Advanced Prediction Models

Today's Outline

- Unsupervised Learning Landscape
- Autoencoders and Variational Autoencoders (VAE)
- Generative Adversarial Networks (GAN)

Unsupervised Learning Landscape

Unsupervised Learning

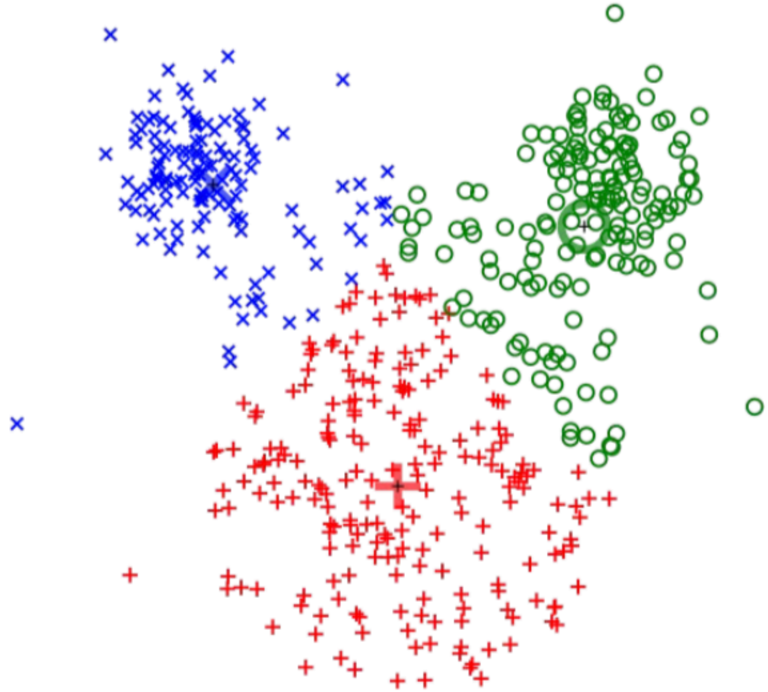
- Supervised learning
  - Involves feature and label pairs as training data
  - Goal is to find a map from feature to label/value

- Unsupervised learning
  - Involves only feature vectors
    - Example: images
  - Goal is to learn some patterns of data
  - There is no objective measure of success

[1]Reference: CS231n (Stanford, Spring 17)

Unsupervised Learning Tasks

- Clustering
- Association rules
- Dimensionality reduction
- Density estimation
- Embedding
- Sampling



K-means clustering

[1]Reference: CS231n (Stanford, Spring 17)

Unsupervised Learning Tasks

- Clustering
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[1] Figure:mathworks.com/matlabcentral/mlc-downloads/downloads/submissions/42541/versions/3/screenshot.jpg

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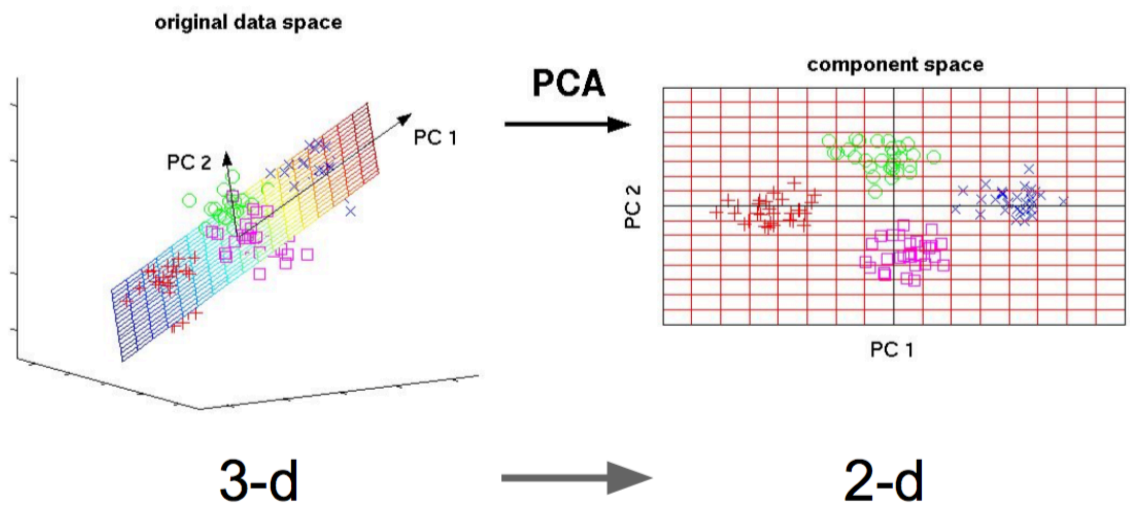

[1]Reference: CS231n (Stanford, Spring 17)

Unsupervised Learning Tasks

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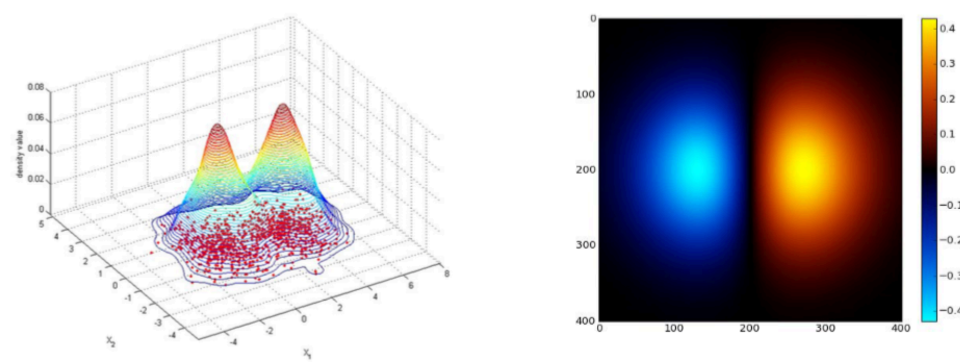
1-d density estimation



2-d density estimation

[1]Reference: CS231n (Stanford, Spring 17)

Unsupervised Learning Tasks

- Clustering
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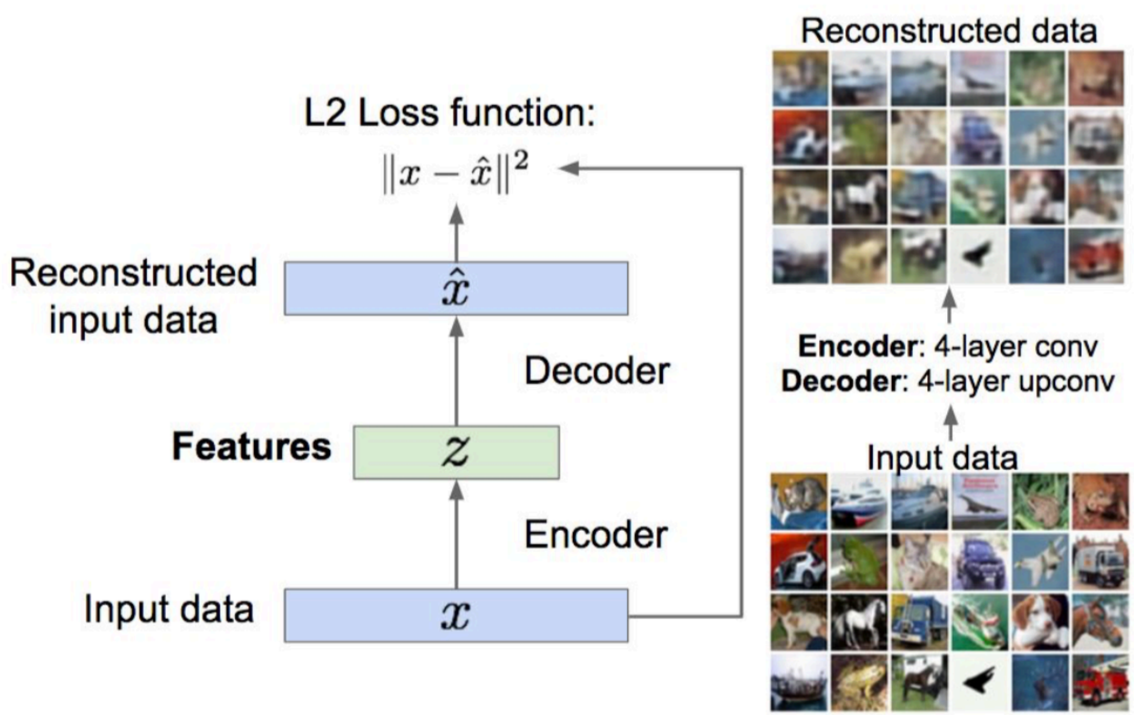
- Sampling



[1]Reference: CS231n (Stanford, Spring 17)

Unsupervised Learning Tasks

- Clustering
- Association rules
- Dimensionality reduction
- Density estimation
- Embedding
- Sampling

[1]Reference: https://www.youtube.com/watch?v=rs3aI7bACGc

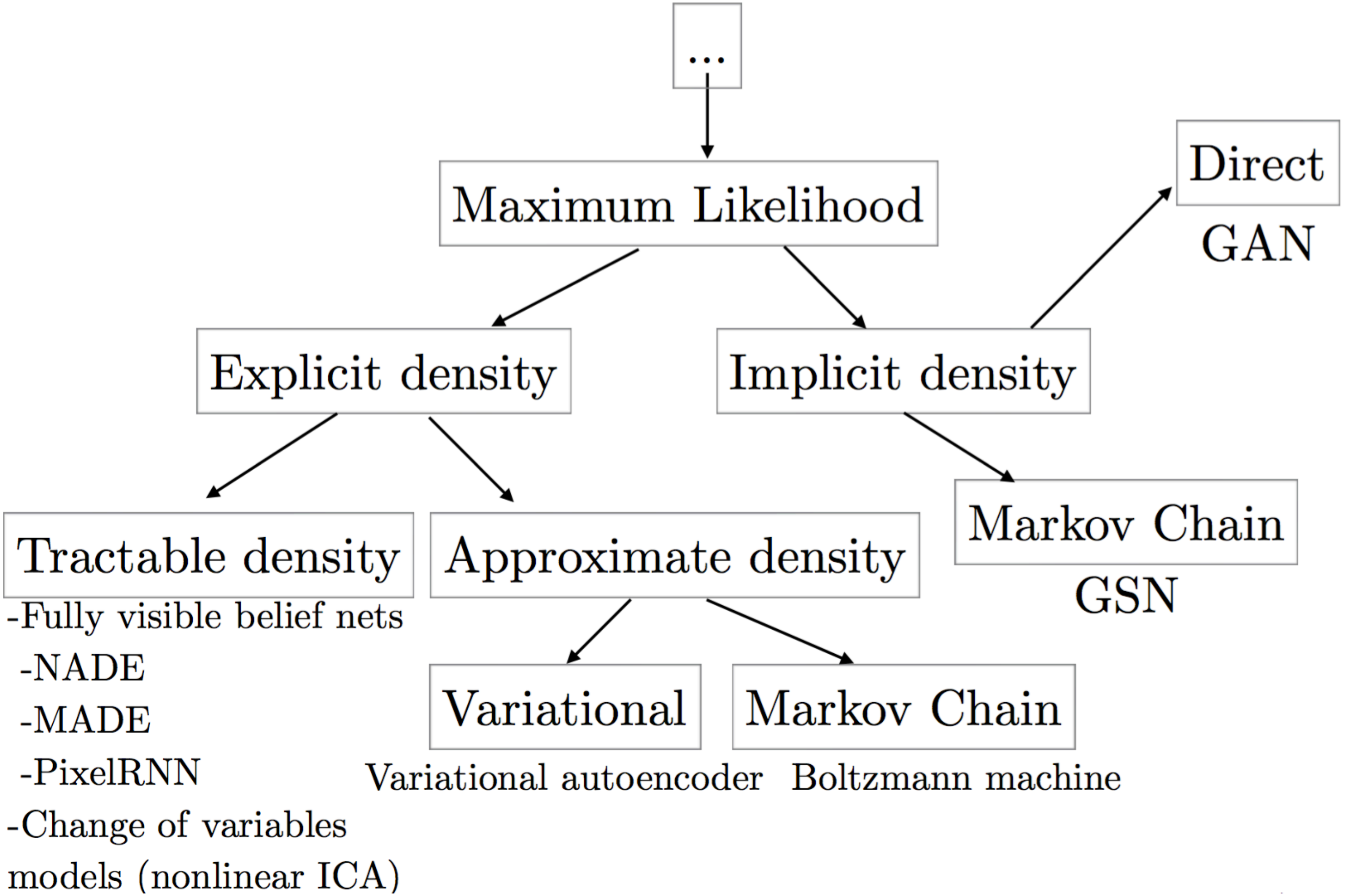
Learning a Distribution

- Given (large amount of) data drawn from P_d, we want to estimate P_m such that samples from P_m are as similar as possible to samples from P_d

- Two approaches:
  - Explicit
    - If we construct P_m explicitly, we can address all the other tasks mentioned
  - Implicit
    - We can directly generate a sample from P_m without explicitly defining it!

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

Explicit and Implicit Approaches



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

Explicit and Implicit Approaches

- When would we be okay with an implicit approach
  - Simulate possible futures for planning
  - When samples themselves are useful for other tasks…

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

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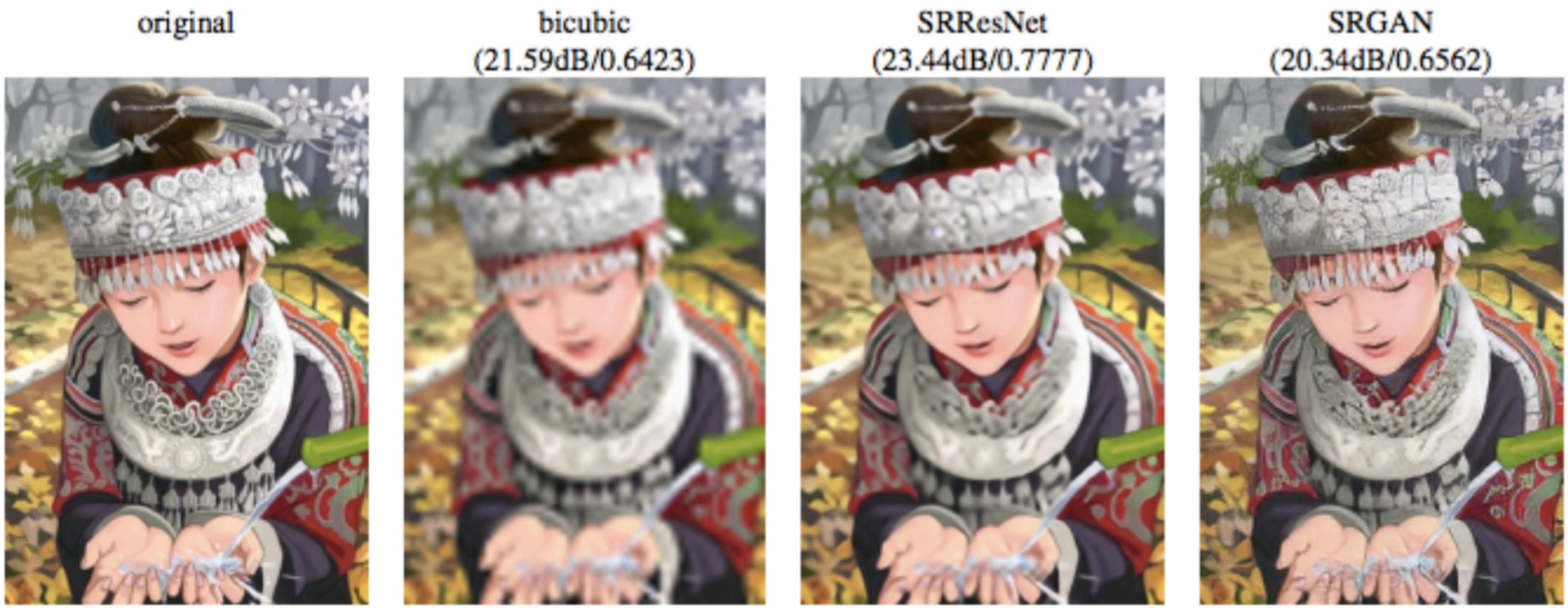

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial), Ledig et al. 2016

Explicit and Implicit Approaches

- When would we be okay with an implicit approach
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[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

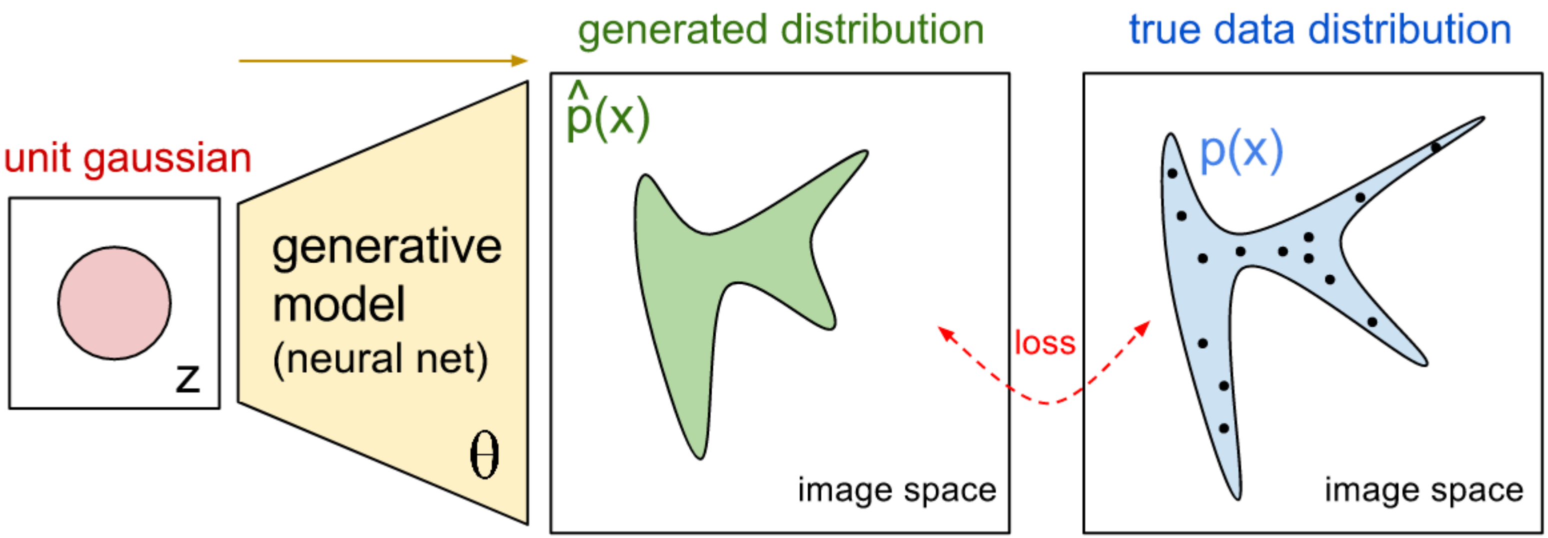
Explicit and Implicit Approaches

- We will look at one model under each approach and work with image data
  - Explicit: Variational Autoencoders (VAE)
  - Implicit: Generative Adversarial Networks (GAN)
- Both use neural networks as a core object

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

More than Memorization

- Either model (VAE or GAN) will essentially build the yellow box below:



[1] Reference: https://blog.openai.com/generative-models/

Questions?

Today's Outline

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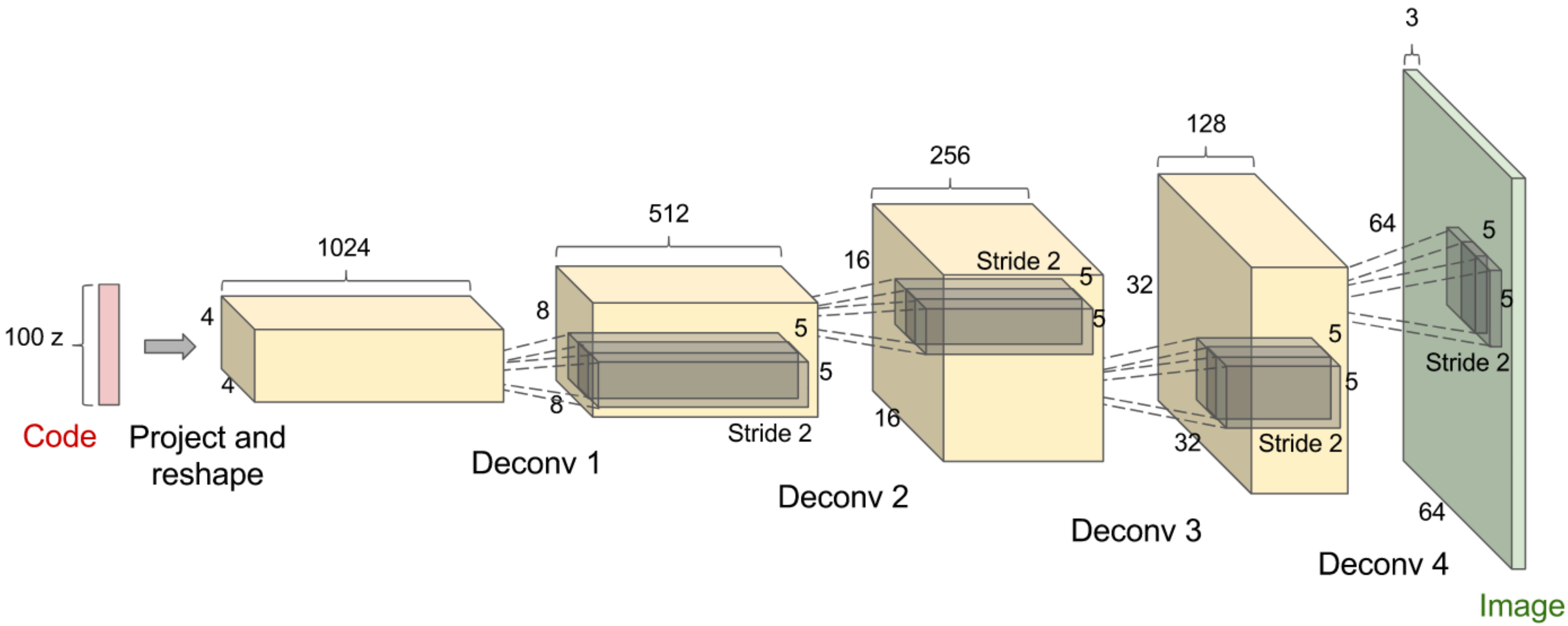
Autoencoders and Variational Autoencoders

Neural Net as a Transformation Map

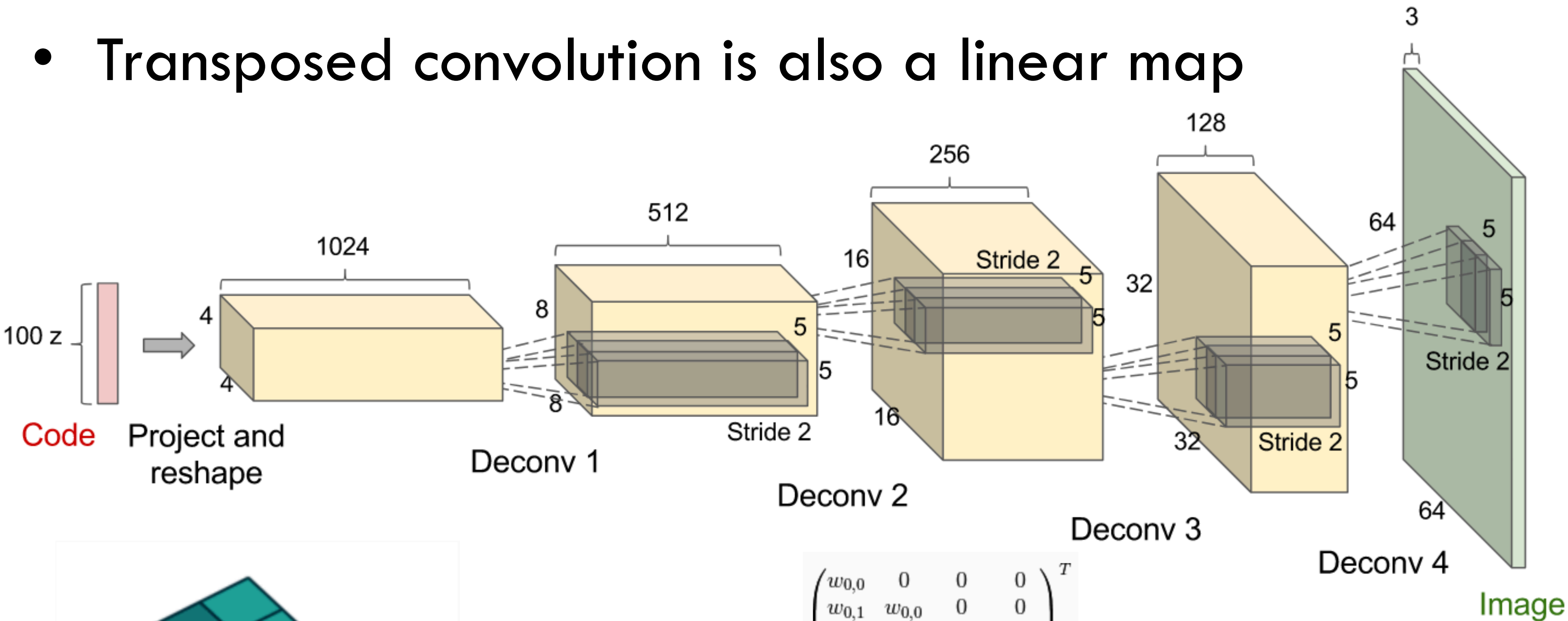
- NN is a function that maps an input to output
- Here is a ~~deconvolutional~~/transposed-convolutional network

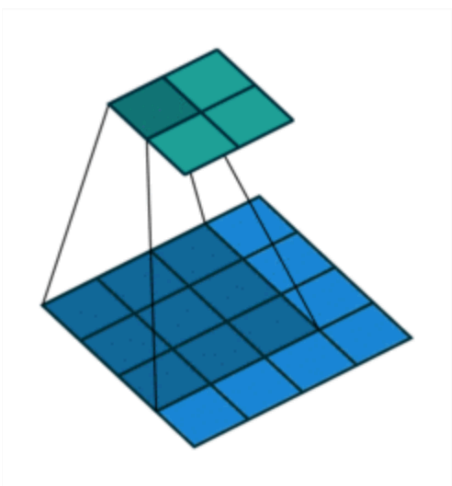


[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Neural Net as a Transformation Map

- Transposed convolution is also a linear map



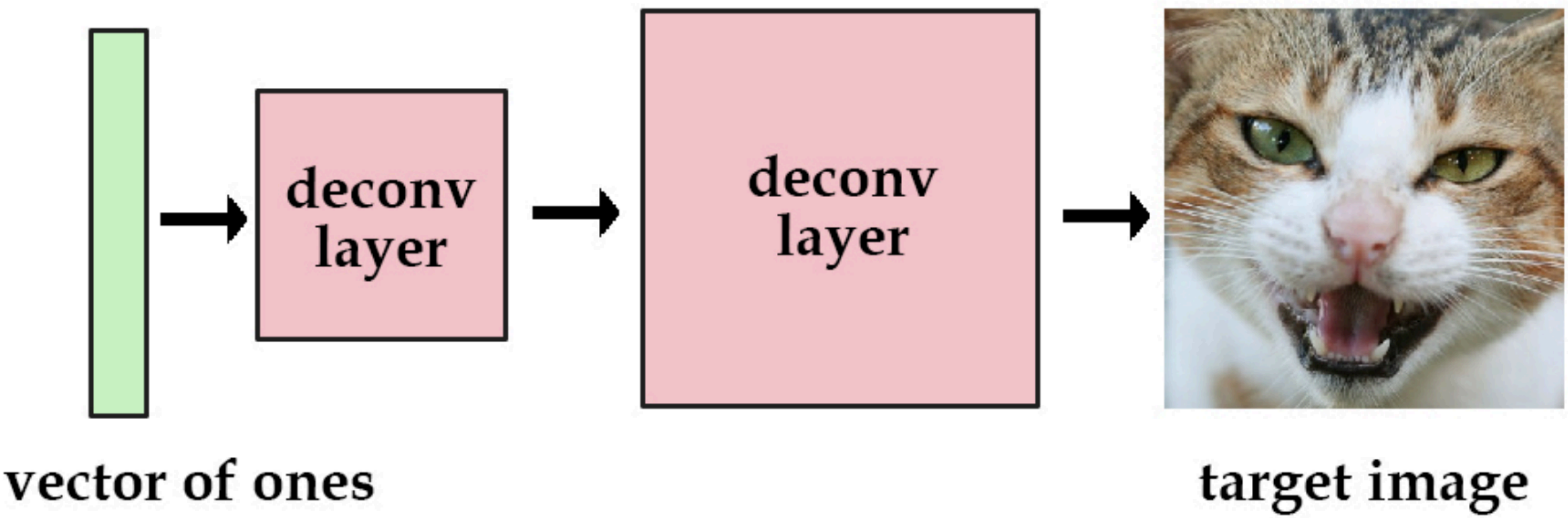


$$\text{16-dim vec} = \begin{pmatrix} w_{0,0} & 0 & 0 & 0 \\ w_{0,1} & w_{0,0} & 0 & 0 \\ w_{0,2} & w_{0,1} & 0 & 0 \\ 0 & w_{0,2} & 0 & 0 \\ w_{1,0} & 0 & w_{0,0} & 0 \\ w_{1,1} & w_{1,0} & w_{0,1} & w_{0,0} \\ w_{1,2} & w_{1,1} & w_{0,2} & w_{0,1} \\ 0 & w_{1,2} & 0 & w_{0,2} \\ w_{2,0} & 0 & w_{1,0} & 0 \\ w_{2,1} & w_{2,0} & w_{1,1} & w_{1,0} \\ w_{2,2} & w_{2,1} & w_{1,2} & w_{1,1} \\ 0 & w_{2,2} & 0 & w_{1,2} \\ 0 & 0 & w_{2,0} & 0 \\ 0 & 0 & w_{2,1} & w_{2,0} \\ 0 & 0 & w_{2,2} & w_{2,1} \\ 0 & 0 & 0 & w_{2,2} \end{pmatrix}^T * \text{4-dim vec}$$

[1] Reference: http://deeplearning.net/software/theano_versions/dev/tutorial/conv_arithmetic.html#transposed-convolution-arithmetic

Transformation from a Single Vector

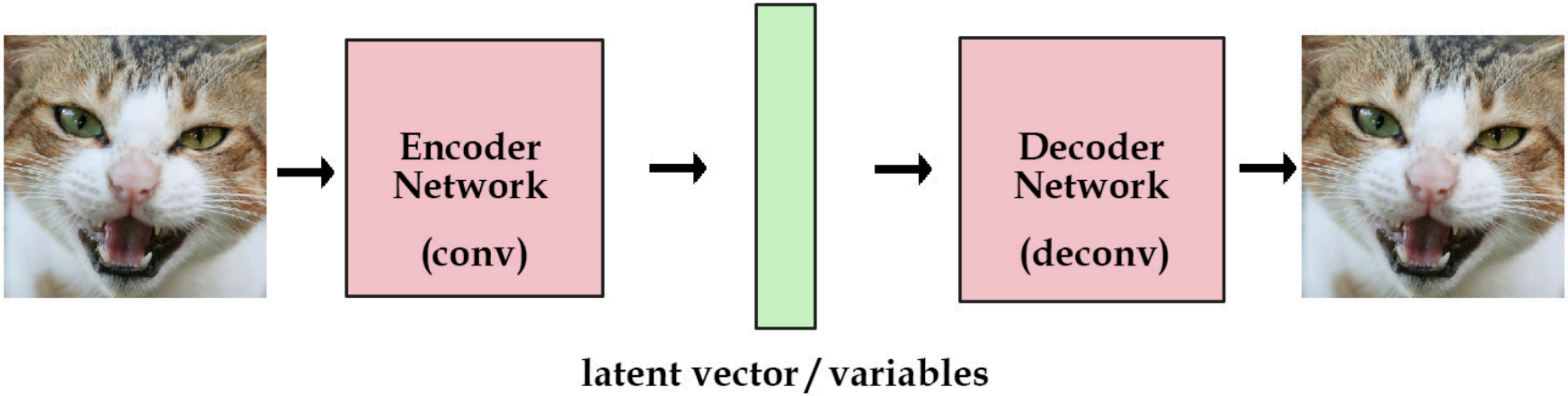
- For example, set inputs to all ones
- Train network to reduce MSE between its output and target image
- Then information related to image is captured in network parameters



[1] Reference: http://kvfrans.com/variational-autoencoders-explained/

Transformation from Multiple Vectors

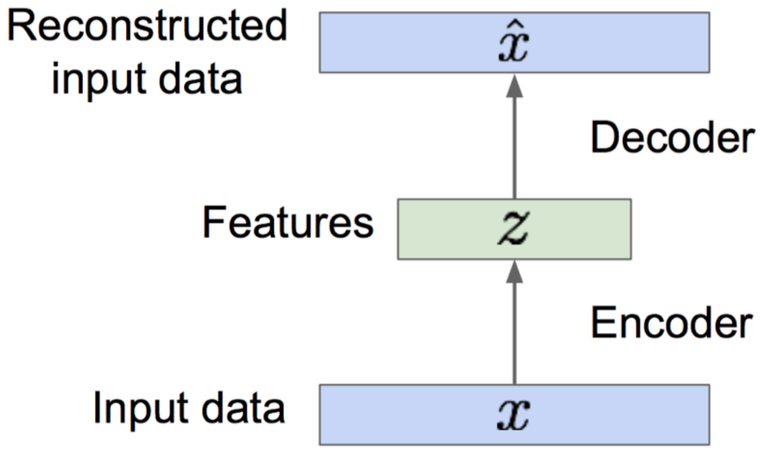
- Do the same with multiple input vectors (e.g., one hot encoded)
- These input vectors are called codes. The network is called a decoder.
- In an autoencoder, we also have an 'encoder' that takes original images and 'codes' them



[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Autoencoder: The Objective

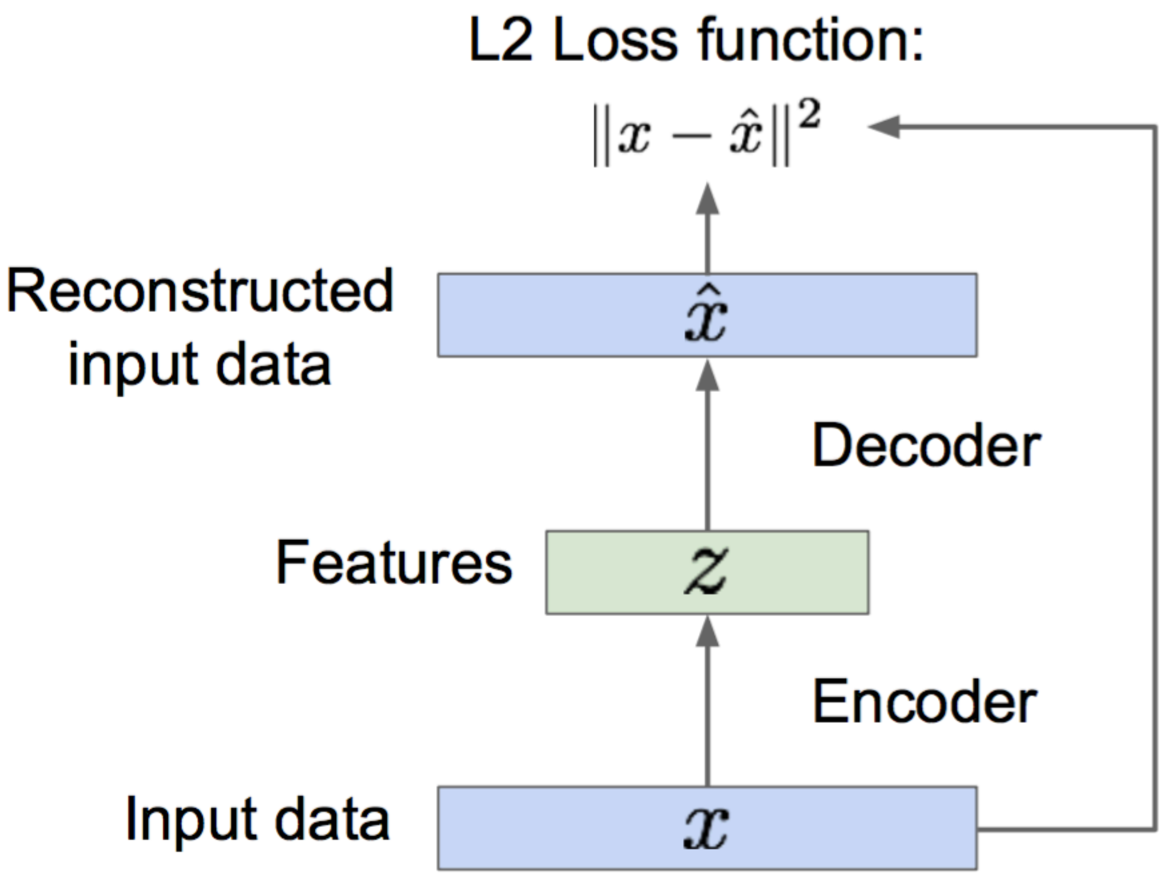
- Captures information in training data
- The latent variable z (also called code) can be thought of as embedding
- Keep the dimension of z smaller than input x, otherwise we have a trivial solution
  - If we choose a larger dimension, add noise to x during training (this is called a denoising autoencoder)



[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

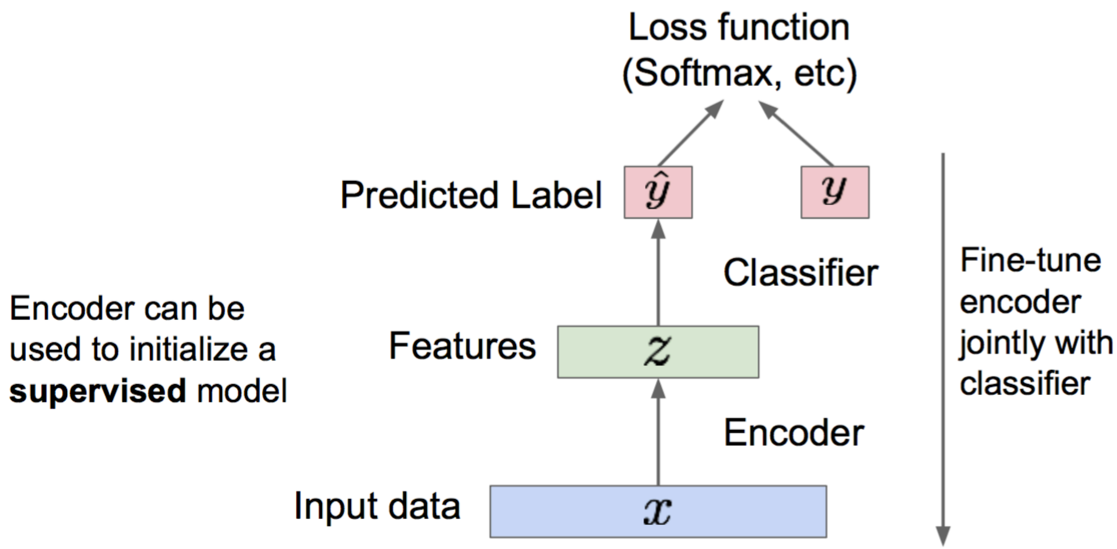
Autoencoder: The Architecture

- No labels are needed here



[1]Reference: CS231n (Stanford, Spring 2017)

Autoencoder: Uses



- Reduction in dimension achieved by the encoder is useful
  - Just like PCA
  - Captures meaningful variations in the data via the embeddings
- Named 'autoencoder' because it attempts to reconstructs original data
- Cannot generate new samples yet!

[1]Reference: CS231n (Spring 2017)

Variational Autoencoder

- Probabilistic extension of autoencoding
- The intuitive idea is to make z random, and in particular make P_z a Gaussian
  - If we can manage this, then we can sample from P_z and generate new images

- Two high level changes needed
  - Architecture
  - Loss function

[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Variational Autoencoder: Loss

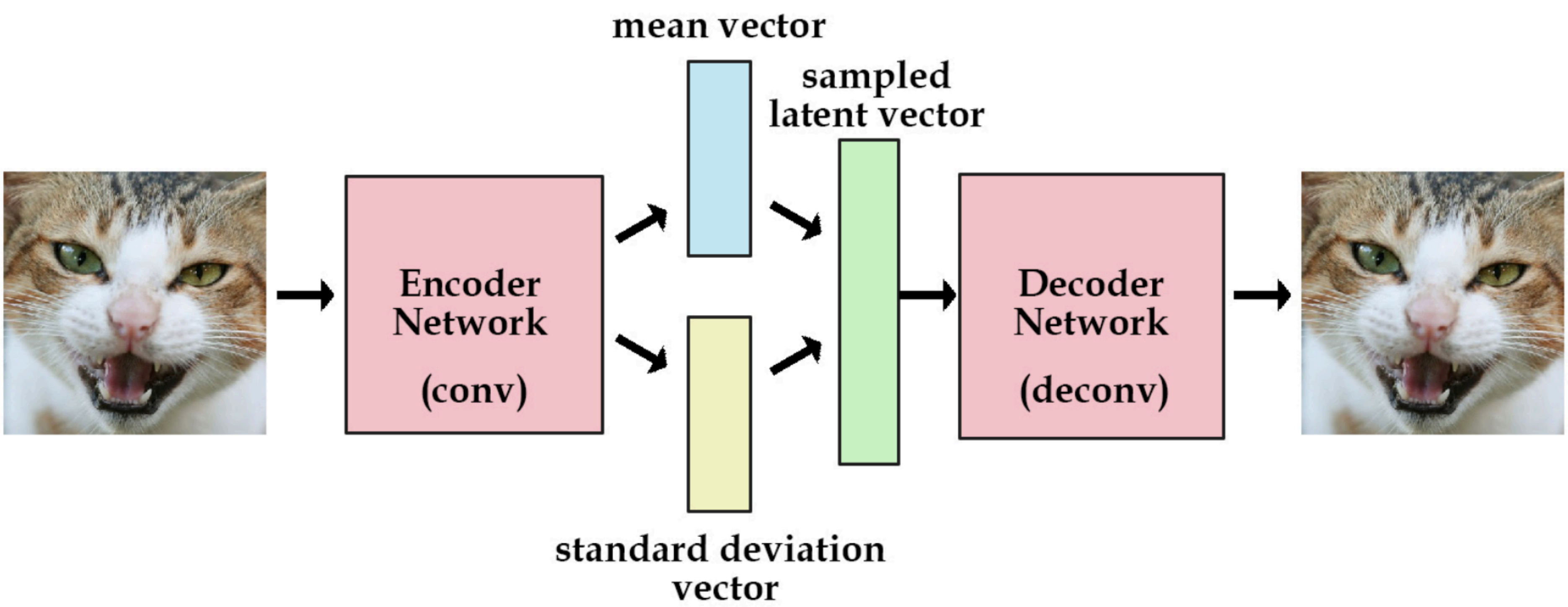
- Loss will be sum of two losses
  - Reconstruction loss
  - Latent loss (how far from Gaussian the distribution obtained from encoder is)
    - Measured using KL divergence
    - Encoder generates the mean and covariance of the Gaussian

- We will look at the math behind this shortly

[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Variational Autoencoder: Architecture

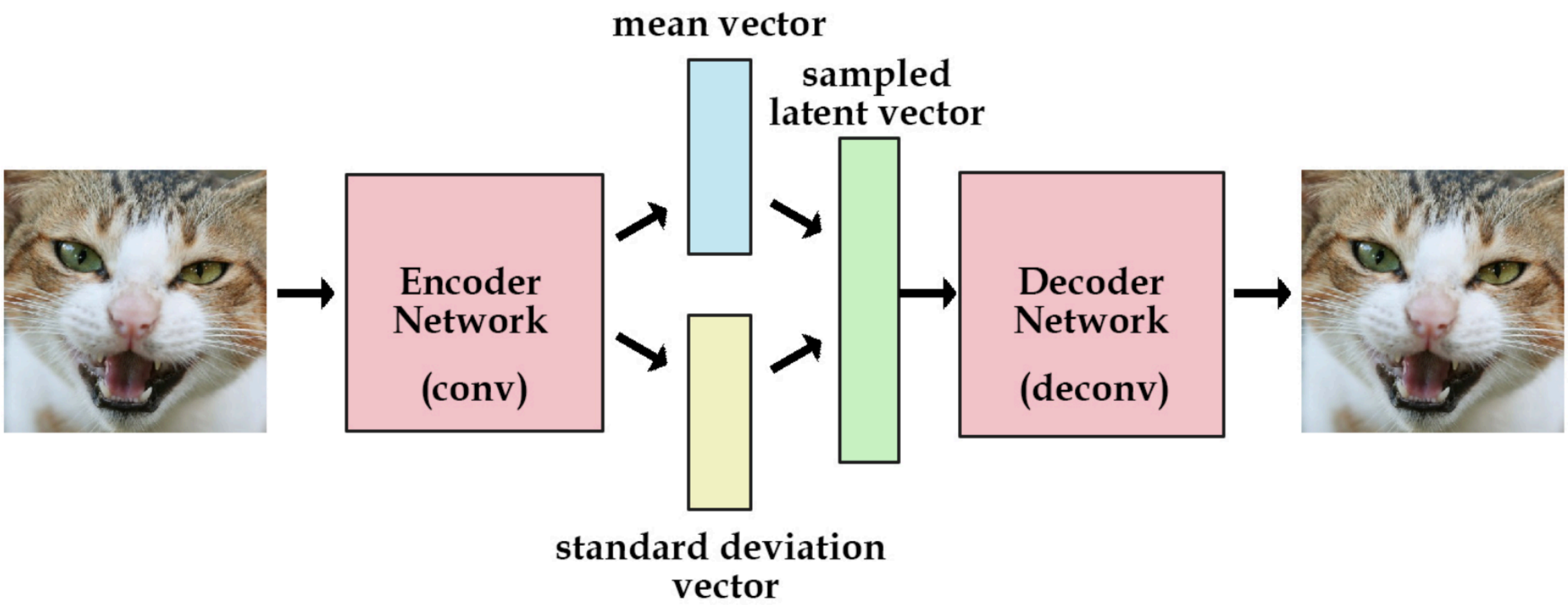
- Architecture involves a sampling in between



[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Variational Autoencoder: Architecture

- Architecture involves a sampling in between
- Can still backprop given realized sample



[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

Variational Autoencoder: Generalization

- This sampling allows for generalization
  - Gaussian noise ensures we are not remembering only the training data
- Once we have trained, we can sample from a Gaussian and pass it through the decoder to get a new image

[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

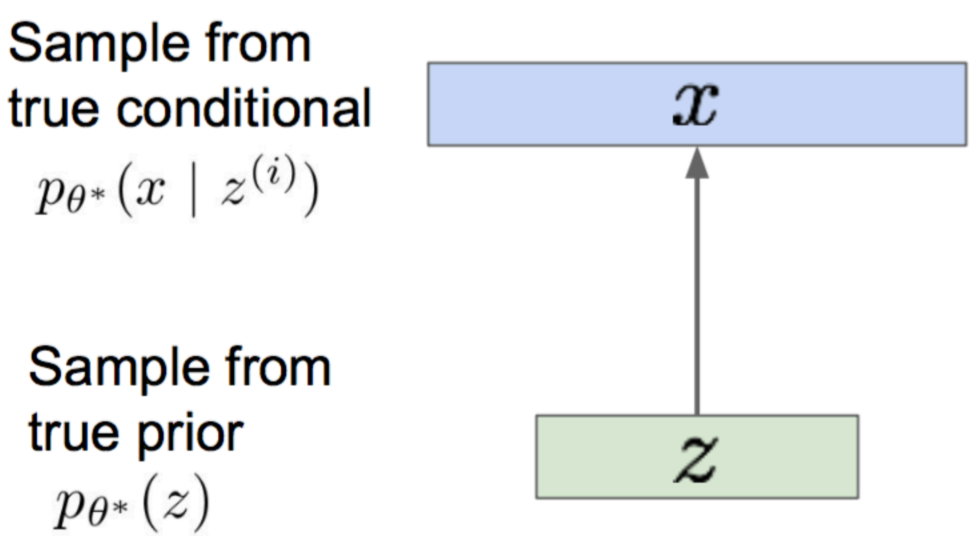
Variational Autoencoder: Samples

- Experiments on MNIST
  - Samples generated during training (left, center) and original data

[1]Reference: http://kvfrans.com/variational-autoencoders-explained/

VAE: Derivation

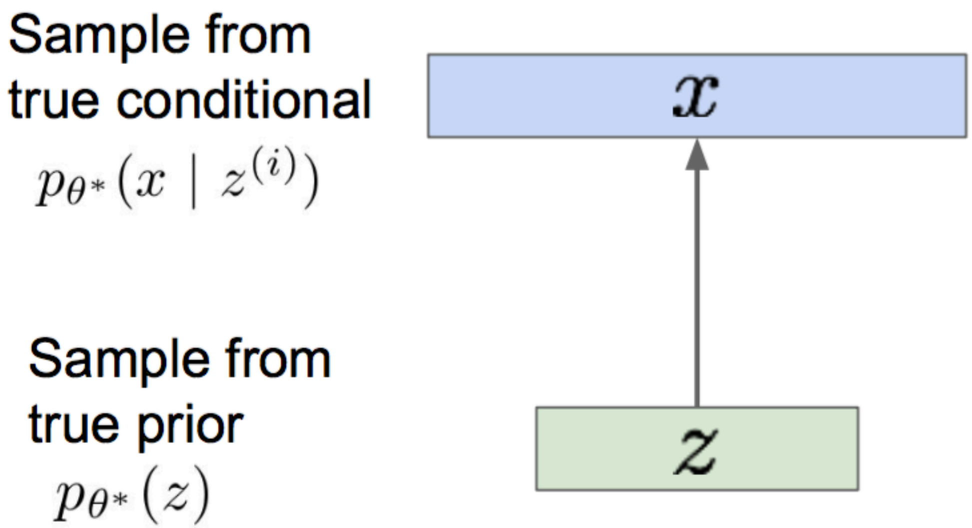
- Assume a model as below
- Variable x represents image, z represents the latent variable
- We want to estimate θ^*



[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

- Let P_z be Gaussian
- Let $P(x|z)$ be a neural network: decoder
- We can train by maximizing likelihood of training data $p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$



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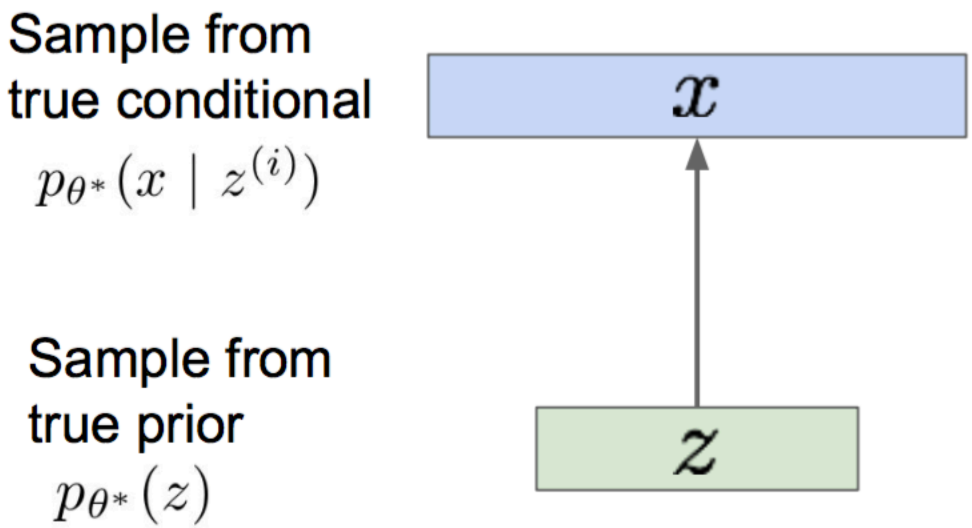
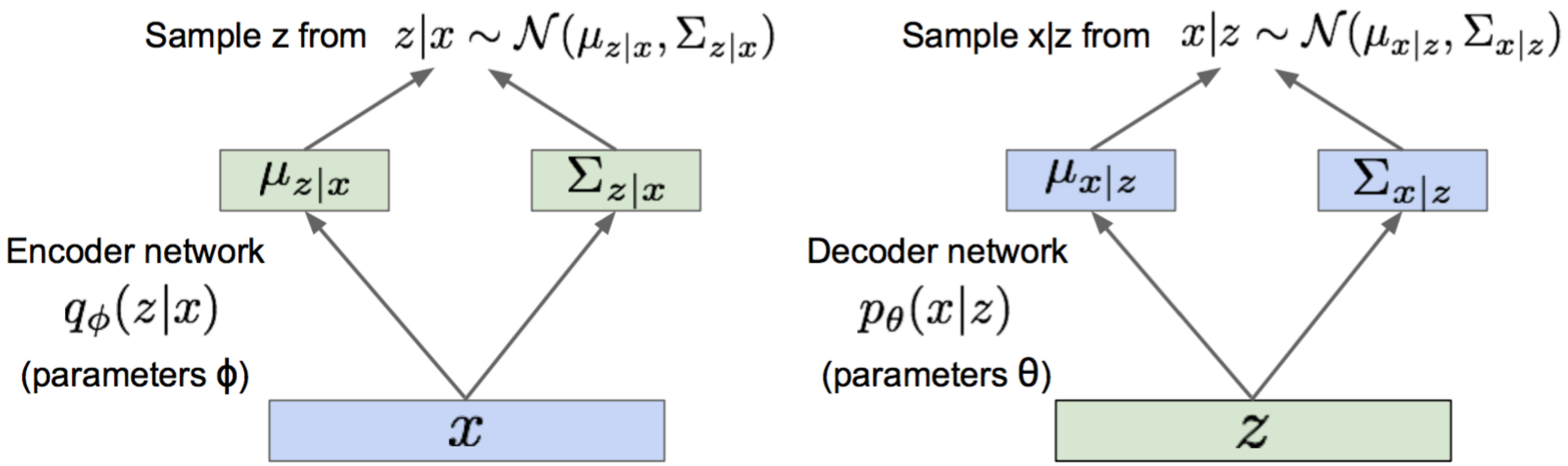


[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

- We will also make the encoder probabilistic



[1]Reference: CS321n (Stanford, Spring 2017)

Aside: Notion of Information

- Information: $-\log P(x)$
- Entropy: $-\sum P(x) \log P(x)$
- KL divergence:
  - A notion of dissimilarity between two distributions
  - $D_{KL}(p||q) = \sum P(x) \log \frac{P(x)}{Q(x)}$

[1] Reference: Ian Goodfellow (NIPS 2016 Tutorial)

VAE: Derivation

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

[1]Reference: CS321n (Stanford, Spring 2017)

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

[1]Reference: CS321n (Stanford, Spring 2017)

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

[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

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

[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

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

[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

- The first two terms constitute a lower bound for the data likelihood that we can maximize tractably

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

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

Variational lower bound ("ELBO")

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

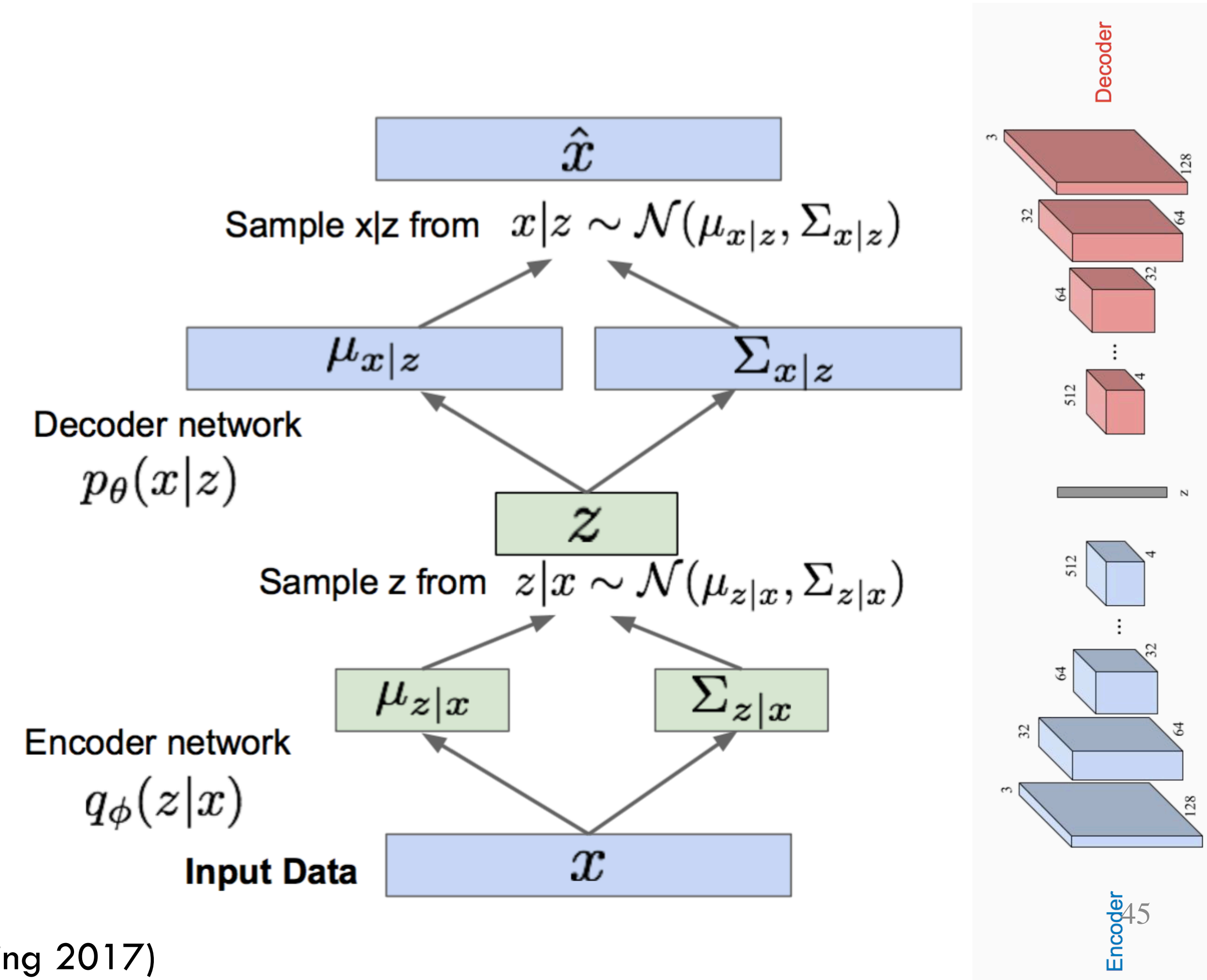
Training: Maximize lower bound

- The first term of $\mathcal{L}$ is essentially reconstruction error
- The second term of $\mathcal{L}$ is making the encoder network close to Gaussian prior

[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Derivation

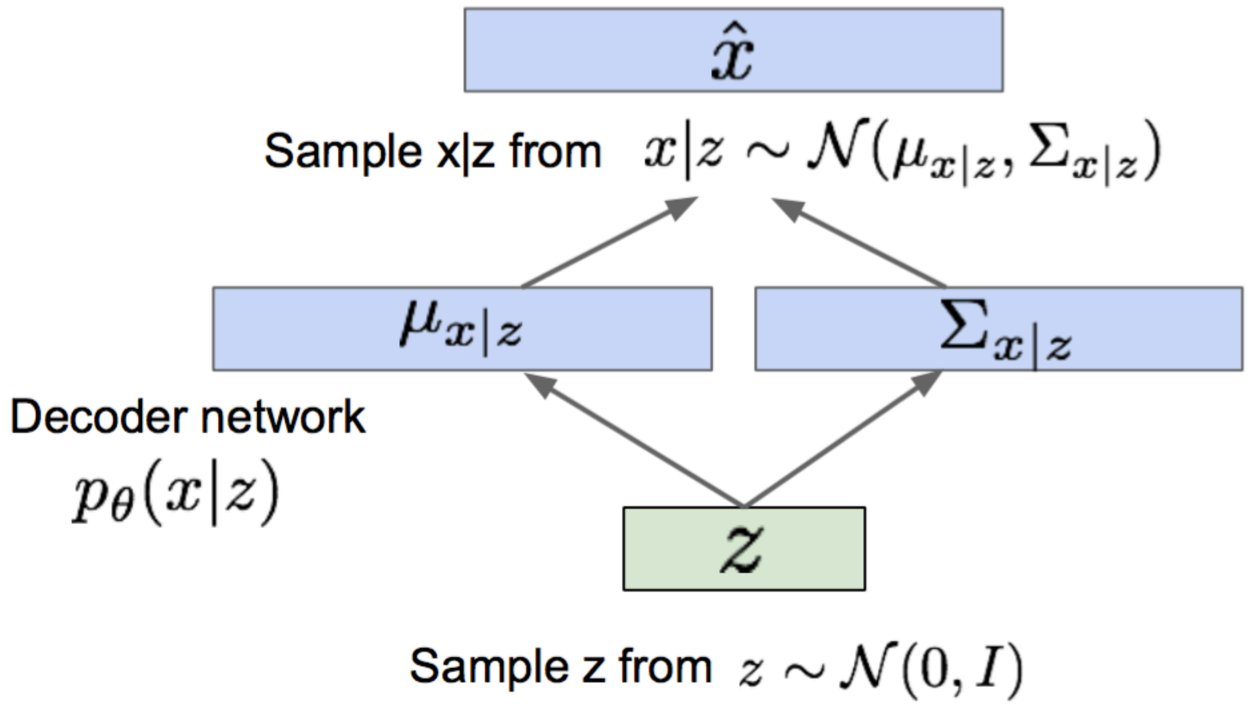
- In summary,



[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Samples

- We can create new samples!

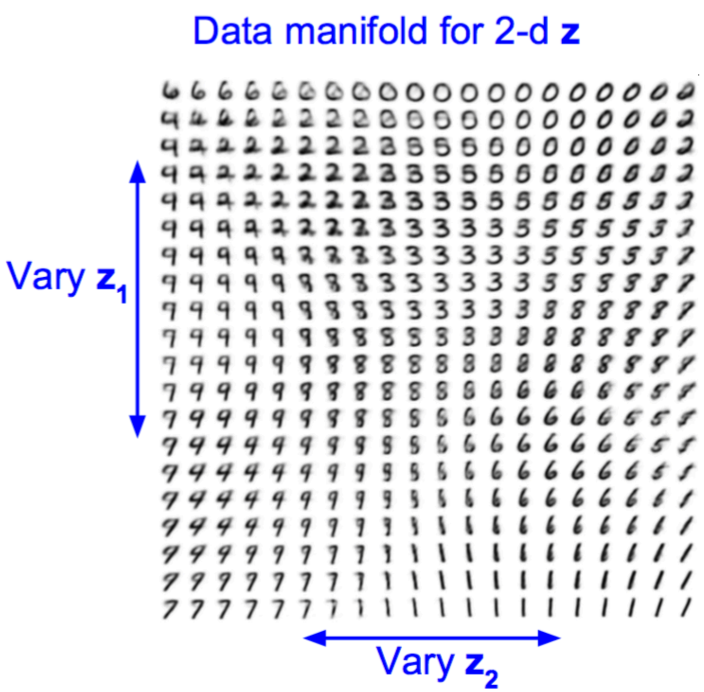


Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

[1]Reference: CS321n (Stanford, Spring 2017)

VAE: Experiments

- Some generated samples




32x32 CIFAR-10


Labeled Faces in the Wild

Further reading: https://arxiv.org/pdf/1606.05908.pdf

[1]Reference: CS321n (Stanford, Spring 2017)

Questions?

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- Generative Adversarial Networks (GAN)

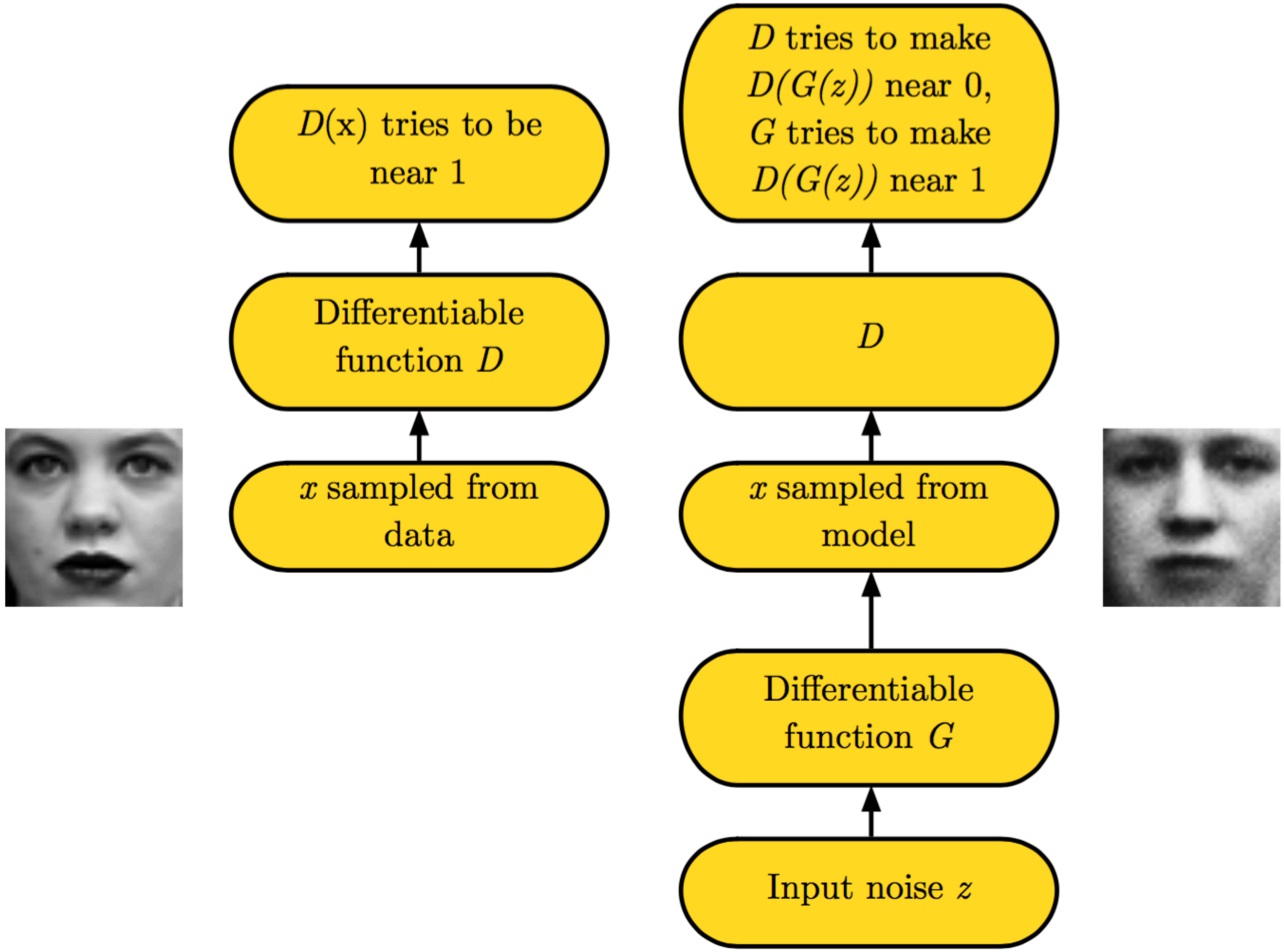
Generative Adversarial Networks

GANs: Two Scenarios

- Overall Idea: Instead of working with an explicit density function, GANs take an 'adversarial' or 'game-theoretic' approach

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

GANs: Two Scenarios

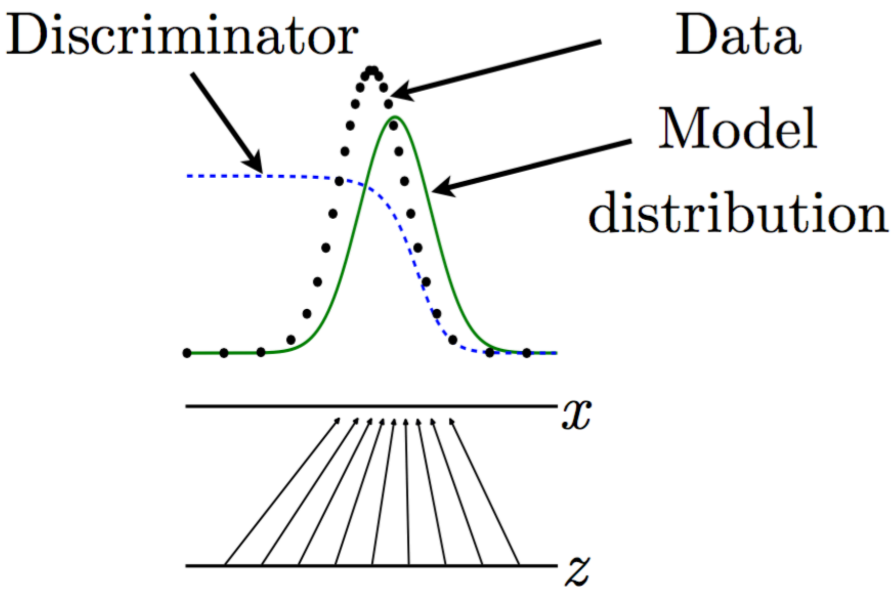


[1] Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Generator and the Discriminator

- Assume $X = G_{\theta_g}(z)$
- Differentiable

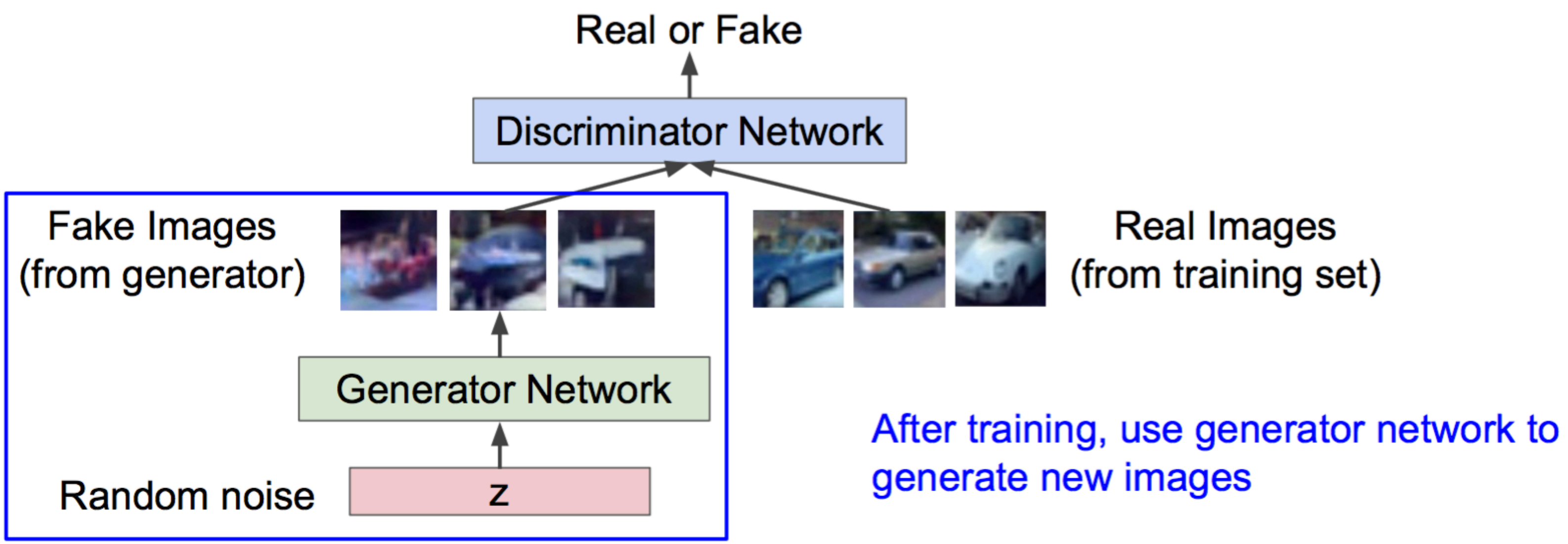
- $D_{\theta_d}(X)$ takes values in $\{0,1\}$



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

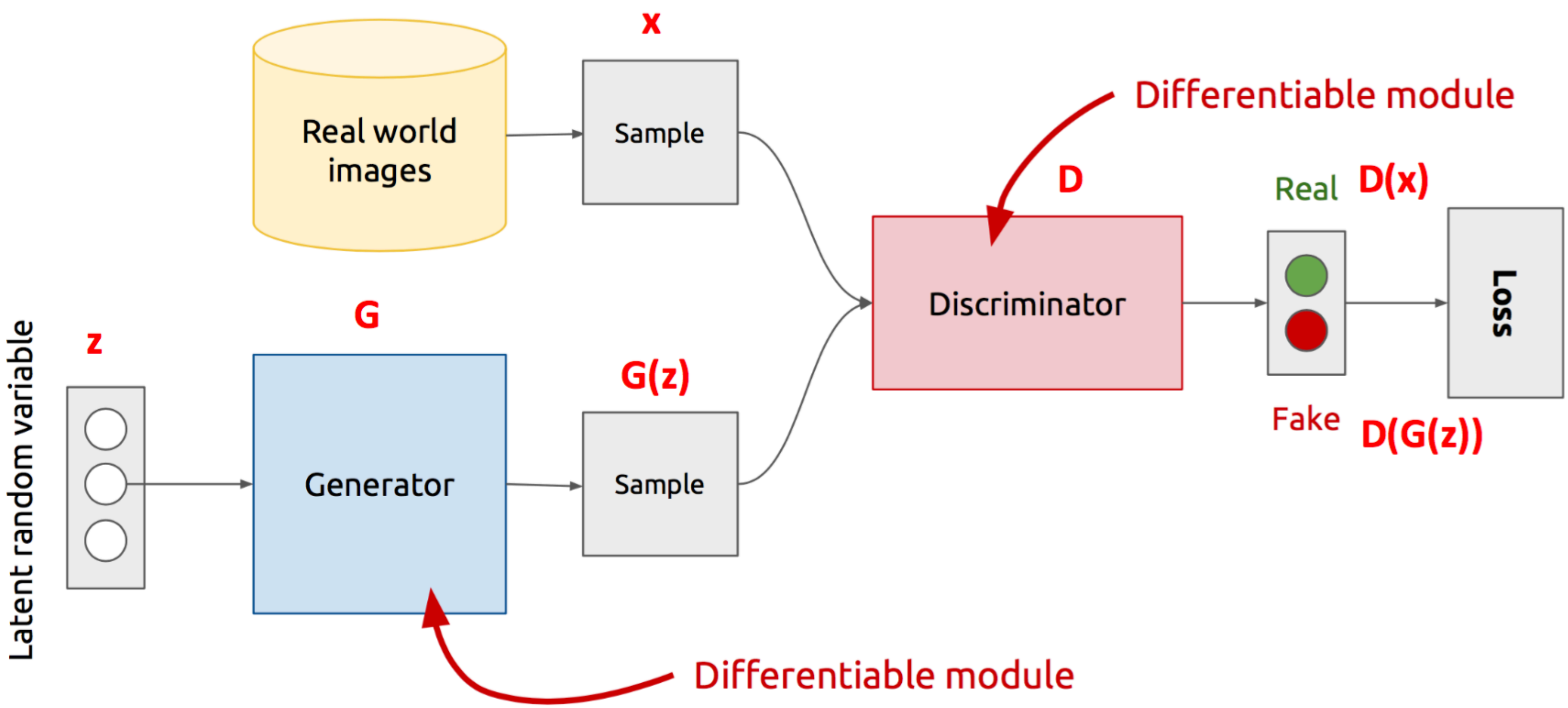
The Generator and the Discriminator

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



[1]Reference: CS231n (Stanford, Spring 2017)

The Generator and the Discriminator



[1]Reference: https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

The Objectives

- The generator and the discriminator are playing a minimax game.

- $J(D) = -E_{P_d} \log D(x) - E_{P_m} \log(1 - D(x))$
  - Where $P_m(x)$ is the derived distribution using $G(z)$ and P_z
- $J(G) = -J(D)$

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Objectives

- The optimal strategy for the discriminator at equilibrium is
  - $D(x) = \frac{P_d(x)}{P_d(x)+P_m(x)}$

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Objectives

- The optimal strategy for the discriminator at equilibrium is
  - $D(x) = \frac{P_d(x)}{P_d(x)+P_m(x)}$
- The optimal strategy for the generator is to find parameters such that
  - $P_d = P_m$

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Training Procedure

- Create a minibatch of real data
- Create a minibatch of generated data
- Score the discriminator
- Backprop to update the parameter θ_d
- Score the generator
- Backprop to update the parameter θ_g

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Training Procedure

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

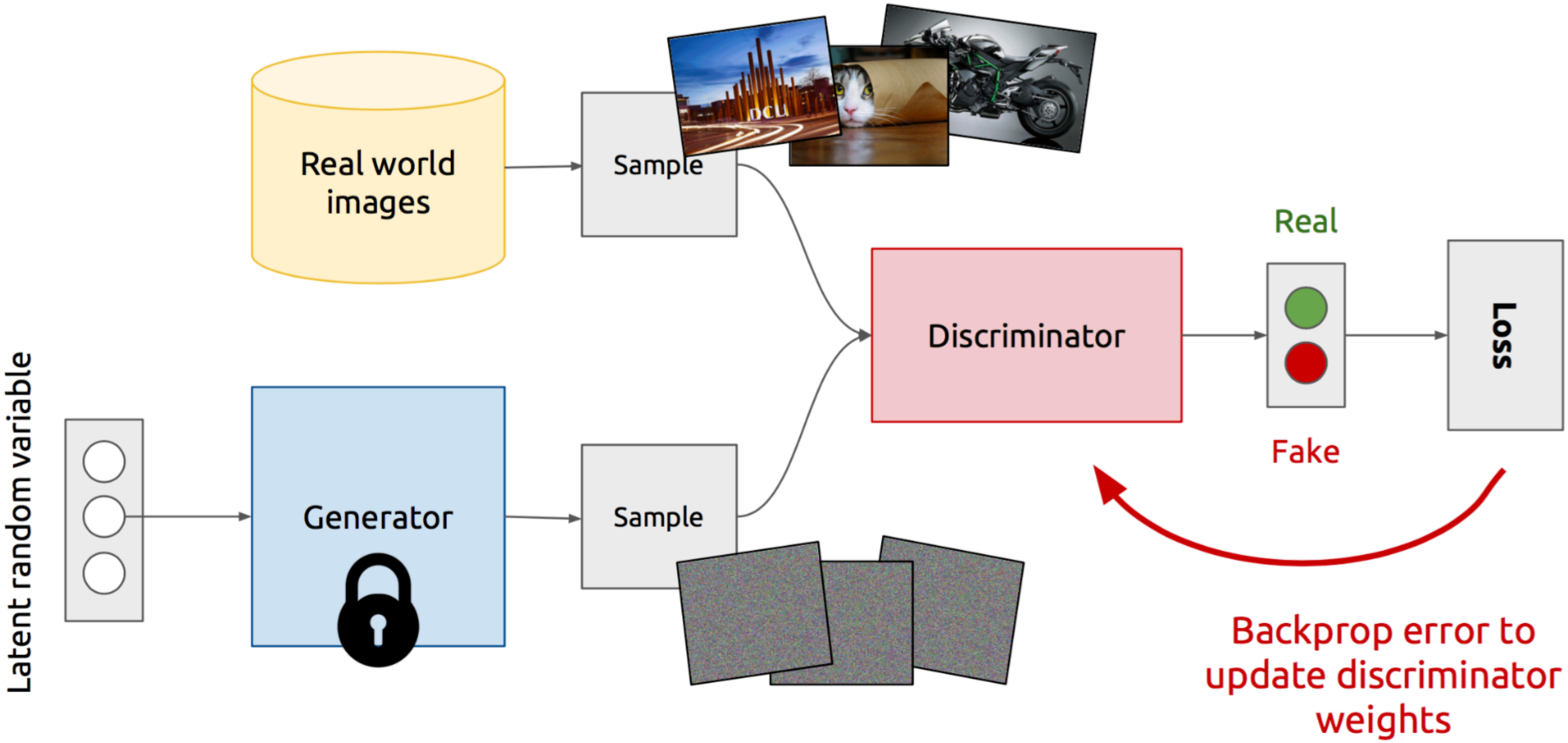
$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

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

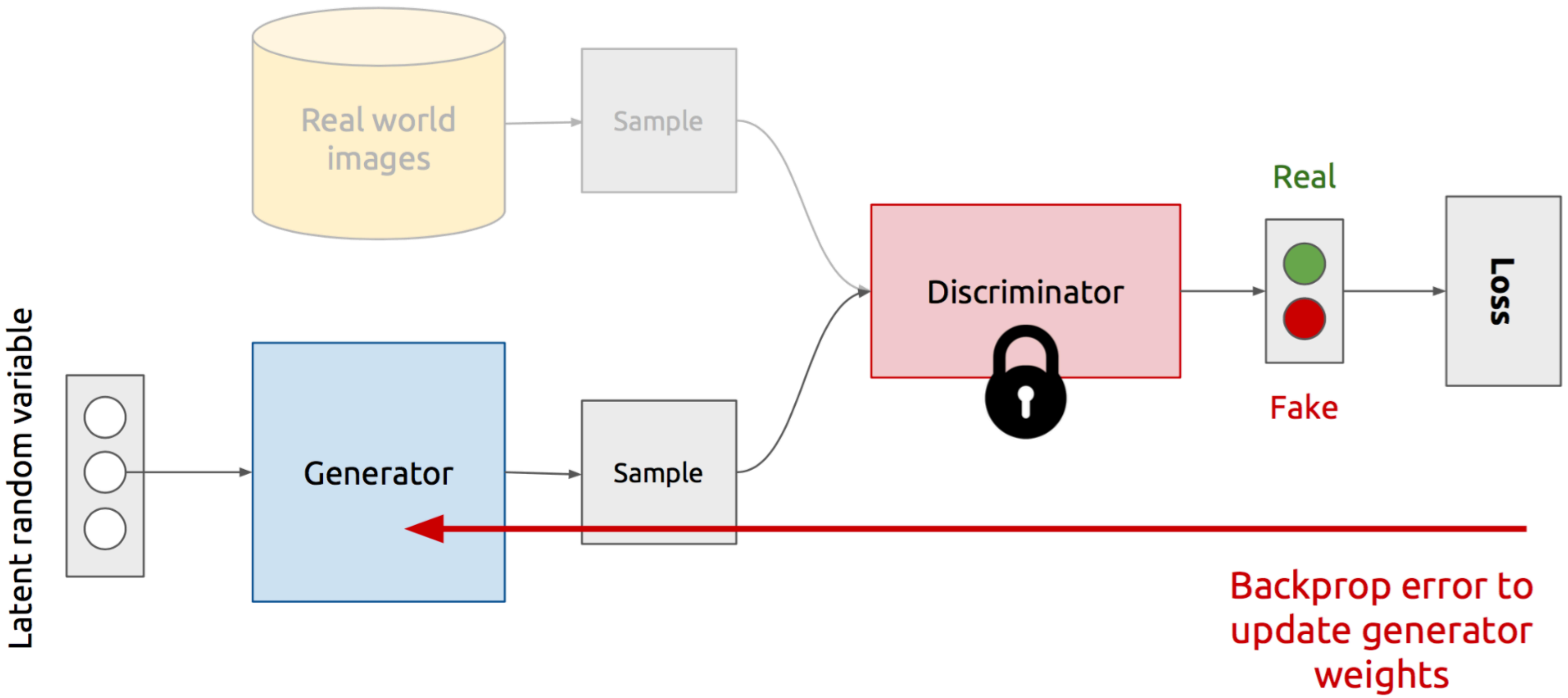
[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

The Training Procedure



[1]Reference: https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

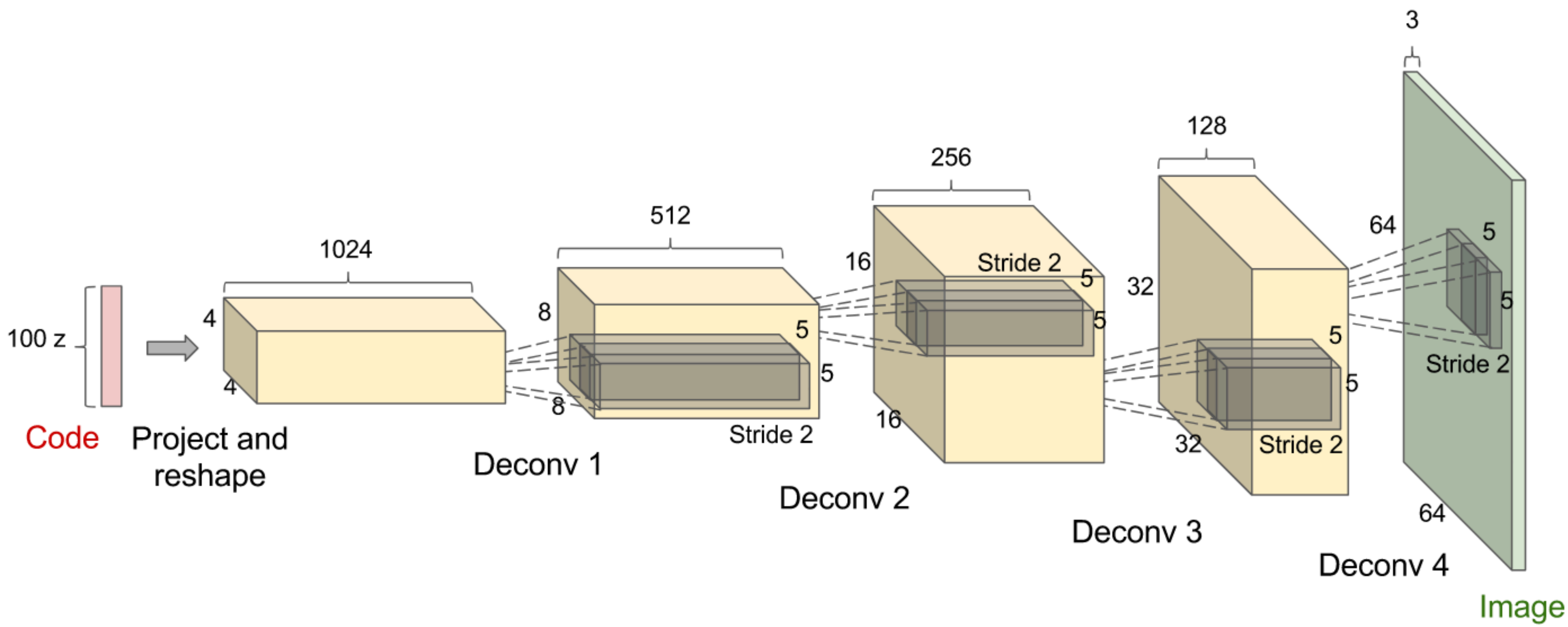
The Training Procedure



[1]Reference: https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

Example Generator Architecture

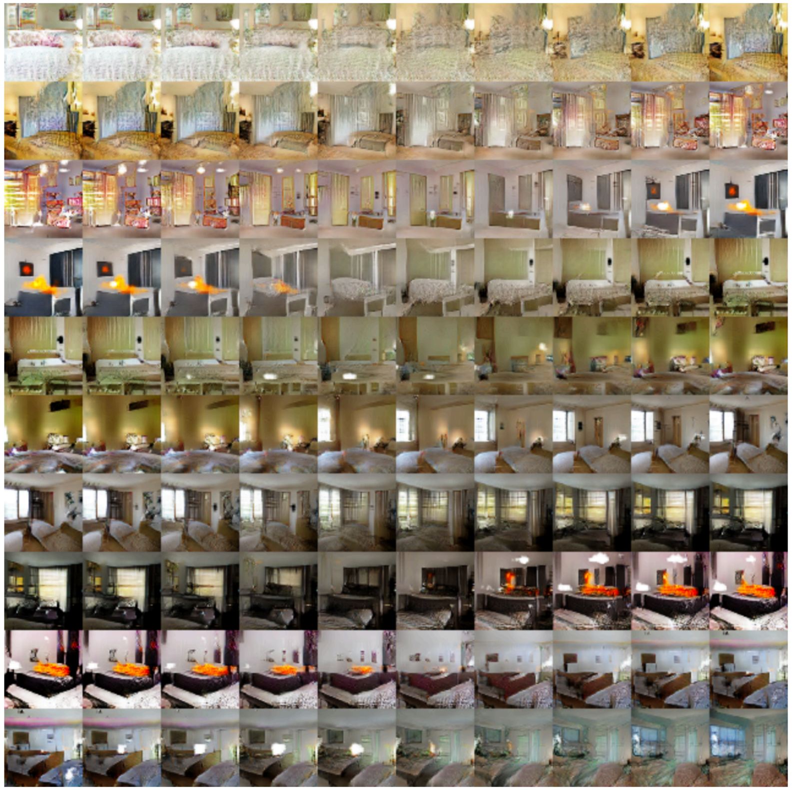
- DCGAN



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

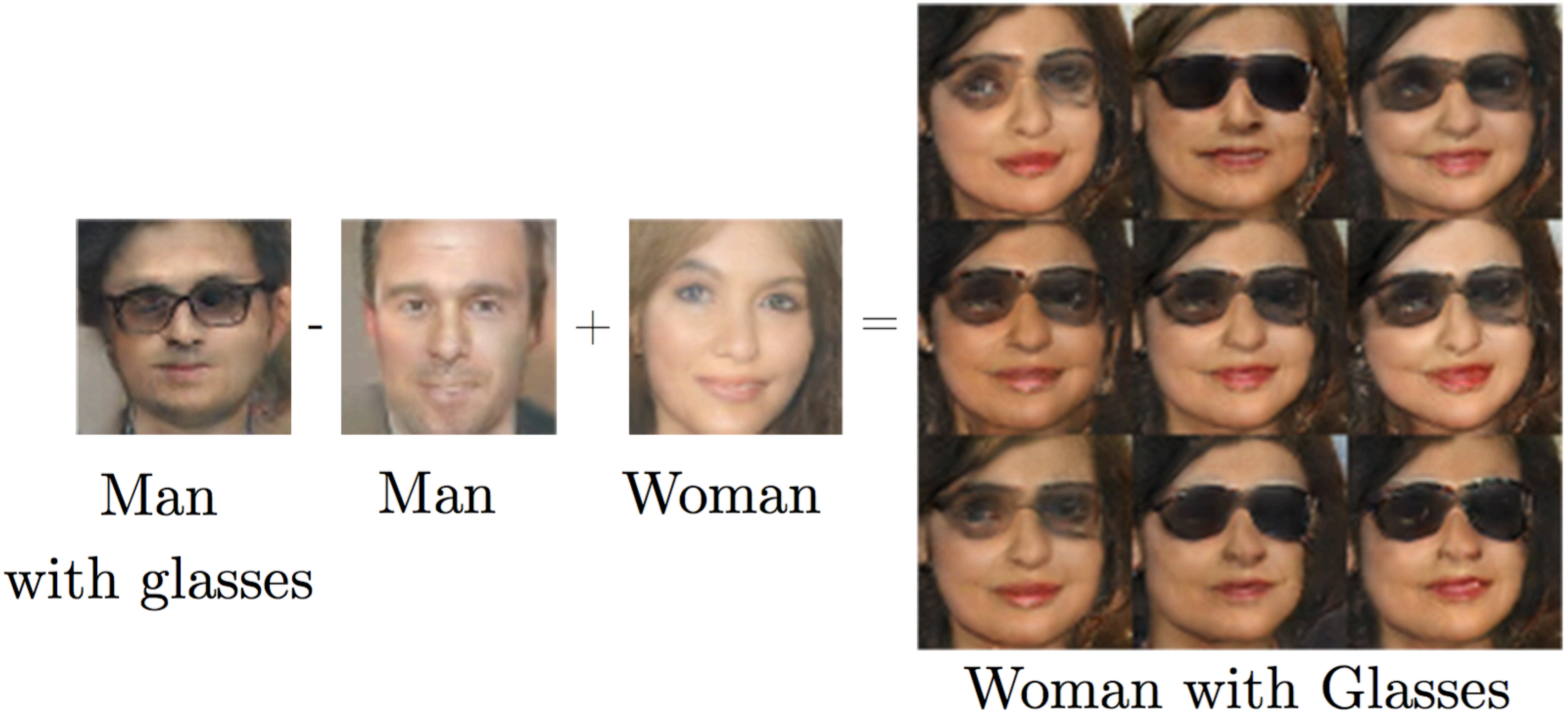
GAN Properties: Latent Space

- Consider Deep Convolutional Generative Adversarial Network (DCGAN)
  - You can walk from one point to another in the bedroom latent space (e.g., 6th and 10th rows)



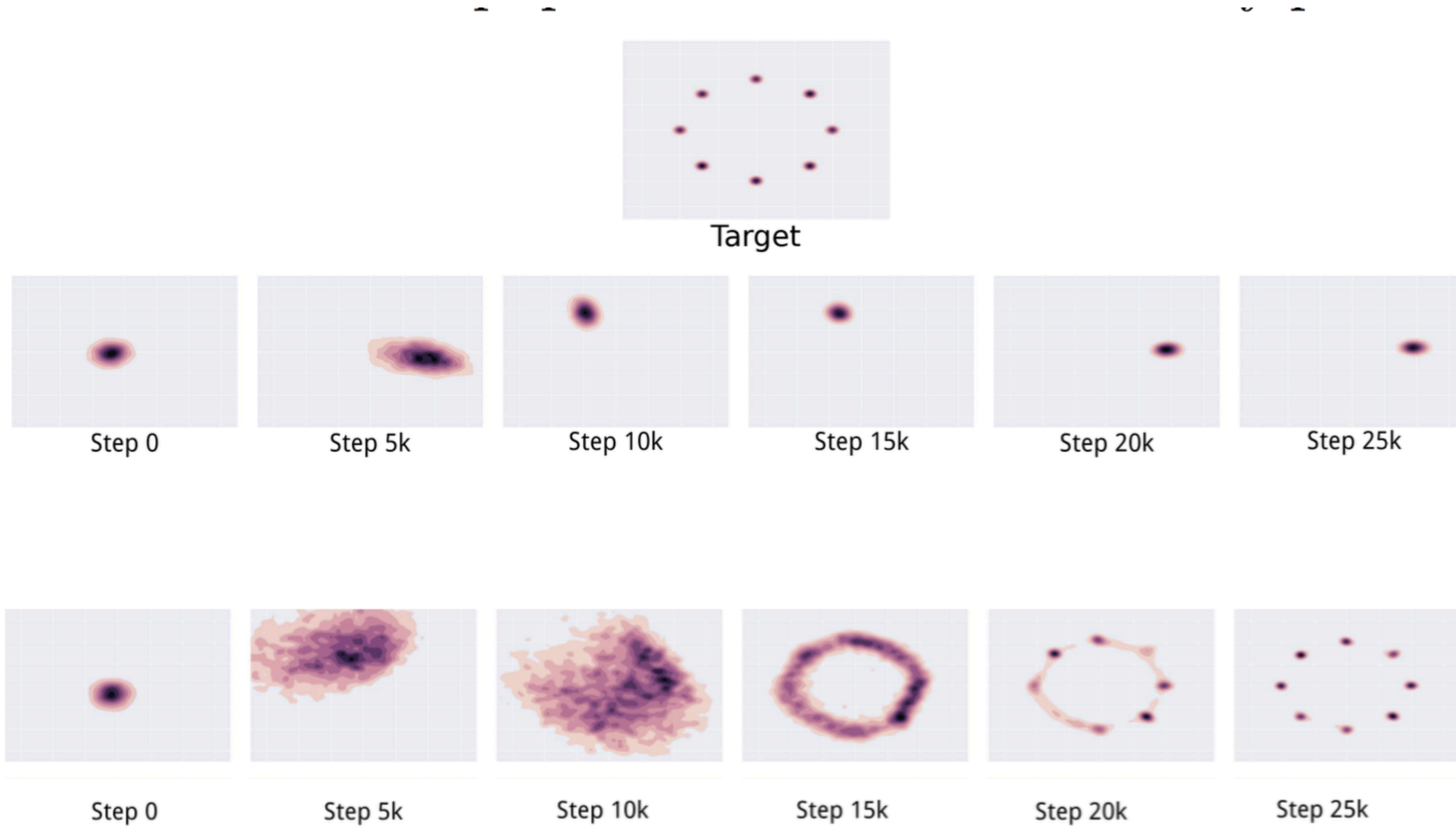
[1]References: http://arxiv.org/abs/1511.06434 and https://github.com/Newmu/dcgan_code

GAN Properties: Latent Space Arithmetic as a Byproduct



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

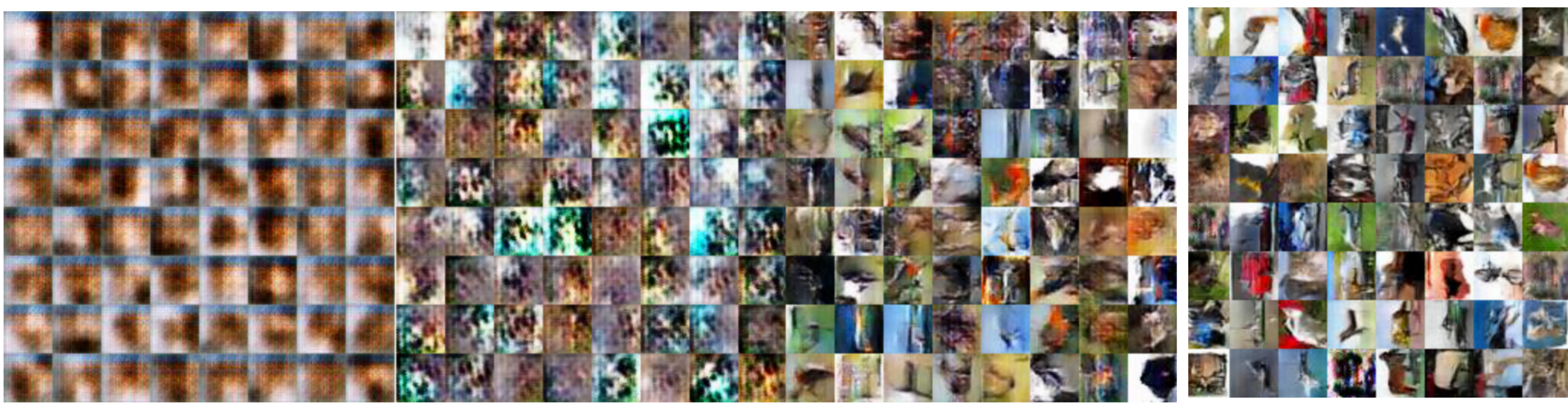
GAN Properties: Mode Collapse Issue



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

GAN: Experiments

- Experiments on CIFAR-10 (only generated images below)
  - Code: https://github.com/kvfrans/generative-adversial



[1]Reference: http://kvfrans.com/generative-adversial-networks-explained/

Questions?

VAE and GAN

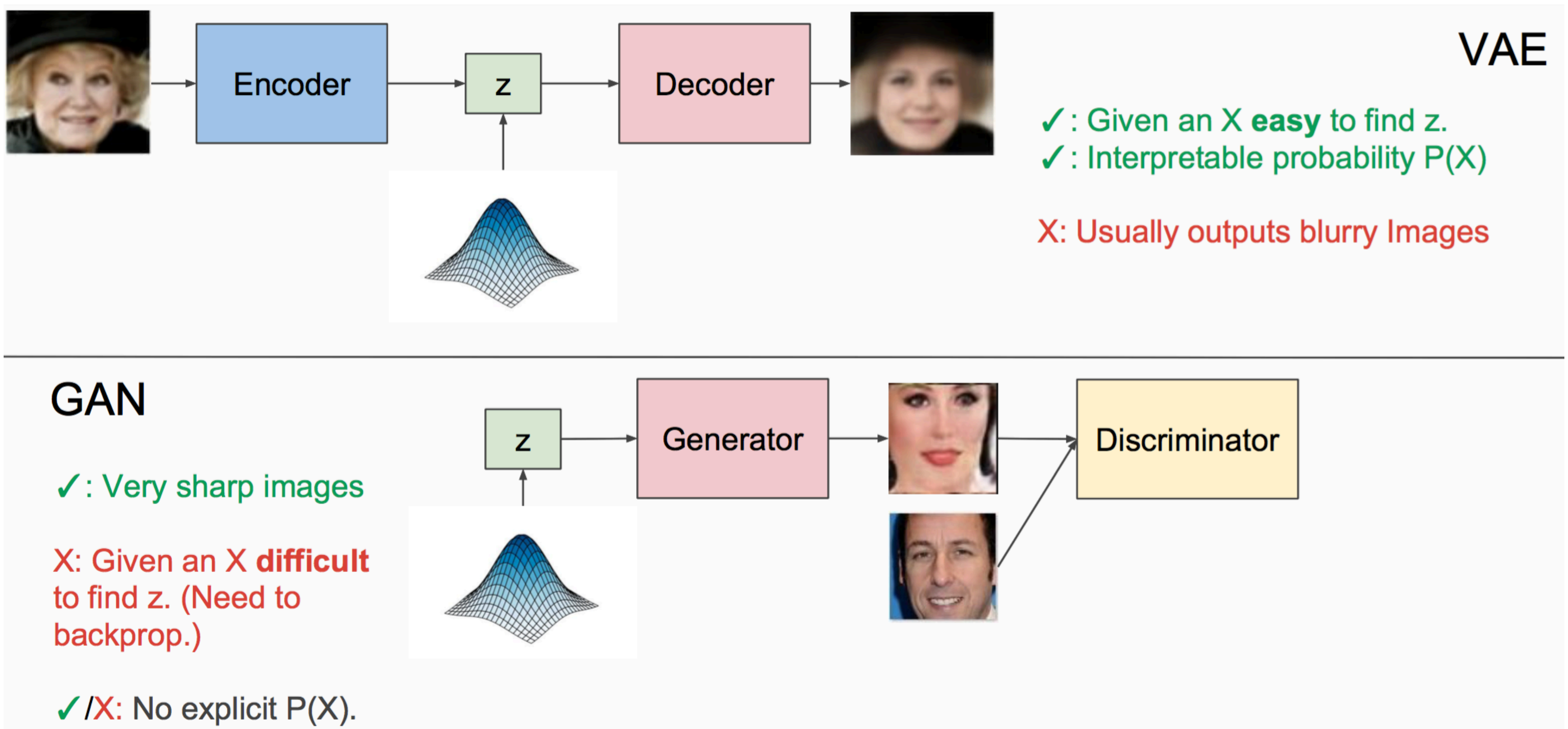
- VAEs
  - Are generative models that use regularized log likelihood to approximate performance score
  - Tend to achieve higher likelihoods of data, but the generated samples don't have real-world properties like sharpness
  - Can compare generated images with original images, which is not possible with GANs
  - Part of graphical models with principled theory

VAE and GAN

- GANs
  - Are generative models that use a supervised learning classifier to approximate performance score
    - No constraint that a 'bed' should look like a 'bed'
  - Try to solve an intractable game, vastly more difficult to train
  - Tend to have sharper image samples
  - Start with latent variables and transform them deterministically
  - There is no Markov chain style of sampling required
  - They are asymptotically consistent (will converge to P_d), whereas VAEs are not
  - Many many variations have been proposed in the past 3 years (>150!)

[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

VAE and GAN


Encoder
z
Decoder
VAE
✓: Given an X **easy** to find z.
✓: Interpretable probability P(X)
X: Usually outputs blurry Images
GAN
z
Generator
Discriminator
✓: Very sharp images
X: Given an X **difficult** to find z. (Need to backprop.)
✓/X: No explicit P(X).

Summary

- Both models are recent (VAEs from 2013, GANs from 2014) and have initiated very exciting new directions in machine learning and AI
- Useful in many applications such as
  - Image denoising
  - Image Super-resolution
  - Reinforcement learning
  - Generating embeddings
  - Artistic help

- Eventually help the computer understand the world better

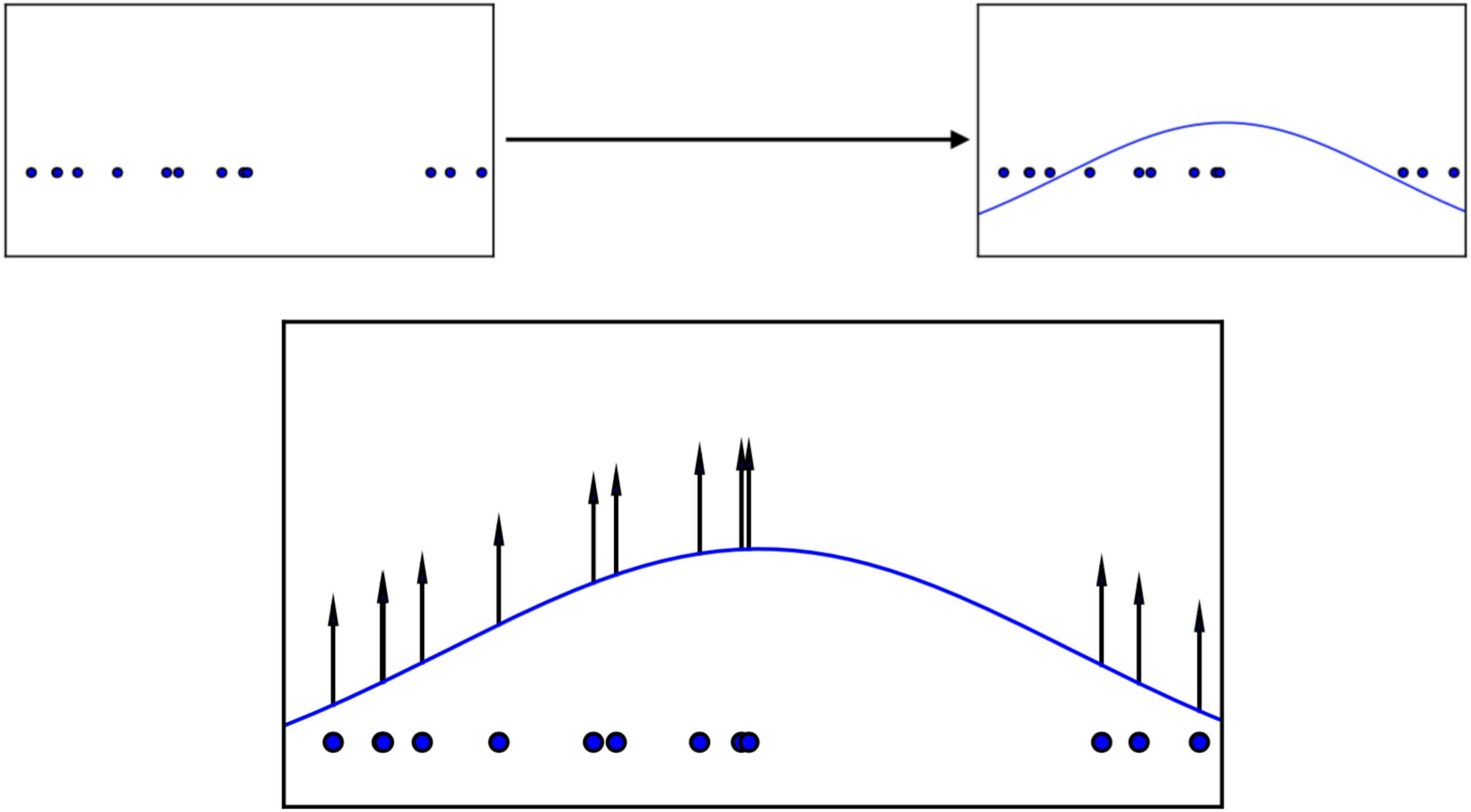
[1]Reference: https://blog.openai.com/generative-models/

Appendix

Sample Exam Questions

- What are the uses of generative models?
- What is the difference between a regular autoencoder and a variational autoencoder?
- What is the qualitative objective of the discriminator in a GAN? What is the qualitative objective of the generator?
- Describe some differences between a VAE model and a GAN.

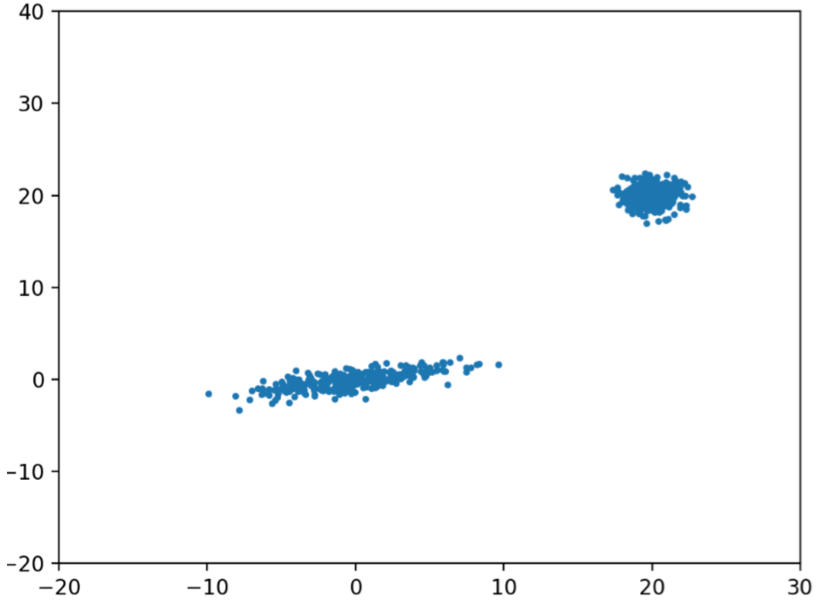
Maximum Likelihood Estimation I



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)

Maximum Likelihood Estimation II

Step 1: observe a set of samples



Step 2: assume a GMM model

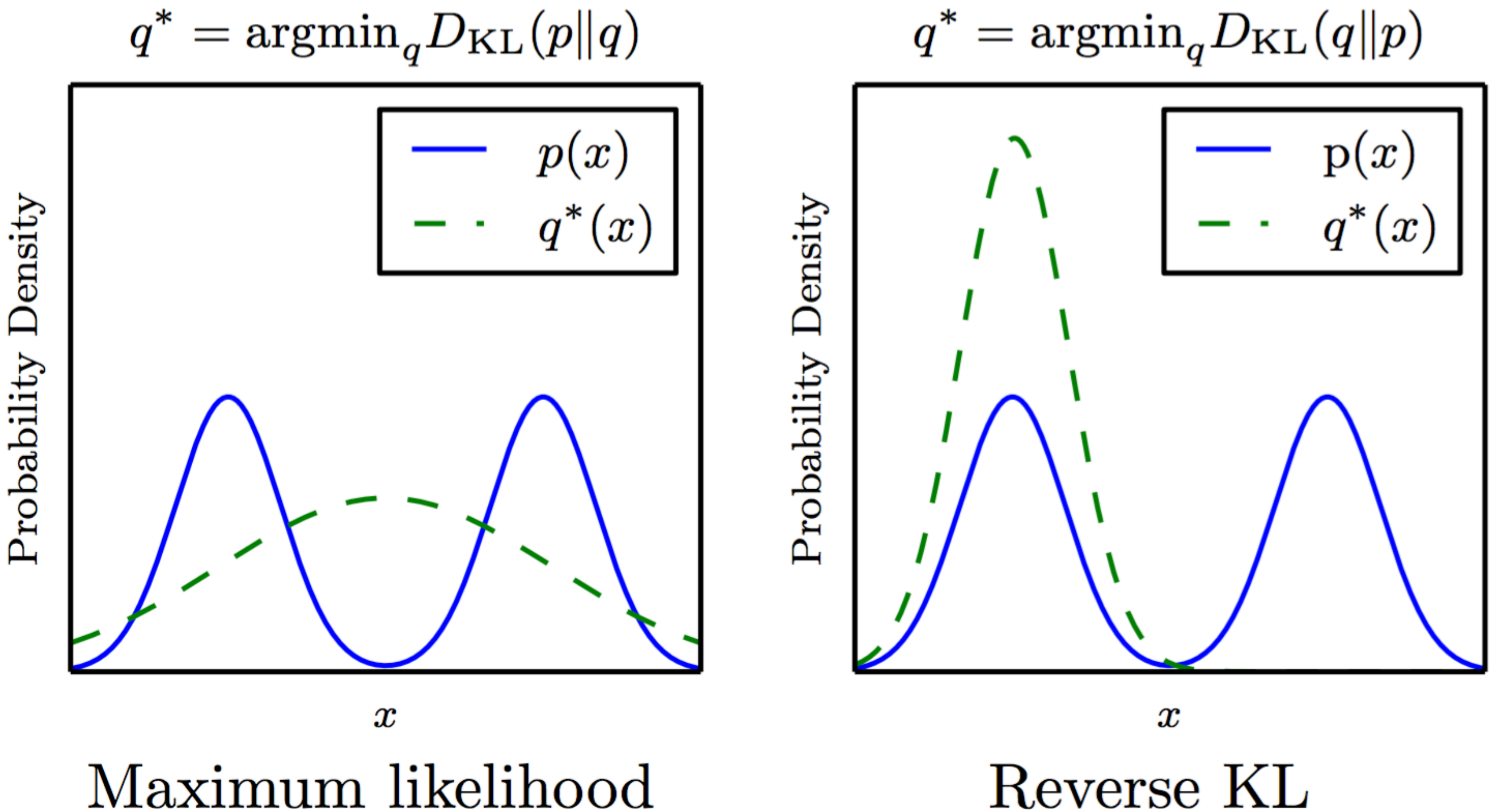
$$p(x|\theta) = \sum_i \pi_i \mathcal{N}(x|\mu_i, \Sigma_i)$$

Step 3: perform maximum likelihood learning

$$\max_\theta \sum_{x^{(j)} \in \text{Dataset}} \log p(\theta|x^{(j)})$$

[1]Reference: ICCV 2017 GAN Tutorial, Ming-Yu et al.

KL Divergence



[1]Reference: Ian Goodfellow (NIPS 2016 Tutorial)