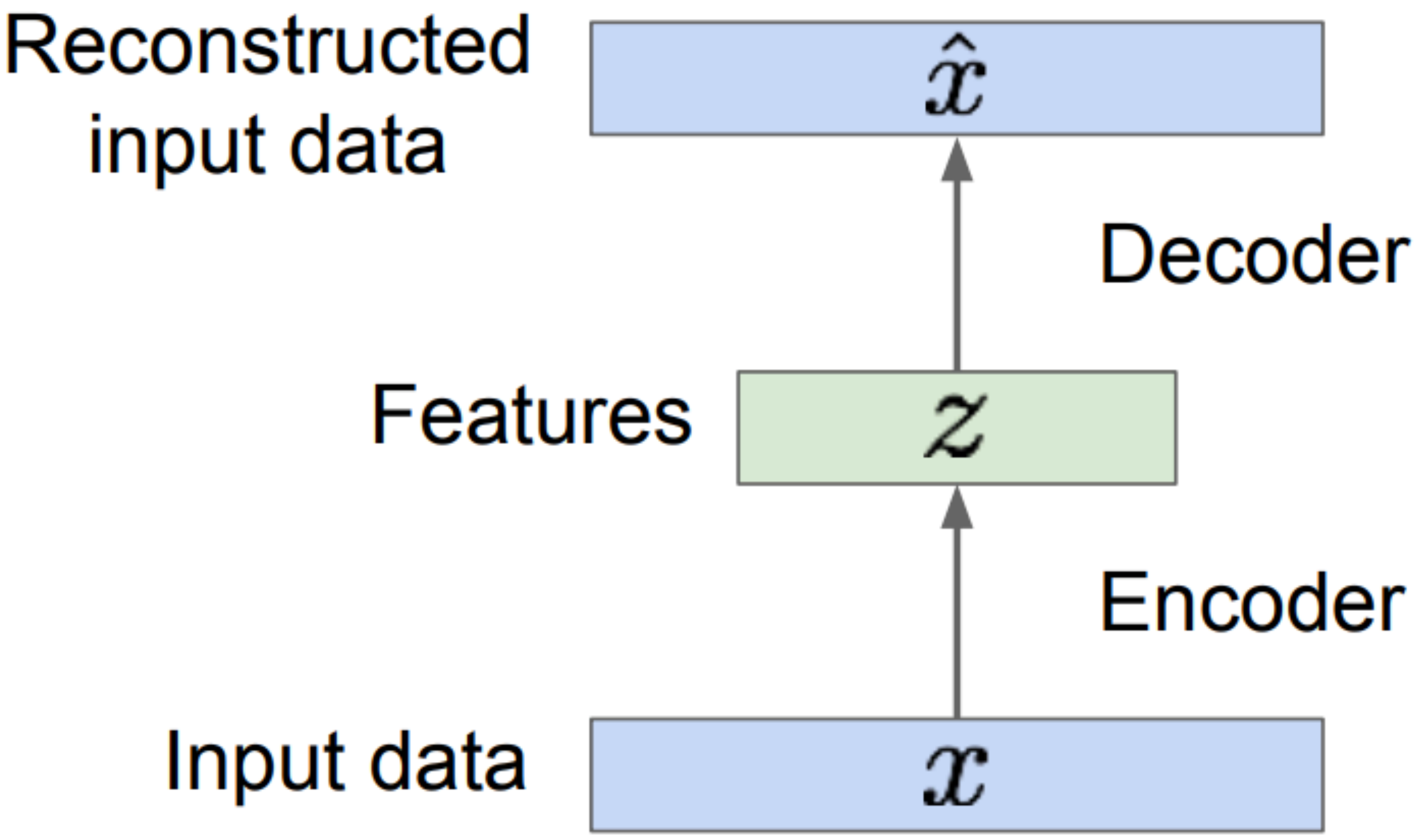
Used with permission from Justin Johnson

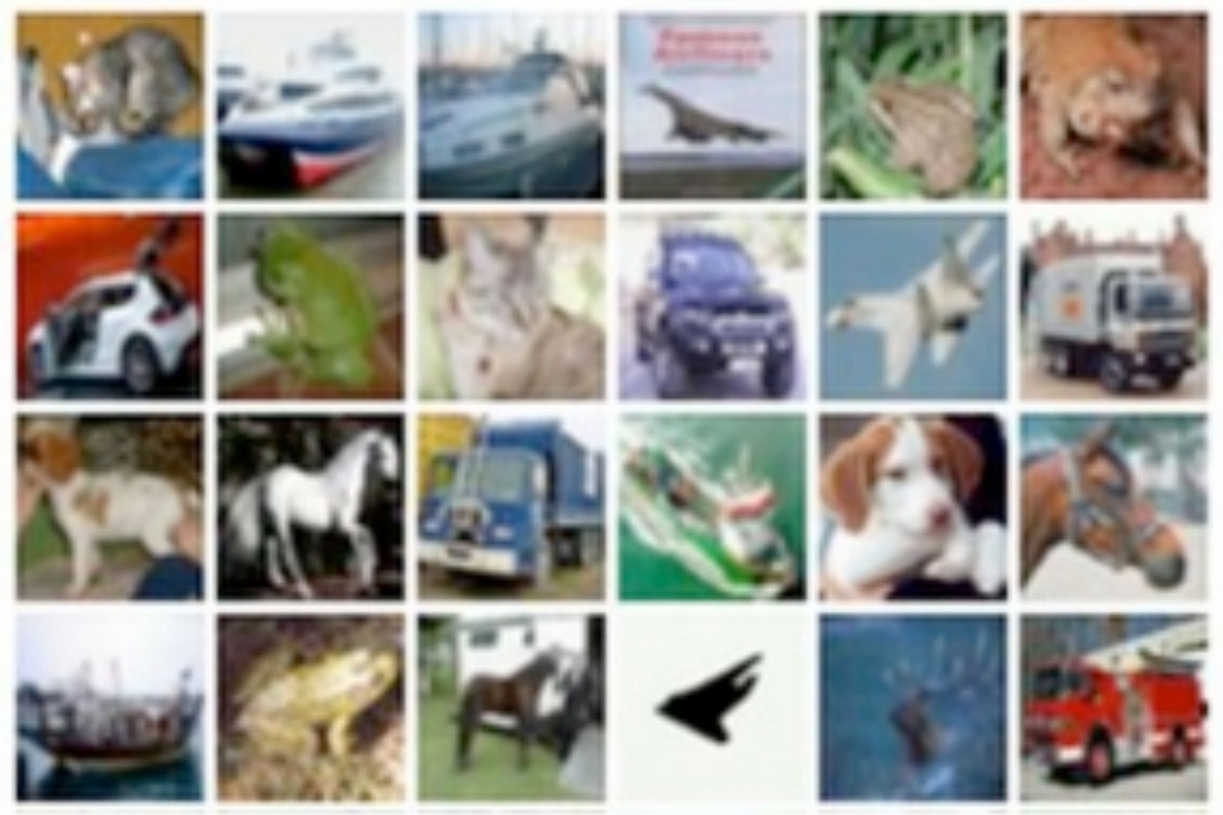
Some background first: Autoencoders

How to learn this feature representation?

Train such that features can be used to reconstruct original data

“Autoencoding” - encoding itself

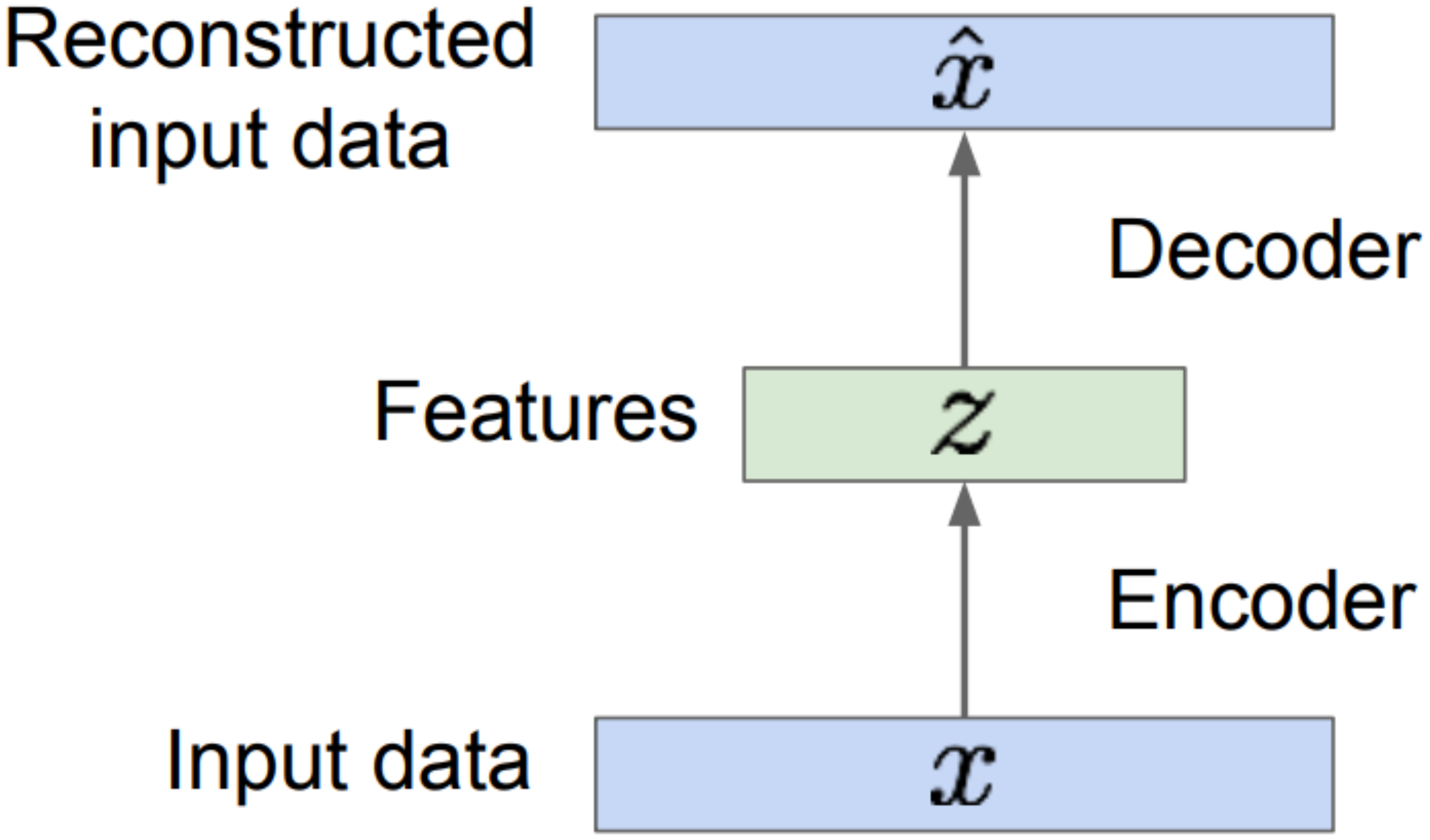




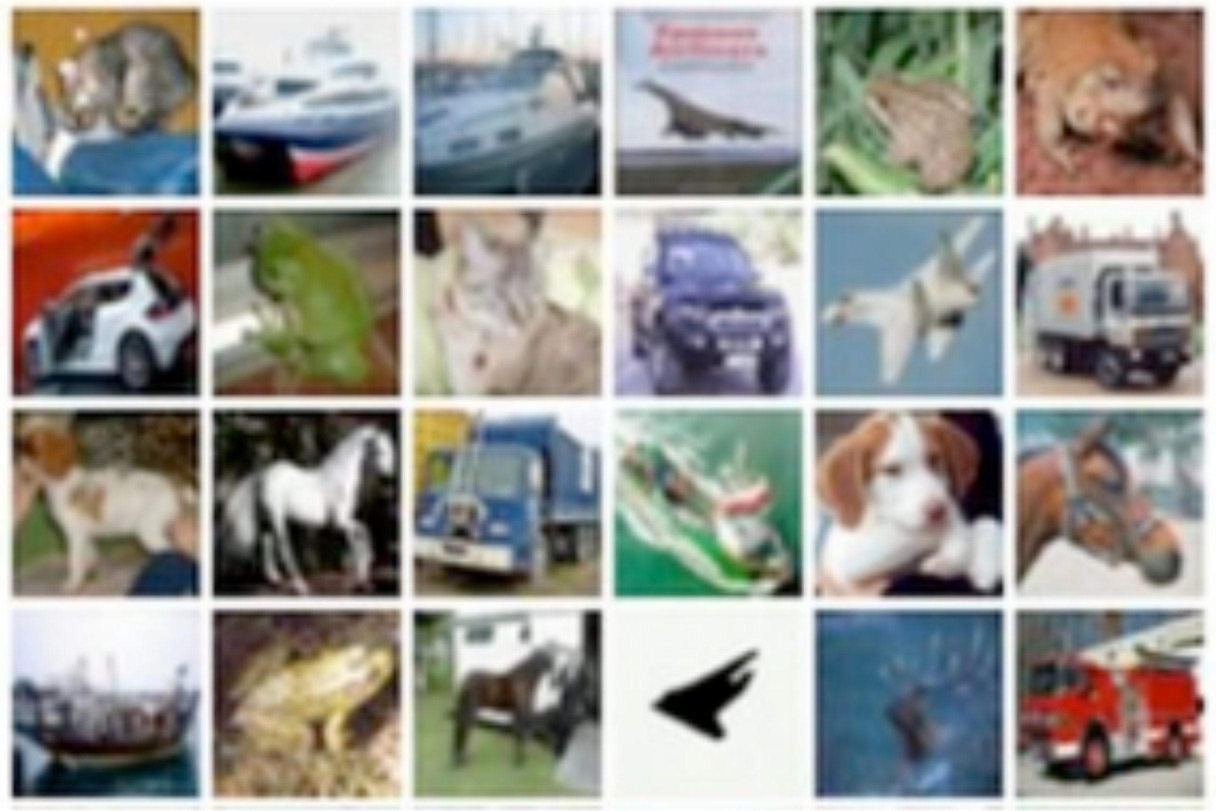
Used with permission from Justin Johnson

Some background first: Autoencoders

How to learn this feature representation?
Train such that features can be used to reconstruct original data
"Autoencoding" - encoding itself



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

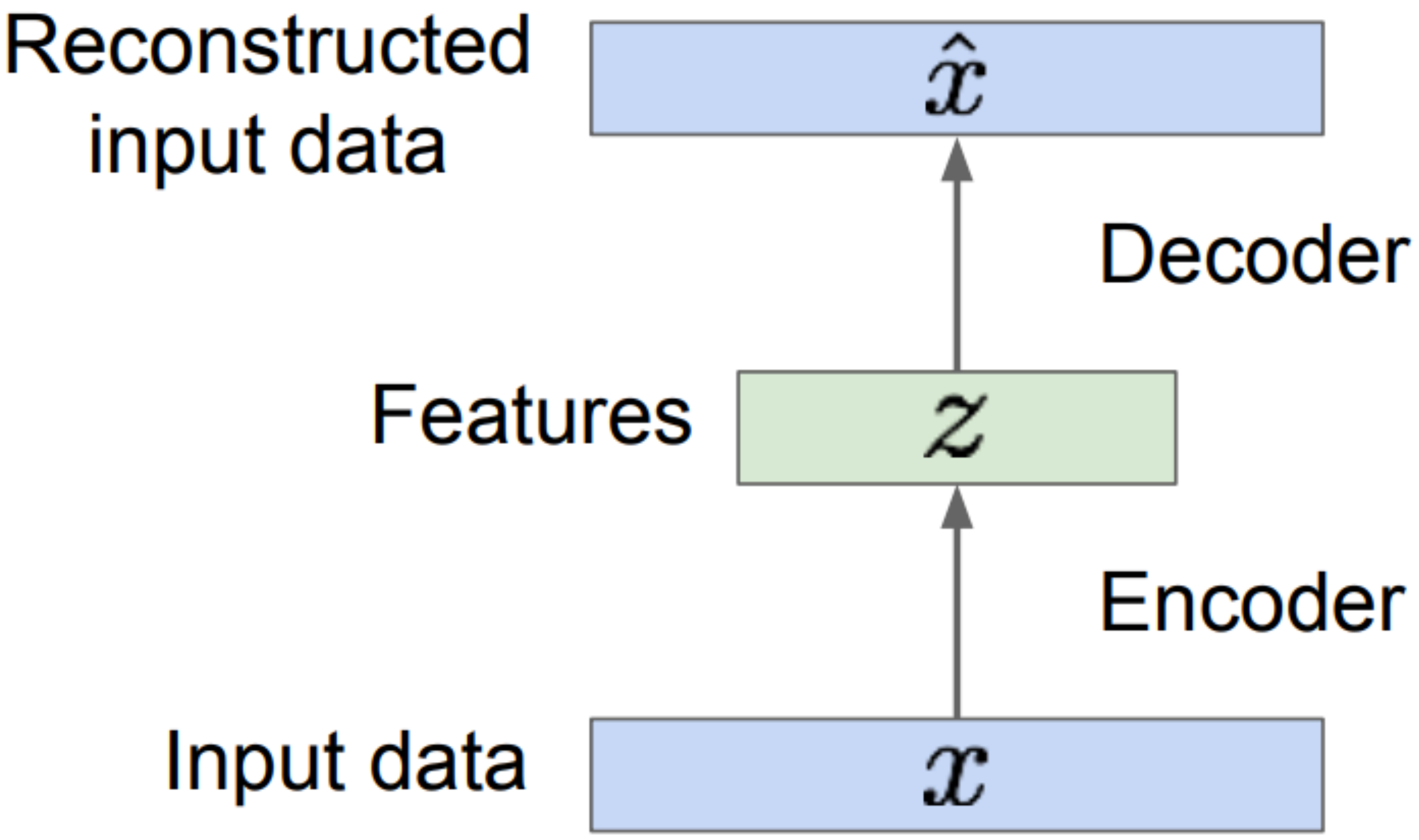


Some background first: Autoencoders

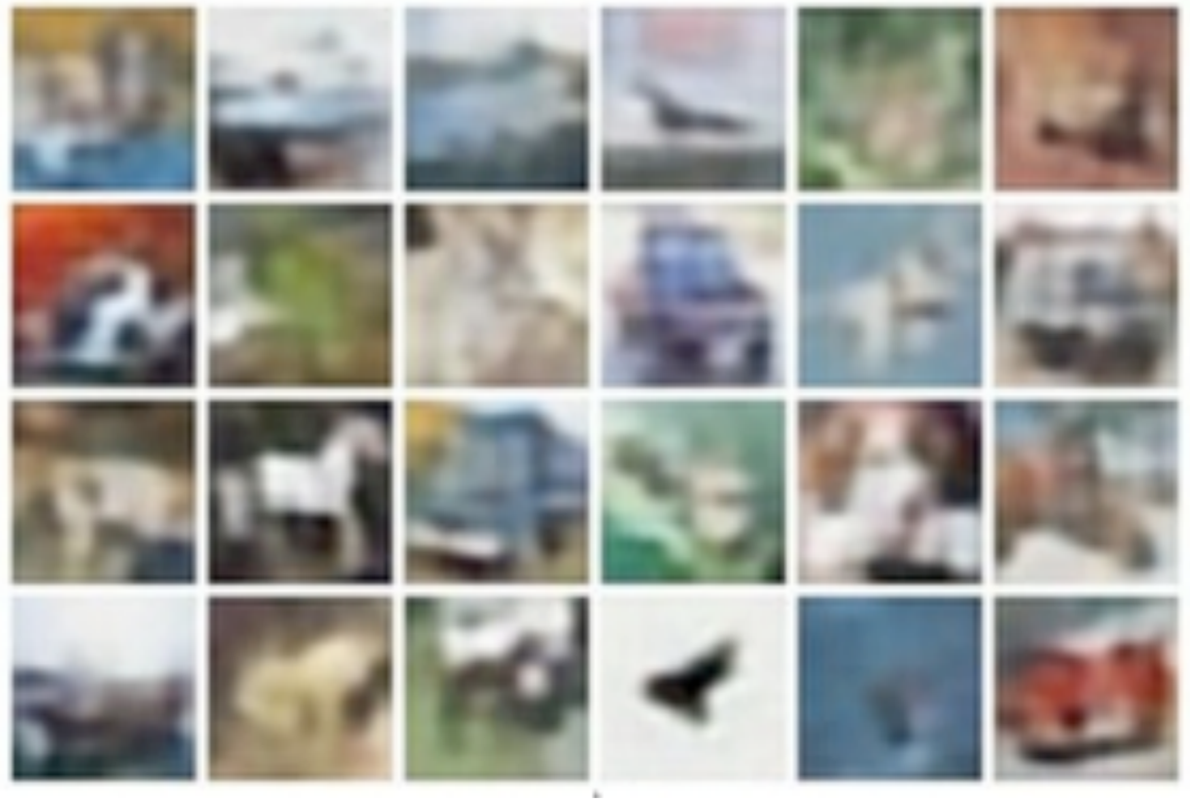
How to learn this feature representation?

Train such that features can be used to reconstruct original data

“Autoencoding” - encoding itself



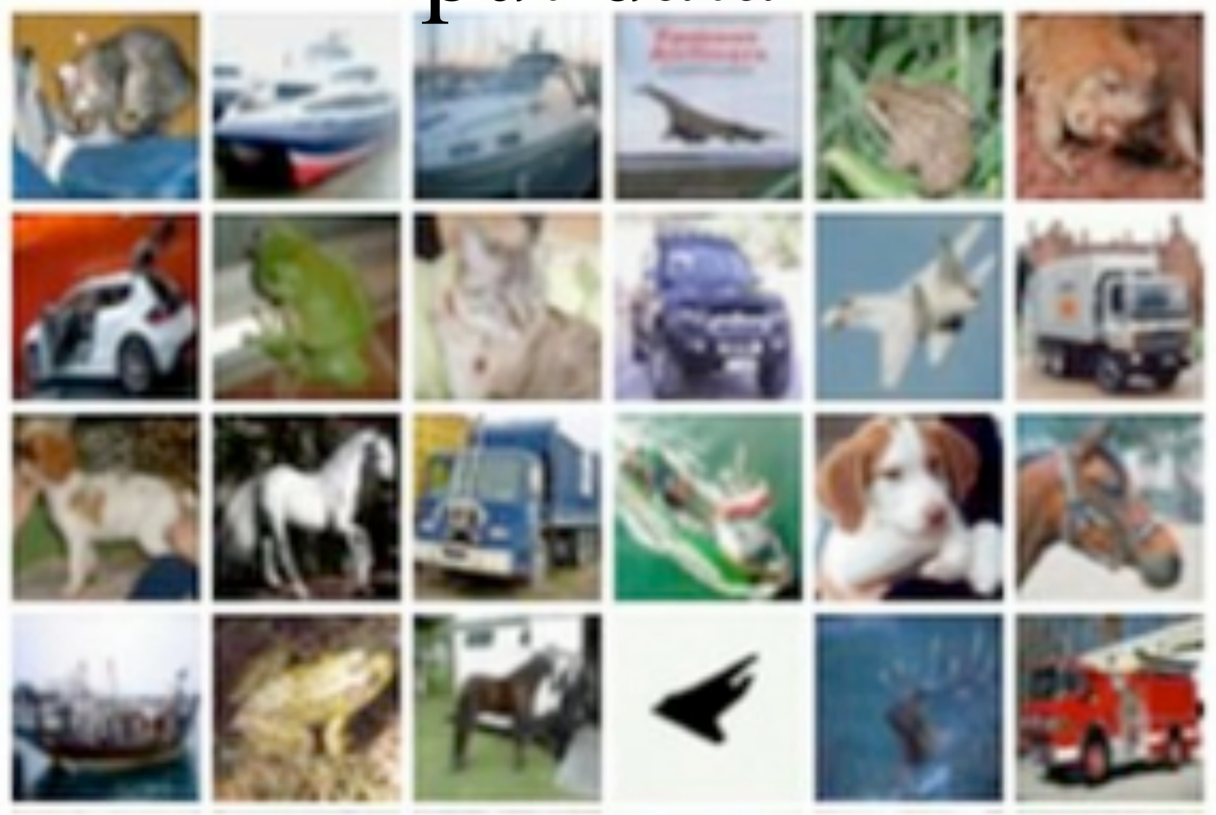
Reconstructed data



Encoder : 4-layer conv

Decoder : 4-layer upconv

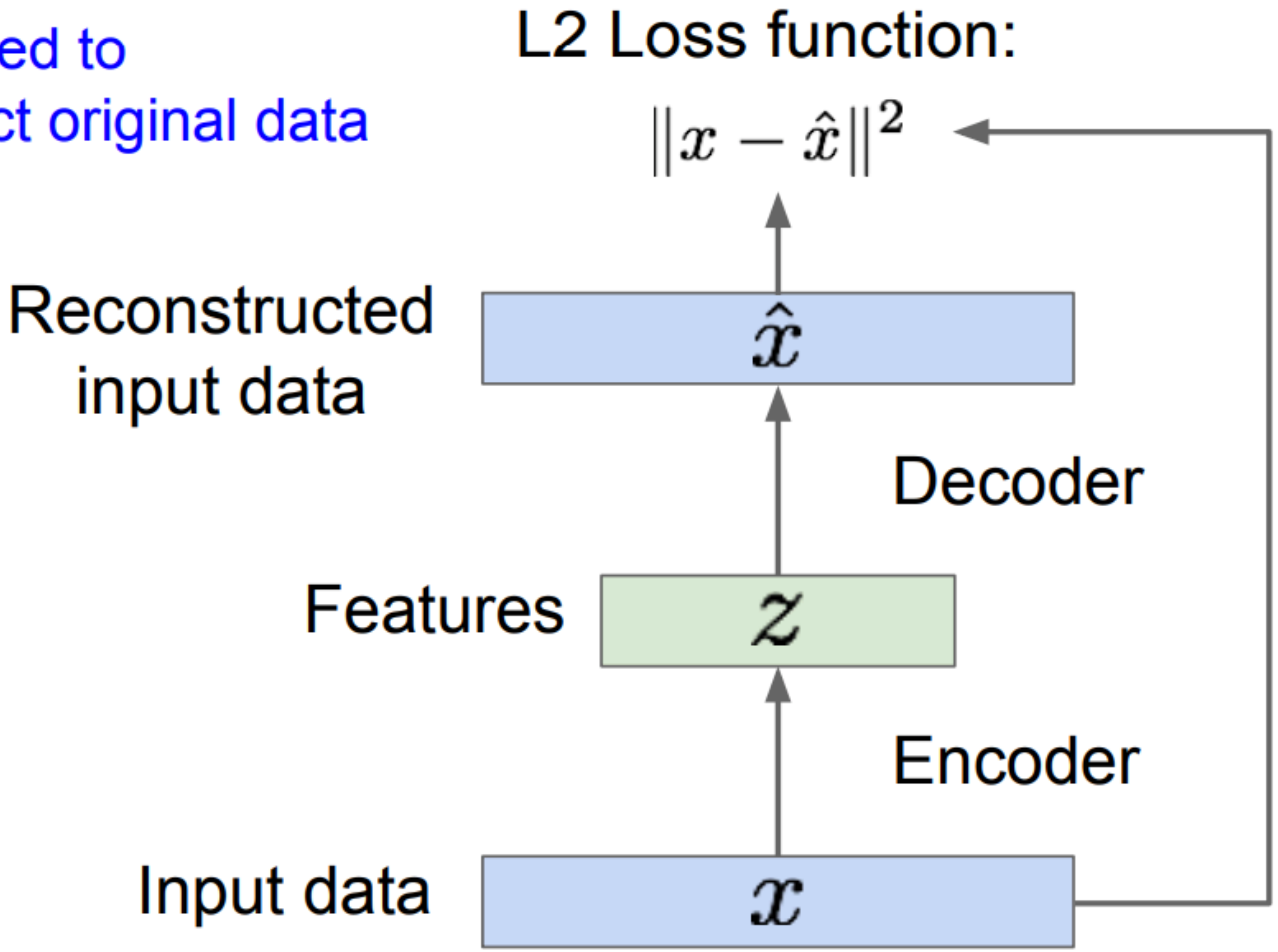
Input data



Some background first: Autoencoders

Train such that features can be used to reconstruct original data

Doesn't use labels!

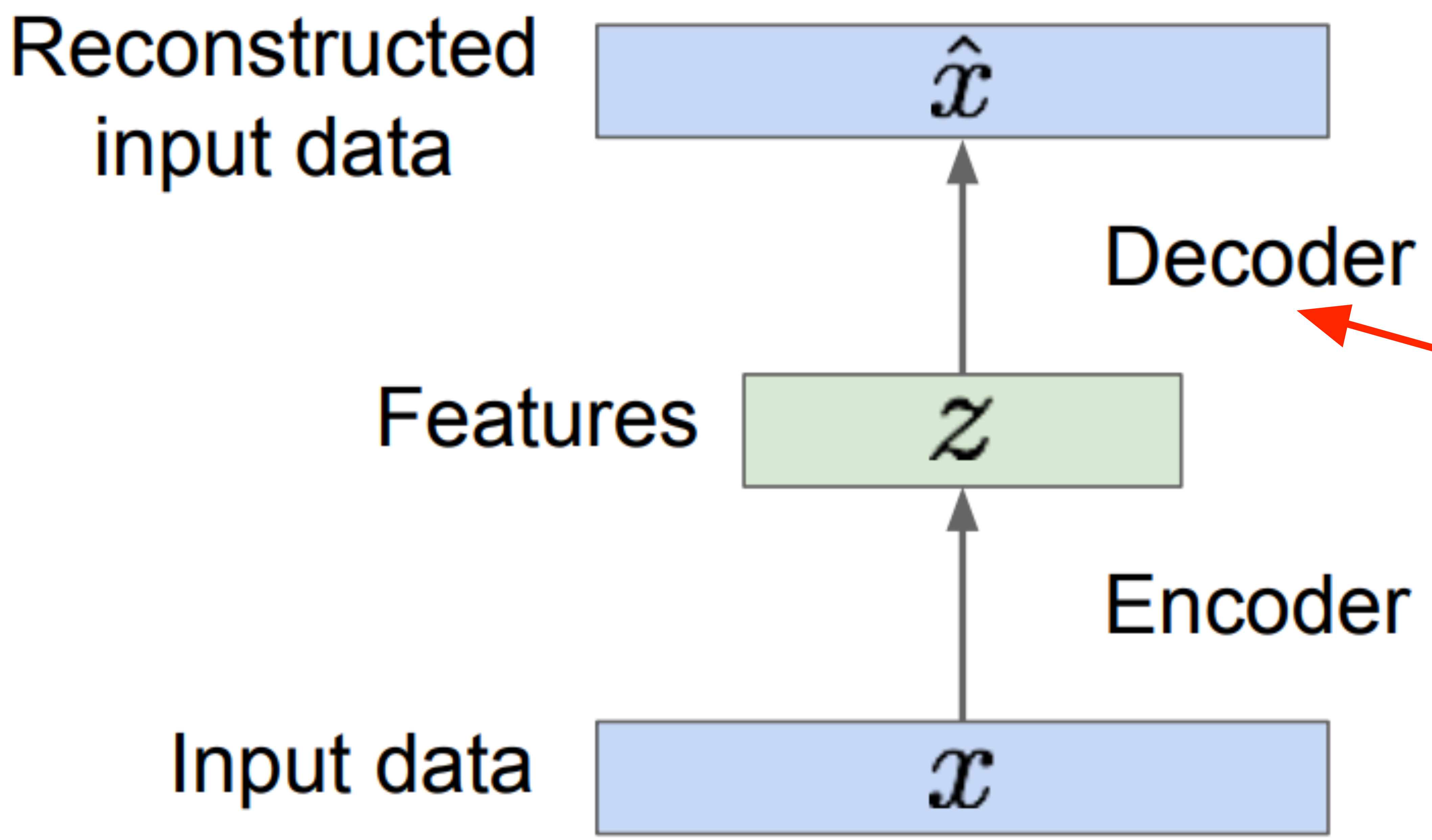


Reconstructed data

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

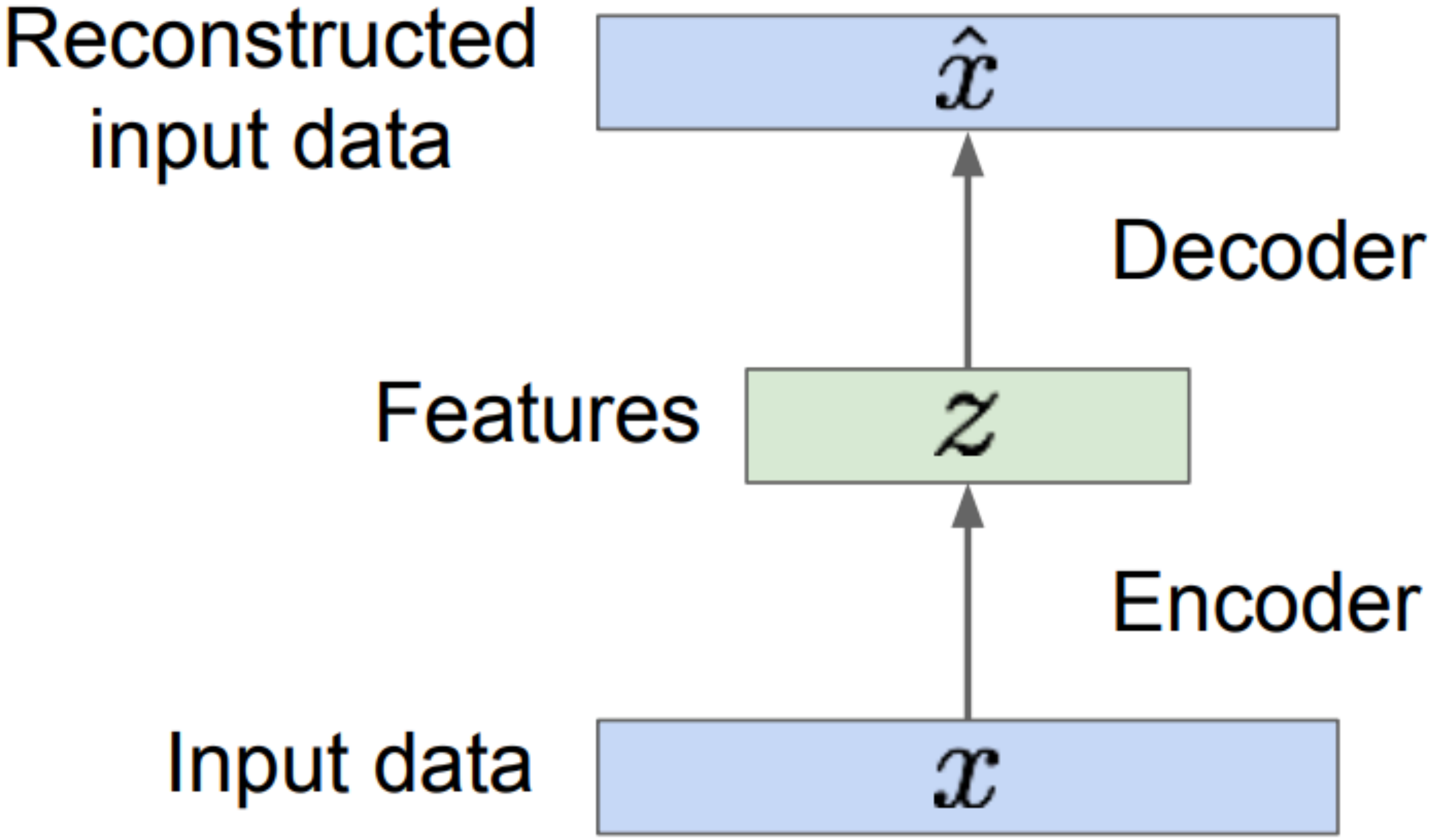
Input data

Some background first: Autoencoders



After training,
throw away 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. Can we generate new images from an autoencoder?

Variational Autoencoders

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

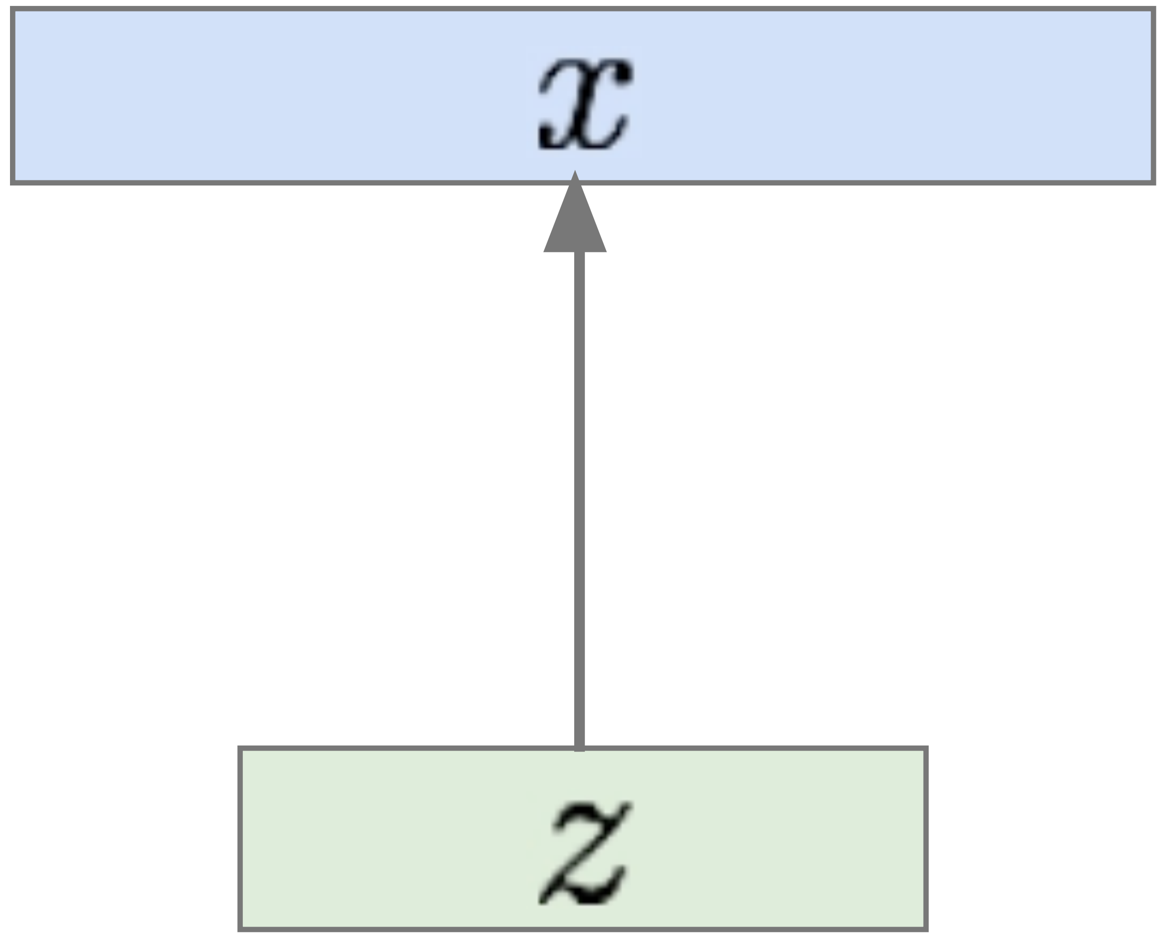
Variational Autoencoders

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 underlying unobserved (latent) representation **z**

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

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



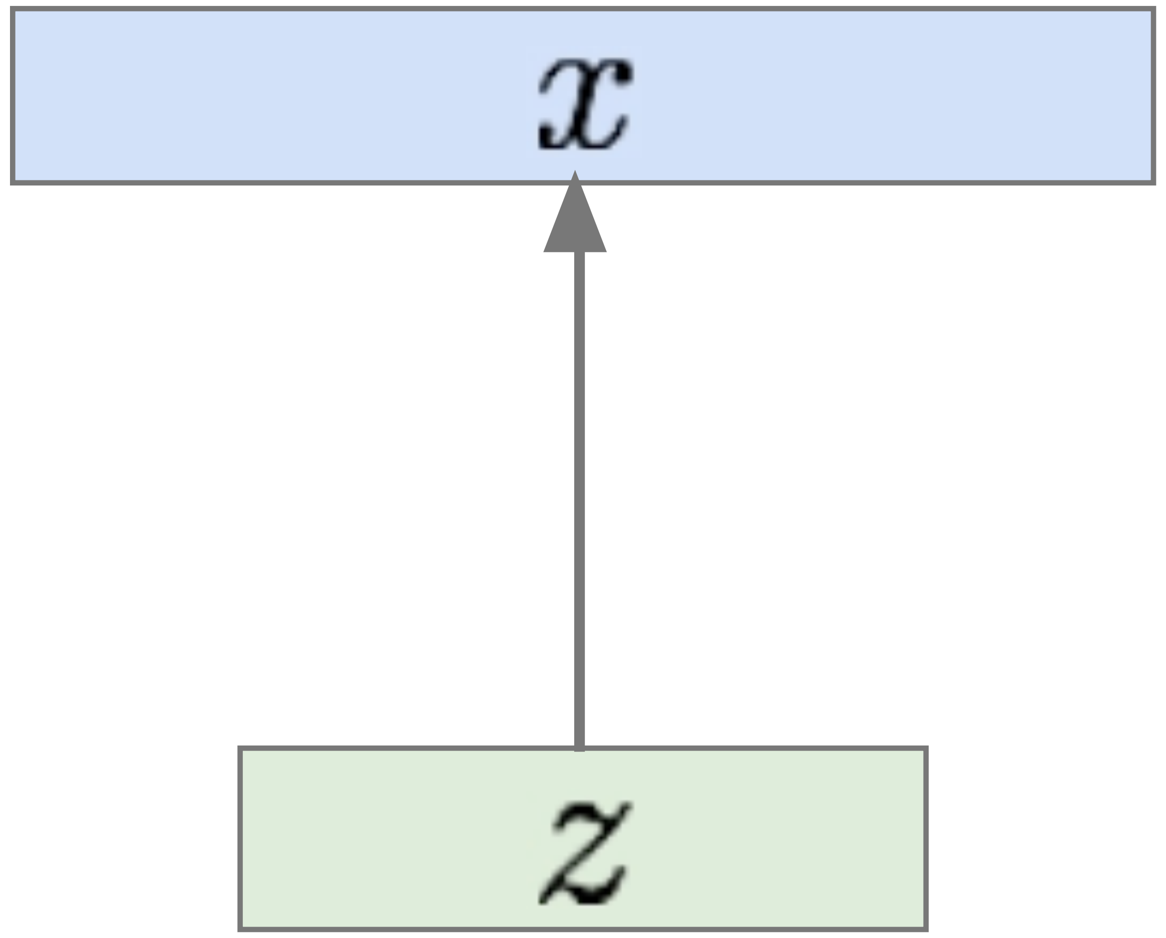
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

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 underlying unobserved (latent) representation **z**

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



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

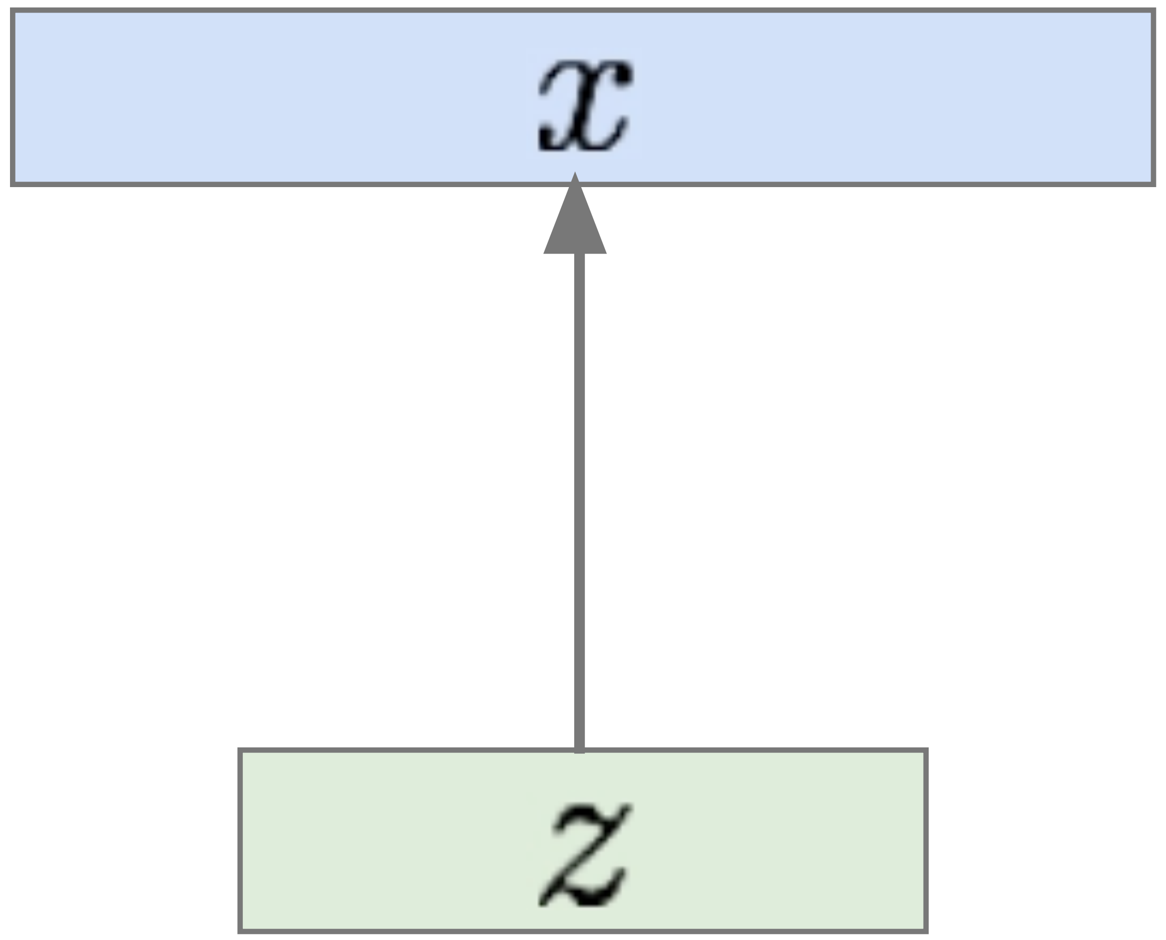
Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

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

Variational Autoencoders

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

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



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

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

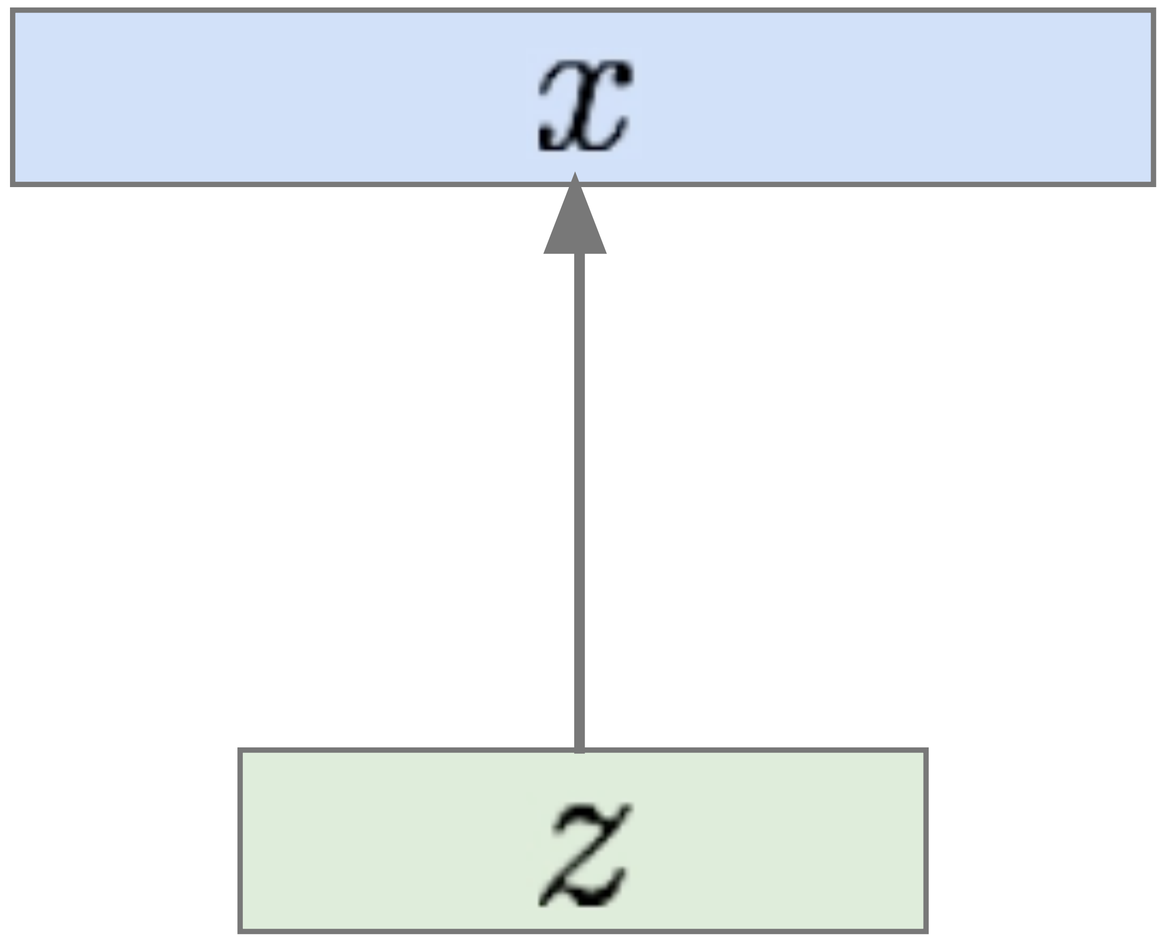
Variational Autoencoders

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

How should we represent this model?

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

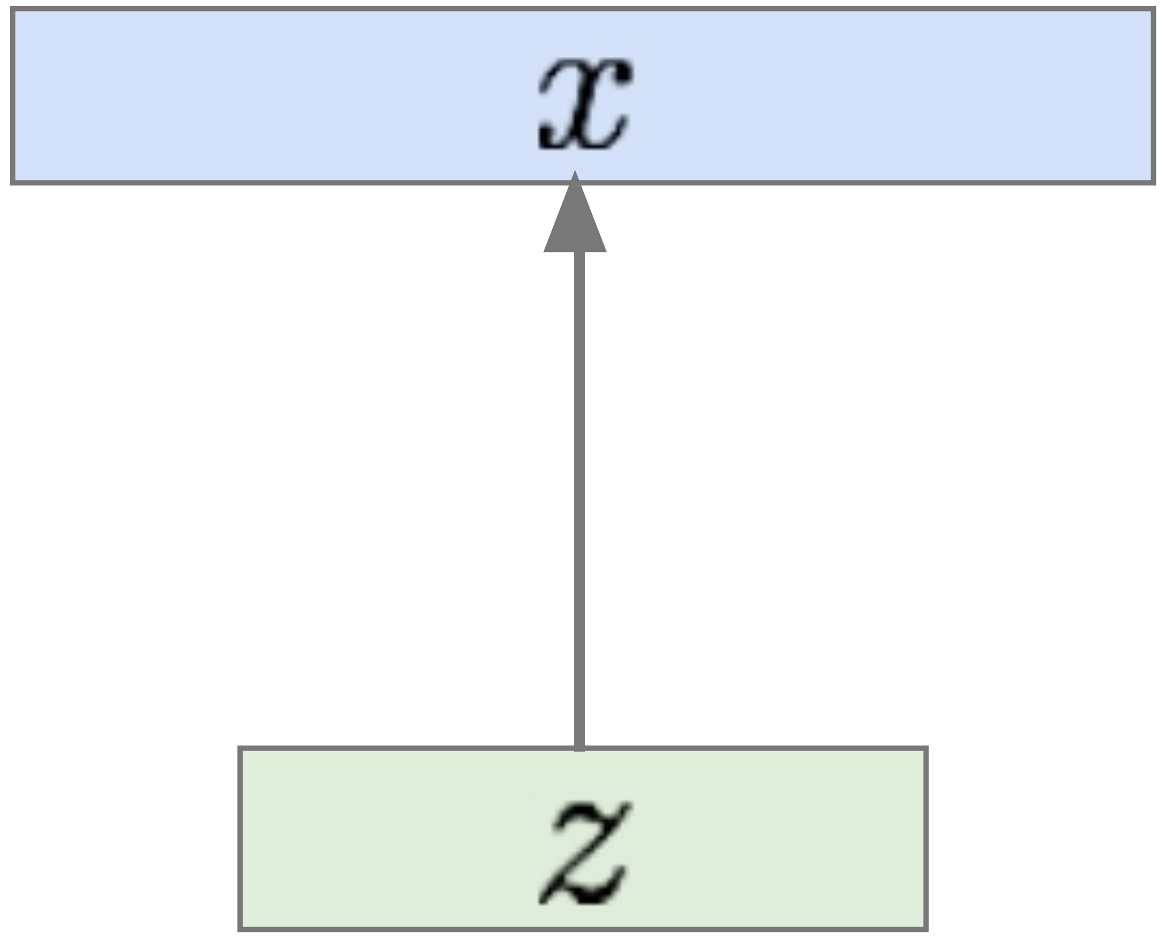
Sample from true prior
$p_{\theta^*}(z)$



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. Reasonable for latent attributes, e.g. pose, how much smile.

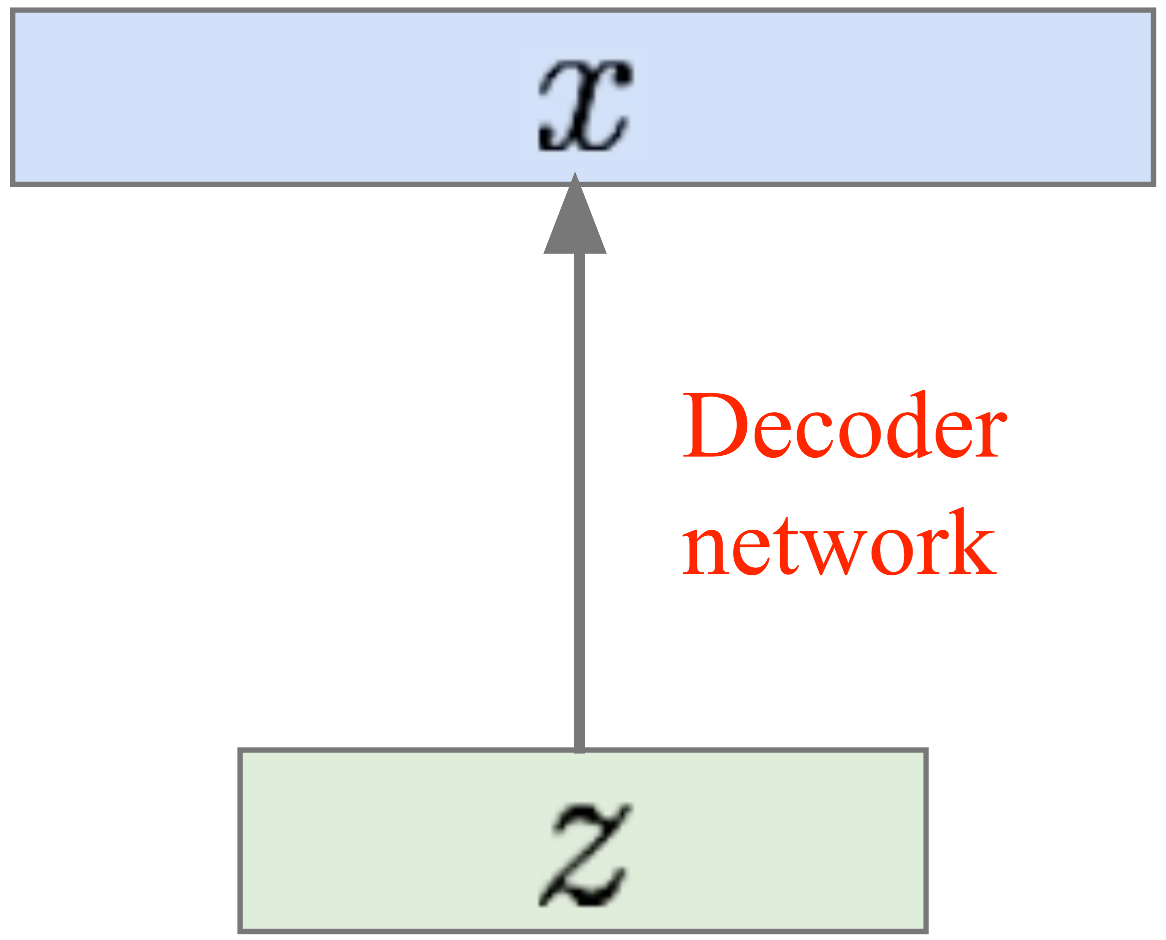
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

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

Sample from true conditional

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



Sample from true prior

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

How should we represent this model?

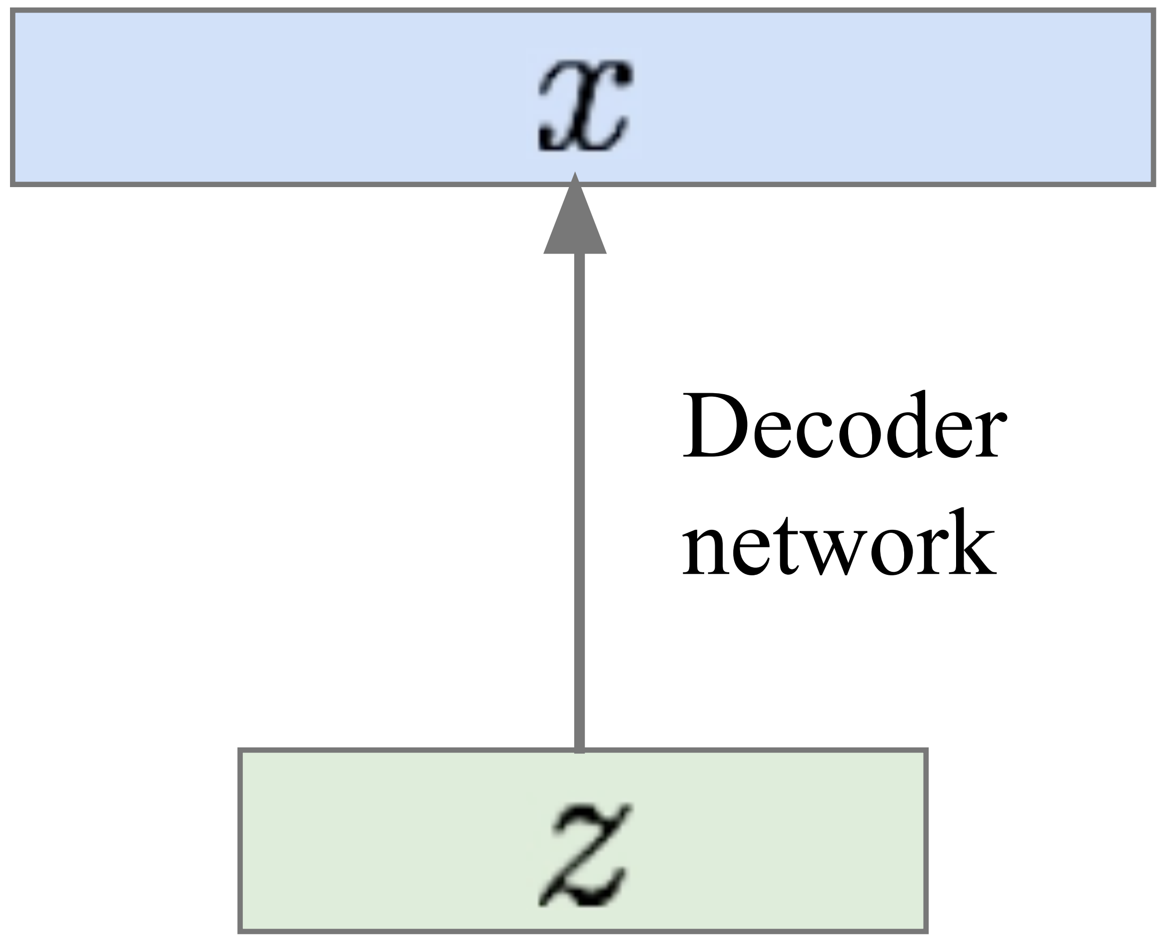
Choose prior p(z) to be simple, e.g. Gaussian.

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

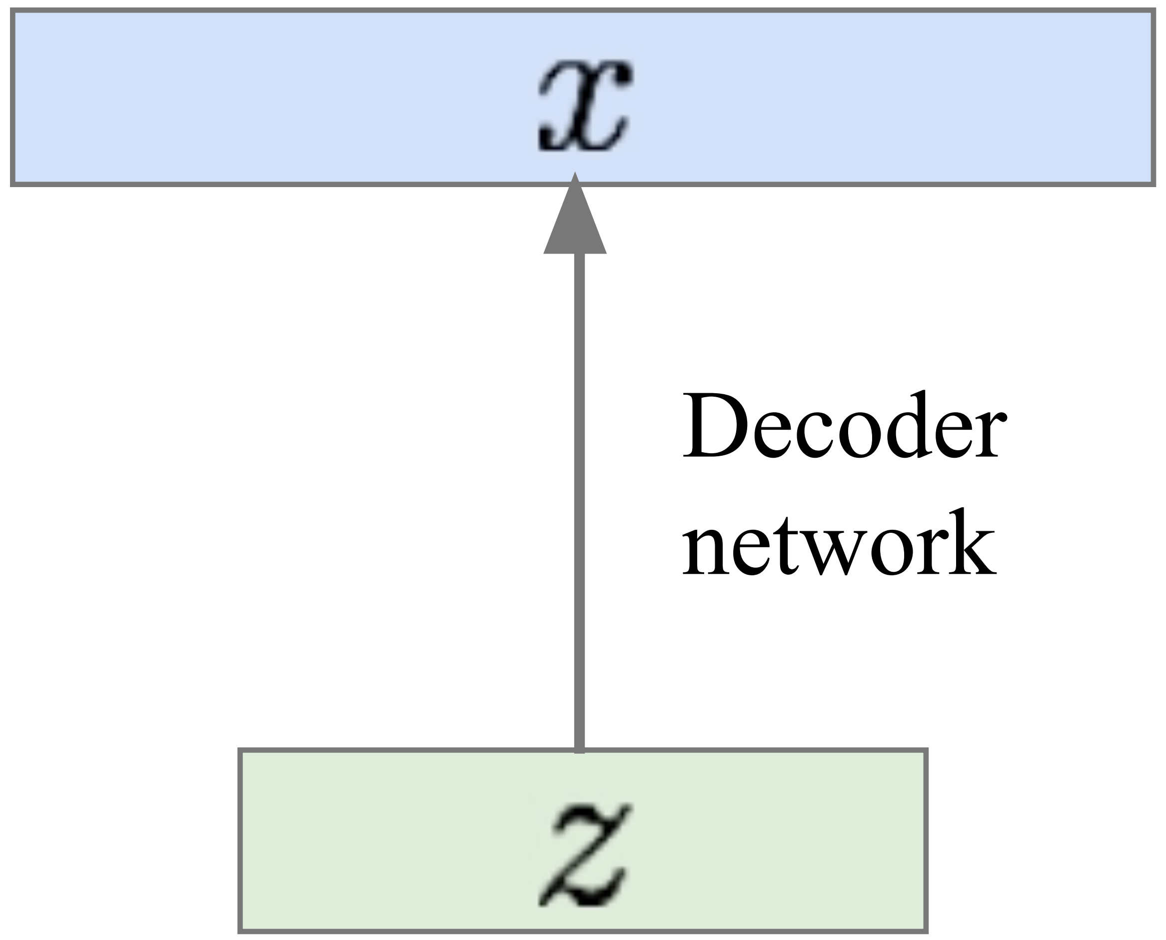
We want to estimate the true parameters θ^*
of this generative model.

How to train the model?

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 to train the model?

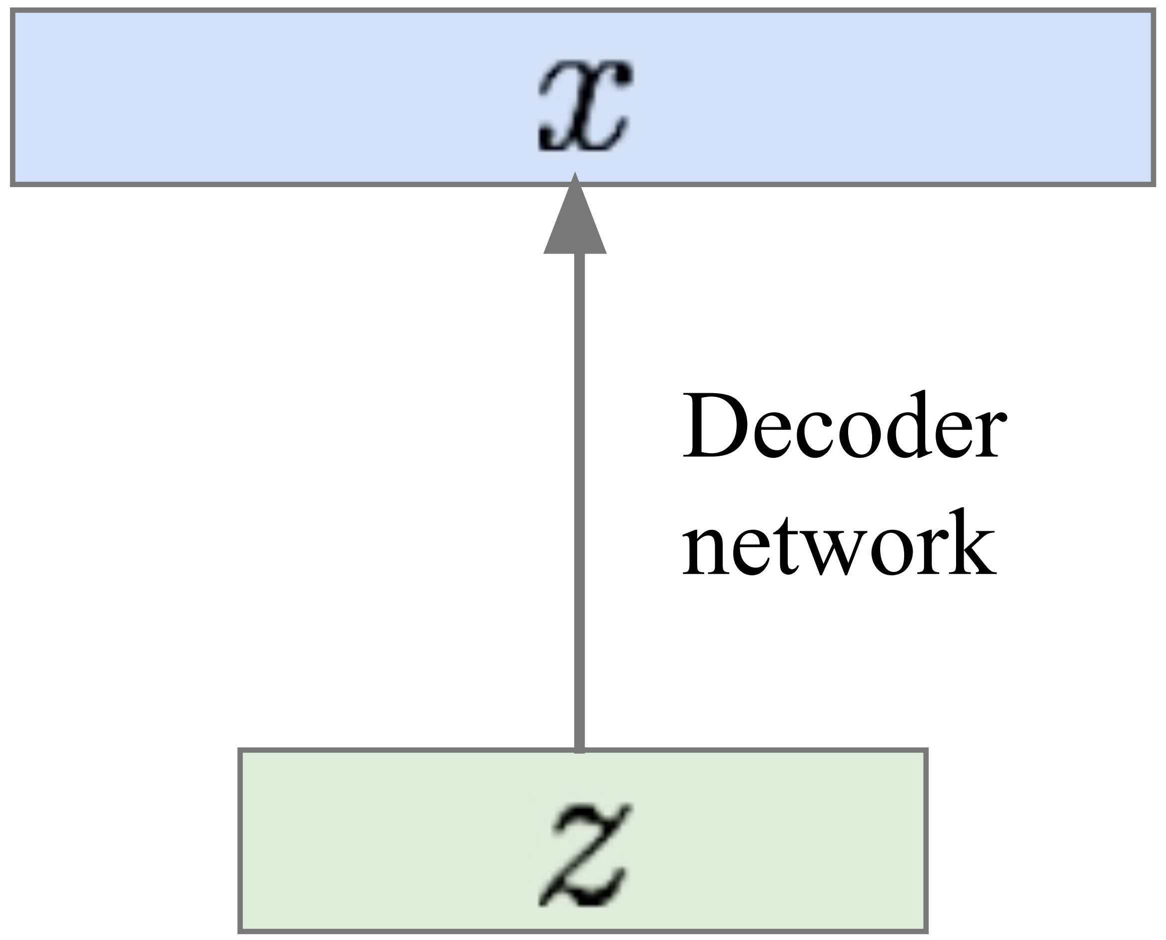
Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

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

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

Variational Autoencoders

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



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

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

How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

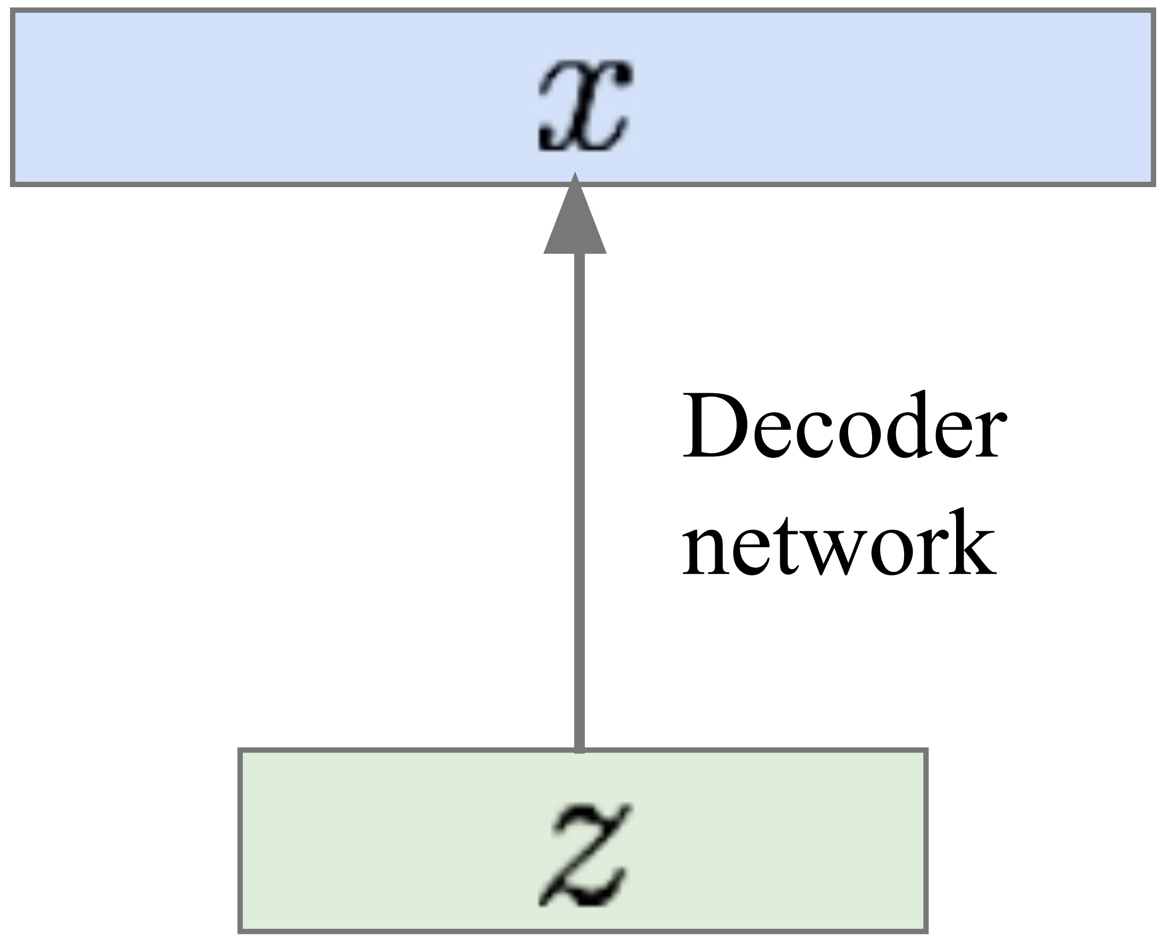
$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Now with latent z

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

Variational Autoencoders

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



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

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

How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

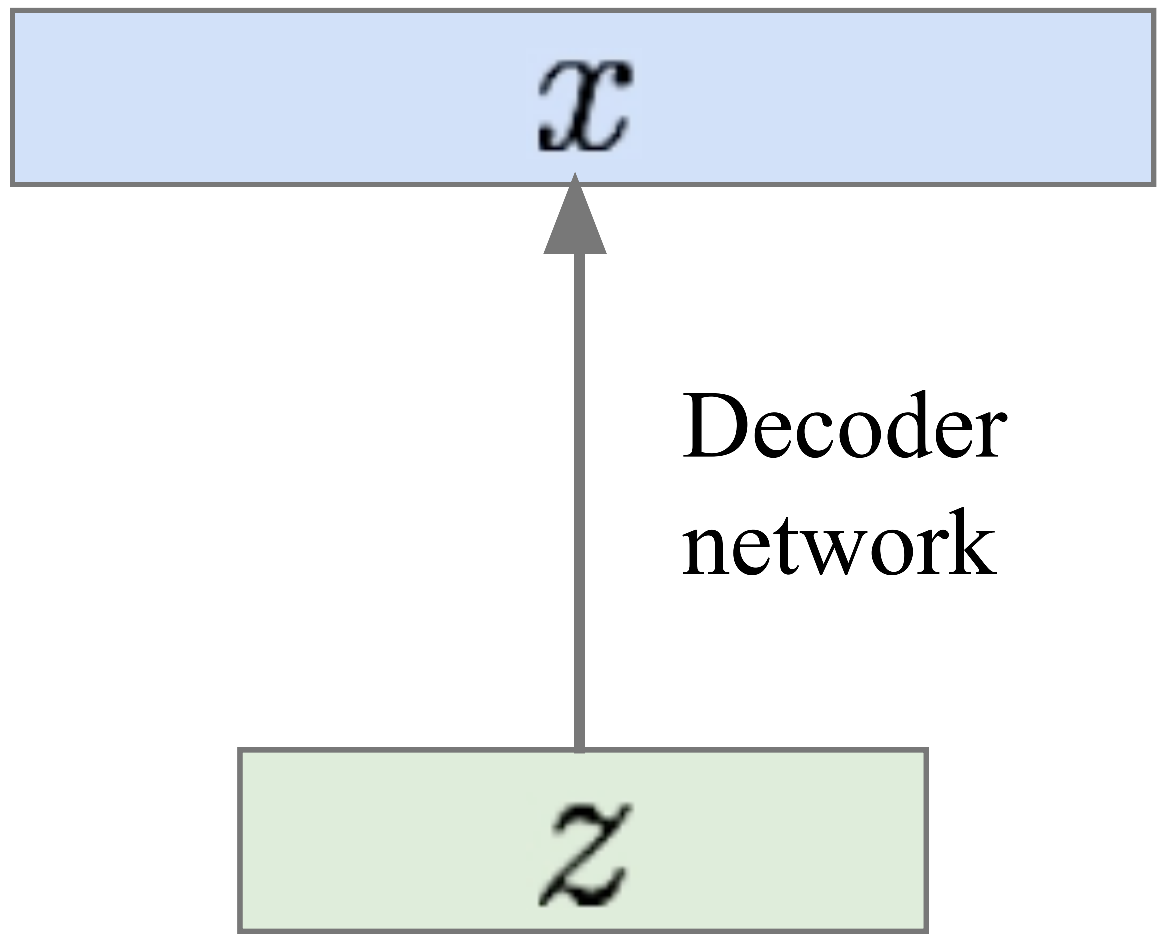
$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Q: What is the problem with this?

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 to train the model?

Remember strategy for training generative models from FVBNs. 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?

A: 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 Autoencoders: Intractability

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

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

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 $_\theta(z|x)$

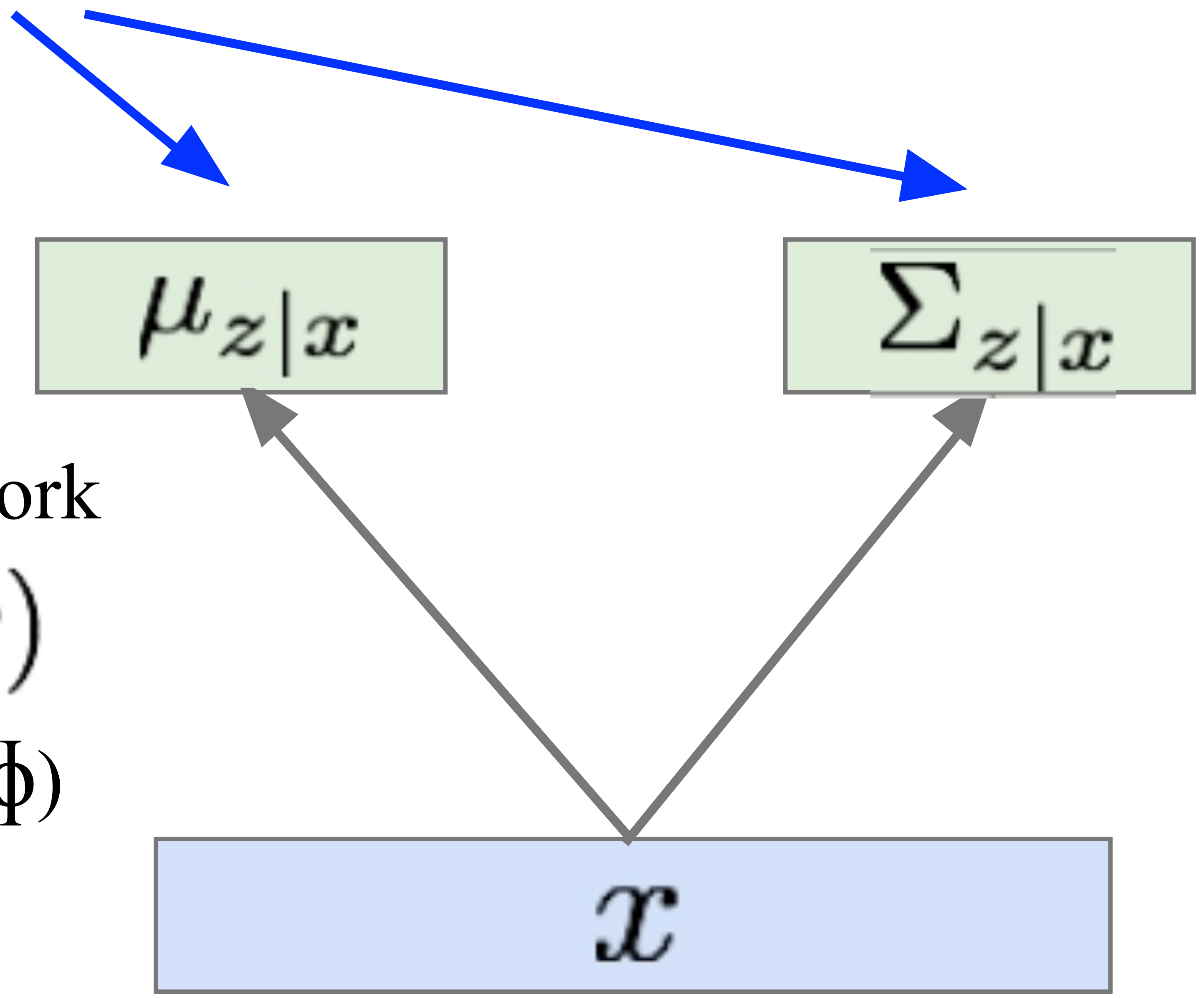
Will see that this allows us to derive a lower bound on the data likelihood that is tractable, which we can optimize

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**

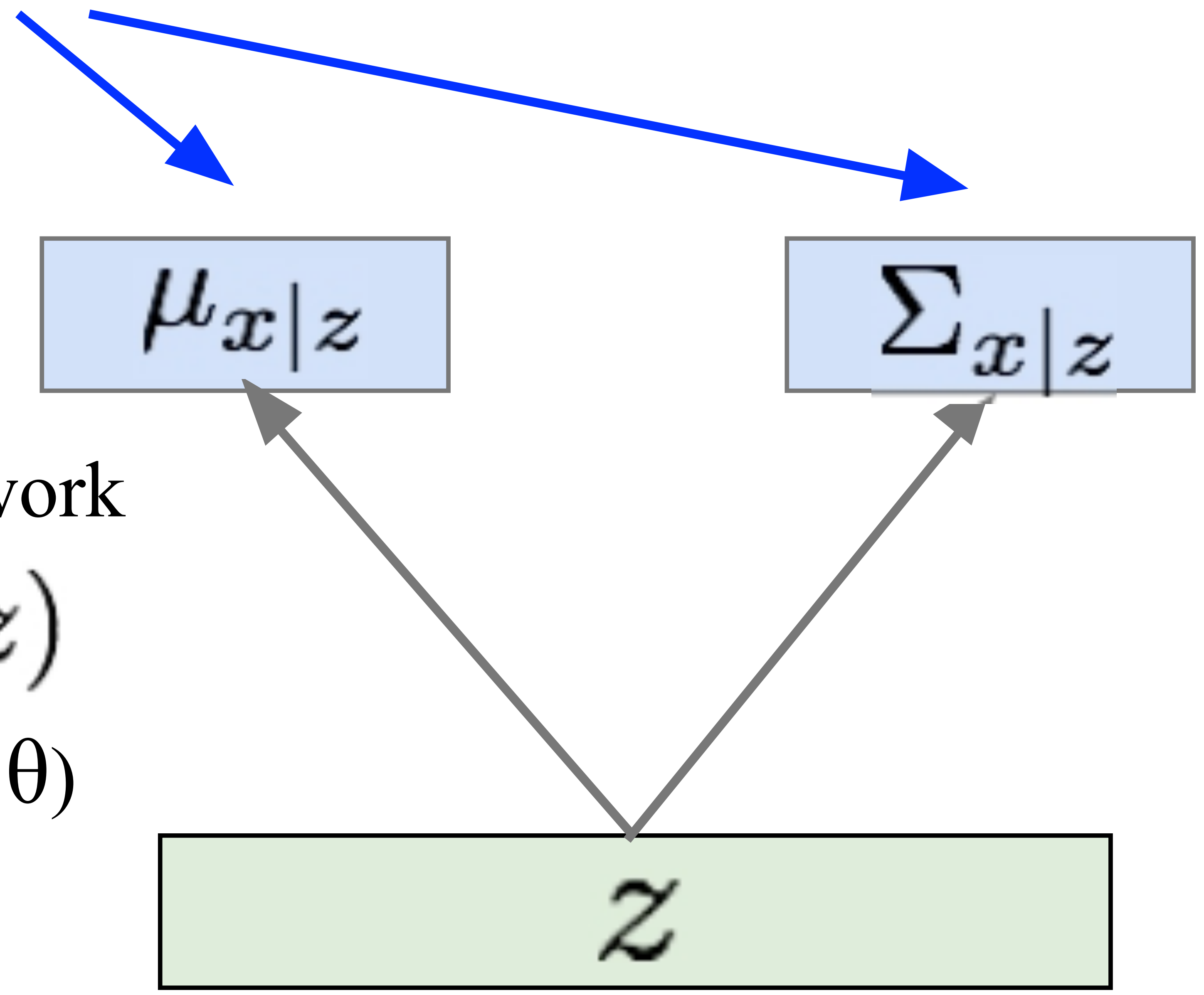


Encoder network

$q_\phi(z|x)$

(parameters ϕ)

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



Decoder network

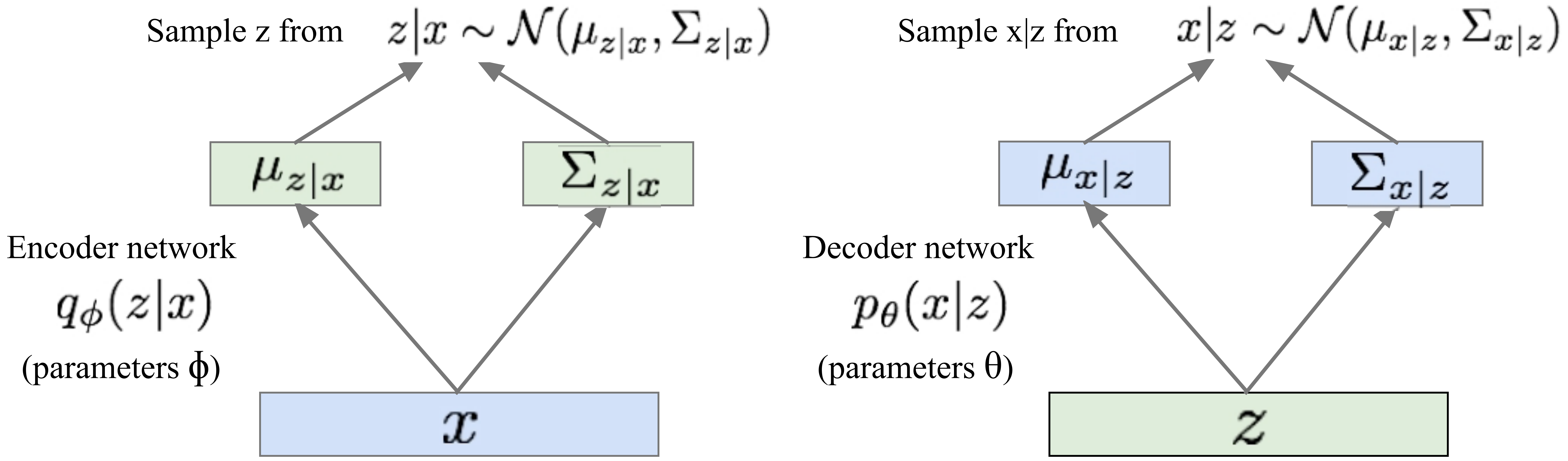
$p_\theta(x|z)$

(parameters θ)

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

Variational Autoencoders

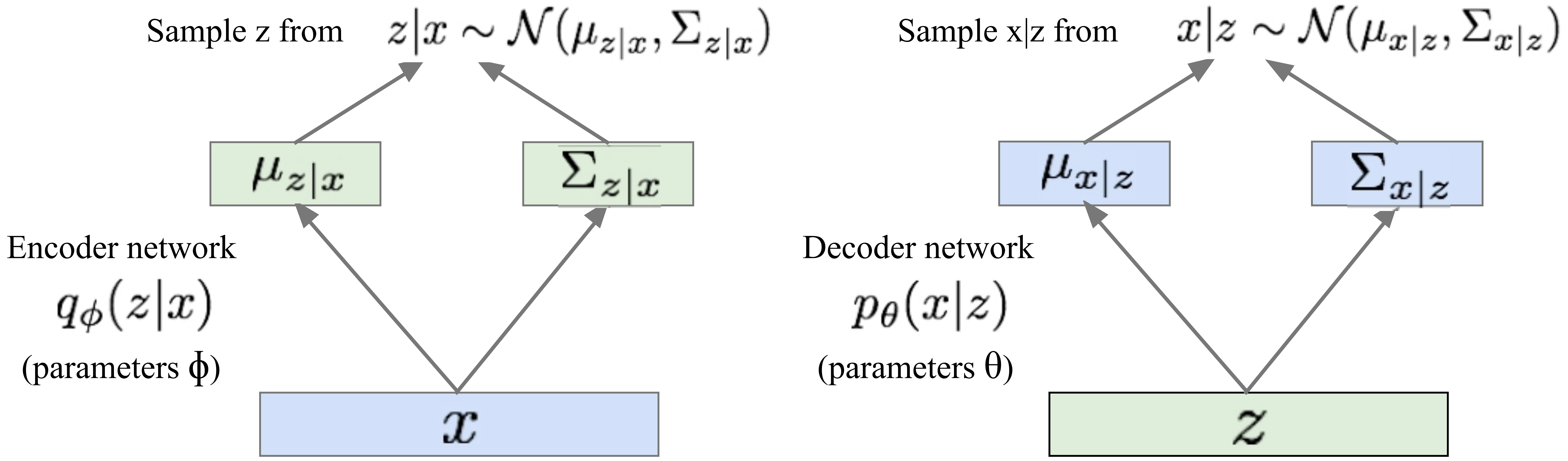
Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



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:

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

Variational Autoencoders

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

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

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:

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

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

Variational Autoencoders

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

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

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

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

Variational Autoencoders

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

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

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

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

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

Variational Autoencoders

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

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

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

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

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

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

Variational Autoencoders

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

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

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:

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

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

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

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

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

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:

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

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

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

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

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

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:

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

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

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

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

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

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

Variational lower bound ("ELBO")

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

Variational Autoencoders

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

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

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

Reconstruct the input data

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

Make approximate posterior distribution close to prior

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

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

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

Variational lower bound ("ELBO")

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

Used with permission from Justin Johnson

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

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

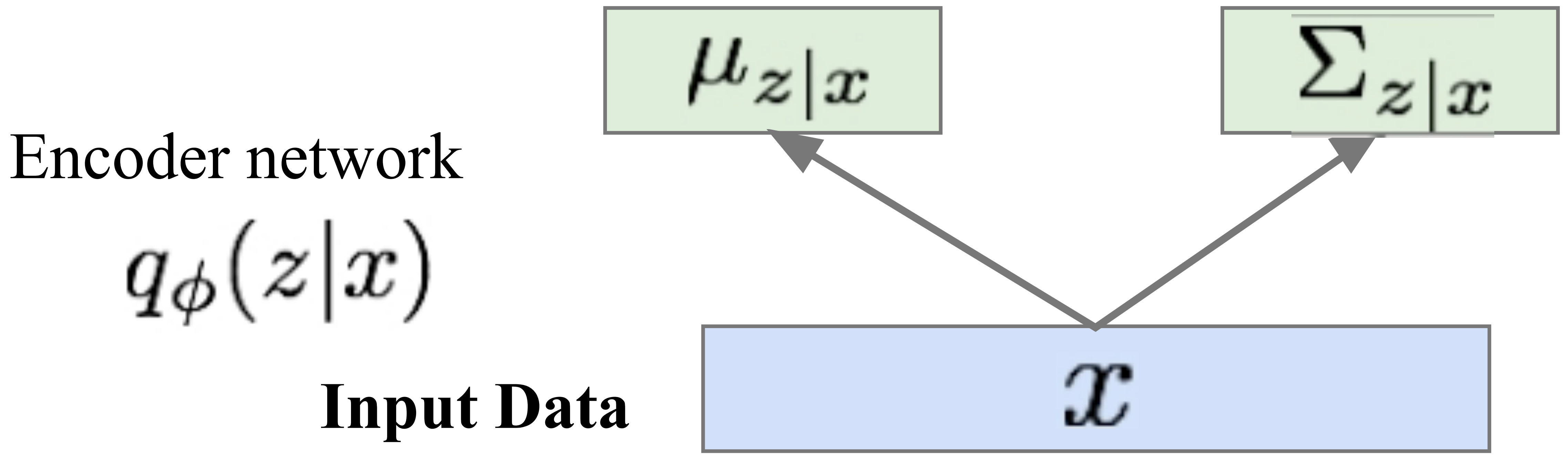
Let's look at computing the bound (forward pass) for a given minibatch of input data

Input Data $\boxed{x}$

Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

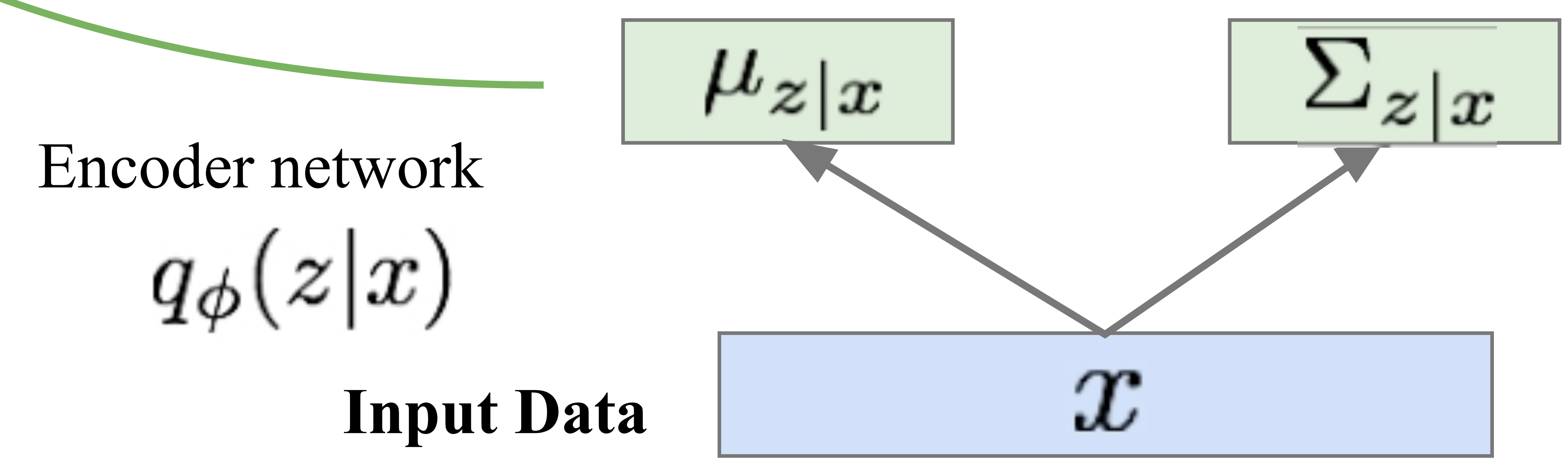


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

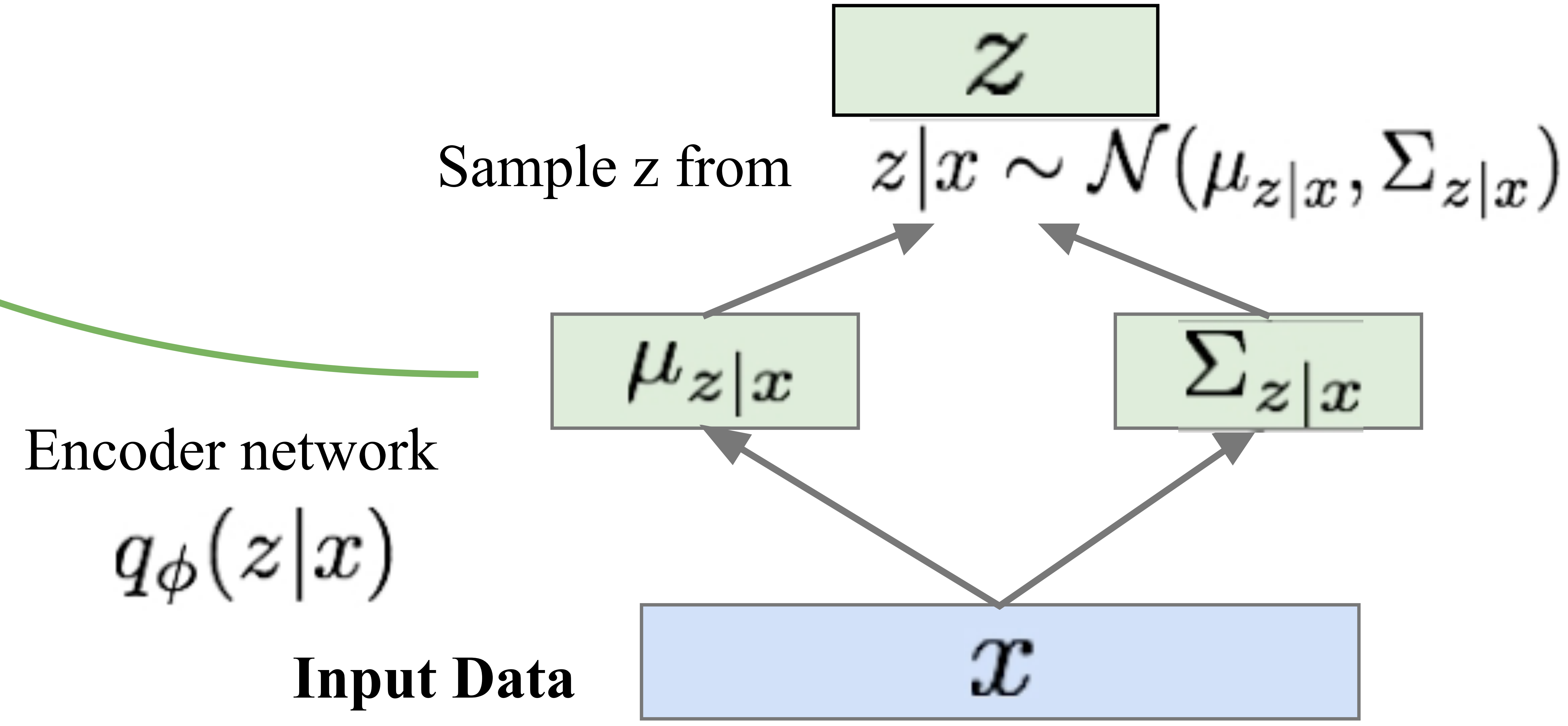


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior

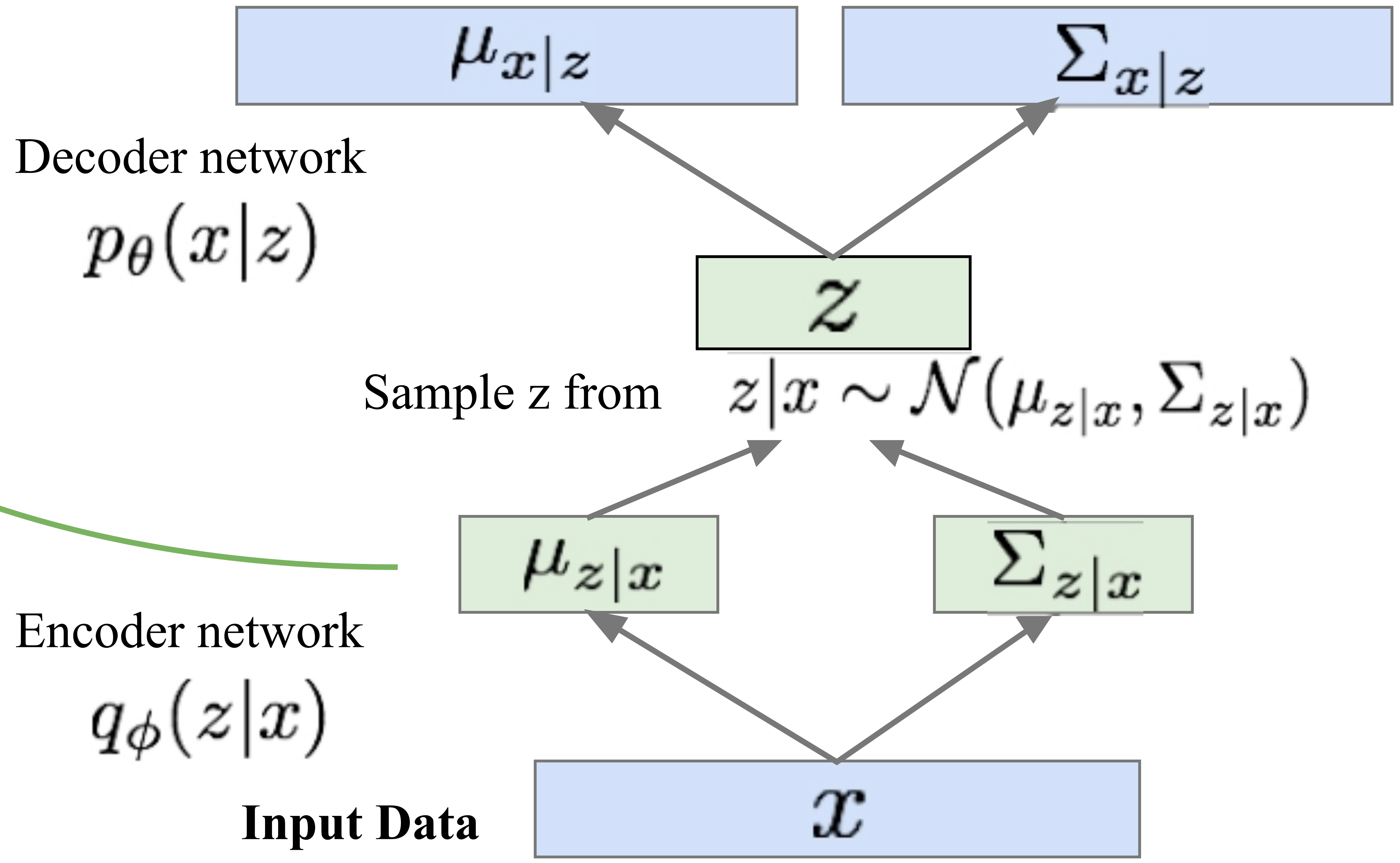


Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Make approximate posterior distribution close to prior



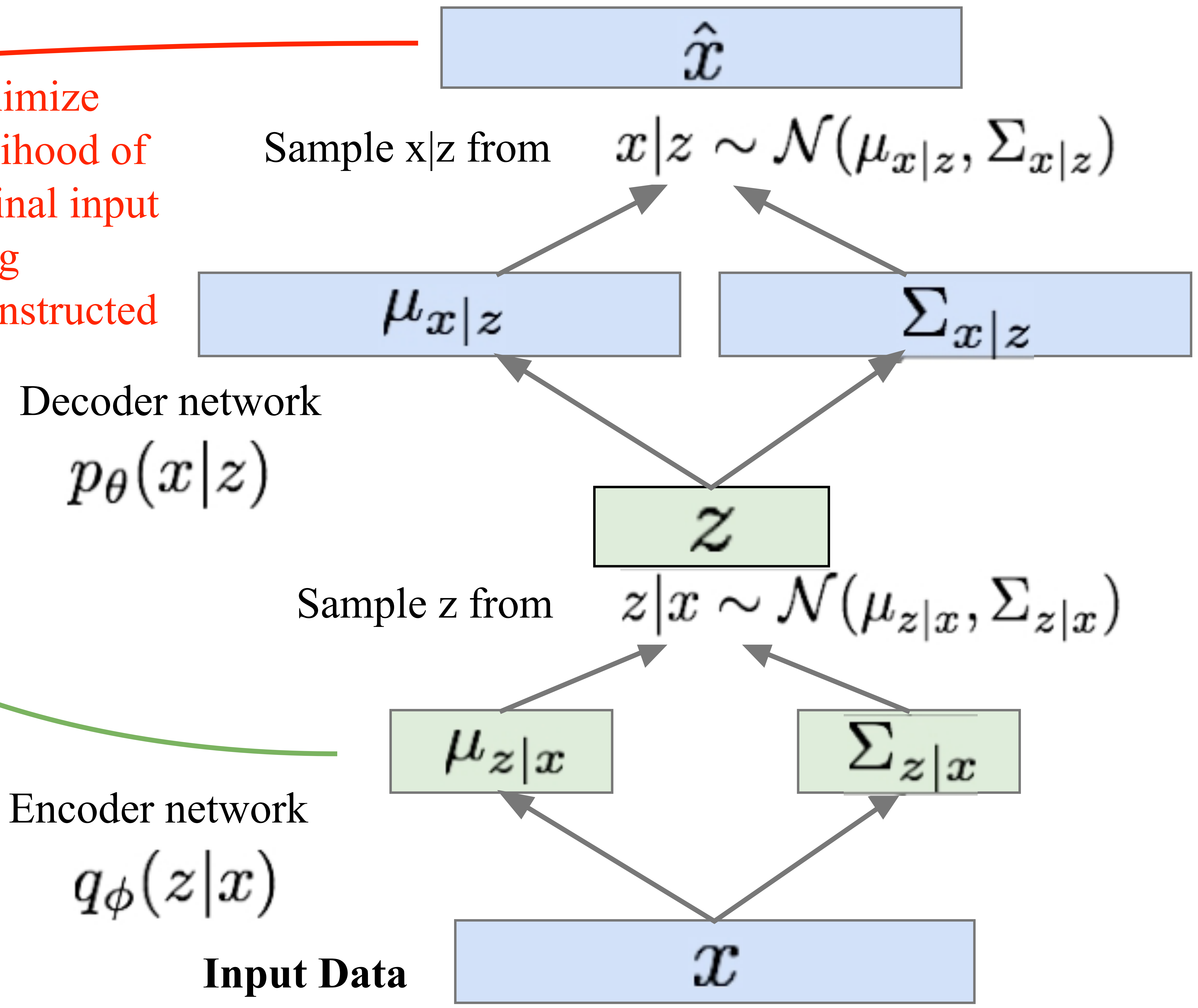
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Maximize likelihood of original input being reconstructed

Make approximate posterior distribution close to prior



Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

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

Maximize likelihood of original input being reconstructed

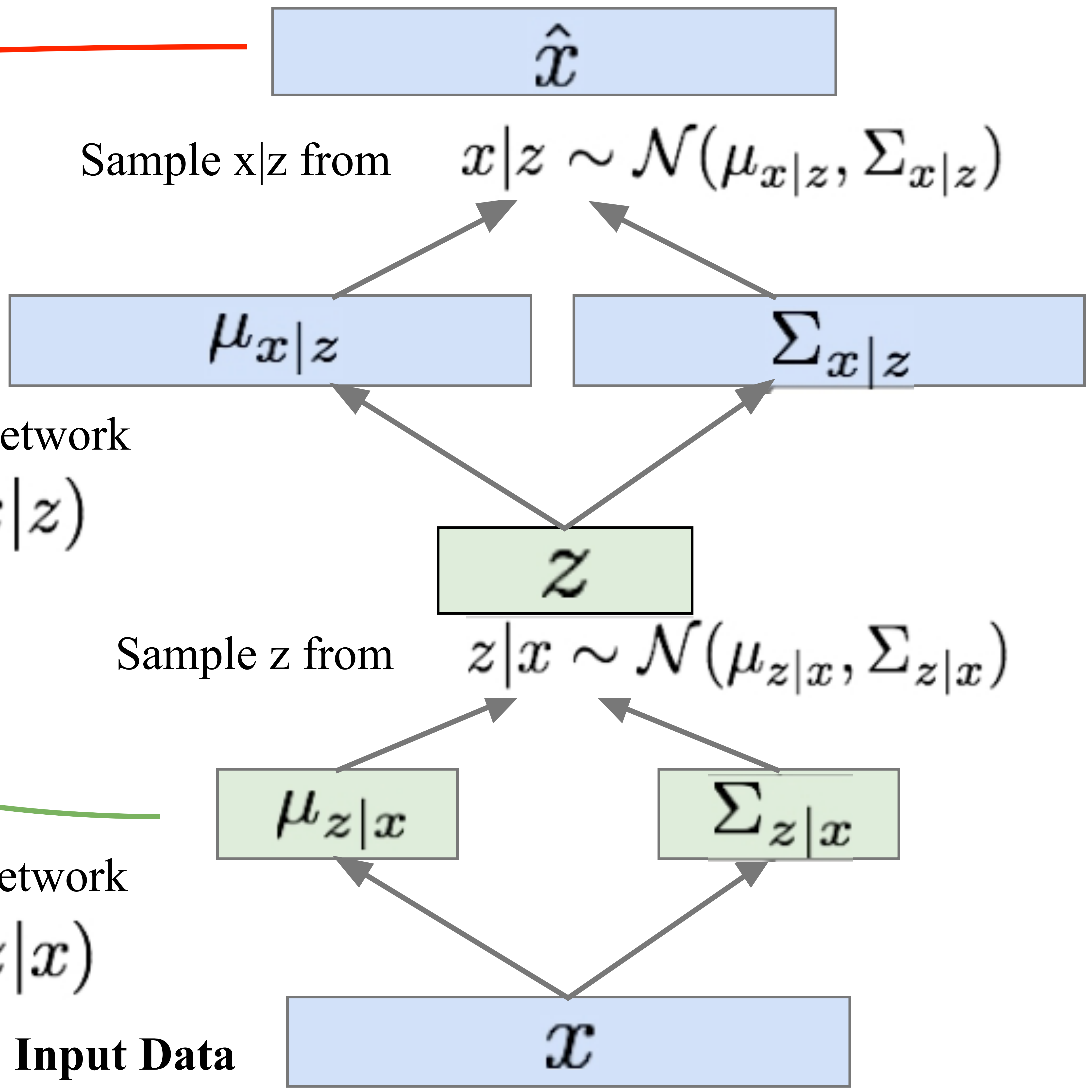
Make approximate posterior distribution close to prior

Decoder network

$p_\theta(x|z)$

Encoder network

$q_\phi(z|x)$

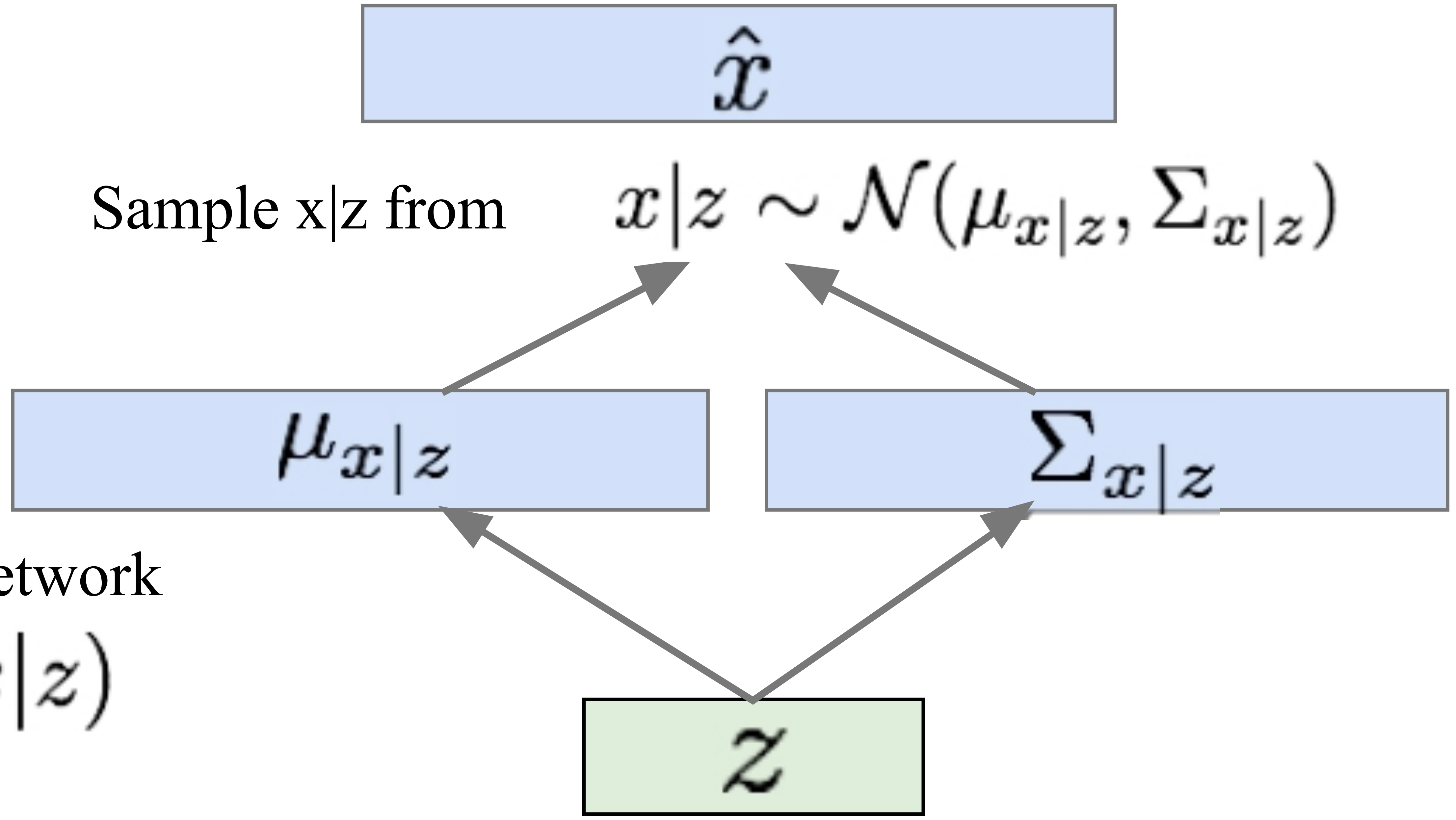


For every minibatch of input data: compute this forward pass, and then backprop!

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$



Decoder network

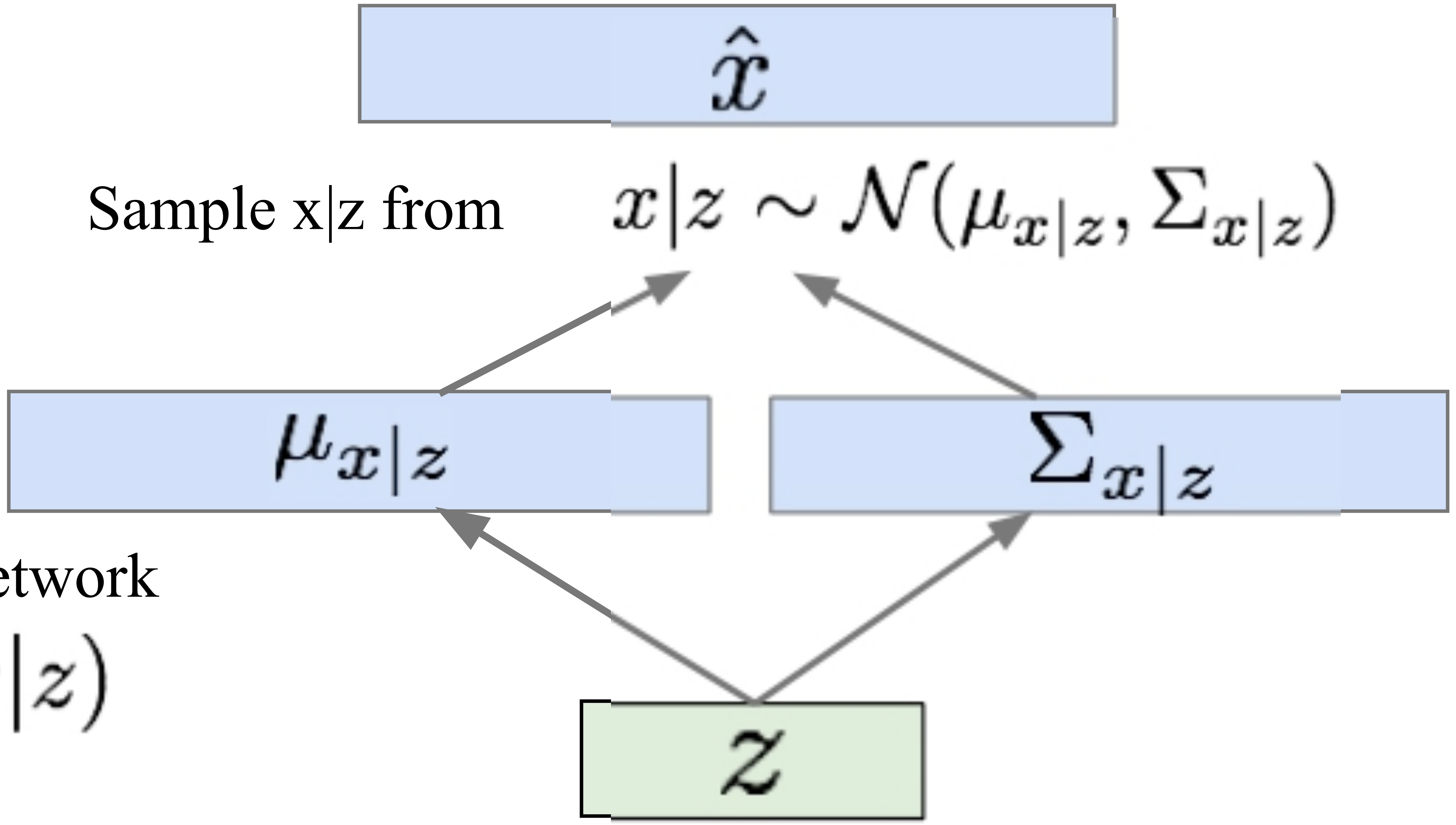
$p_\theta(x|z)$

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

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

Variational Autoencoders: Generating Data!

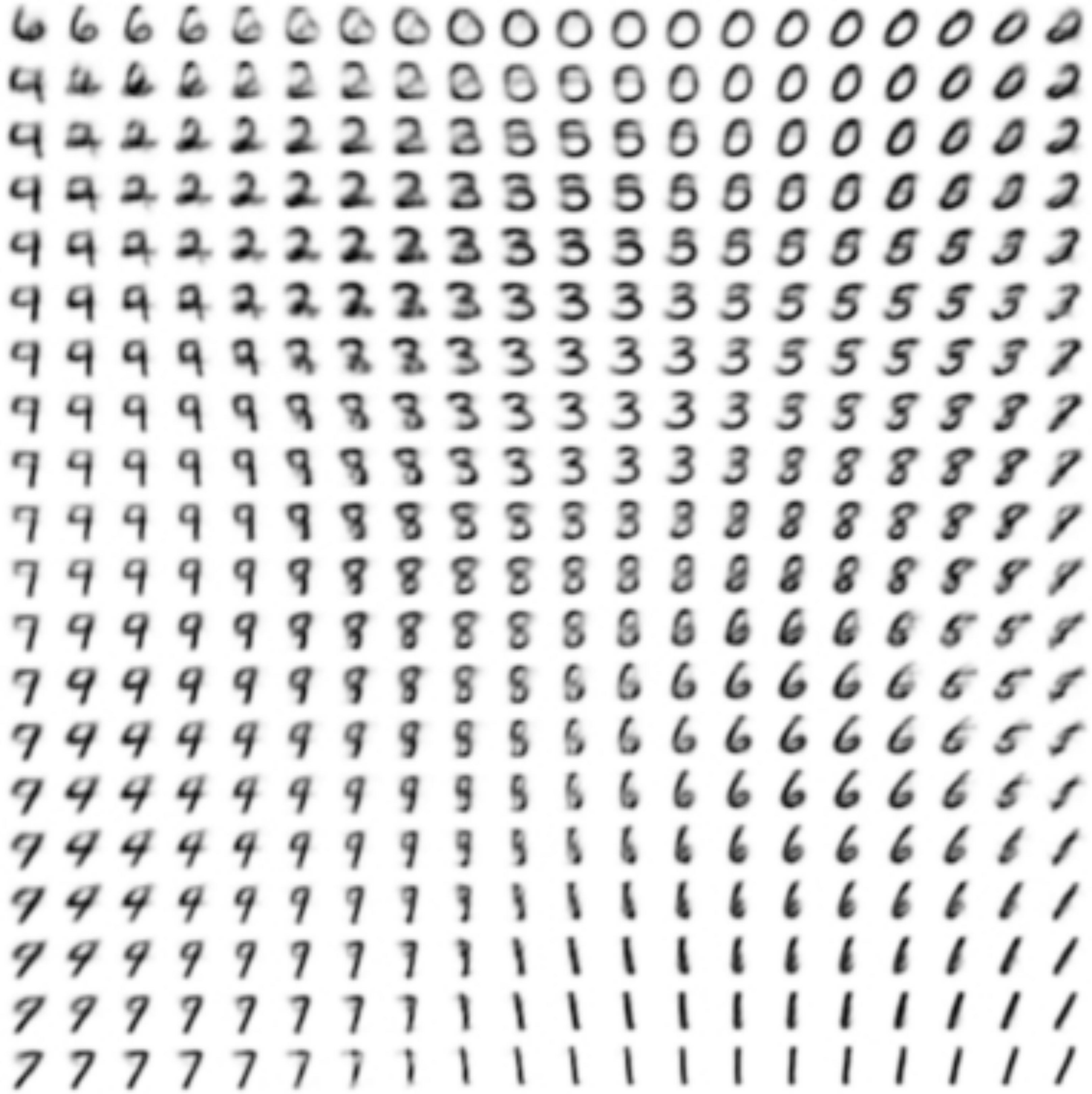
Use decoder network. Now sample z from prior!



Decoder network

$p_\theta(x|z)$

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



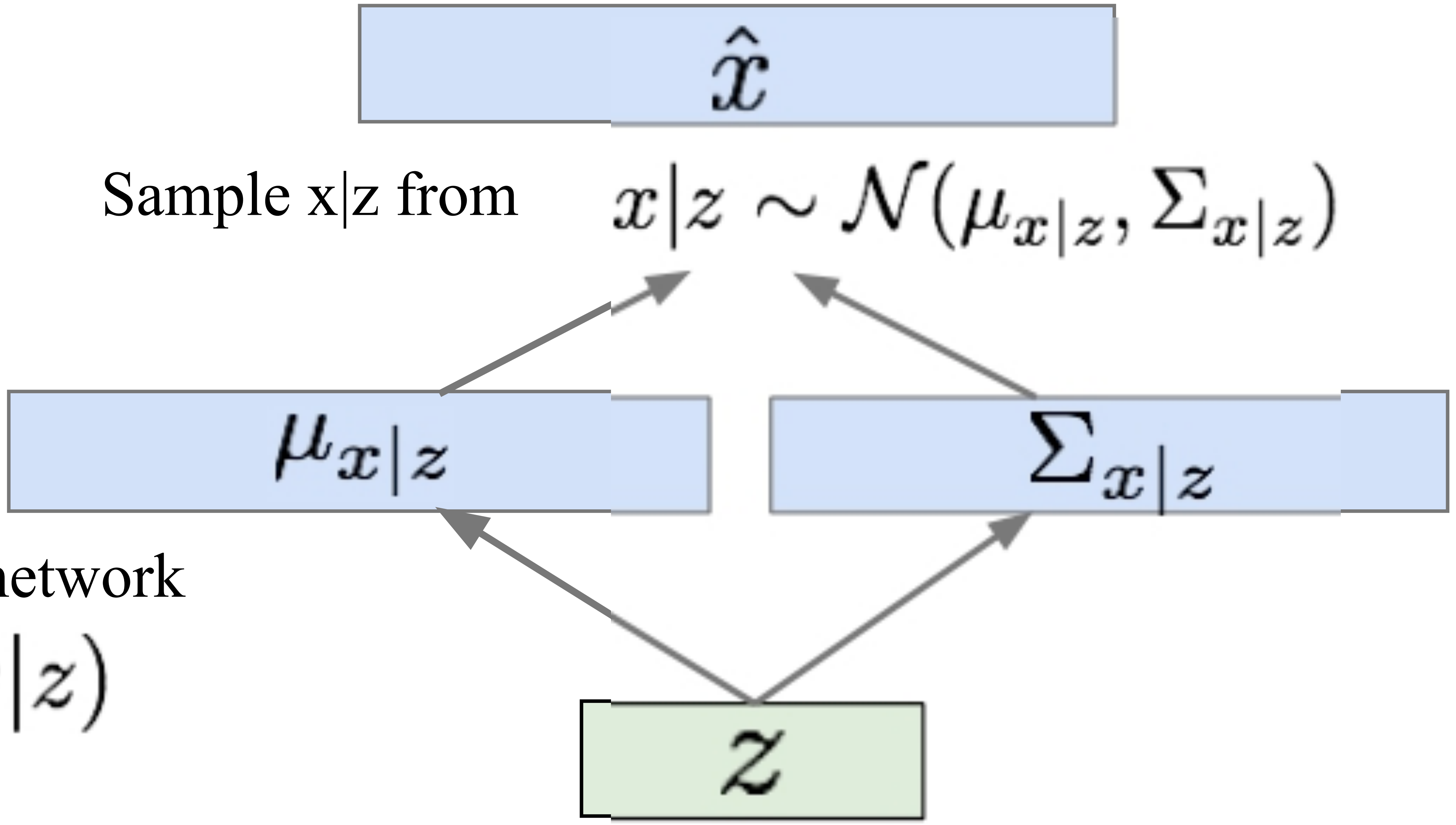
Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!

Data manifold for 2-d **z**

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$



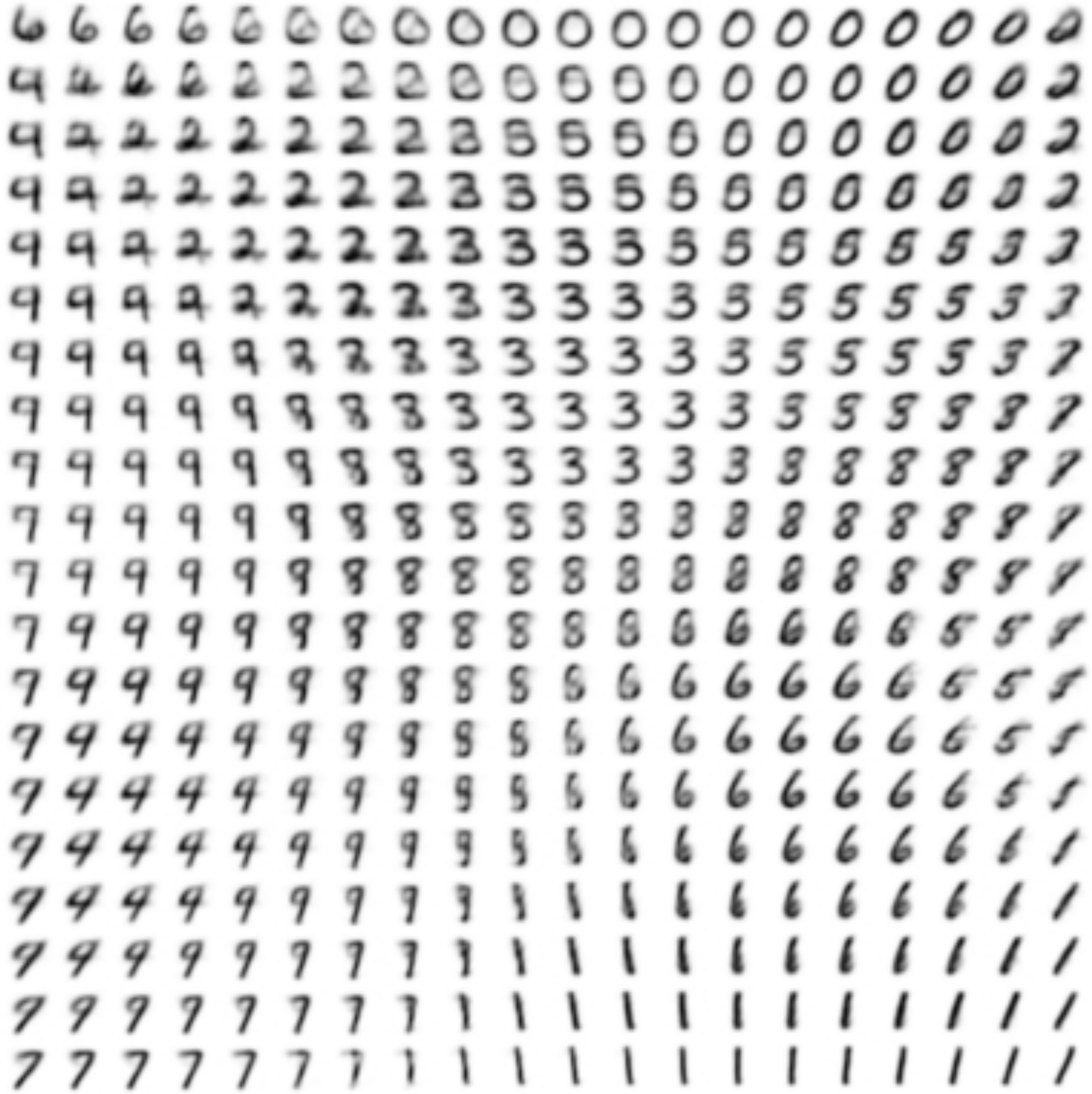
Decoder network

$p_\theta(x|z)$

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

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

Vary $\mathbf{z_1}$



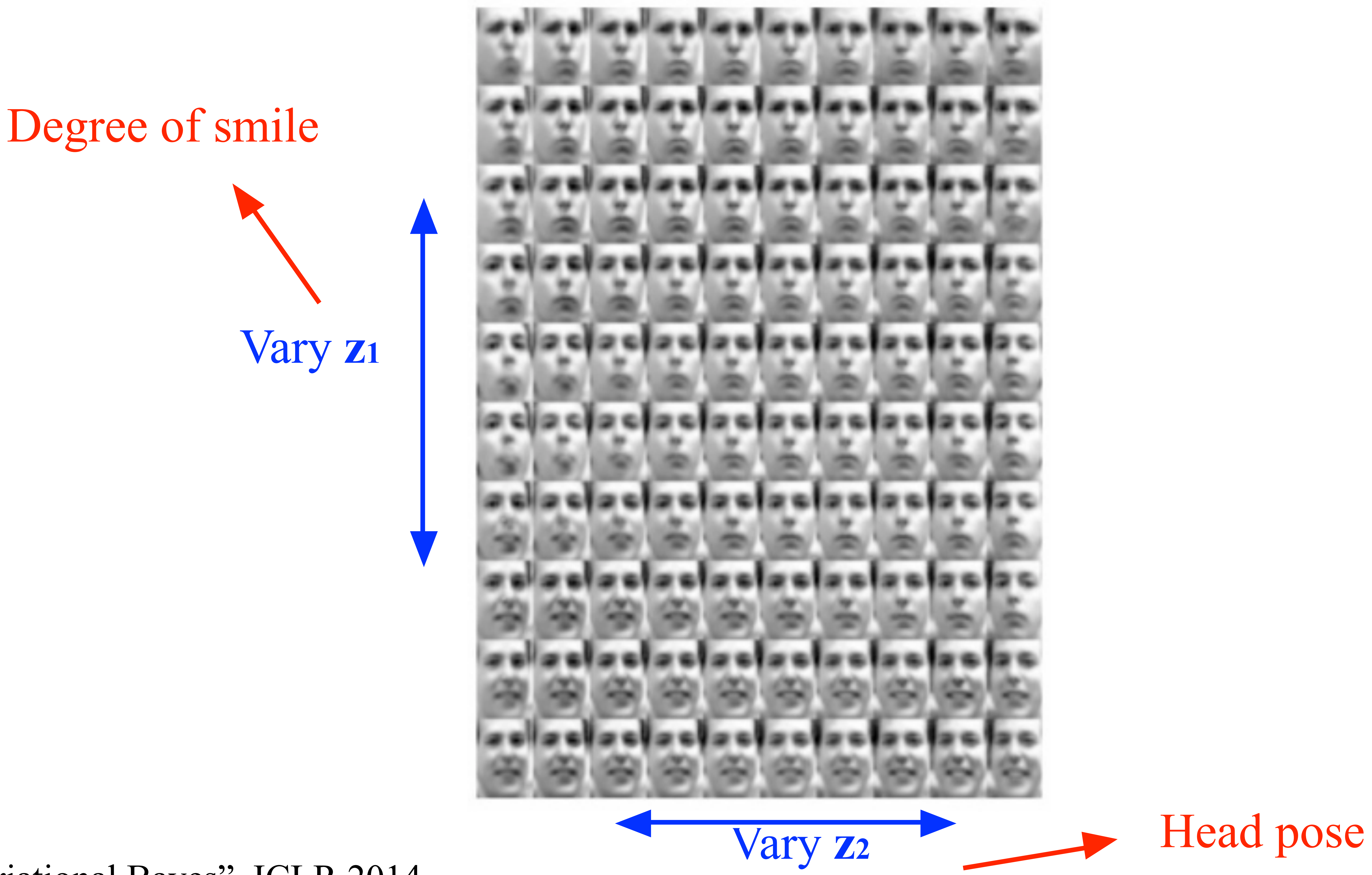
Vary $\mathbf{z_2}$

Variational Autoencoders: Generating Data!

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

Different
dimensions of **z**

encode
interpretable factors
of variation



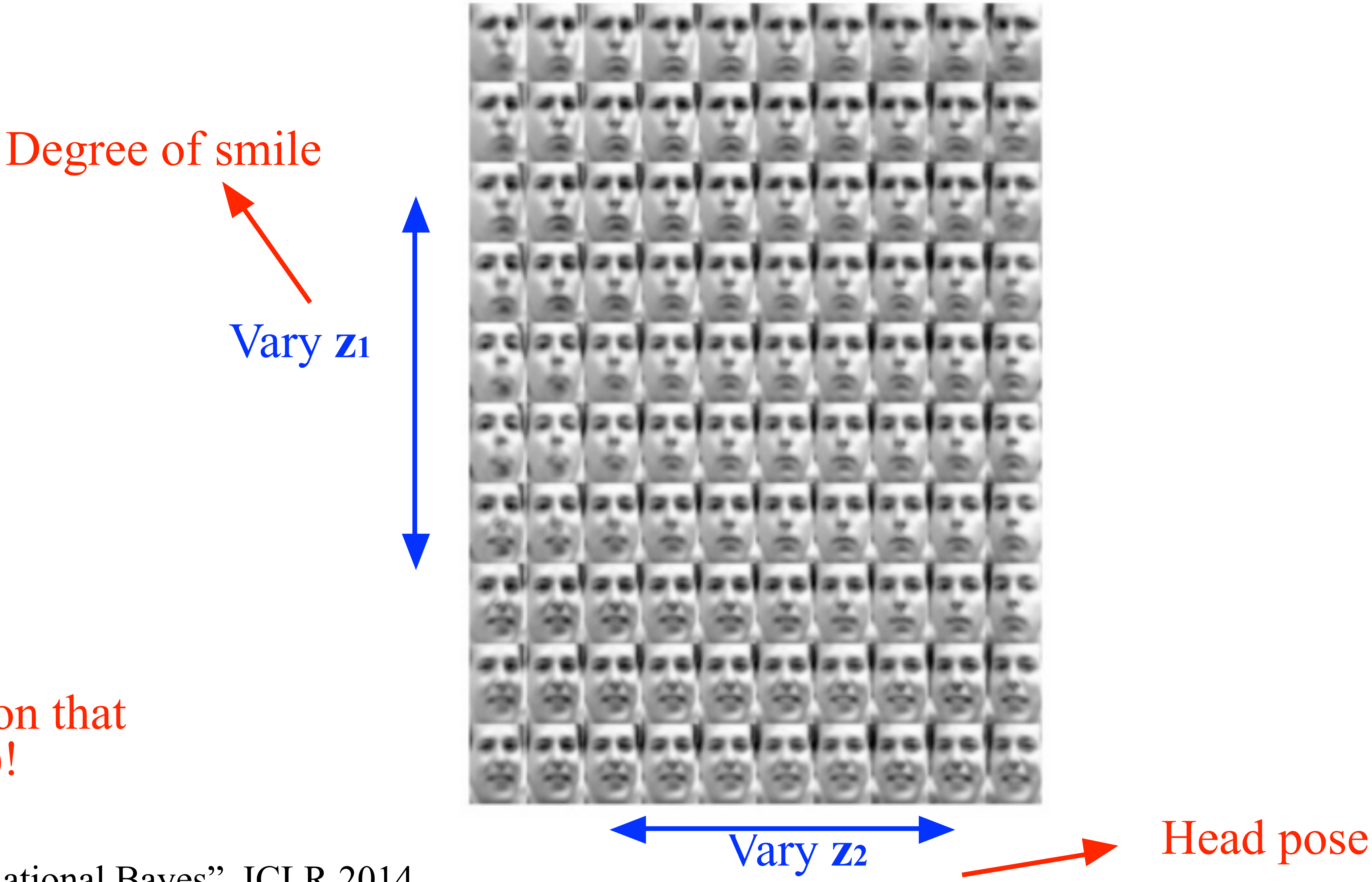
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders: Generating Data!

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

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

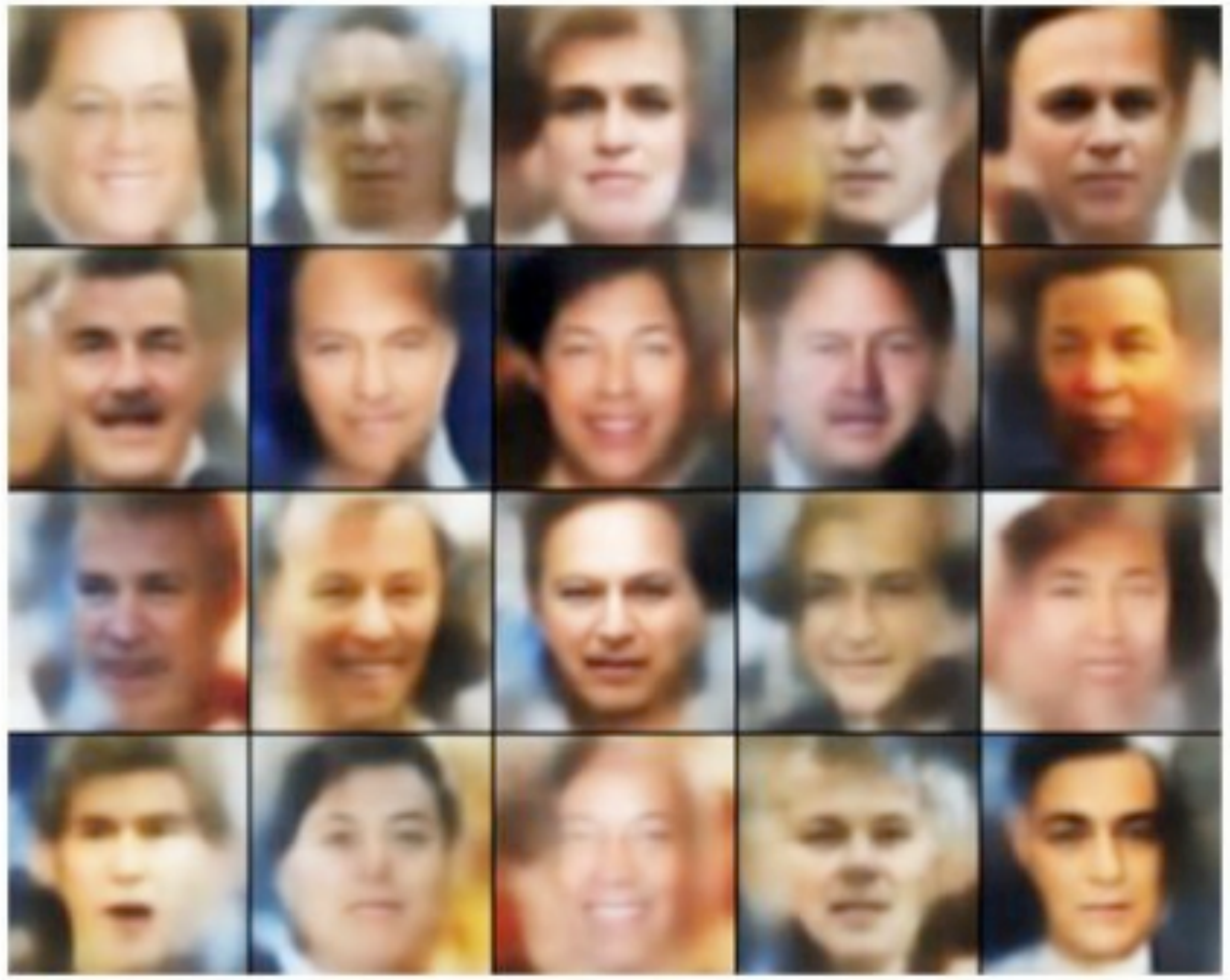
Also good feature representation that
can be computed using $q_\phi(z|x)$!



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

Cons:

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

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian
- Incorporating structure in latent variables