Generative Models

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Slides are based on Fei Fei Li and colleagues lectures, cs231n, Stanford 2017.

Supervised Learning

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

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

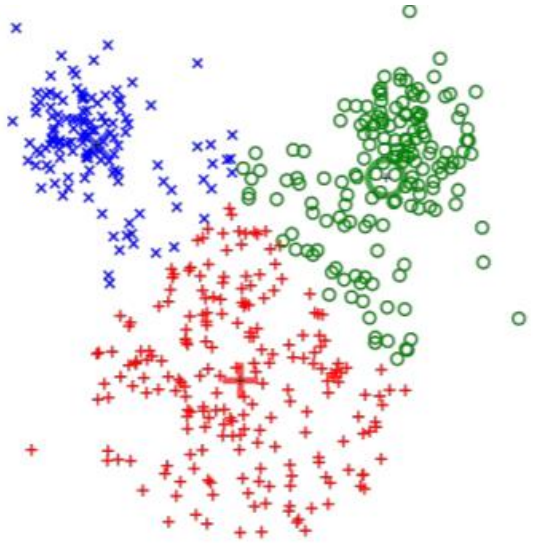
- Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

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.



K-means clustering

Unsupervised Learning

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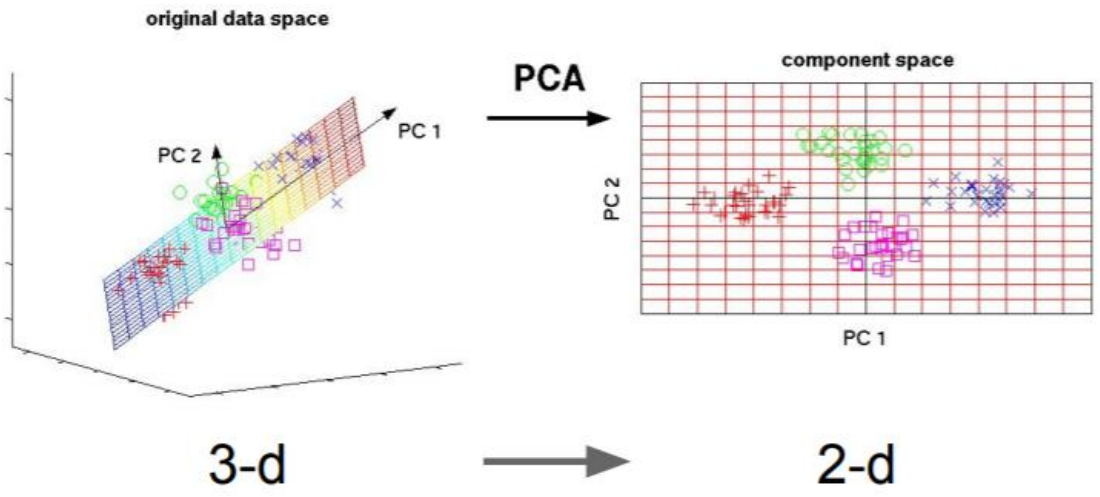
- Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.



Principal Component Analysis
(Dimensionality reduction)

Unsupervised Learning

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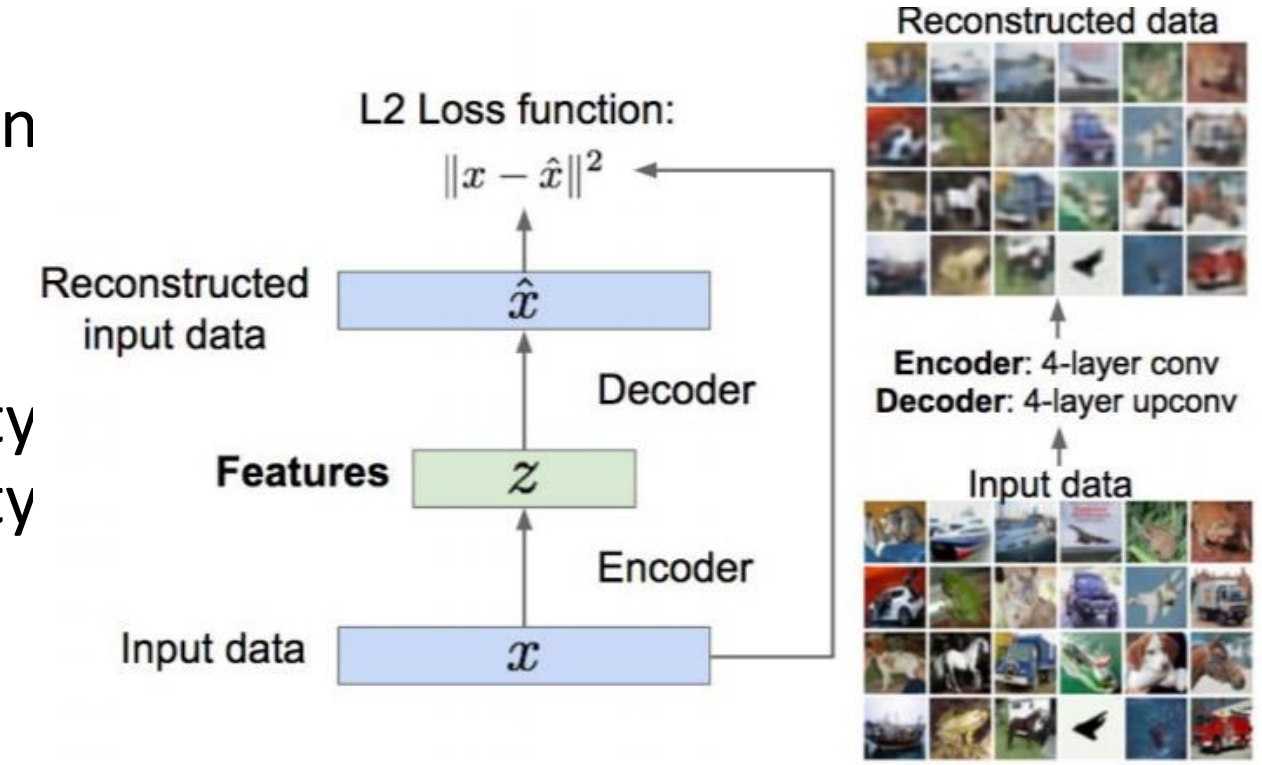
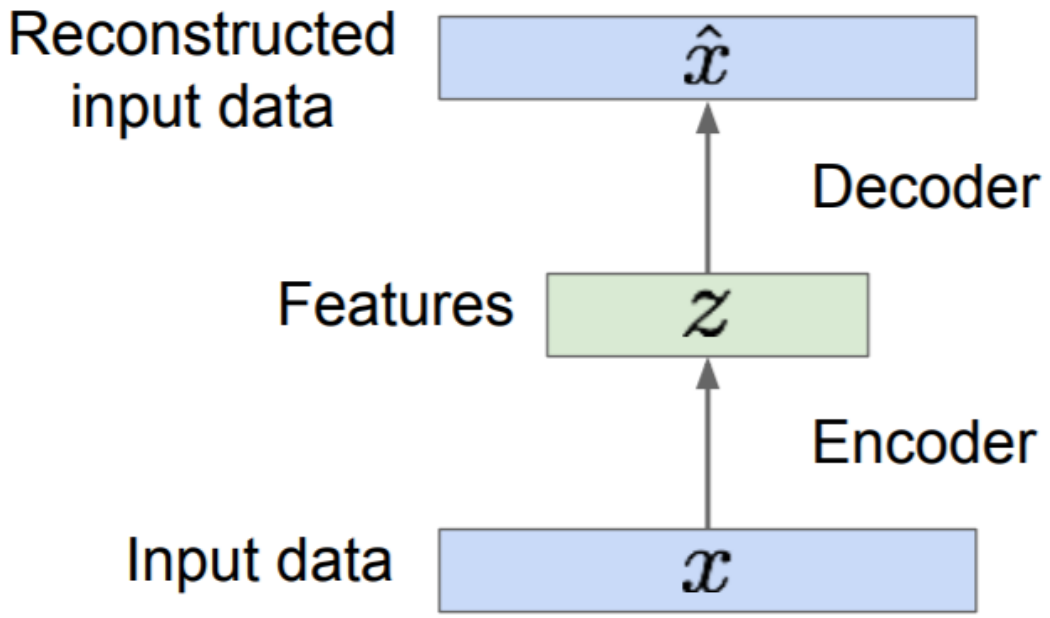
- Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.



Autoencoders
(Feature learning)

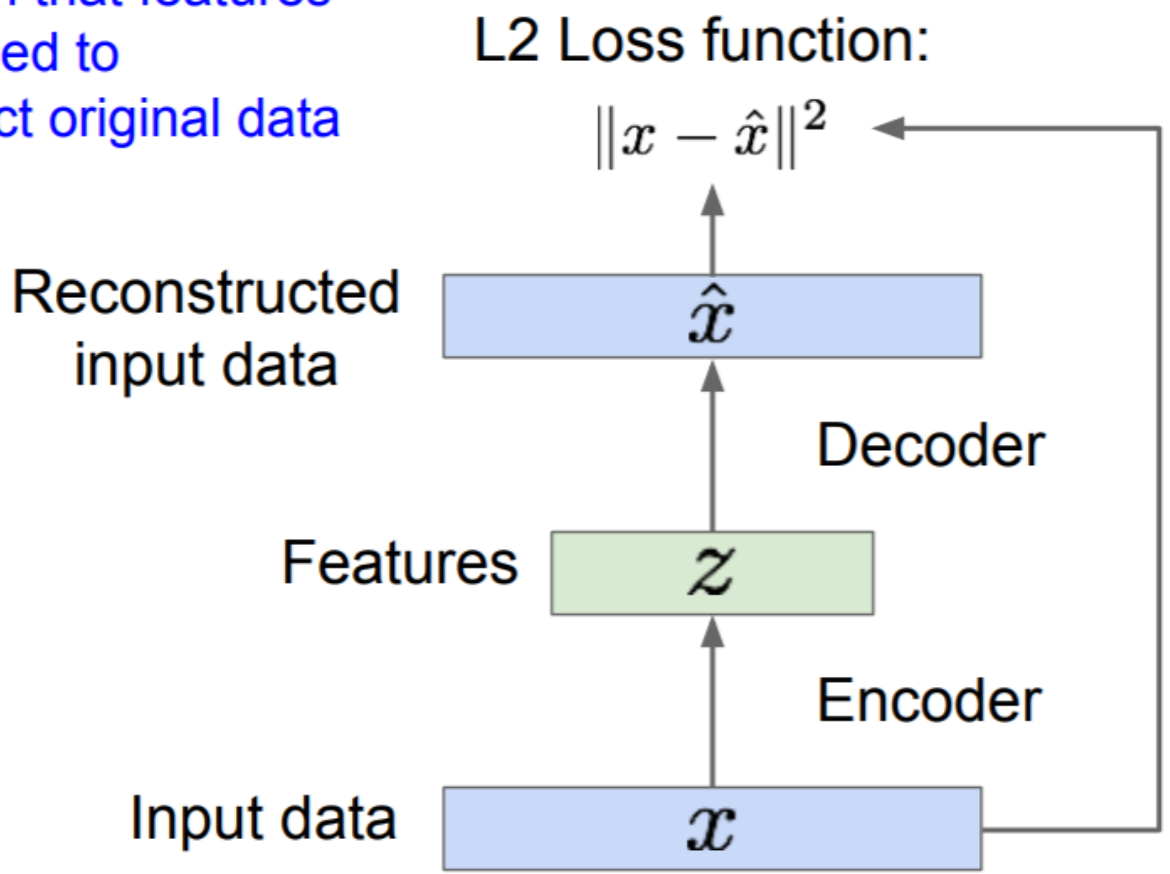
Autoencoders

- 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

Train such that features can be used to reconstruct original data



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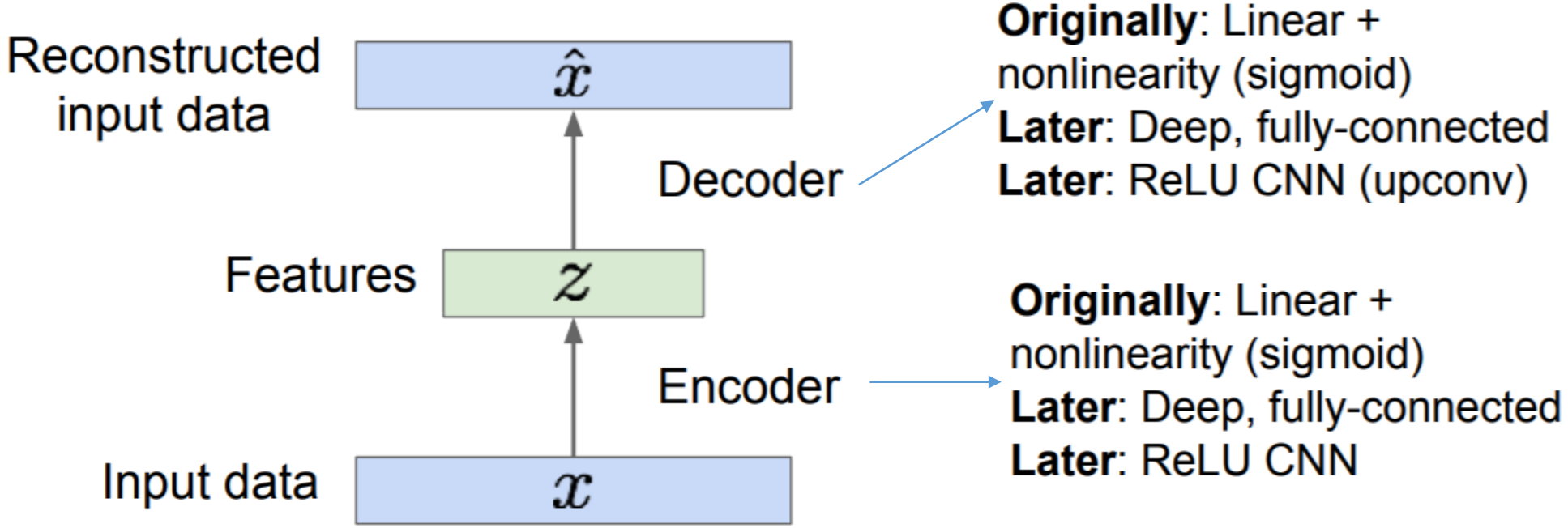

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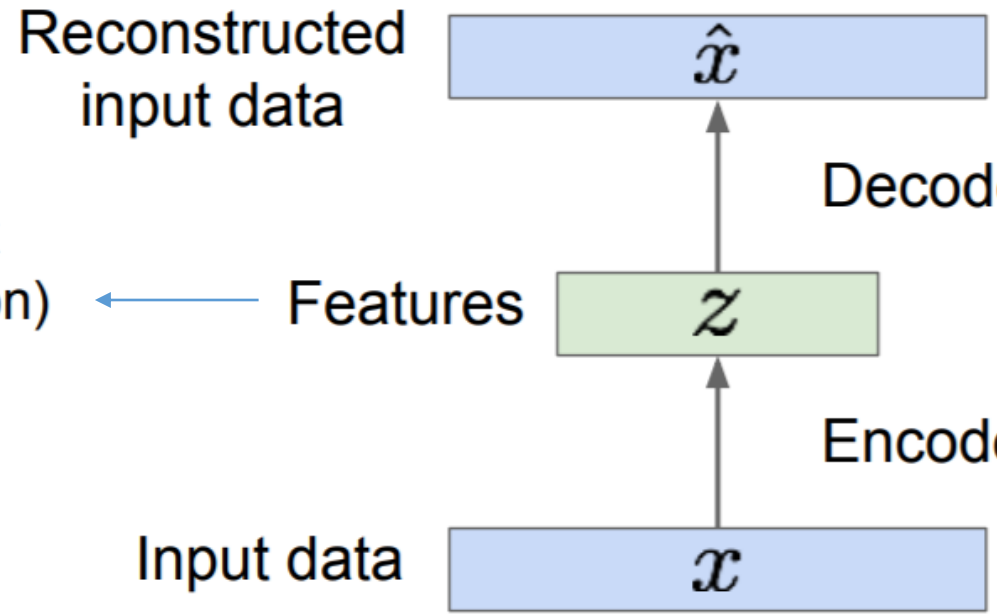


Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN (upconv)

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

Train such that features can be used to reconstruct original data

Doesn't use labels!

L2 Loss function:

$\|x - \hat{x}\|^2$

Reconstructed input data

$\hat{x}$

Decoder

Features

z

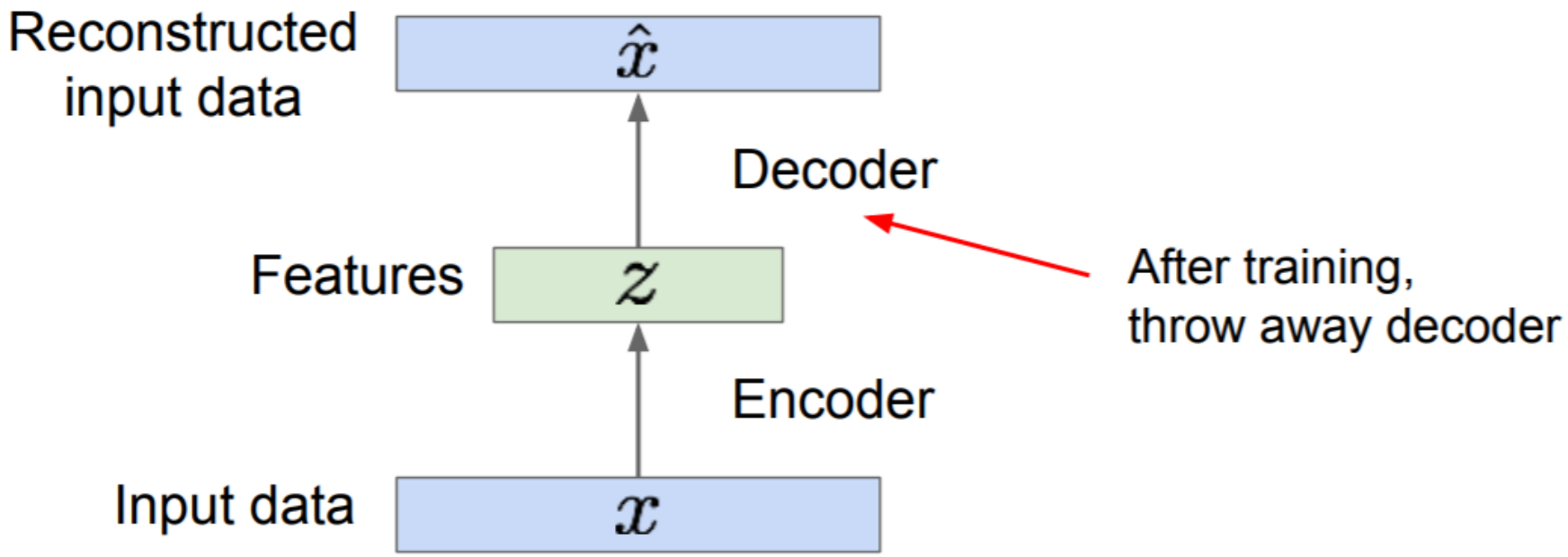
Encoder

Input data

x

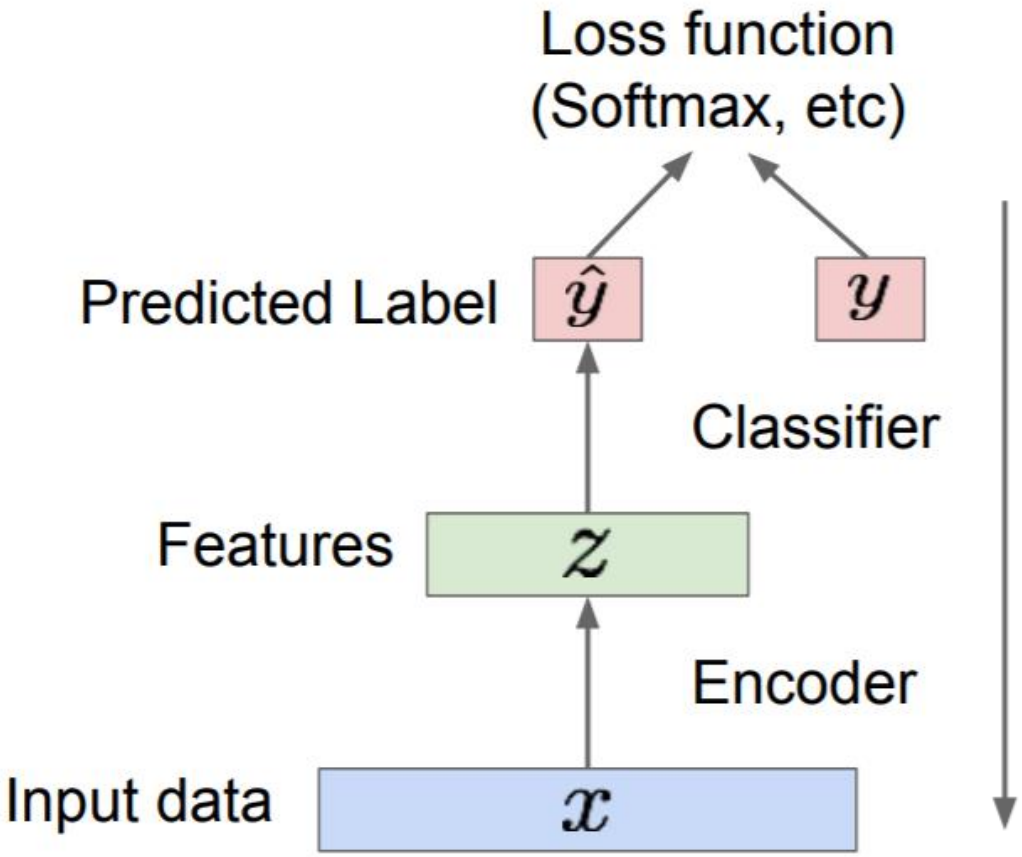
Encoder: 4-layer conv
Decoder: 4-layer upconv

Autoencoders



Autoencoders

- Pre-train the encoder with (unlabeled) data



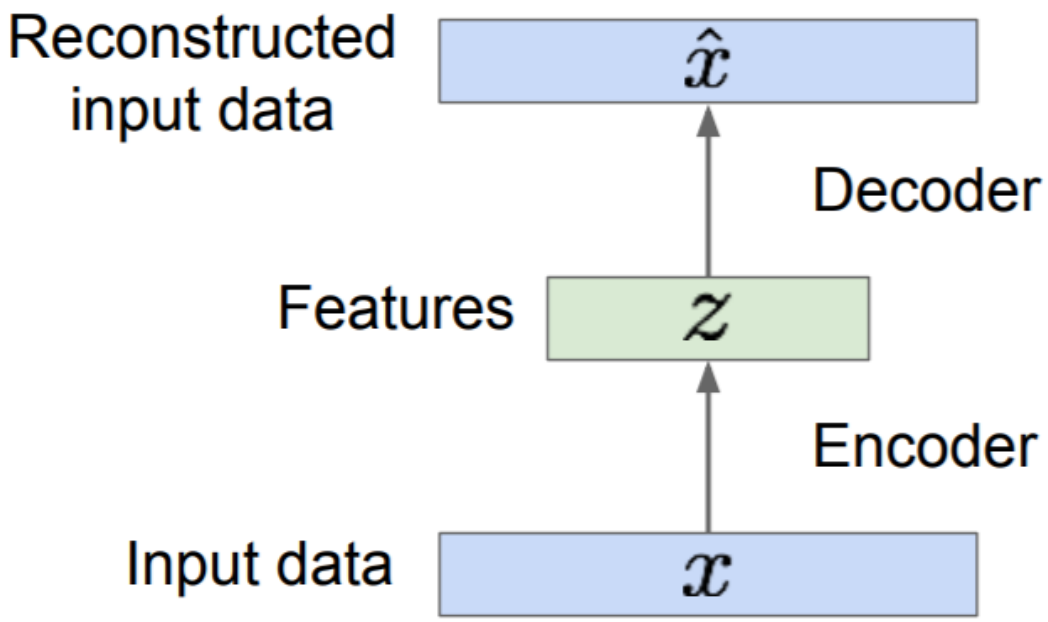
Encoder can be used to initialize a **supervised** model

Fine-tune encoder jointly with classifier

bird plane
dog deer truck

Train for final task (sometimes with small data)

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?

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.

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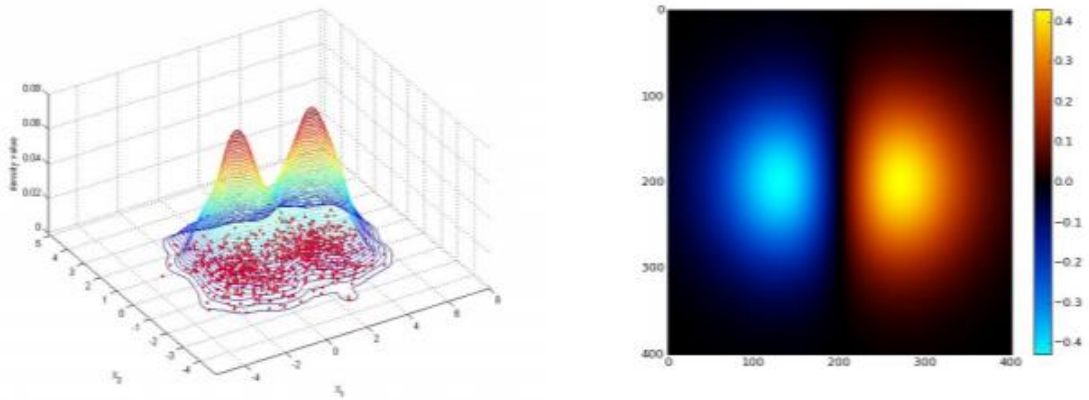
1-d density estimation



2-d density estimation

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

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

Generative Models

- Task: Given a dataset of images {X1,X2...} can we learn the distribution of X?

- Typically generative models implies modelling P(X).
  - Very limited, given an input the model outputs a probability

- More Interested in models which we can sample from distribution of data.
  - producing examples that are similar to the training examples but not exactly the same.
    - synthesize new, unseen examples similar to the seen ones

Taxonomy of Generative Models

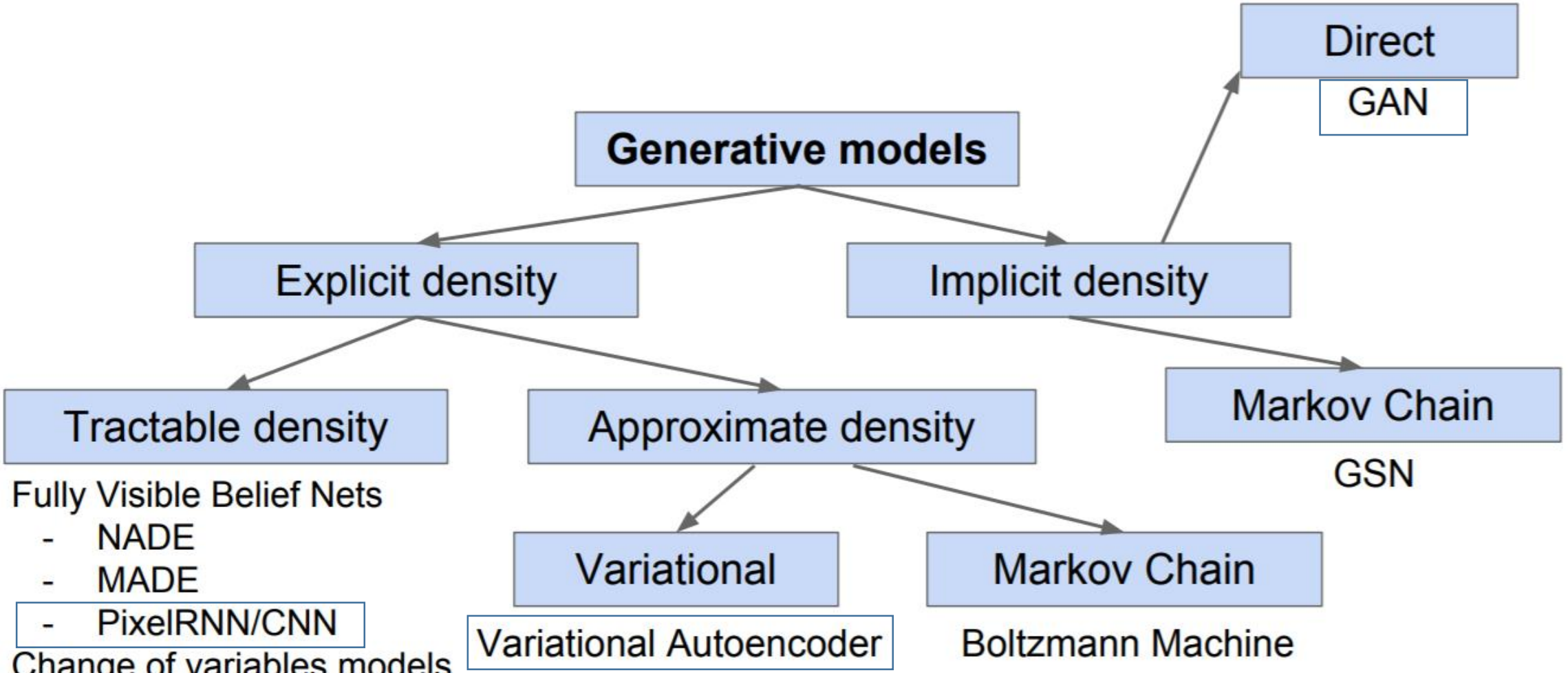


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

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

Fully visible belief network

Explicit density model

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

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

Likelihood of image x

Probability of i'th pixel value given all previous pixels

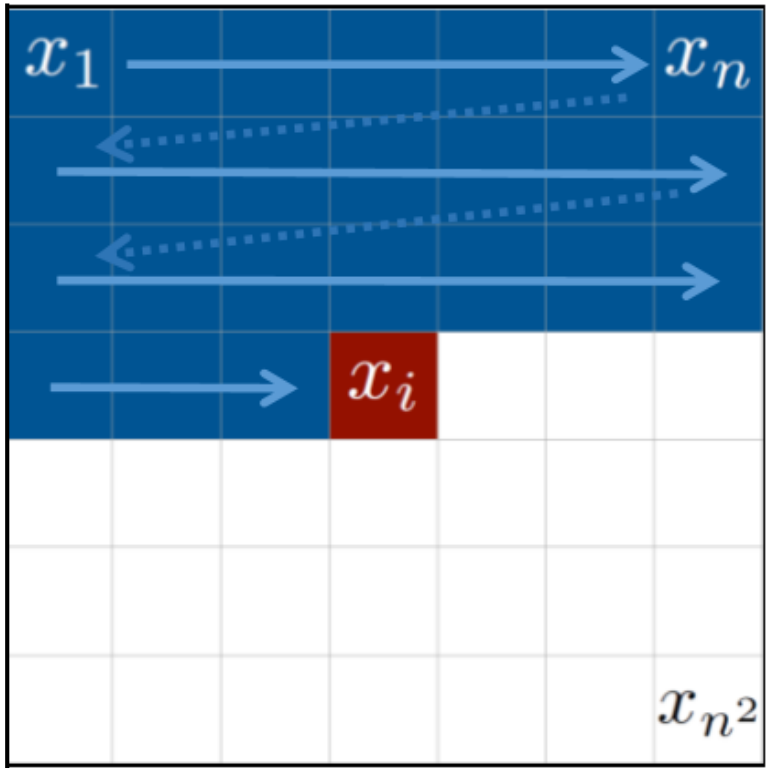
Then maximize likelihood of training data

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

Fully visible belief network

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Likelihood of image x

Probability of i'th pixel value given all previous pixels

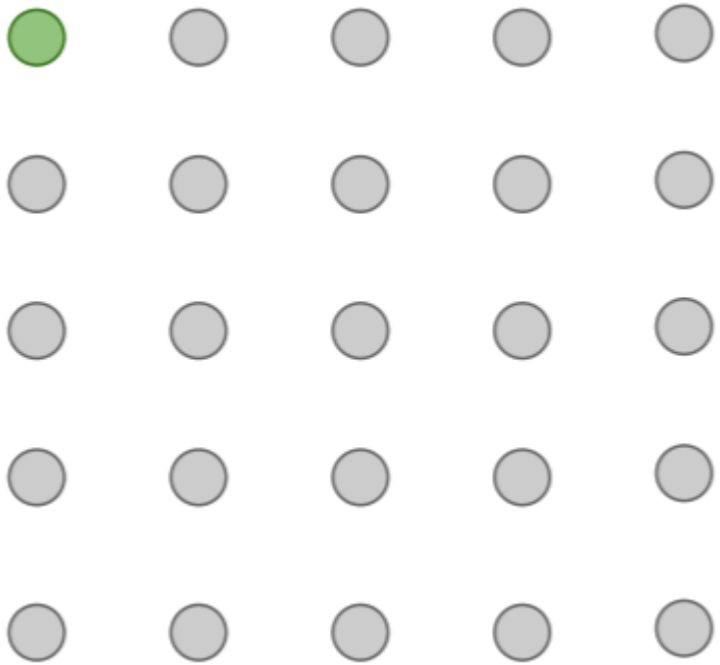
Will need to define ordering of "previous pixels"

Then maximize likelihood of training data

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

PixelRNN

- Generate image pixels starting from corner
- Dependency on previous pixels modeled using an RNN (LSTM)



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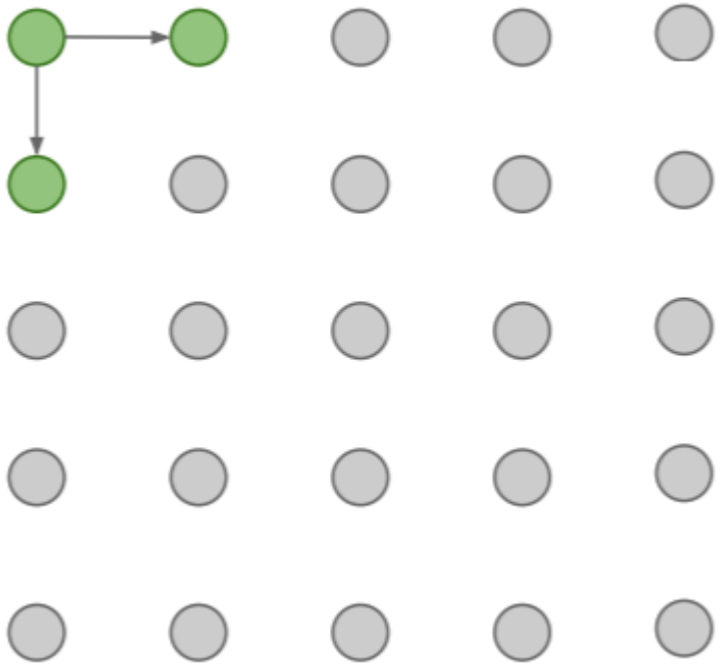

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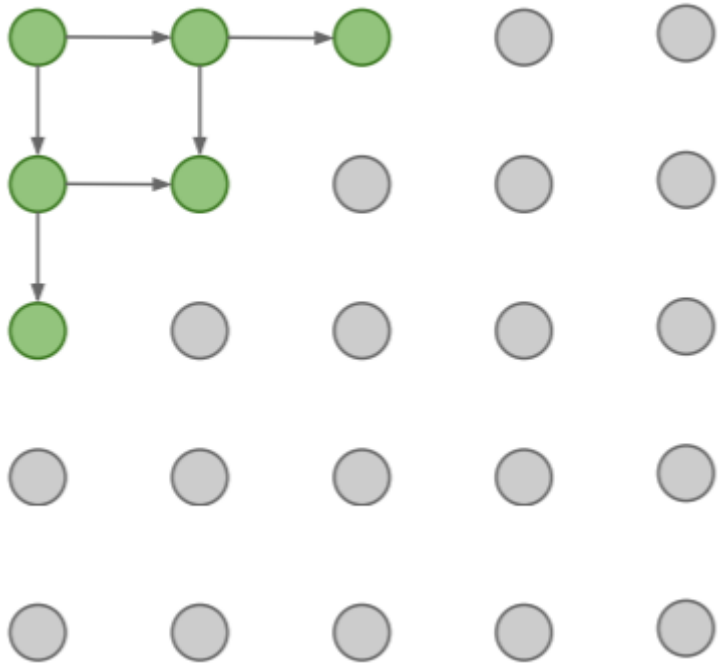
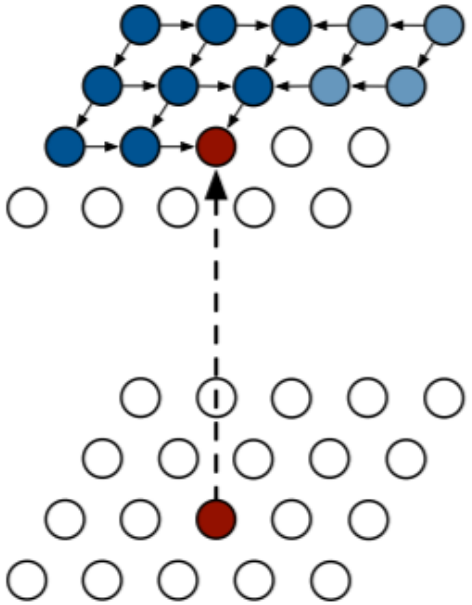


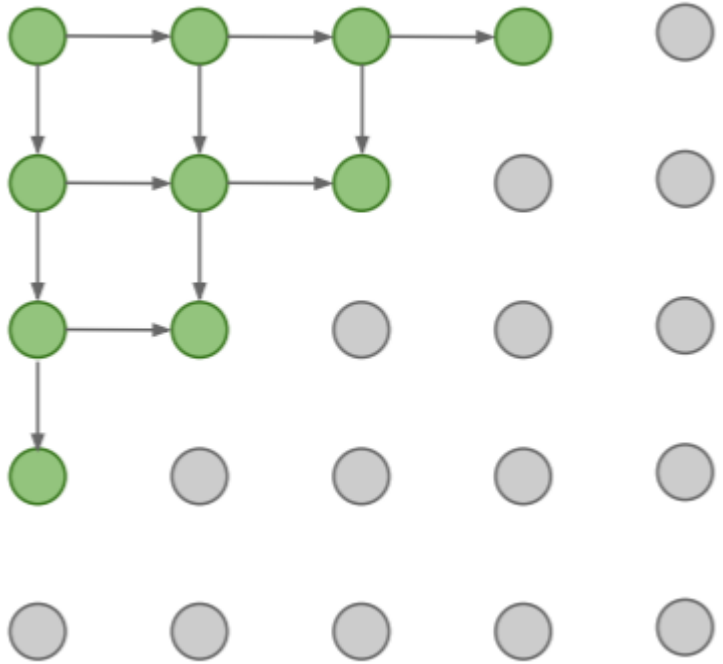
Oord et al., Pixel recurrent neural networks, ICML 2016

PixelRNN

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



Diagonal BiLSTM

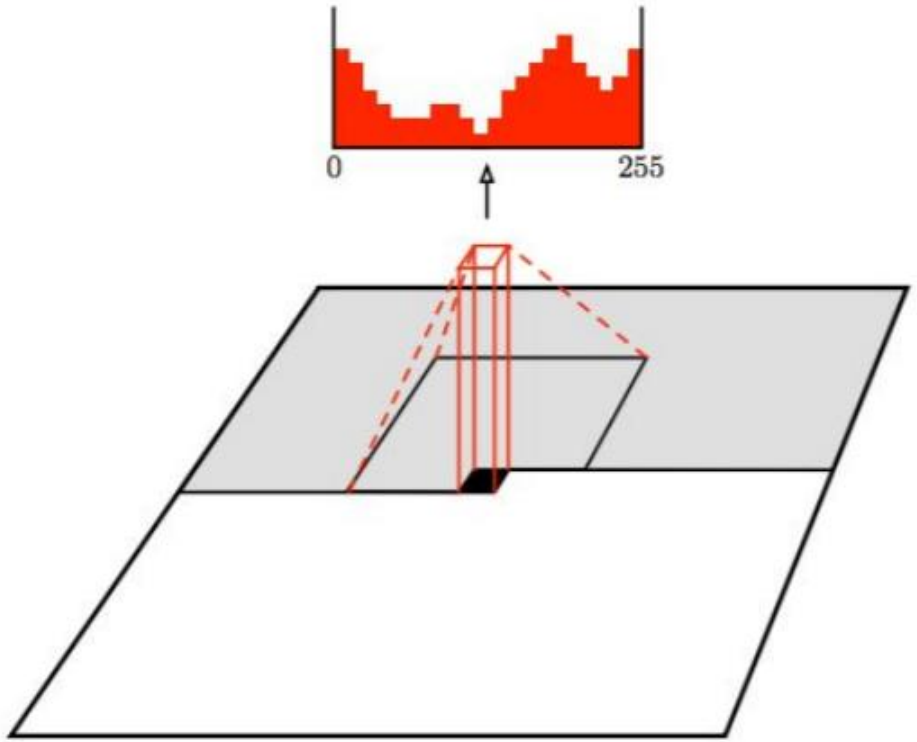


Oord et al., Pixel recurrent neural networks, ICML 2016

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



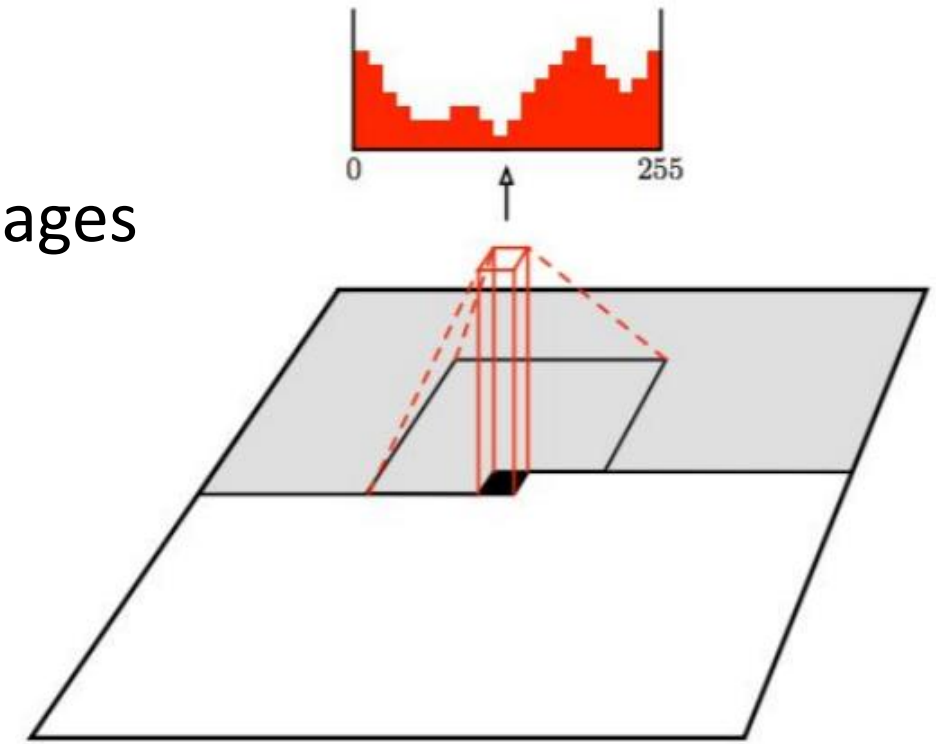
PixelCNN

- 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

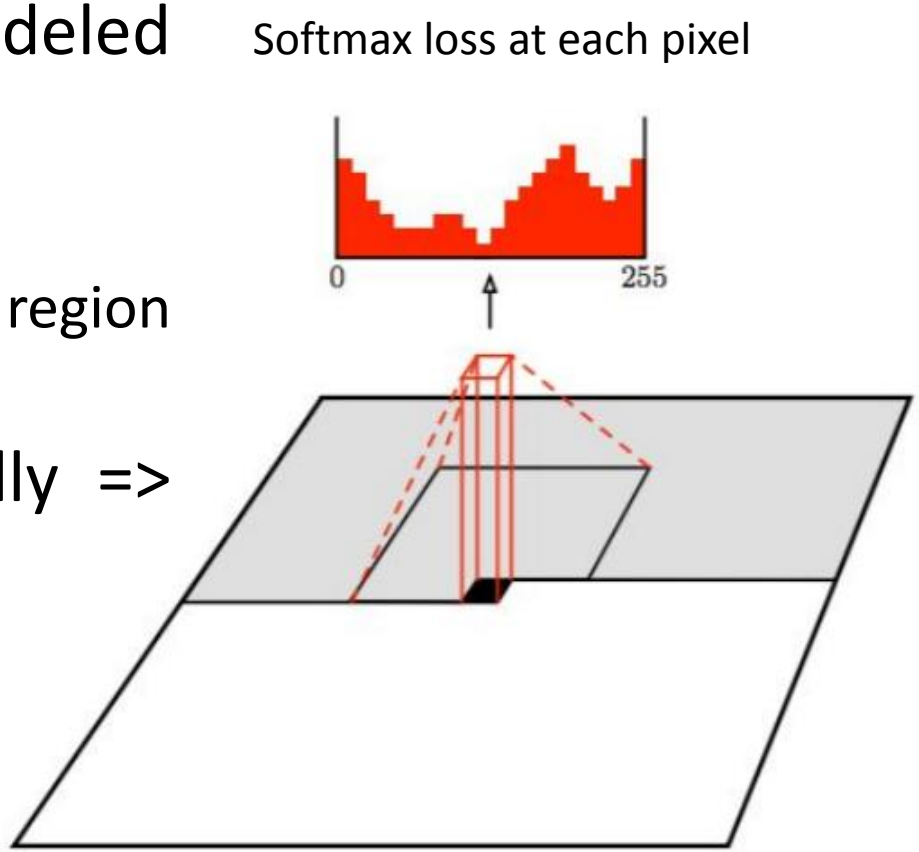
$$p(x) = \prod_{i=1}^{n} p(x_i | x_1, \ldots, x_{i-1})$$

Softmax loss at each pixel



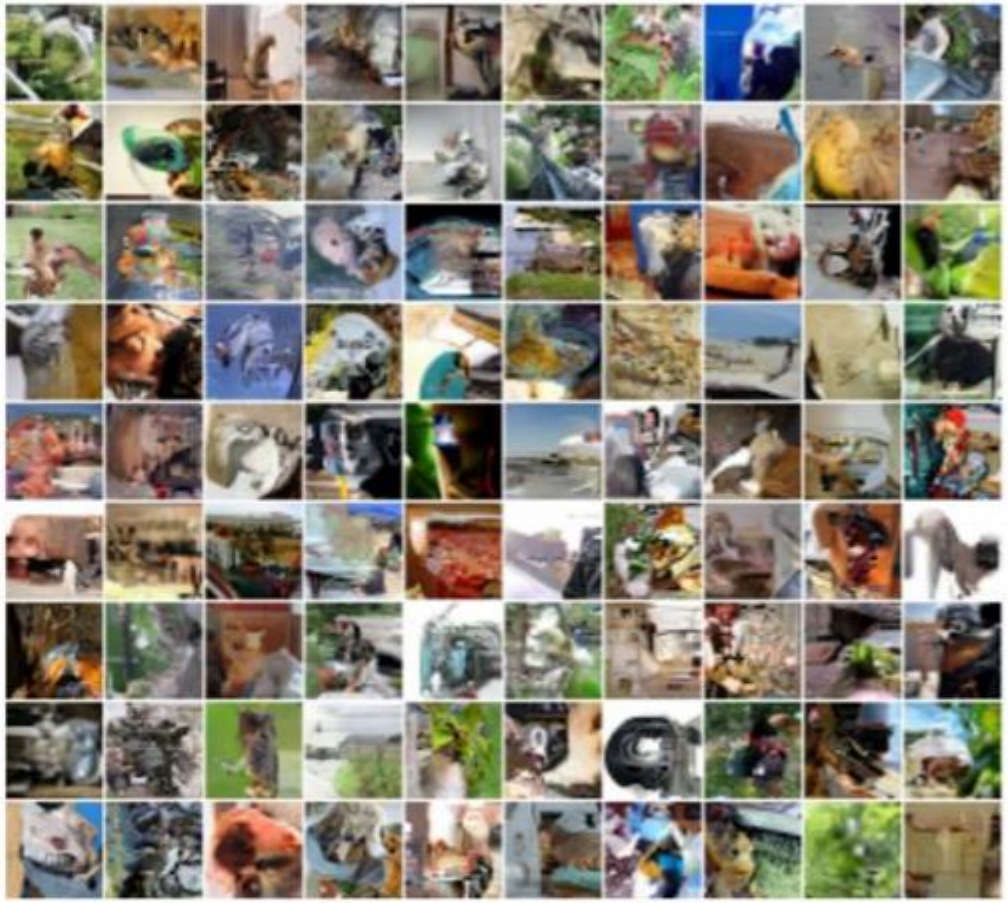
PixelCNN

- 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



Generated 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++)

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

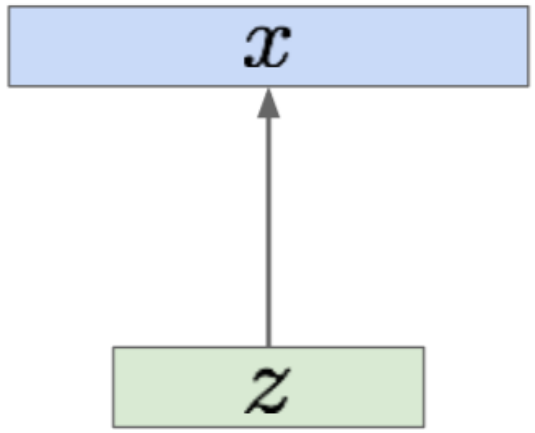
Variational Autoencoders

- 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

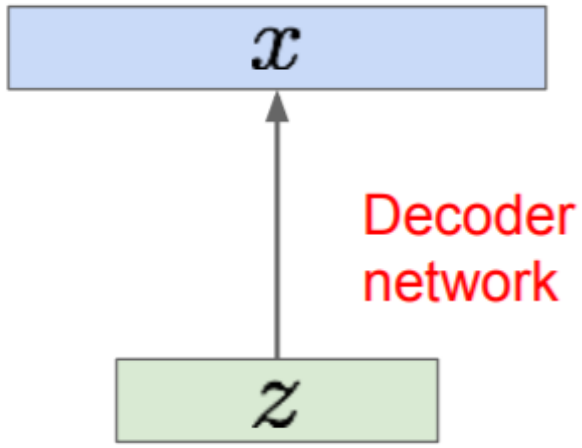
Variational Autoencoders

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

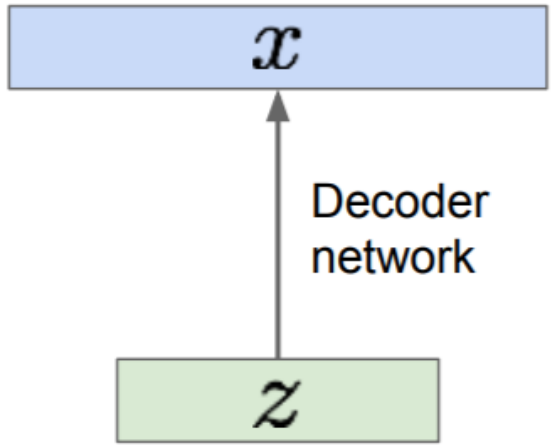
Variational Autoencoders

Sample from true conditional

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

Sample from true prior

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



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

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

Variational Autoencoders: Intractability

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

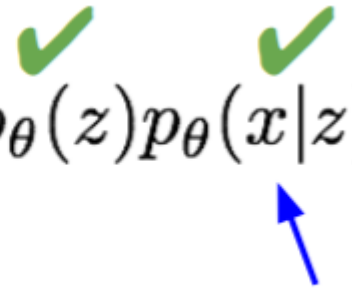
✔

Simple Gaussian prior

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

Variational Autoencoders: Intractability

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



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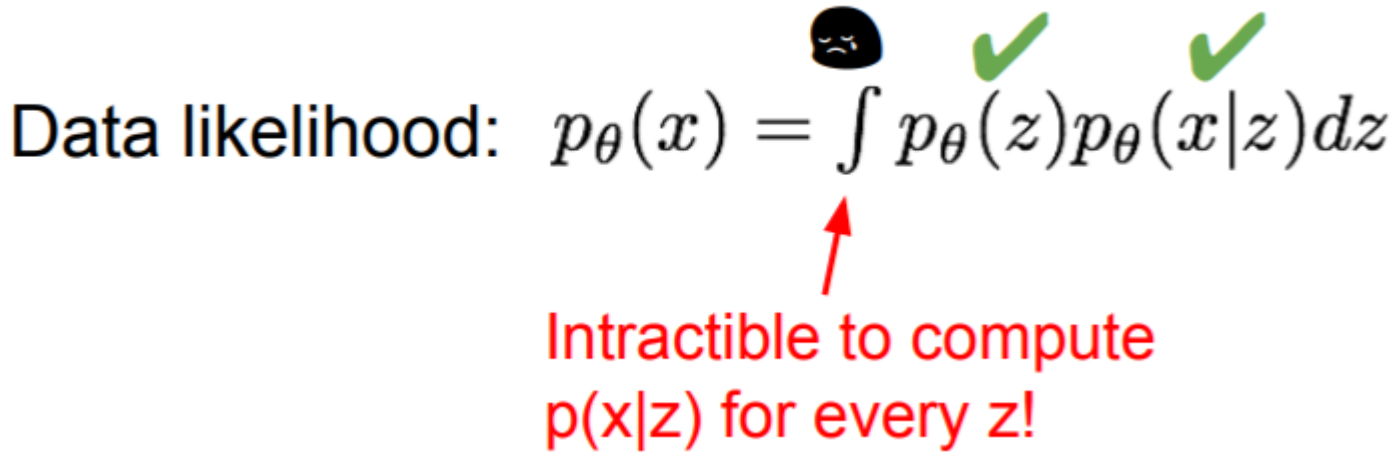
Variational Autoencoders: Intractability



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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

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Intractable data likelihood

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

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

Lower bound for log likelihood

$$\log p(x) = E_{z \sim p(z)}[\log p(x)]$$

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

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

Lower bound for log likelihood

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

Bayes rule

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

Lower bound for log likelihood

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

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

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

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

Variational Autoencoders

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

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

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

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

Variational Autoencoders

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

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

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

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

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

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

Variational Autoencoders

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

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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

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

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

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

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

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

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

Variational Autoencoders

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

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

Variational lower bound ("ELBO")

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

Training: Maximize lower bound

Variational Autoencoders

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

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

Reconstruct the input data

Make approximate posterior distribution close to prior

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

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

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

Variational lower bound ("ELBO")

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

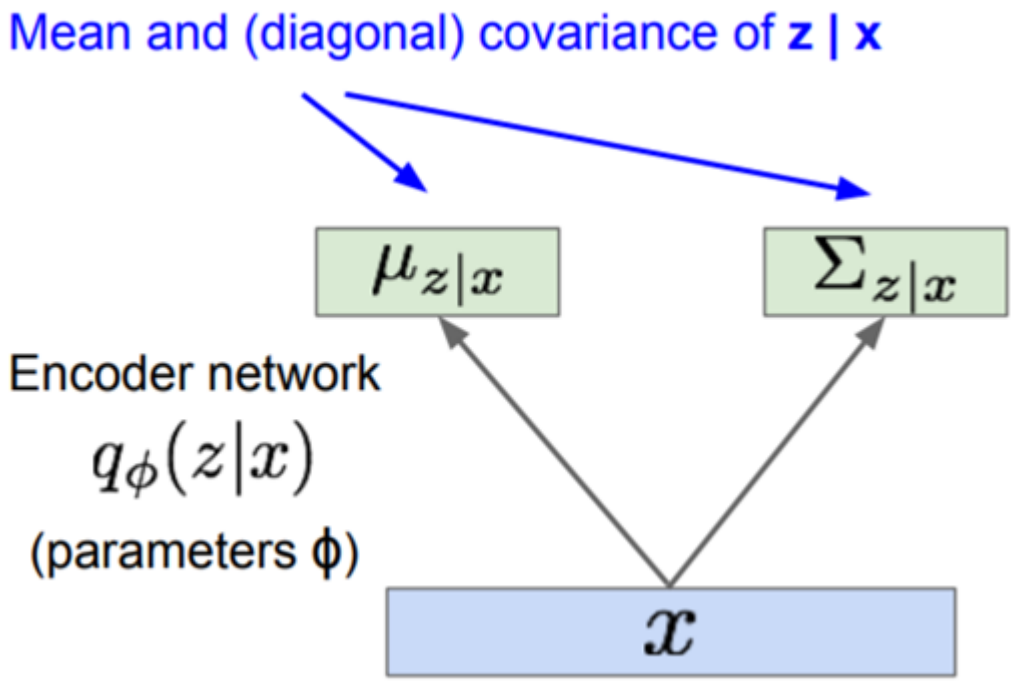
Training: Maximize lower bound

Maximizing ELBO

- Maximizing ELBO composed of:
  - Approximate posterior distribution $q(z|x)$: Best match to true posterior $p(z|x)$
  - 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 $p(z)$.

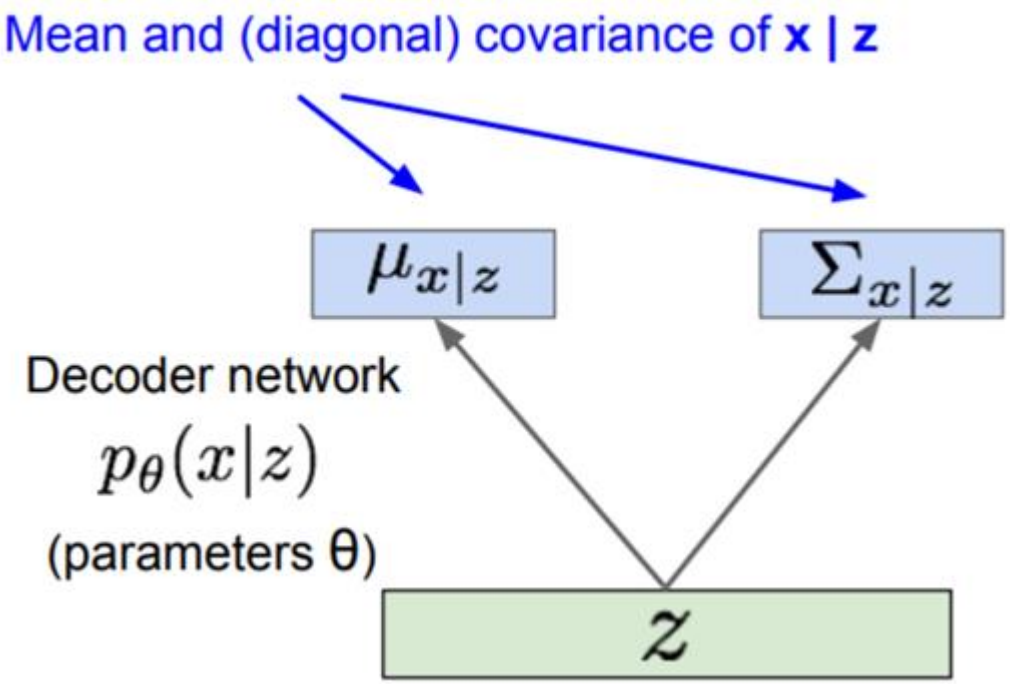
Encoder network

- Model q(z|x) with a neural network (called encoder network)
- Assume q(z|x) to be Gaussian
- Neural network outputs the mean $\mu_{z|x}$ and covariance matrix $\Sigma_{z|x}$



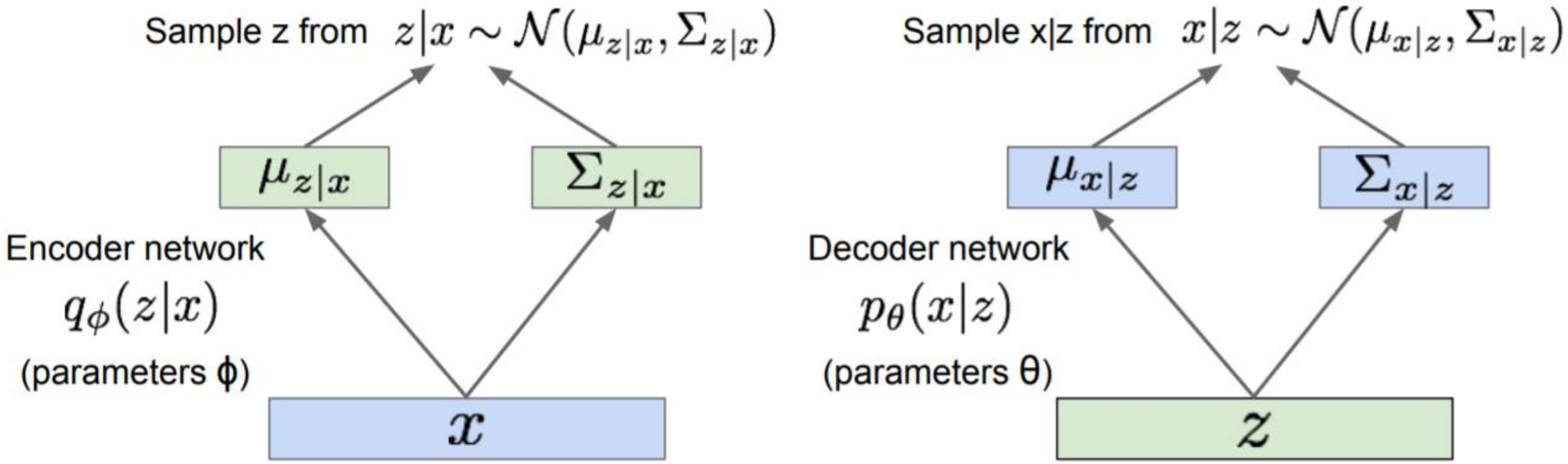
Decoder network

- Model P(x|z) with a neural network (called decoder network)
  - let f(z) be the network output.
  - Assume p(x|z) to be i.i.d. Gaussian, e.g.,
    - x = f(z) + η , where η ~ N(0,I)



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

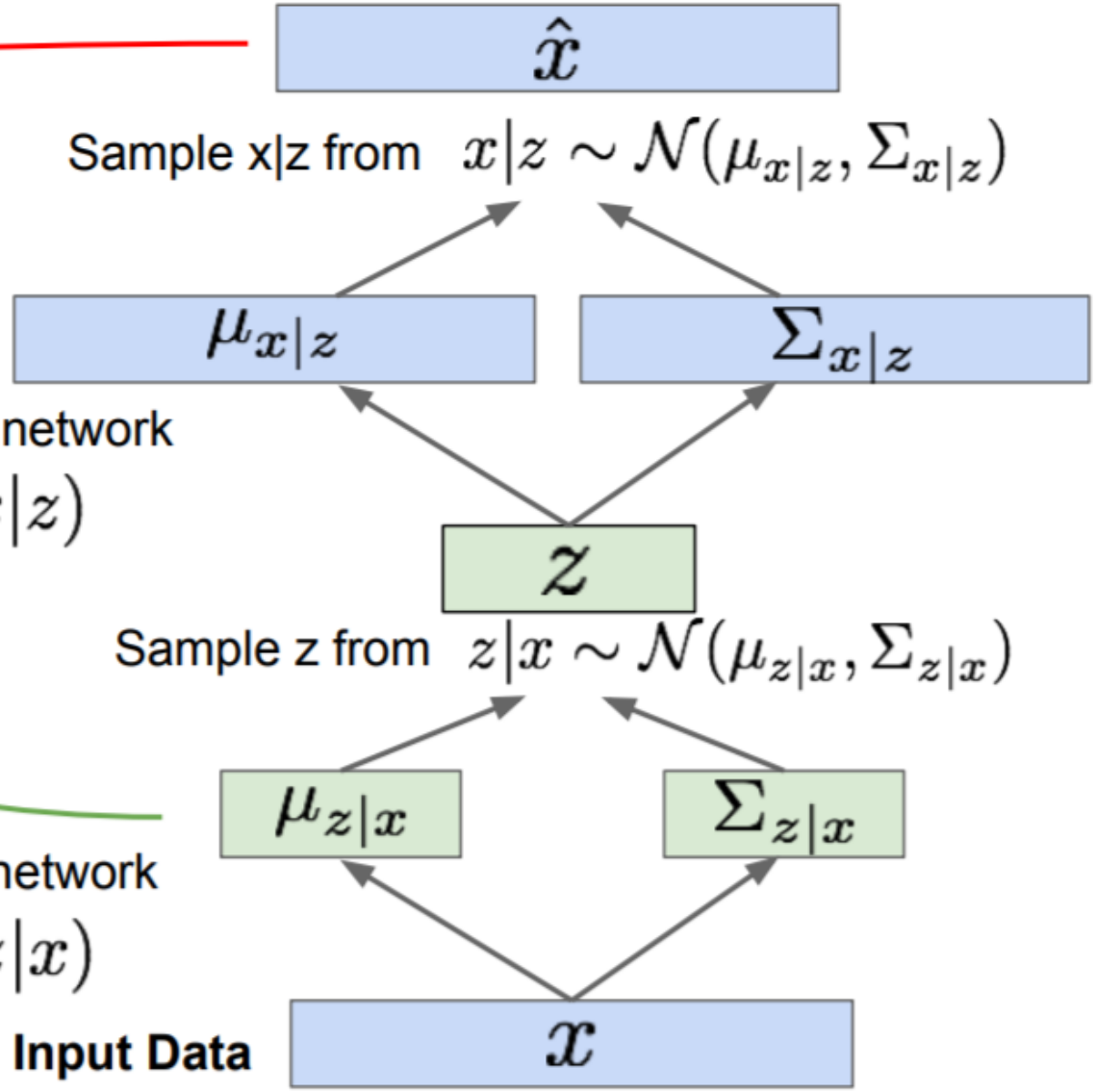
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

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

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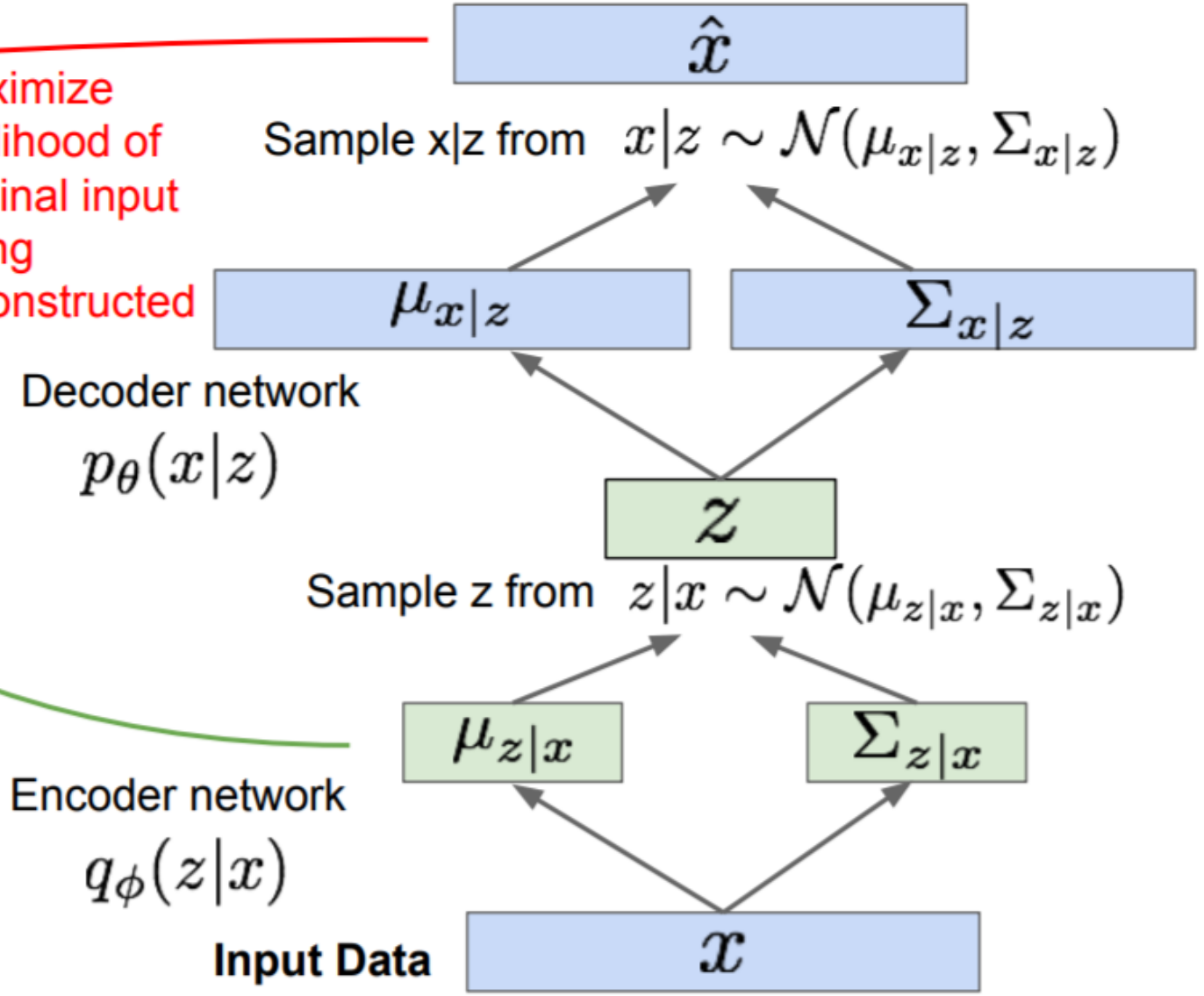


For every minibatch of input data: compute this forward pass, and then backprop!

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

Cost function

If we consider:

$$p(x|z) \sim N(f(z), \sigma^2 I)$$

We have:

$$\log p(x|z) = C - \frac{1}{2\sigma^2} \|x - f(z)\|^2$$

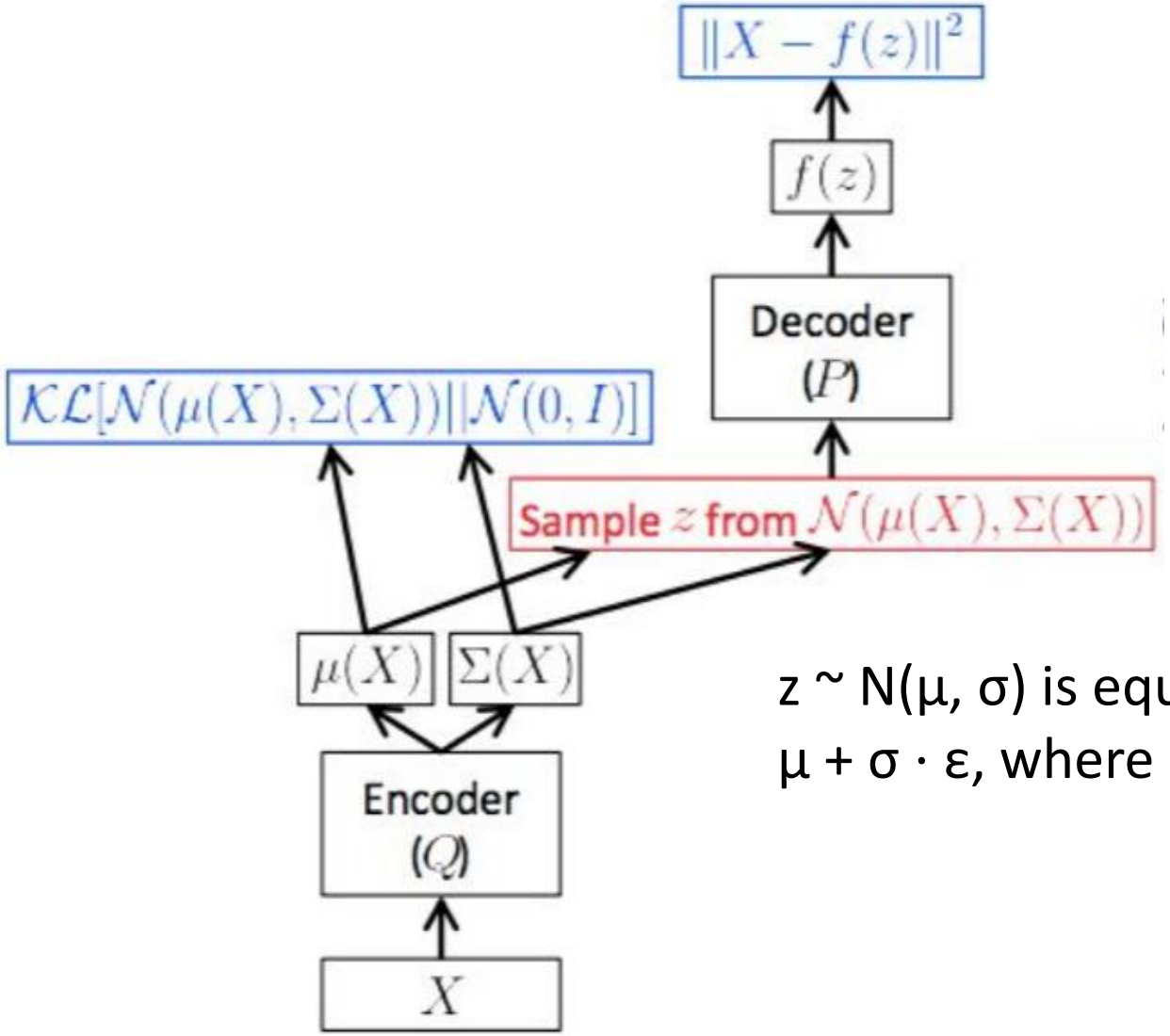
- Putting it all together (given a (x, z) pair):

$$L = \frac{1}{2\sigma^2} \|x - f(z)\|^2 + D[q(z)||p(z)]$$

Corresponding to $E_{z\sim q(z|x)}[\log p(x|z)]$
term since $z\sim q(z|x)$ in the training data

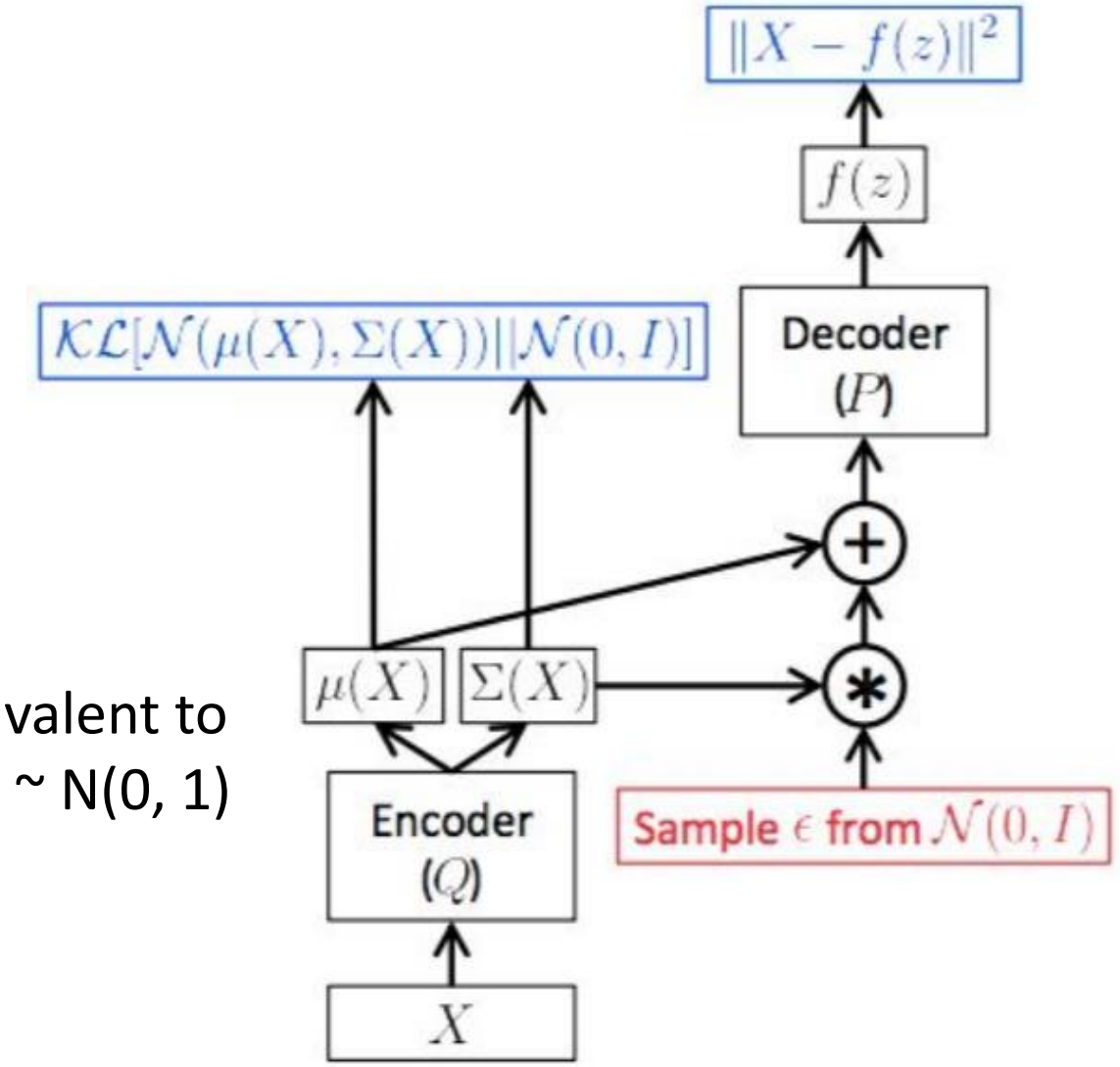
Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Reparametrization Trick



Non-continuous operation and has no gradient

$z \sim N(\mu, \sigma)$ is equivalent to
$\mu + \sigma \cdot \varepsilon$, where $\varepsilon \sim N(0, 1)$

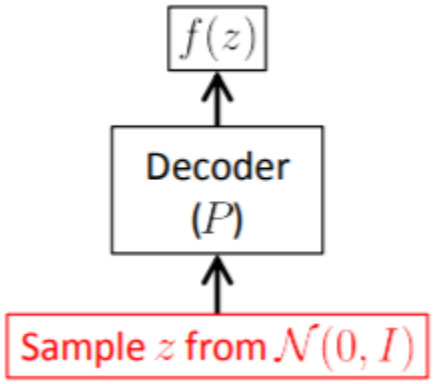


Now we can easily backpropagate the loss to the Encoder.

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

Generate Image: At Test Time

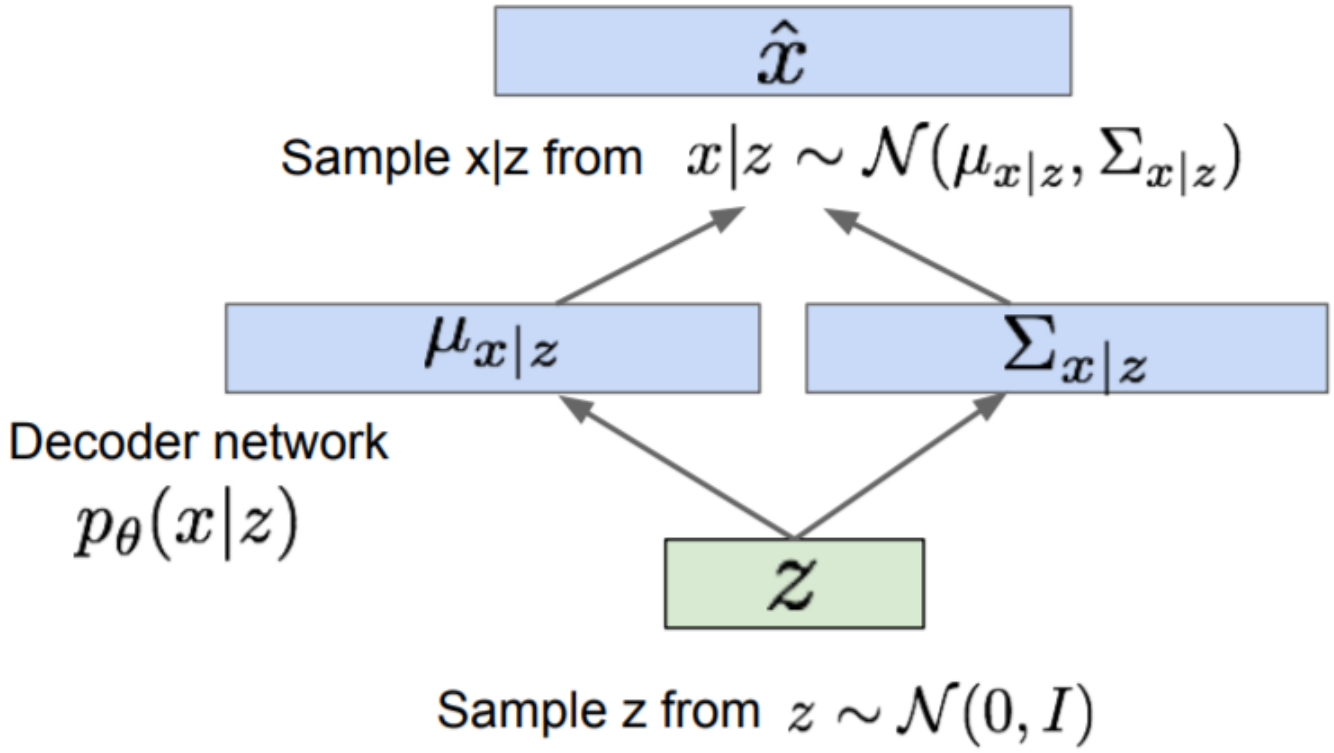
- Remove the Encoder
- Sample z ~ N(0,I) and pass it through the Decoder.
- No good quantitative metric, relies on visual inspection

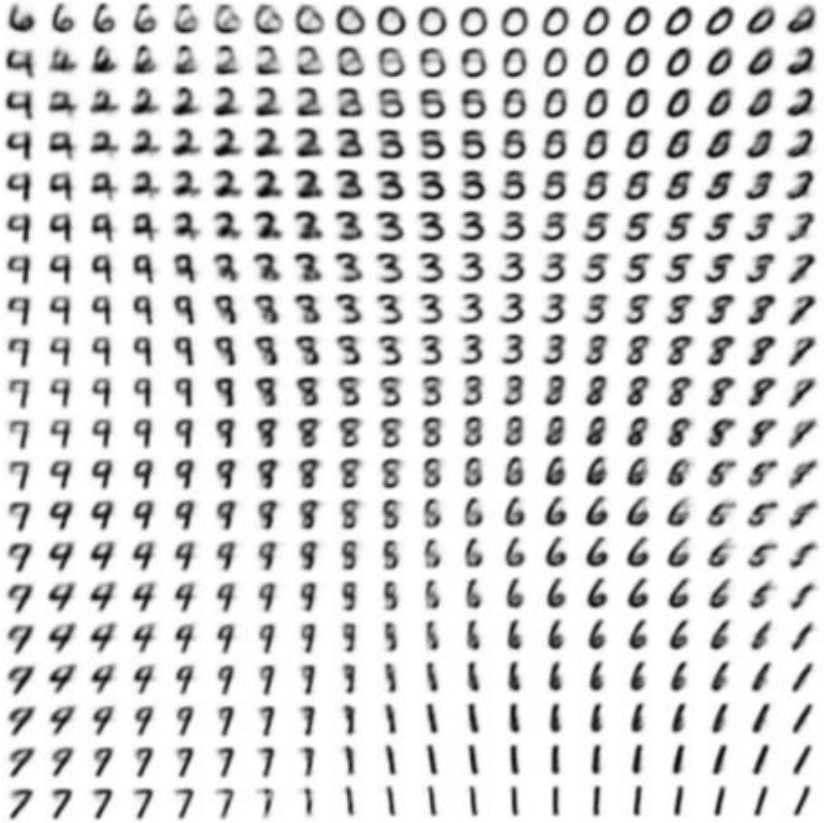


Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!





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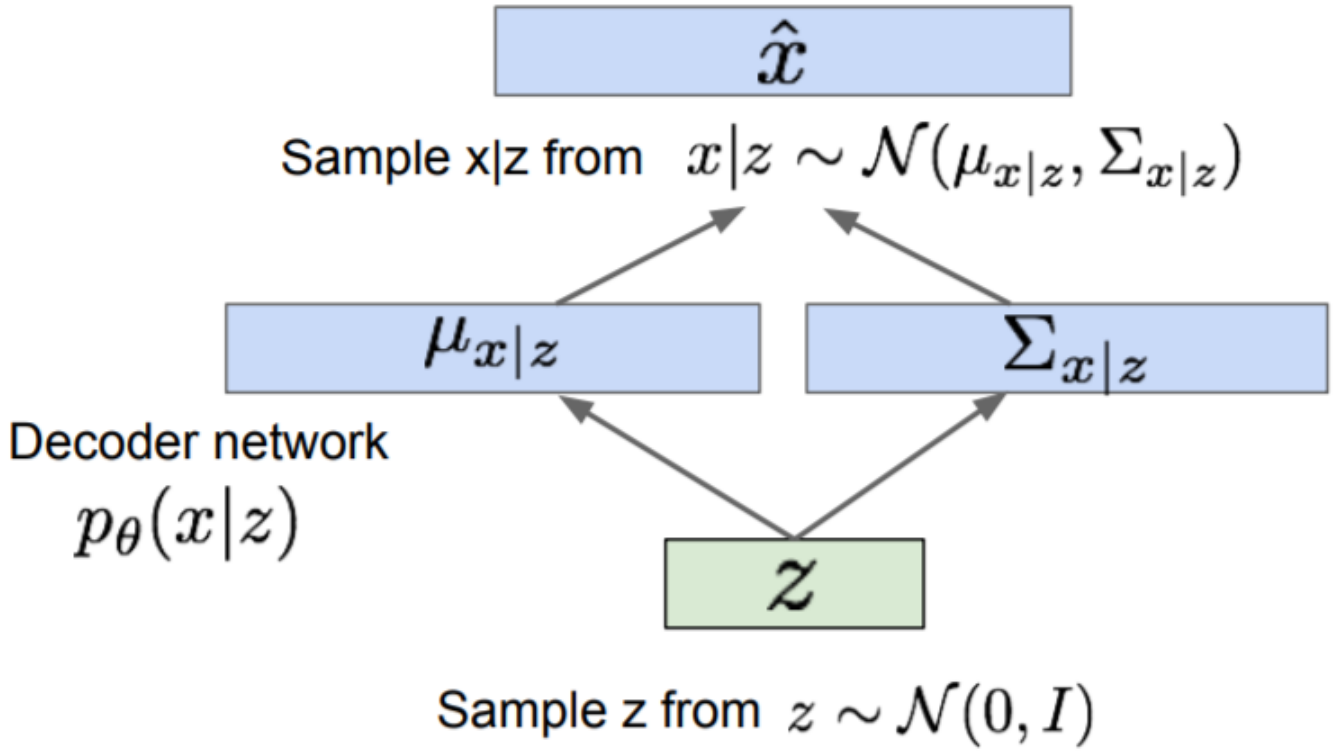
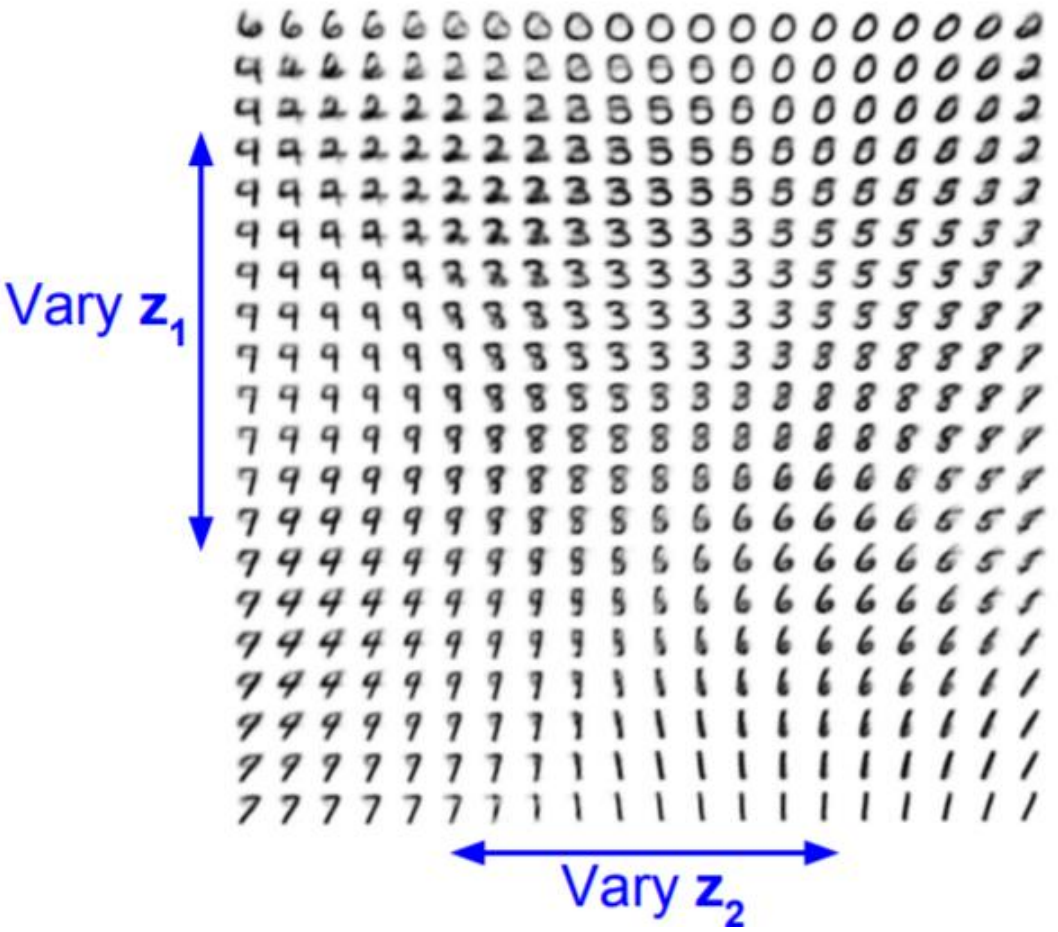
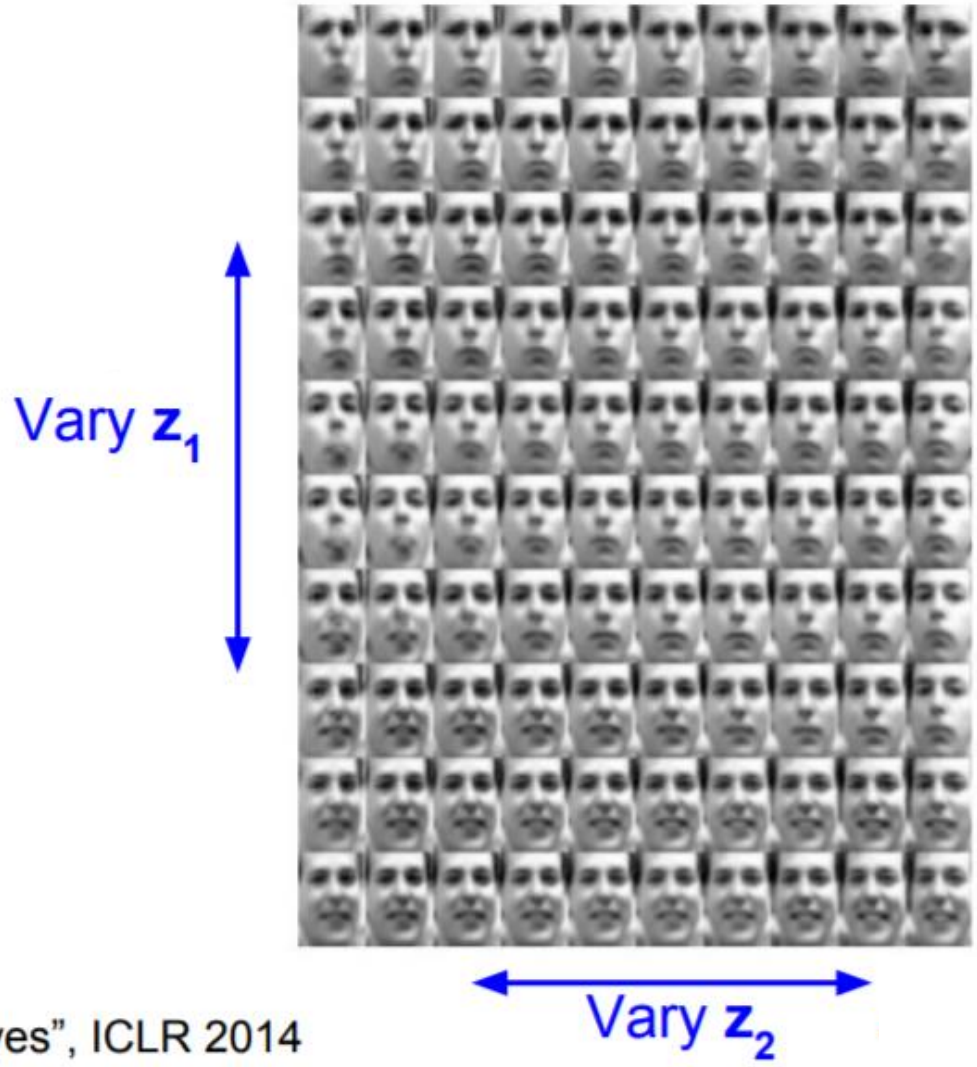


Data manifold for 2-d **z**



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

Variational Autoencoders: Generating Data!

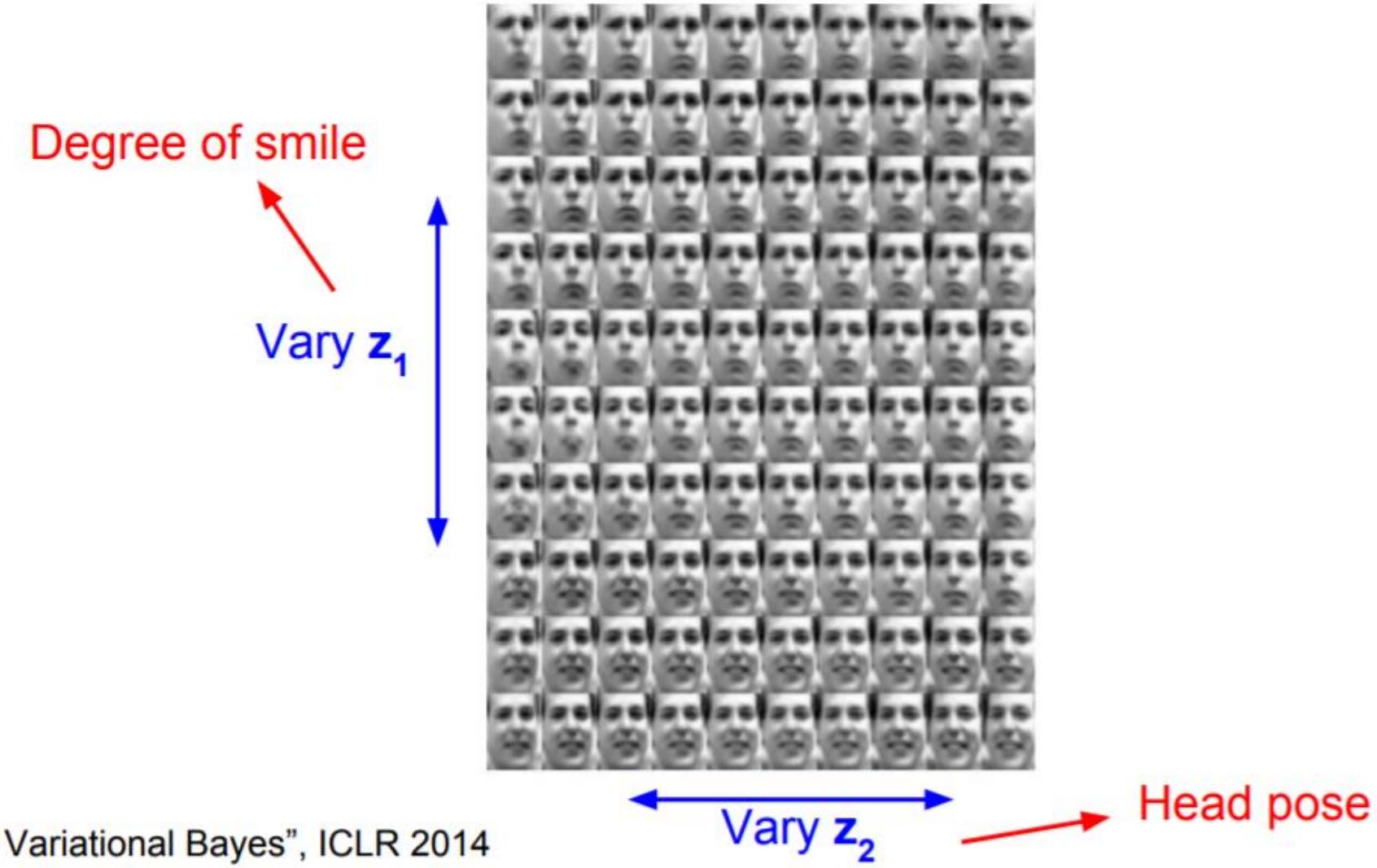


Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!

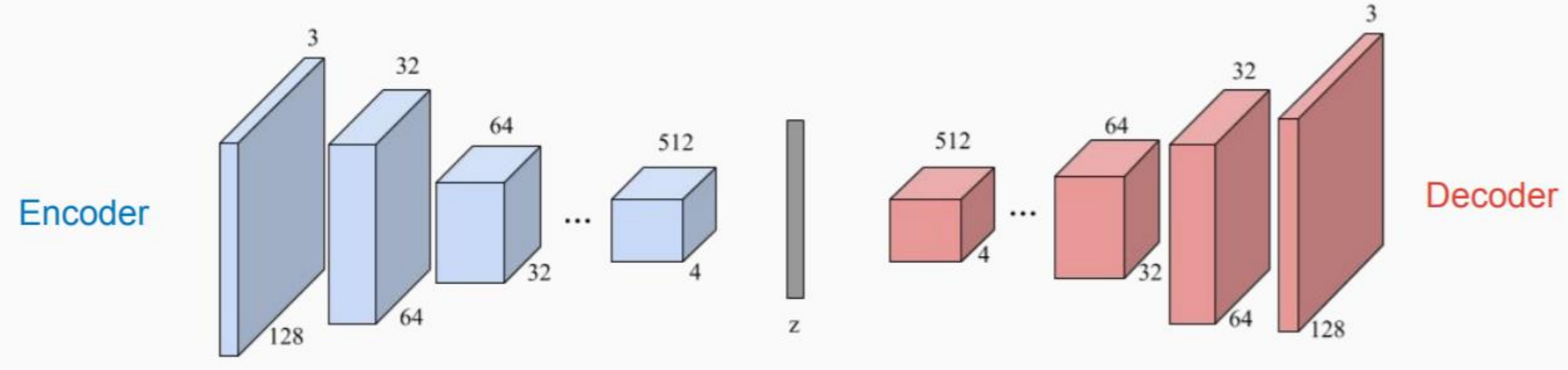
Diagonal prior on **z** => independent latent variables

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

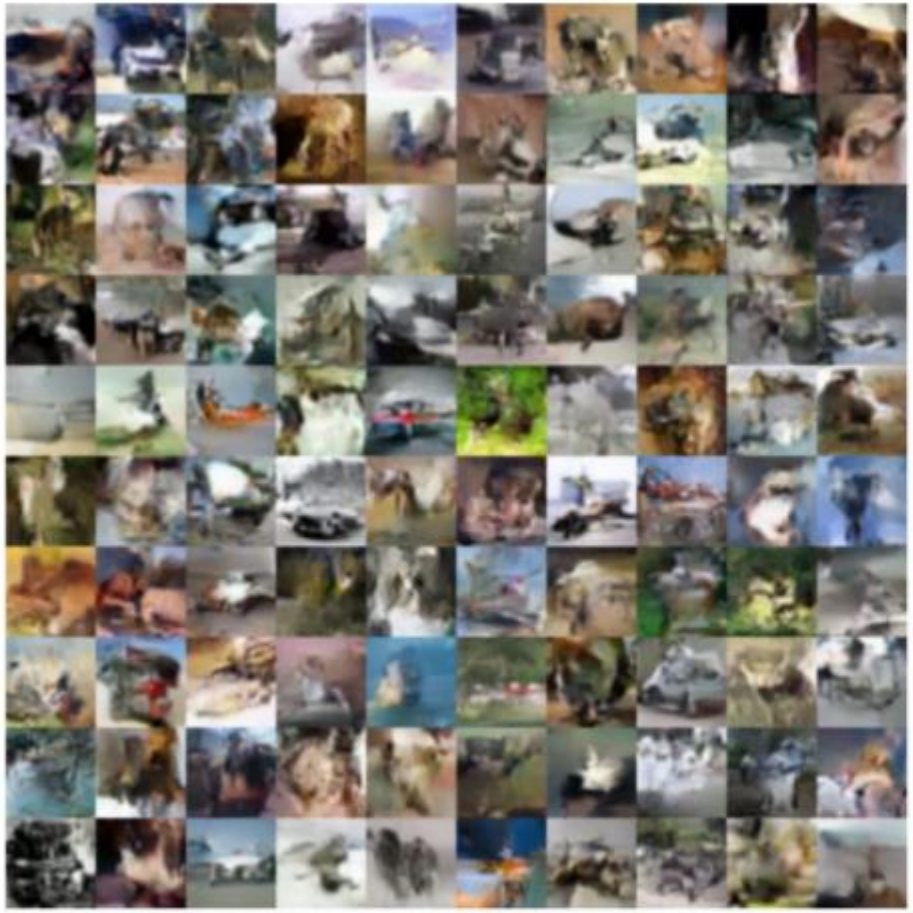


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Common VAE Architecture for Image Generation



Variational Autoencoders: Generating Data!

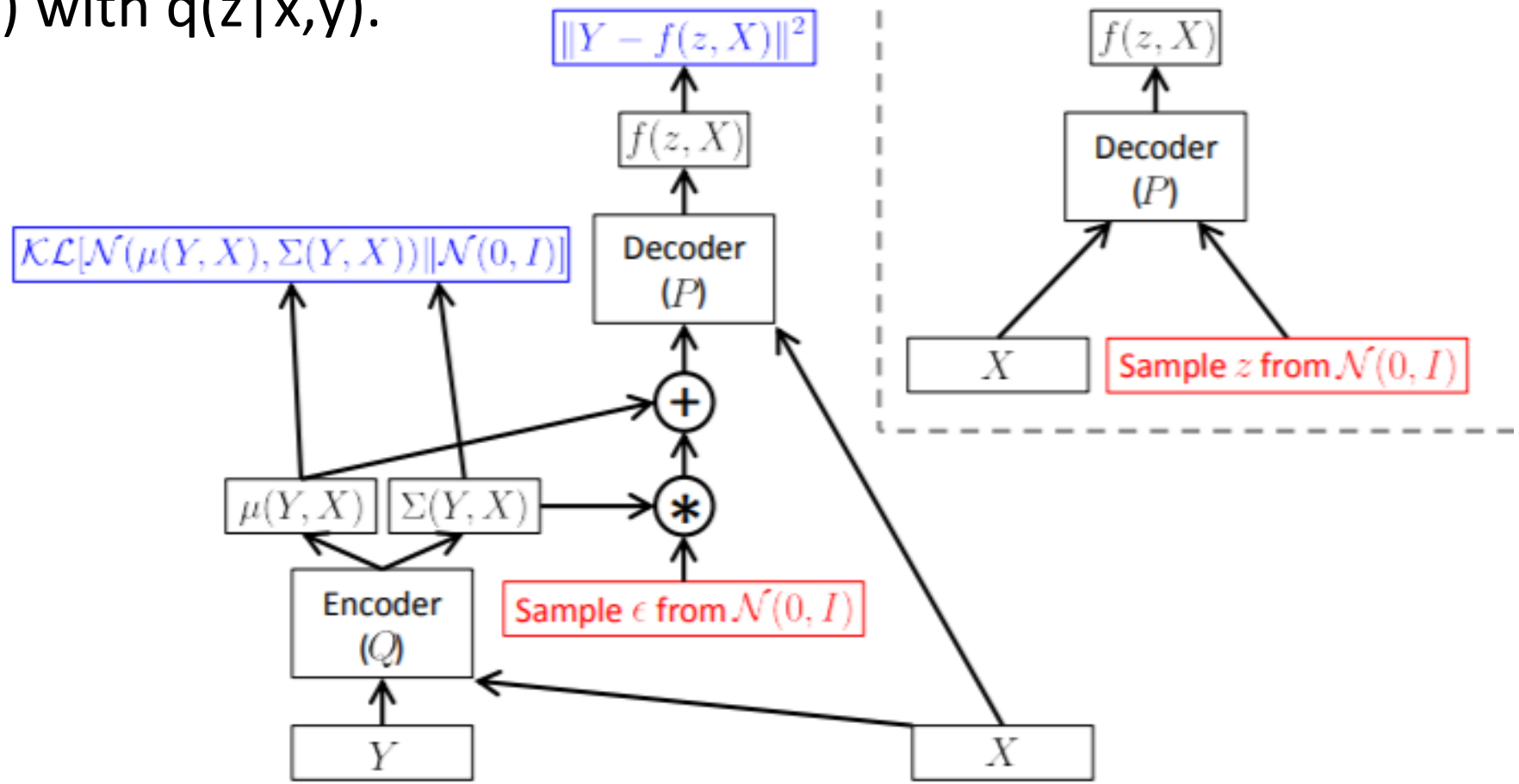


32x32 CIFAR-10

Labeled Faces in the Wild

Conditional VAE (CVAE)

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



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

CVAE

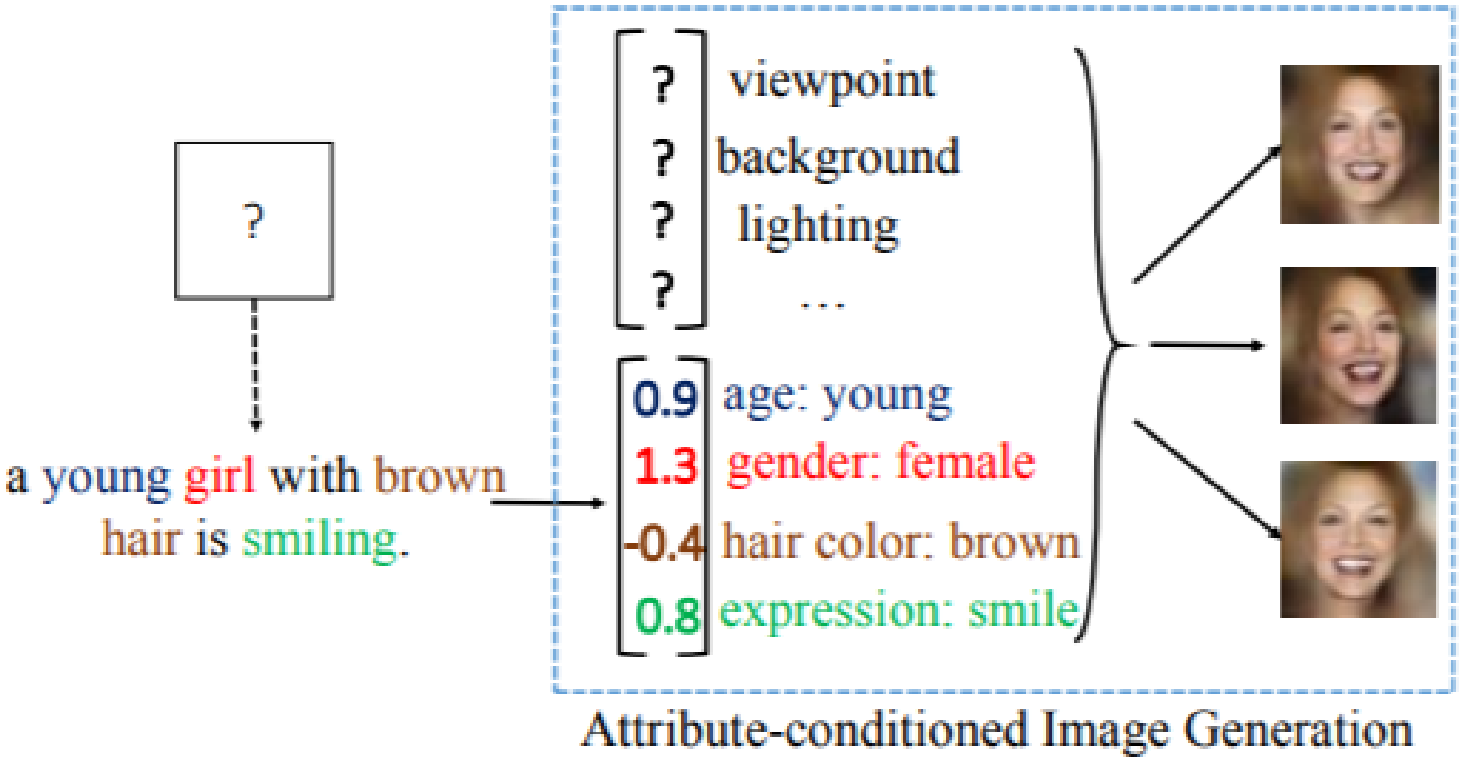
Go through the same KL divergence procedure, to get the same lower bound.

Lower bound of log conditional likelihood:

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

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

Attribute2Image



Xinchen Yan et al., Attribute2Image: Conditional Image Generation from Visual Attributes, 2015.

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

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**:

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

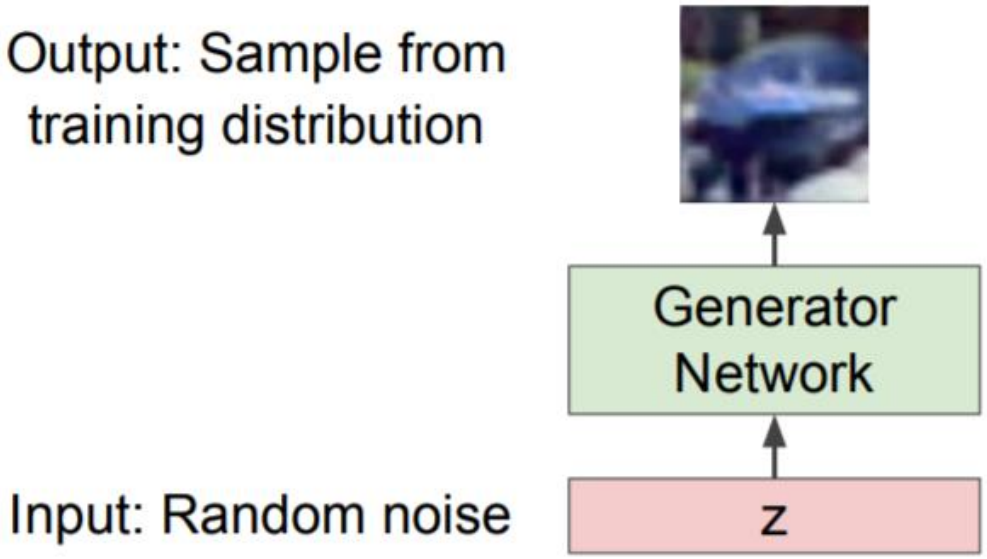
Cannot optimize directly, derive and optimize lower bound on likelihood instead

What if we give up on explicitly modeling density, and just want ability to sample?

GANs: don't work with any explicit density function!
Instead, take game-theoretic approach: learn to generate from training distribution through 2-player game

Generative Adversarial Networks

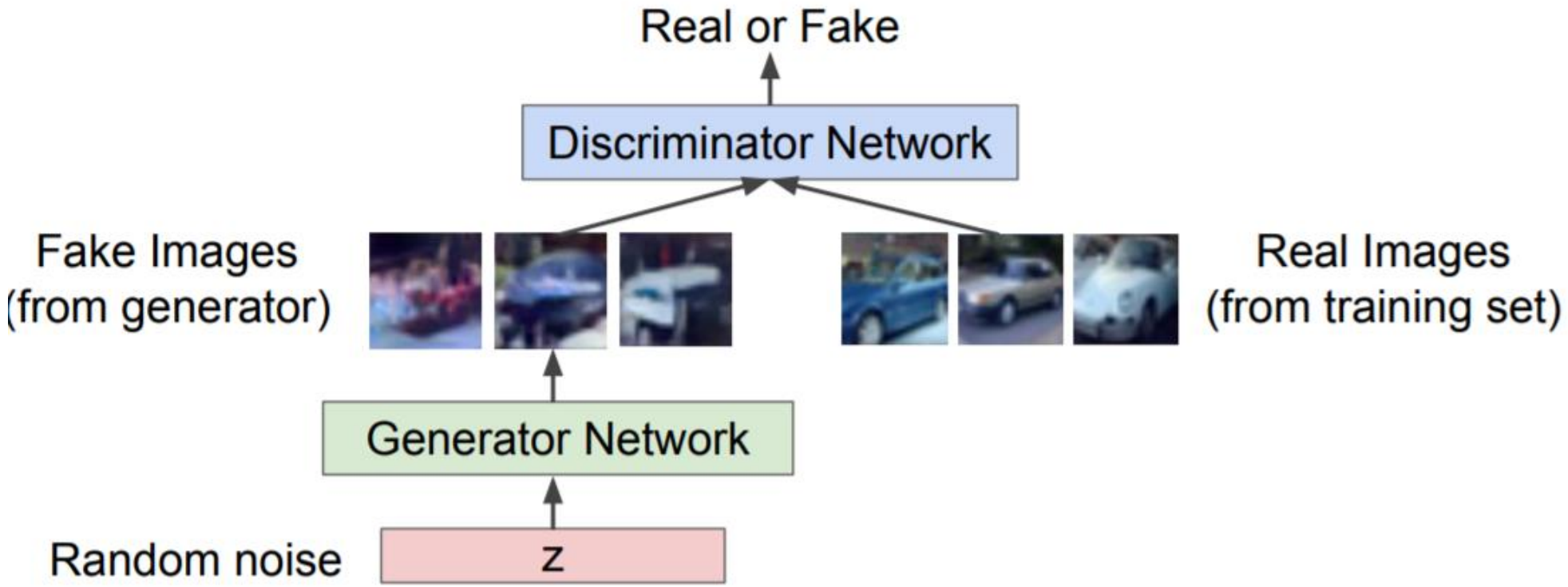
- Problem: Want to sample from complex, high-dimensional training distribution.
  - No direct way to do this!
- Solution:
  - Sample from a simple distribution, e.g. random noise.
  - Then, learn transformation to training distribution.
- Q: What can we use to represent this complex transformation?
  - A neural network!



Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

Training GANs: Two-player game

- Generator network: try to fool the discriminator by generating real-looking images
- Discriminator network: try to distinguish between real and fake images



Training GANs: Two-player game

- Generator network: try to fool the discriminator by generating real-looking images
- Discriminator network: try to distinguish between real and fake images

Train jointly in **minimax game**

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

Training GANs: Two-player game

- Generator network: try to fool the discriminator by generating real-looking images
- Discriminator network: try to distinguish between real and fake images

Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log \underbrace{D_{\theta_d}(x)}_{\text{Discriminator output for real data x}} + \mathbb{E}_{z \sim p(z)} \log(1 - \underbrace{D_{\theta_d}(G_{\theta_g}(z))}_{\text{Discriminator output for generated fake data G(z)}}) \right]$$

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Discriminator outputs likelihood in (0,1) of real image

Minimax objective function:

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Discriminator (θd) wants to maximize objective such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)

Generator (θg) wants to minimize objective such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

Training GANs: Two-player game

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

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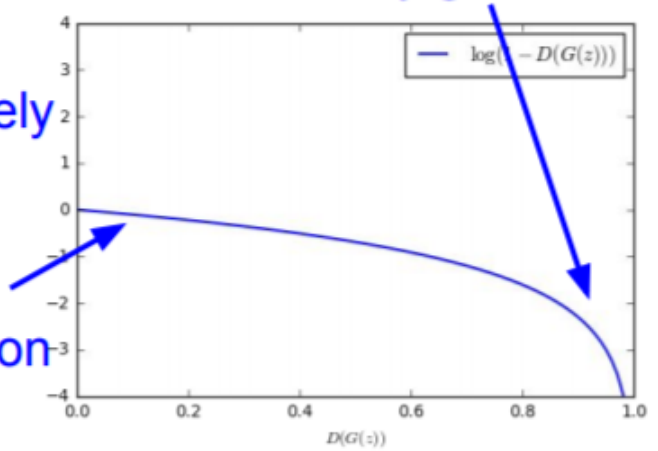
2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!

Gradient signal dominated by region where sample is already good

When sample is likely fake, want to learn from it to improve generator. But gradient in this region is relatively flat!



Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

Training GANs: Two-player game

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Alternate between:

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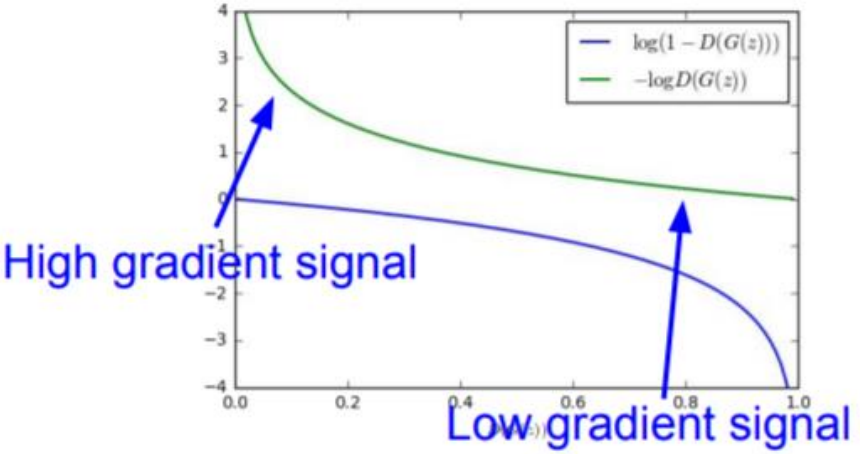
2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.

Aside: Jointly training two networks is challenging, can be unstable. Choosing objectives with better loss landscapes helps training, is an active area of research.



Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

Putting it together: GAN training algorithm

for number of training iterations **do**

  for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$$

  end for

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \ldots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by ascending its stochastic gradient (improved objective):

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

Putting it together: GAN training algorithm

Some find k=1 more stable, others use k > 1, no best rule.

Recent work (e.g. Wasserstein GAN) alleviates this problem, better stability!

for number of training iterations **do**

  for k steps **do**

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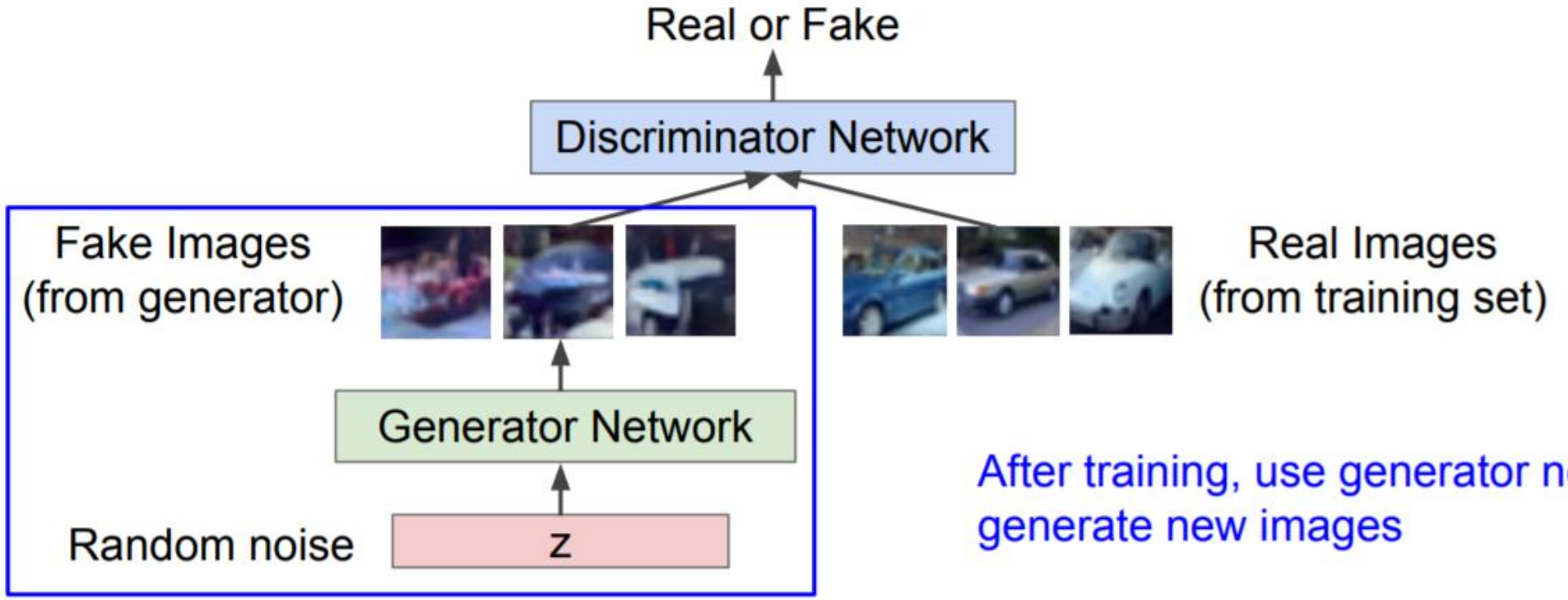
$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$$

end for

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.

GAN: Example Generation

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



After training, use generator network to generate new images

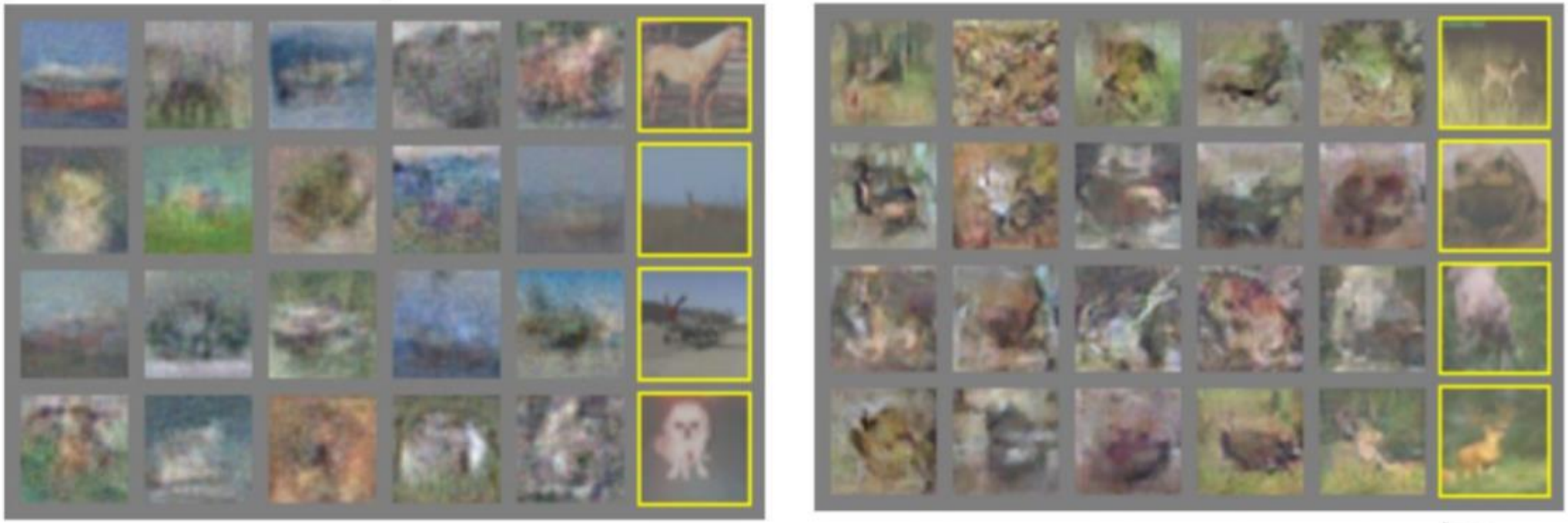
GAN: Example Generation

Generated samples

Nearest neighbor from training set

GAN: Example Generation

Generated samples (CIFAR-10)



Nearest neighbor from training set

Generative Adversarial Nets: Convolutional Architectures

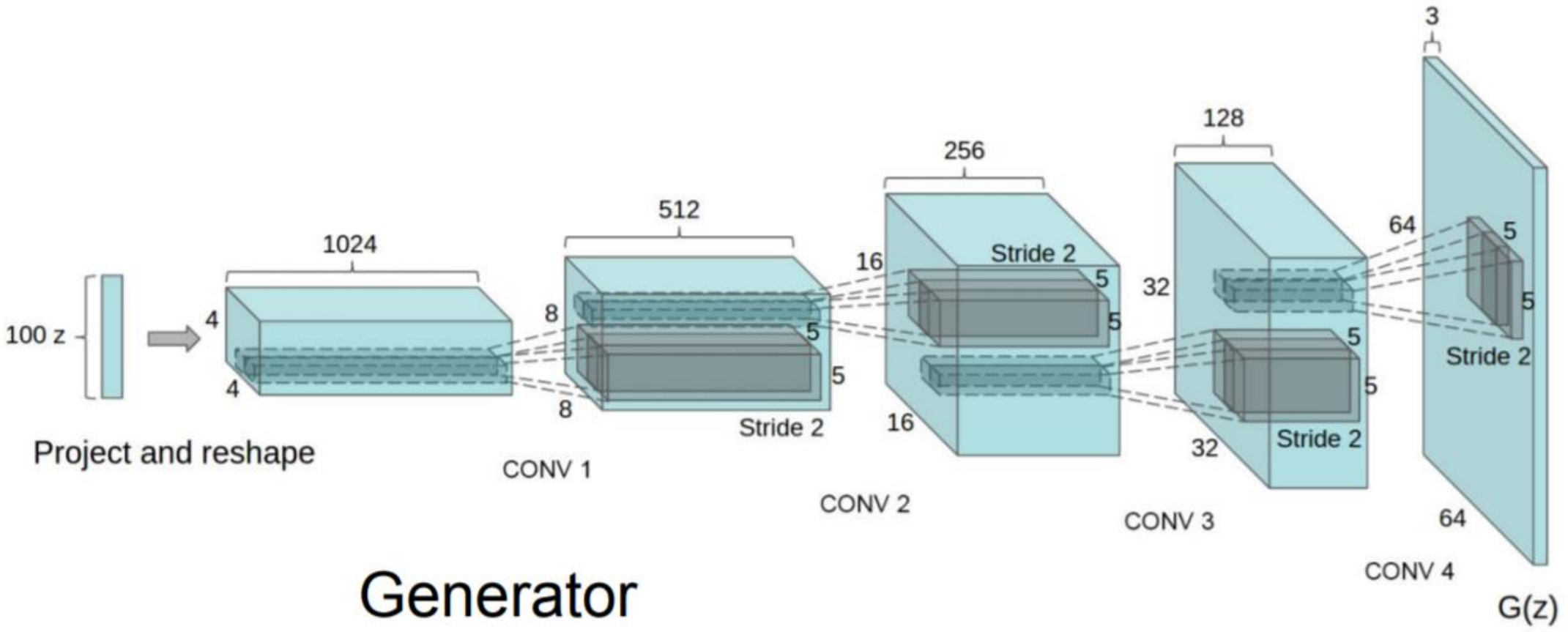
- Generator is an upsampling network with fractionally-strided convolutions Discriminator is a convolutional network

Architecture guidelines for stable Deep Convolutional GANs

- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.
- Use LeakyReLU activation in the discriminator for all layers.

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

DCGAN: Convolutional Architectures



Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Samples from the model look amazing!

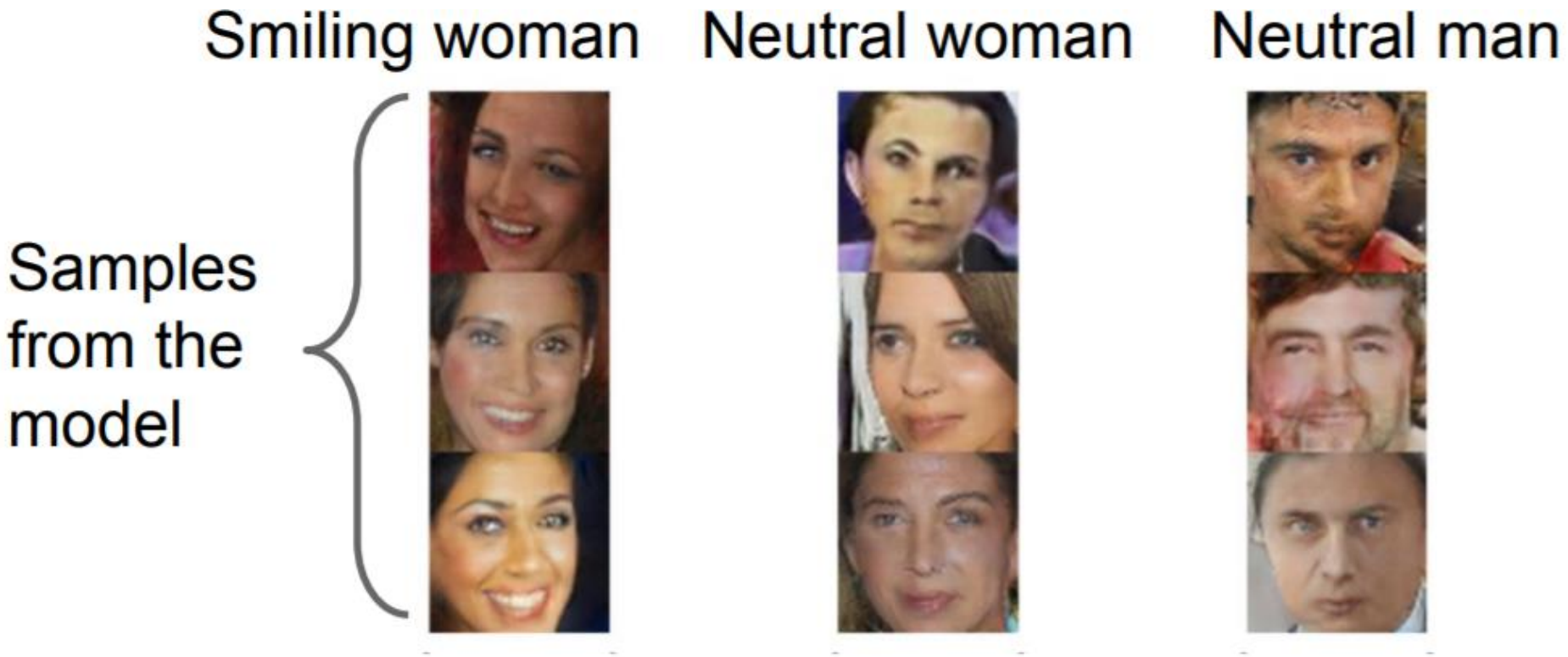
Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in laten space

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math



Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

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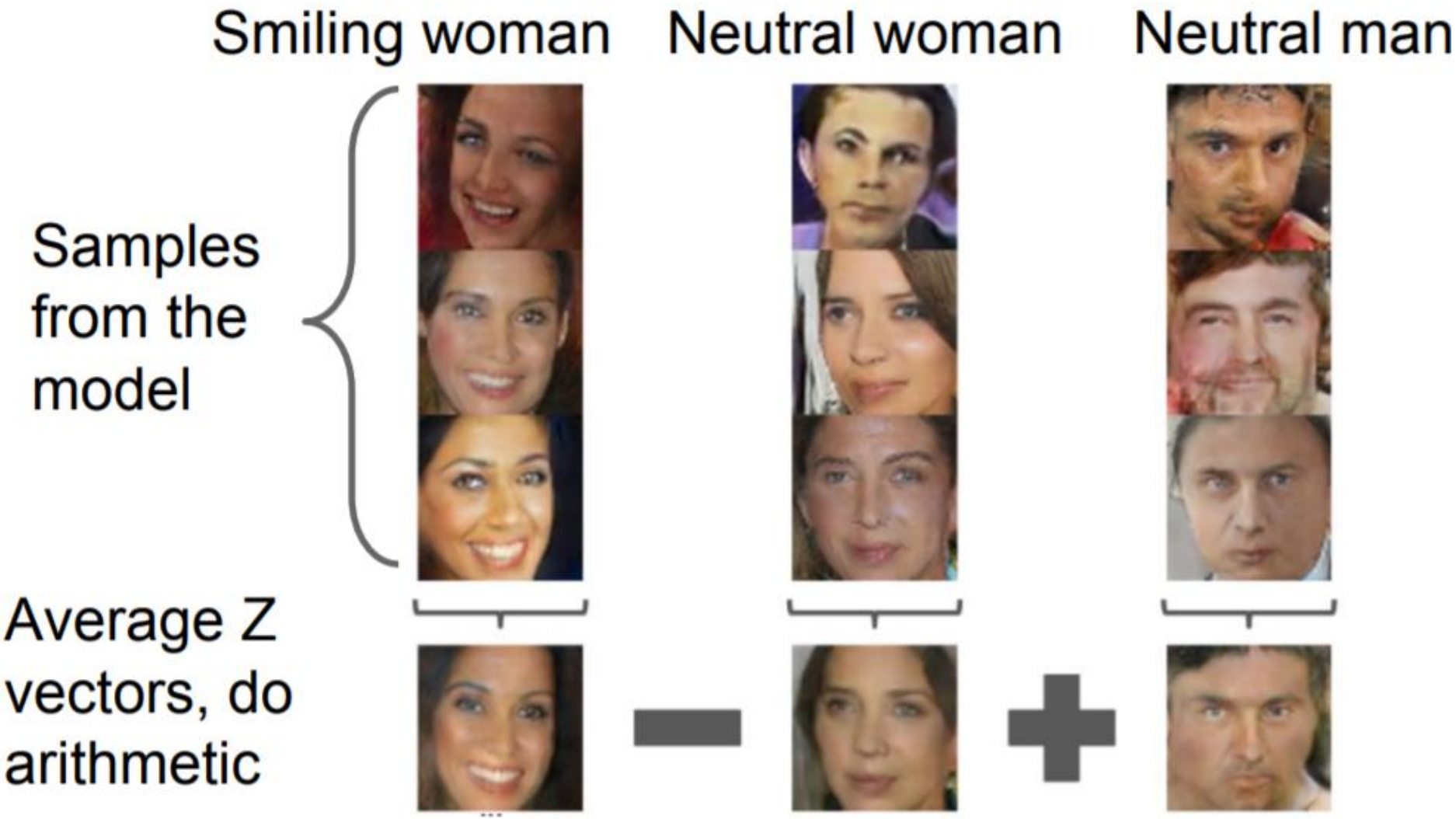

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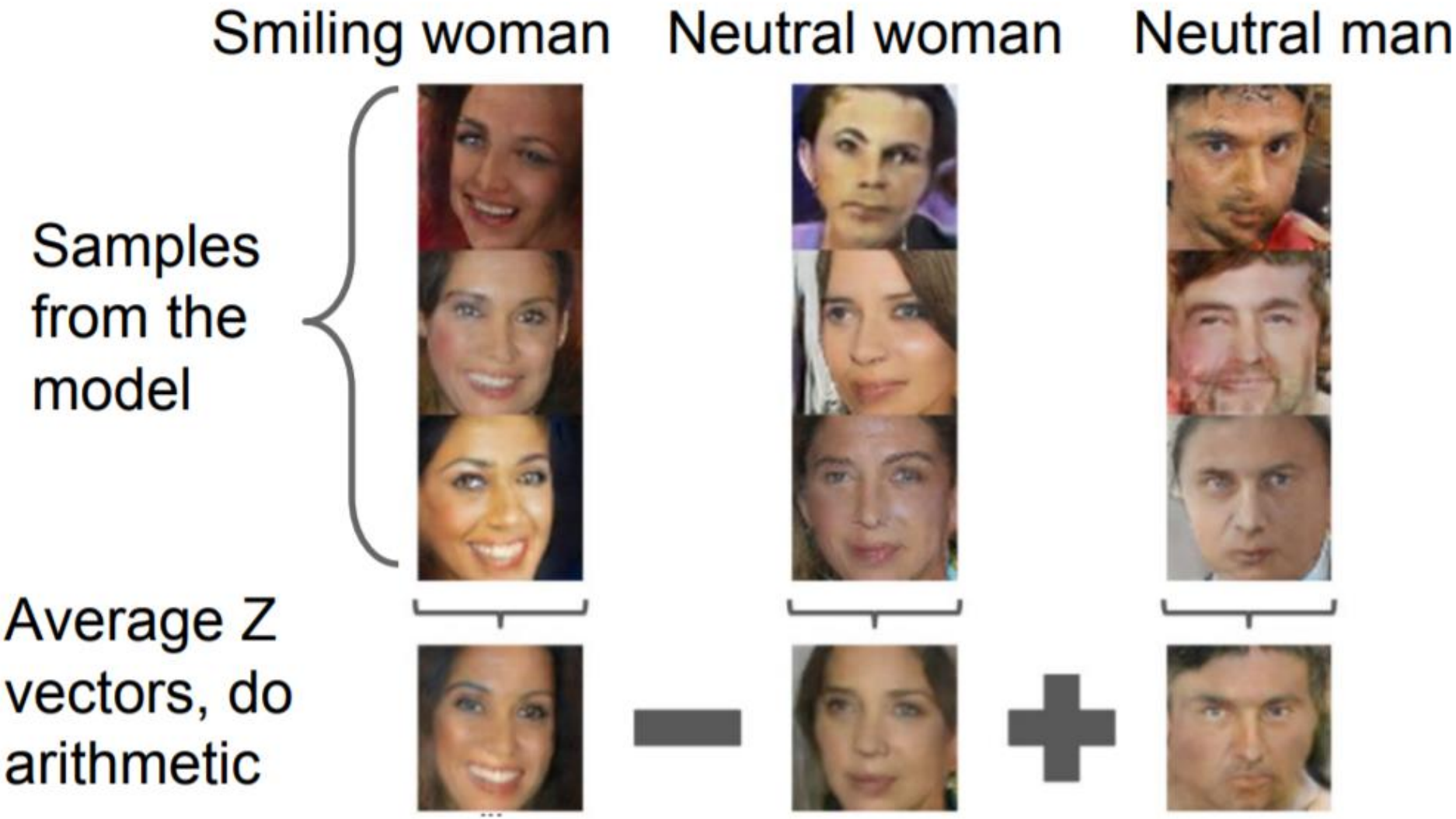

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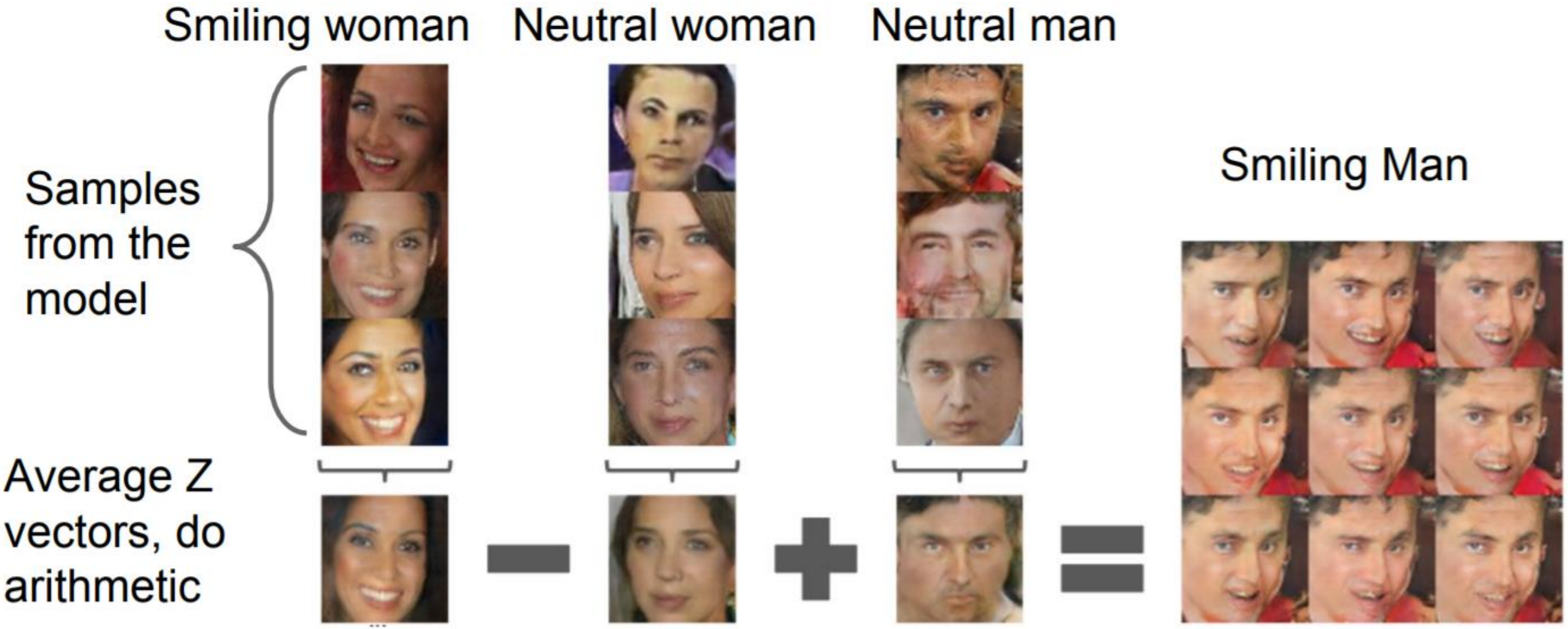

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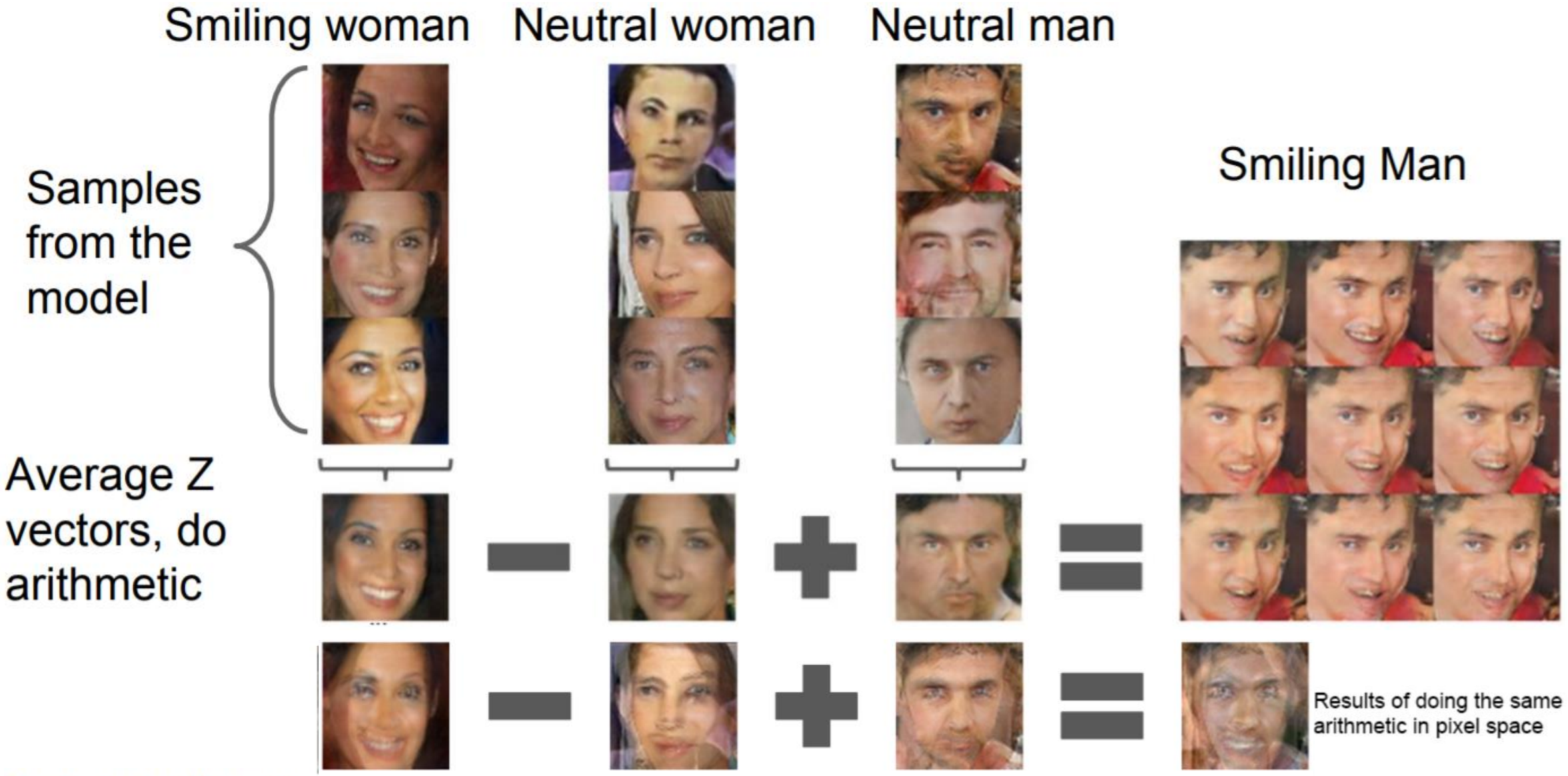

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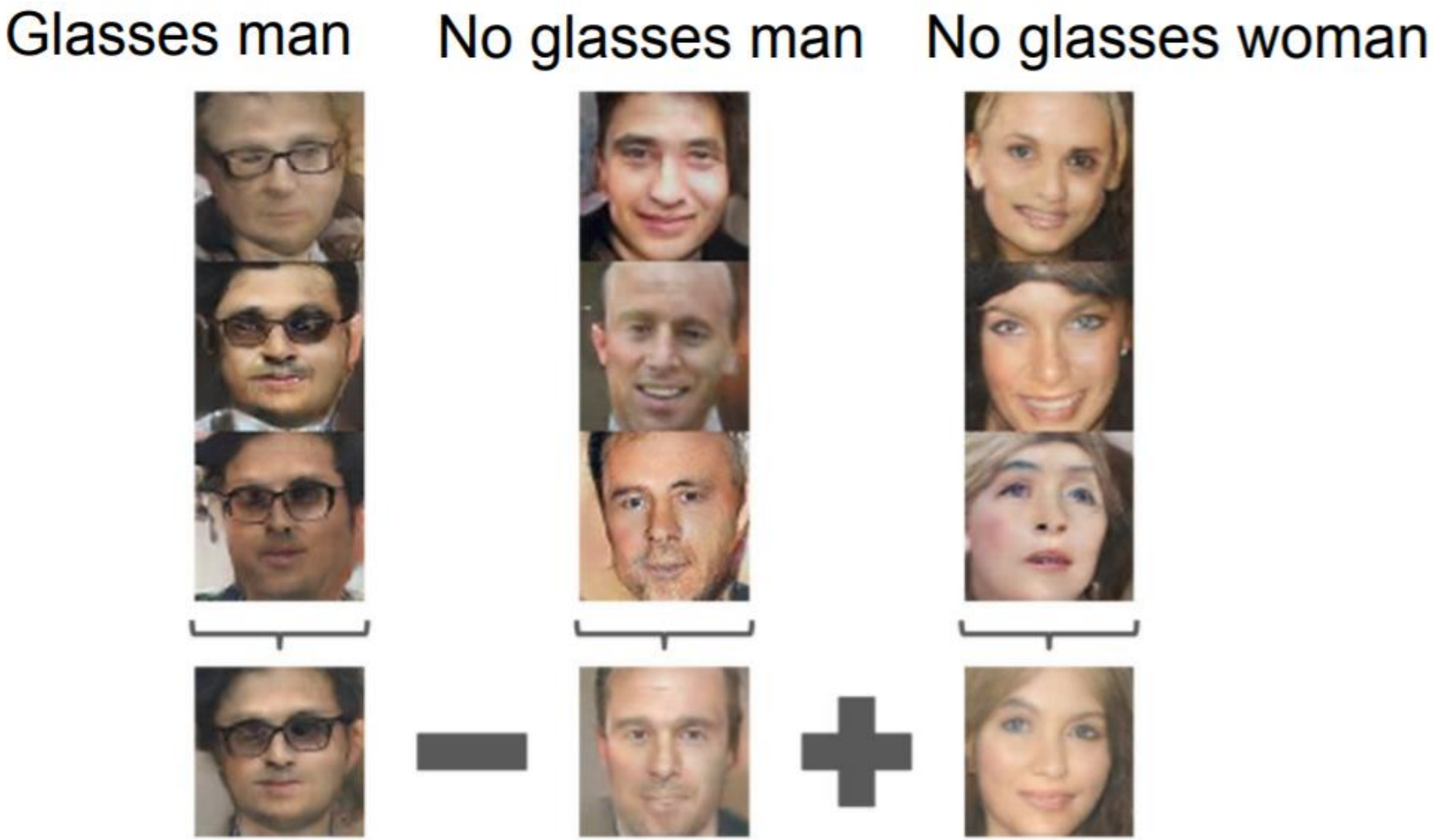

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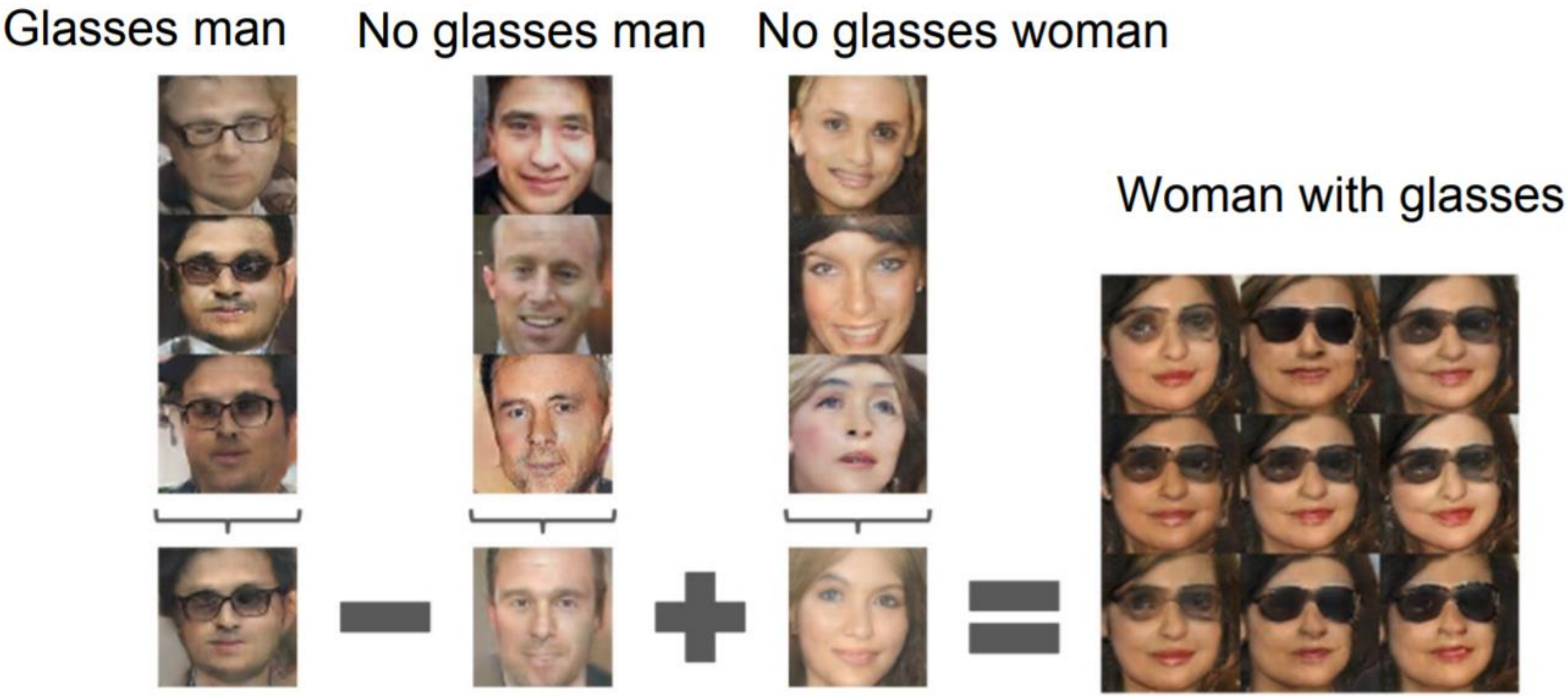
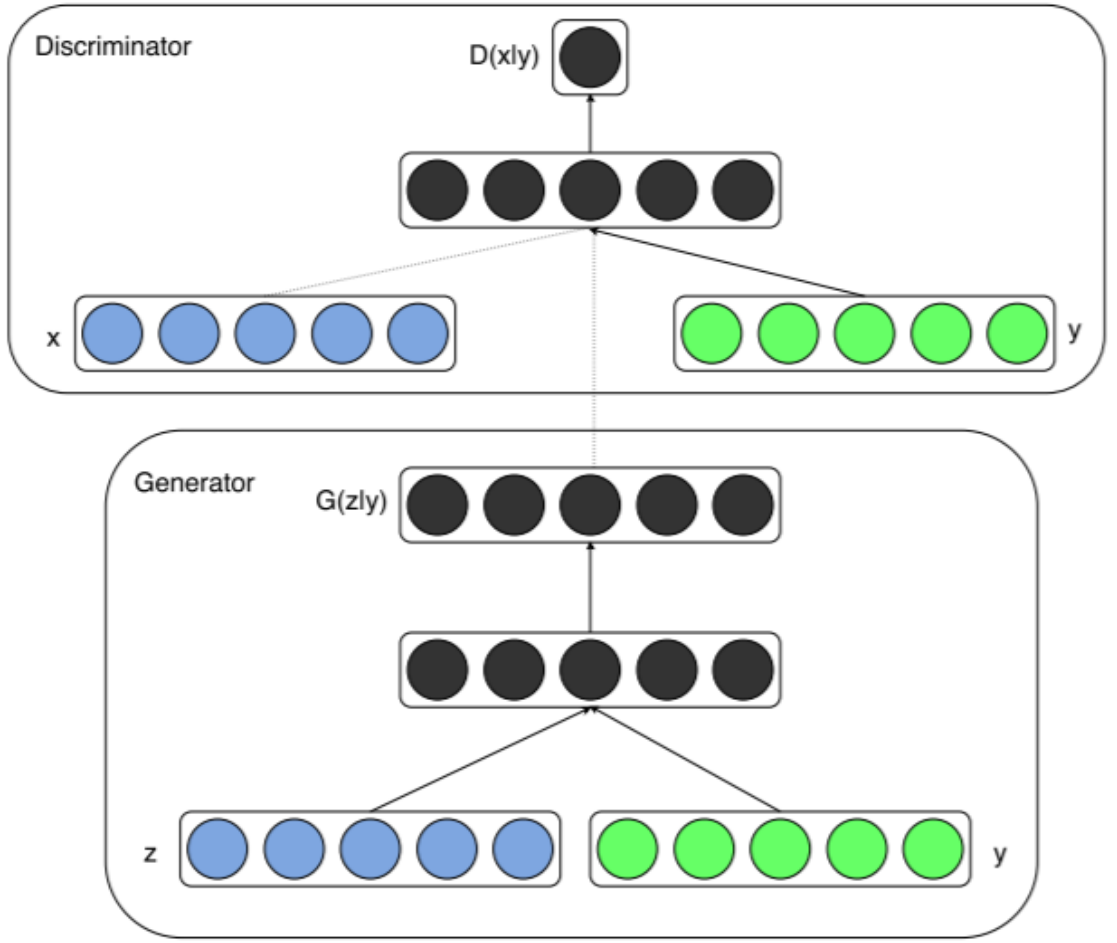


Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Conditional GAN



$$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x}|\boldsymbol{y})] + \mathbb{E}_{\boldsymbol{z}\sim p_z(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z}|\boldsymbol{y})))]$$

M. Mirza, S. Osindero, Conditional Generative Adversarial Nets, 2014.

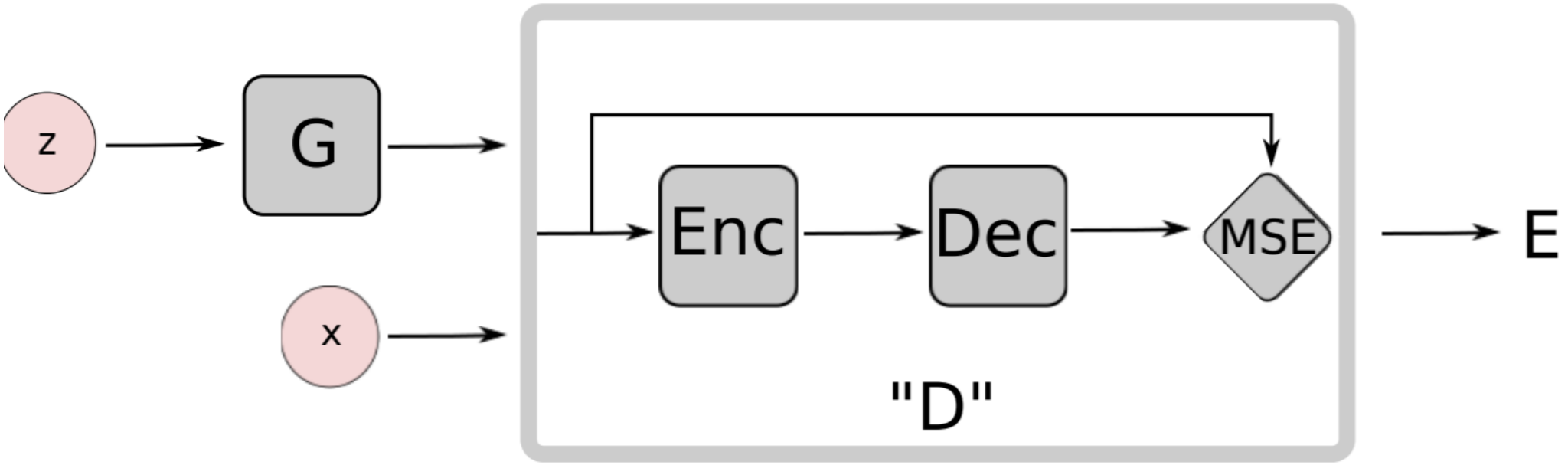
Conditional GAN

Figure 2: Generated MNIST digits, each row conditioned on one label

M. Mirza, S. Osindero, Conditional Generative Adversarial Nets, 2014.

Energy-Based GAN (EBGAN)

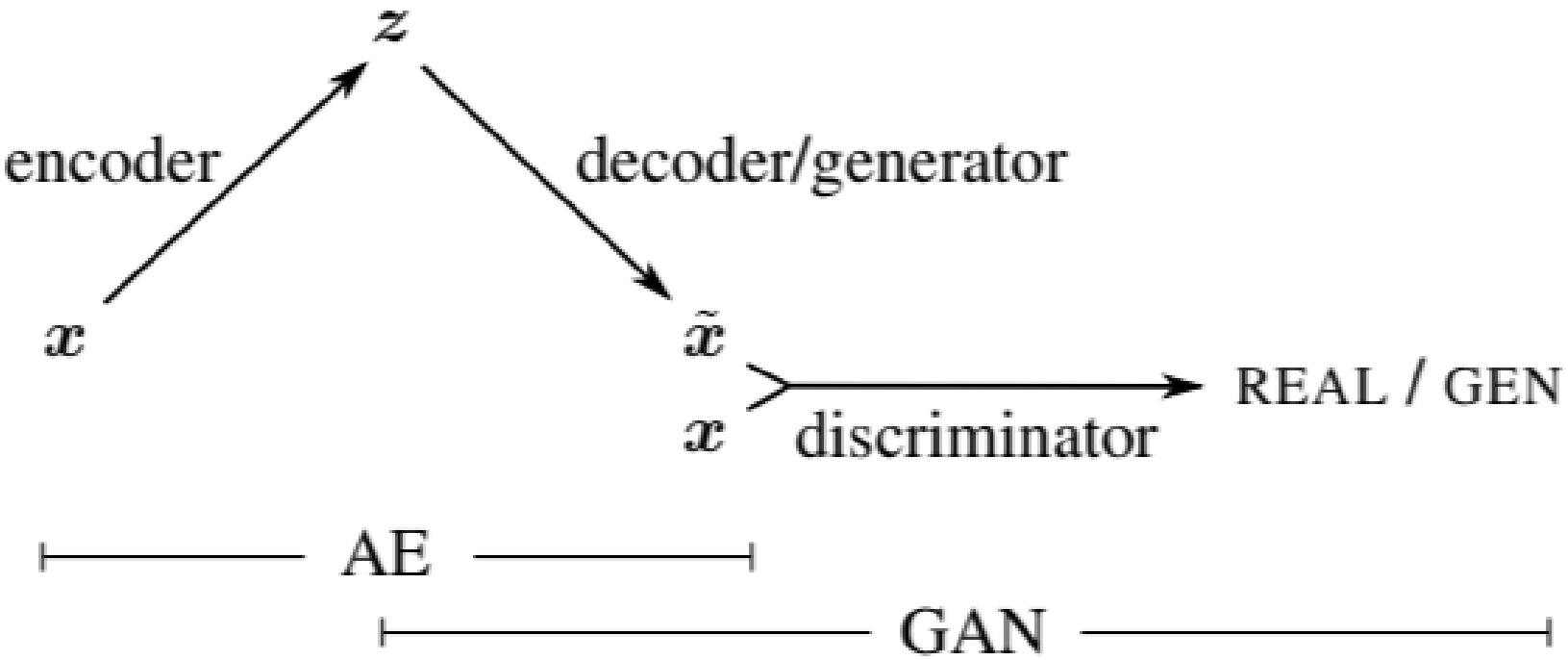
- EBGAN architecture with an auto-encoder discriminator



- auto-encoders have the ability to learn an energy manifold without supervision or negative examples

J. Zhao et al., Energy-based Generative Adversarial Network, 2016.

Combining VAE with GAN



Anders Boesen Lindbo Larse et al., Autoencoding beyond pixels using a learned similarity metric, ICML 2016.

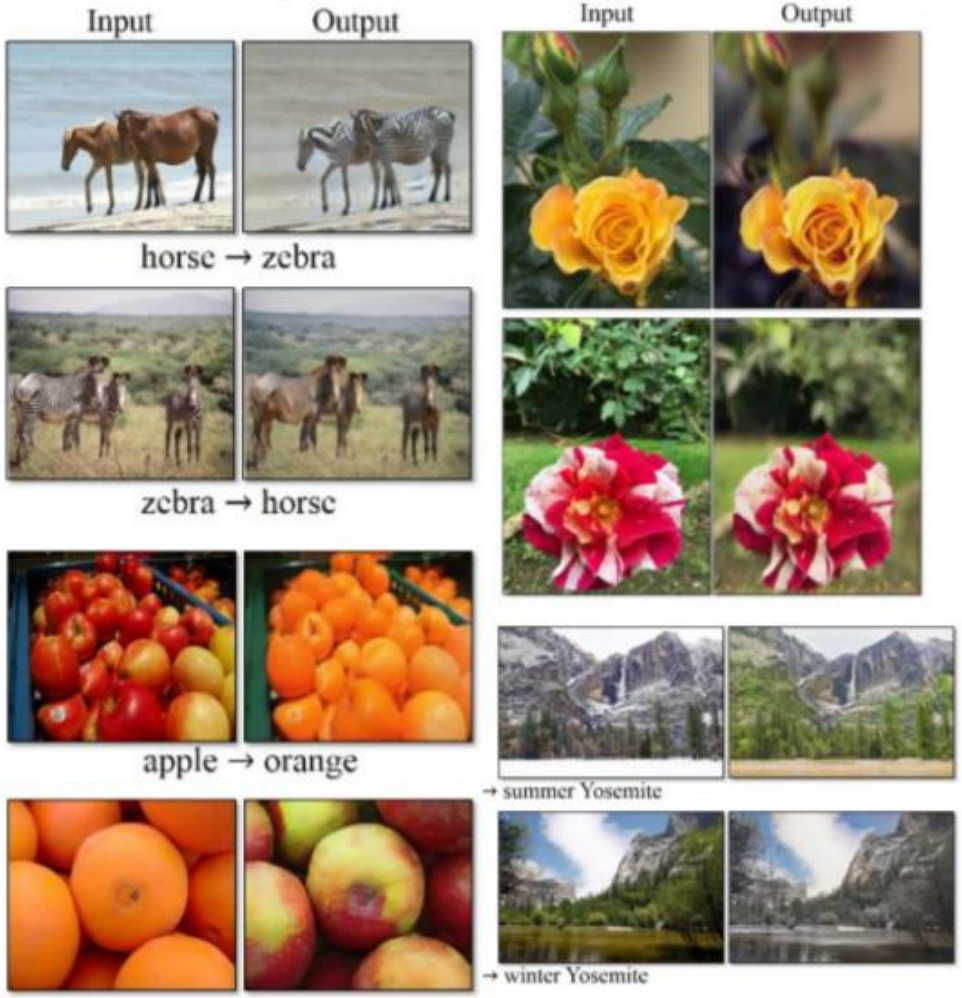
2017: Year of the GAN

Better training and generation

LSGAN. Mao et al. 2017.

BEGAN. Bertholet et al. 2017.

Source->Target domain transfer



CycleGAN. Zhu et al. 2017.

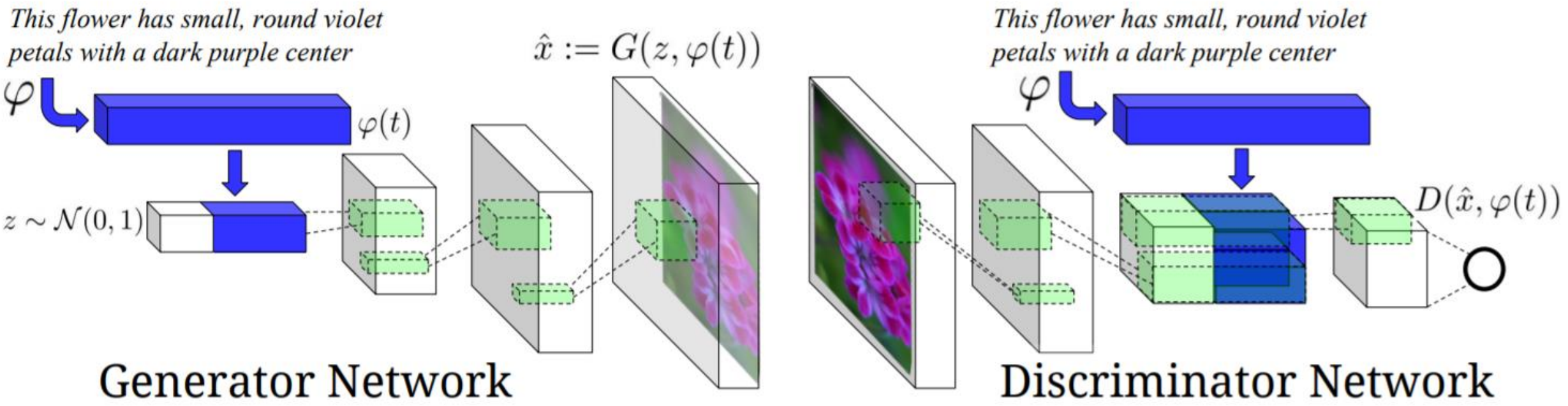
Text -> Image Synthesis

Reed et al. 2017.

Many GAN applications

Pix2pix. Isola 2017. Many examples at https://phillipi.github.io/pix2pix/

Generative Adversarial Text to Image Synthesis



S. Reed et al., Generative Adversarial Text to Image Synthesis, 2016.

“The GAN Zoo”

See also: https://github.com/soumith/ganhacks for tips and tricks for trainings GANs

- GAN - Generative Adversarial Networks
- 3D-GAN - Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling
- acGAN - Face Aging With Conditional Generative Adversarial Networks
- AC-GAN - Conditional Image Synthesis With Auxiliary Classifier GANs
- AdaGAN - AdaGAN: Boosting Generative Models
- AEGAN - Learning Inverse Mapping by Autoencoder based Generative Adversarial Nets
- AffGAN - Amortised MAP Inference for Image Super-resolution
- AL-CGAN - Learning to Generate Images of Outdoor Scenes from Attributes and Semantic Layouts
- ALI - Adversarially Learned Inference
- AM-GAN - Generative Adversarial Nets with Labeled Data by Activation Maximization
- AnoGAN - Unsupervised Anomaly Detection with Generative Adversarial Networks to Guide Marker Discovery
- ArtGAN - ArtGAN: Artwork Synthesis with Conditional Categorial GANs
- b-GAN - b-GAN: Unified Framework of Generative Adversarial Networks
- Bayesian GAN - Deep and Hierarchical Implicit Models
- BEGAN - BEGAN: Boundary Equilibrium Generative Adversarial Networks
- BiGAN - Adversarial Feature Learning
- BS-GAN - Boundary-Seeking Generative Adversarial Networks
- CGAN - Conditional Generative Adversarial Nets
- CaloGAN - CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks
- CCGAN - Semi-Supervised Learning with Context-Conditional Generative Adversarial Networks
- CatGAN - Unsupervised and Semi-supervised Learning with Categorical Generative Adversarial Networks
- CoGAN - Coupled Generative Adversarial Networks
- Context-RNN-GAN - Contextual RNN-GANs for Abstract Reasoning Diagram Generation
- C-RNN-GAN - C-RNN-GAN: Continuous recurrent neural networks with adversarial training
- CS-GAN - Improving Neural Machine Translation with Conditional Sequence Generative Adversarial Nets
- CVAE-GAN - CVAE-GAN: Fine-Grained Image Generation through Asymmetric Training
- CycleGAN - Unpaired Image-to-Image Translation using Cycle-Consistent Adversarial Networks
- DTN - Unsupervised Cross-Domain Image Generation
- DCGAN - Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks
- DiscoGAN - Learning to Discover Cross-Domain Relations with Generative Adversarial Networks
- DR-GAN - Disentangled Representation Learning GAN for Pose-Invariant Face Recognition
- DualGAN - DualGAN: Unsupervised Dual Learning for Image-to-Image Translation
- EBGAN - Energy-based Generative Adversarial Network
- f-GAN - f-GAN: Training Generative Neural Samplers using Variational Divergence Minimization
- FF-GAN - Towards Large-Pose Face Frontalization in the Wild
- GAWWN - Learning What and Where to Draw
- GeneGAN - GeneGAN: Learning Object Transfiguration and Attribute Subspace from Unpaired Data
- Geometric GAN - Geometric GAN
- GoGAN - Gang of GANs: Generative Adversarial Networks with Maximum Margin Ranking
- GP-GAN - GP-GAN: Towards Realistic High-Resolution Image Blending
- IAN - Neural Photo Editing with Introspective Adversarial Networks
- iGAN - Generative Visual Manipulation on the Natural Image Manifold
- IcGAN - Invertible Conditional GANs for image editing
- ID-CGAN - Image De-raining Using a Conditional Generative Adversarial Network
- Improved GAN - Improved Techniques for Training GANs
- InfoGAN - InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets
- LAGAN - Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics Synthesis
- LAPGAN - Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

https://github.com/hindupuravinash/the-gan-zoo

GANs

- Don’t work with an explicit density function
- Take game-theoretic approach: learn to generate from training distribution through 2-player game

- Pros:
  - Beautiful, state-of-the-art samples!
- Cons:
  - Trickier / more unstable to train
  - Can’t solve inference queries such as p(x), p(z|x)
- Active areas of research:
  - Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)
  - Conditional GANs, GANs for all kinds of applications

Recap

Generative Models

- PixelRNN and PixelCNN — Explicit density model, optimizes exact likelihood, good samples. But inefficient sequential generation.
- Variational Autoencoders (VAE) — Optimize variational lower bound on likelihood. Useful latent representation, inference queries. But current sample quality not the best.
- Generative Adversarial Networks (GANs) — Game-theoretic approach, best samples! But can be tricky and unstable to train, no inference queries.

Also recent work in combinations of these types of models! E.g. Adversarial Autoencoders (Makhanzi 2015) and PixelVAE (Gulrajani 2016)

Resources

- Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014.
- Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014.
- Ian Goodfellow, “Generative Adversarial Nets”, NIPS 2016 Tutorial.