Topics:

- Variational Autoencoders

# CS 4803-DL / 7643-A
# ZSOLT KIRA

- **Projects!**
  - Due May 3rd (May 5th with grace period)
  - Cannot extend due to grade deadlines!

- CIOS
  - Please make sure to fill out! Let us know about things you liked and didn’t like in comments so that we can keep or improve!

4803DL

7643A

# Introduction

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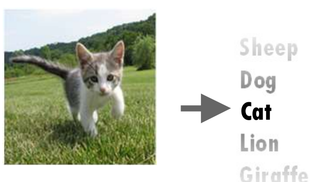
# Spectrum of Low-Labeled Learning

## Supervised Learning

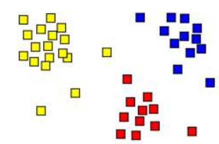
- Train Input: $\{X, Y\}$
- Learning output: $f : X \rightarrow Y$, $P(y|x)$
- e.g. classification

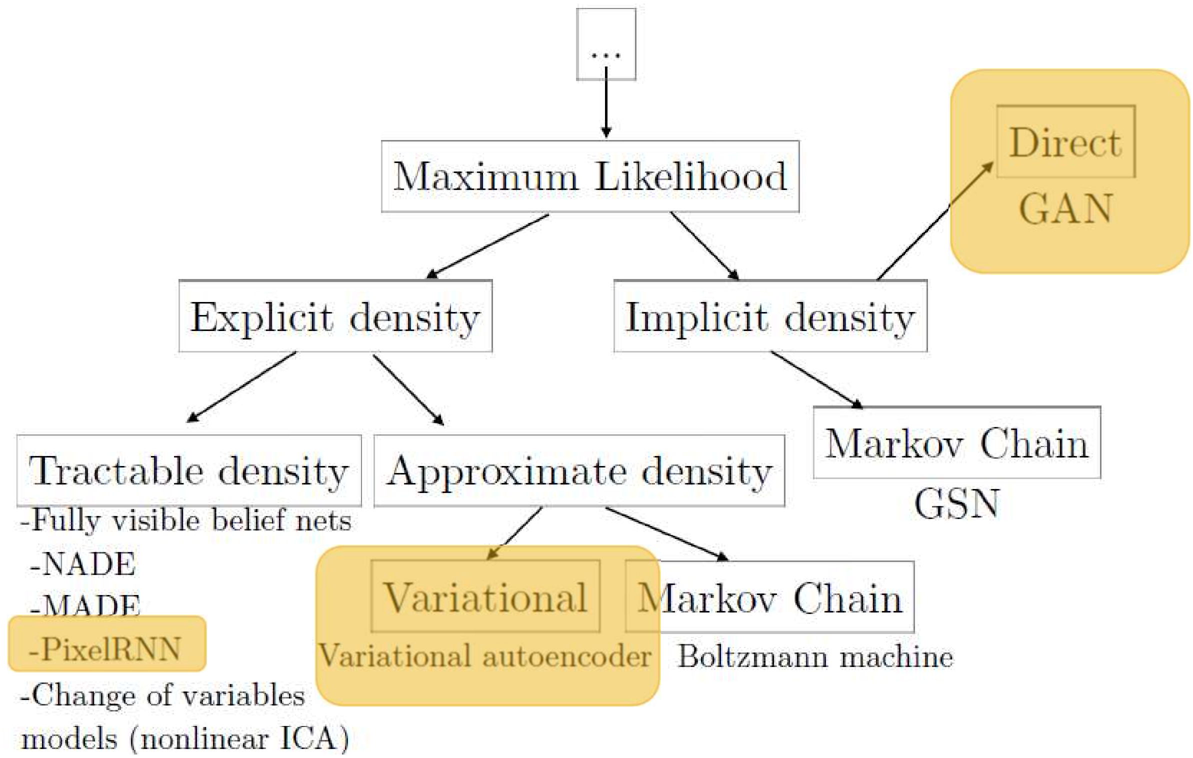



**Less Labels** →

## Unsupervised Learning

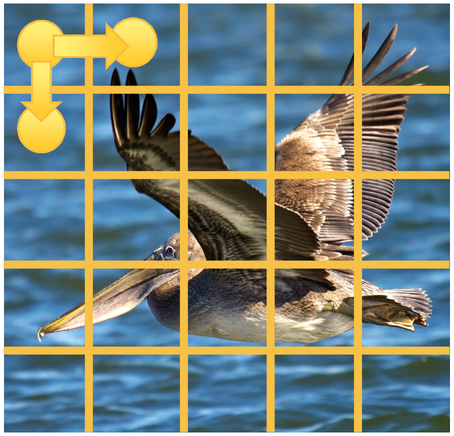
- Input: $\{X\}$
- Learning output: $P(x)$
- Example: Clustering, density estimation, etc.

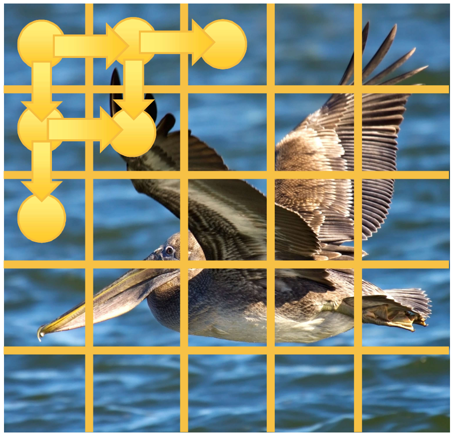





*Goodfellow, NeurIPS 2016 Tutorial: Generative Adversarial Networks*

## Generative Models





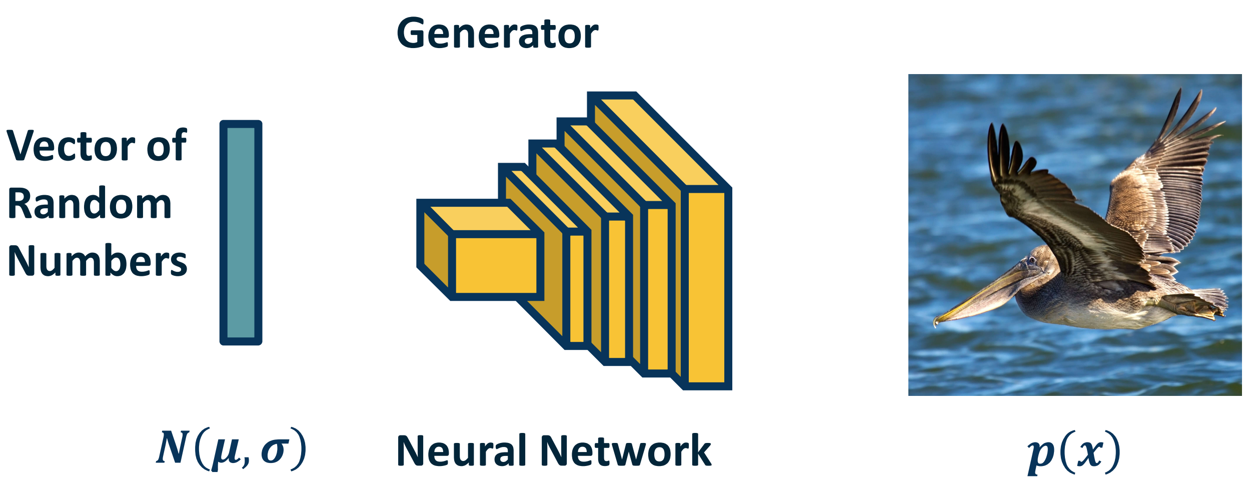
$$p(x) = p(x_1)p(x_2|x_1)p(x_3|x_1)\prod_{i=1}^{n^2} p(x_i|x_1, \ldots, x_{i-1})$$

- Training:
  - We can train similar to language models: Teacher/student forcing
  - Maximum likelihood approach
- Downsides:
  - Slow sequential generation process
  - Only considers few context pixels

*Oord et al., Pixel Recurrent Neural Networks*

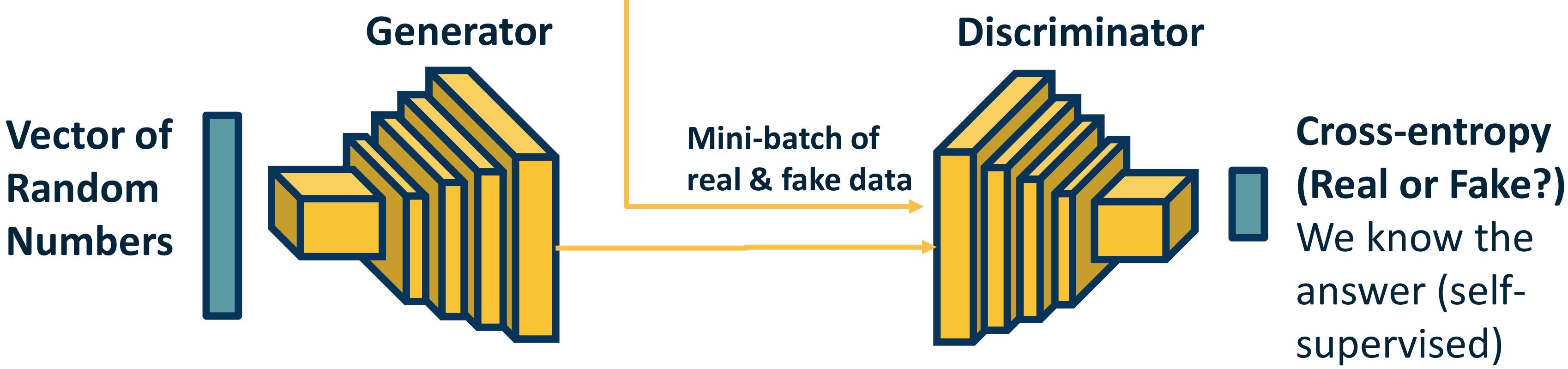
# Factorized Models for Images

- Input can be a vector with (independent) Gaussian random numbers
- We can use a CNN to generate images!

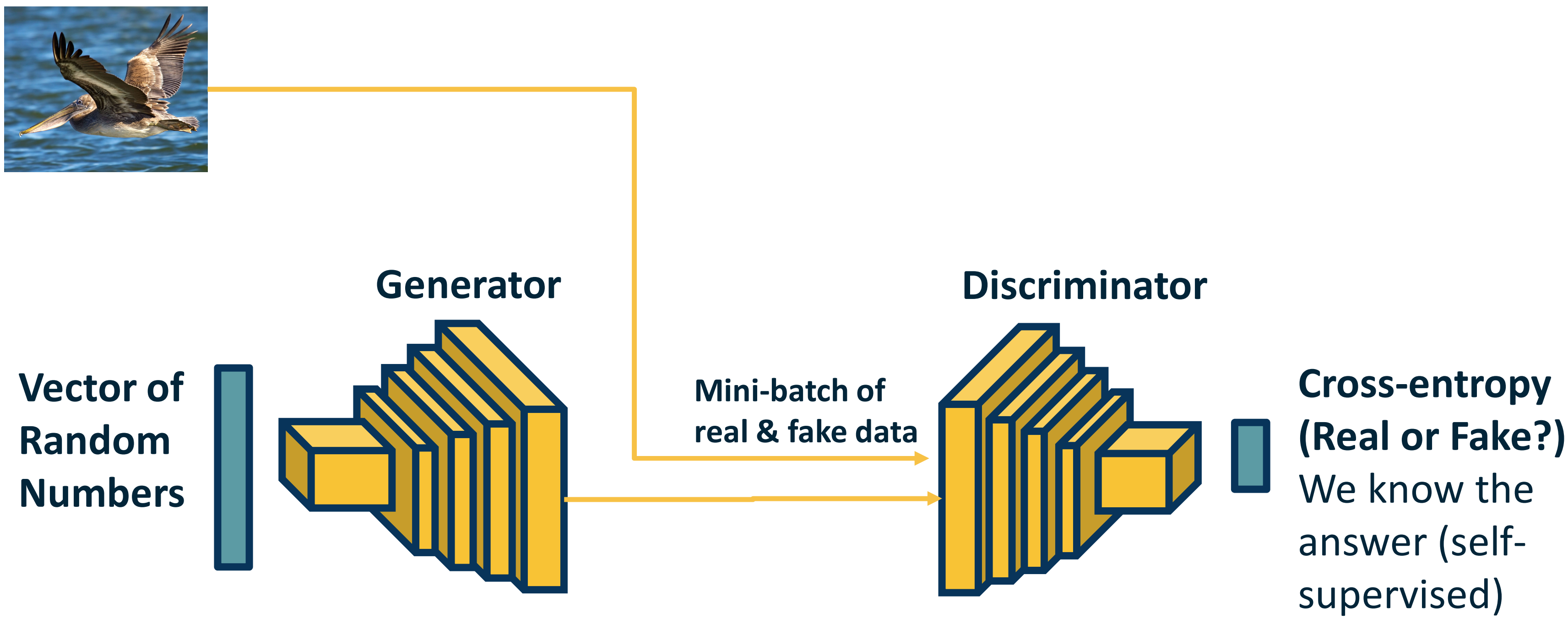



# Generating Images

- **Generator:** Update weights to improve realism of generated images
- **Discriminator:** Update weights to better discriminate




**Question: What loss functions can we use (for each network)?**



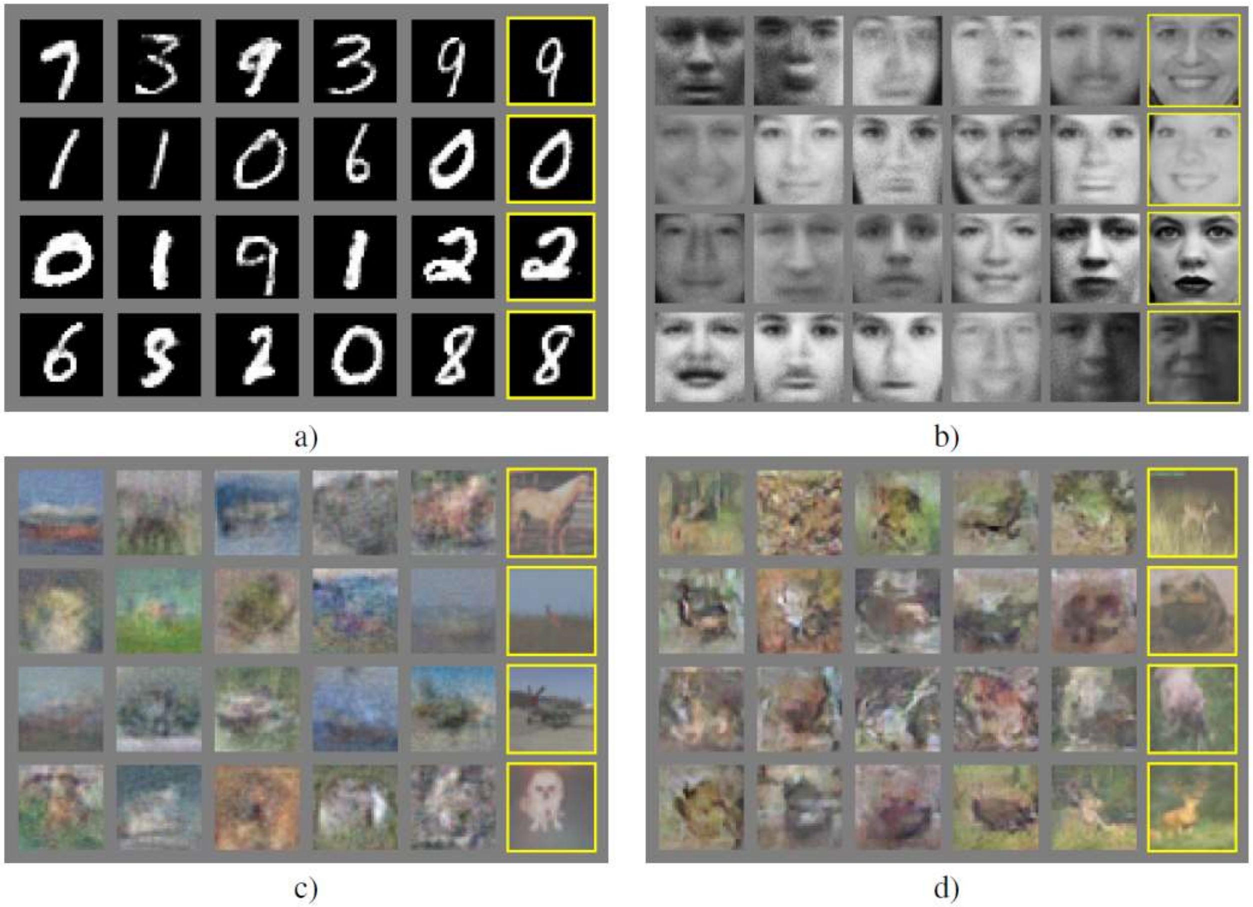

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

**Generator Loss**

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)\right].$$

**Discriminator Loss**

# Generative Adversarial Networks (GANs)




- Low-resolution images but look decent!
- Last column are nearest neighbor matches in dataset

# Early Results

- GANs are very difficult to train due to the mini-max objective

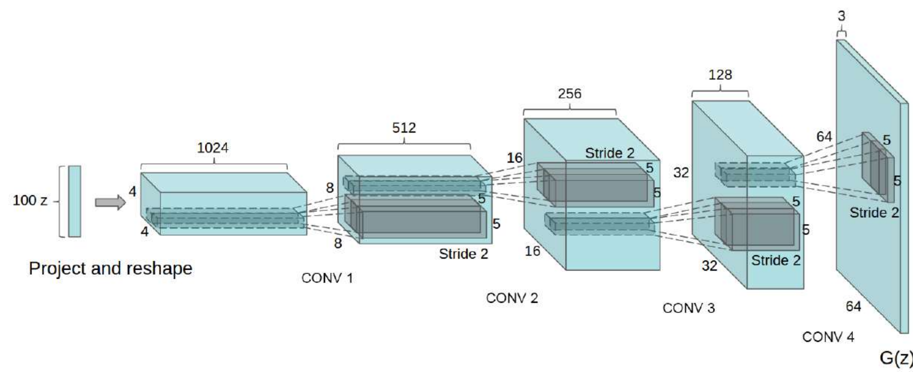
- Advancements include:
  - More stable architectures
  - Regularization methods to improve optimization
  - Progressive growing/training and scaling

*Goodfellow, NeurIPS 2016 Generative Adversarial Nets*

# Difficulty in Training

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*

# DCGAN

- Training GANs is difficult due to:
  - Minimax objective – For example, what if generator learns to memorize training data (no variety) or only generates part of the distribution?
  - Mode collapse – Capturing only some modes of distribution

- Several theoretically-motivated regularization methods
  - Simple example: Add noise to real samples!

$$\lambda \cdot \mathbb{E}_{x \sim P_{real}, \delta \sim N_d(0, cI)} \left[ \|\nabla_{\mathbf{x}} D_\theta(x + \delta)\| - k \right]^2$$

*Kodali et al., On Convergence and Stability of GANs (also known as How to Train your DRAGAN)*

# Generative Adversarial Nets: Convolutional Architectures

Samples from the model look much better!

Radford et al, ICLR 2016

# Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in latent space

Radford et al, ICLR 2016

*Brock et al., Large Scale GAN Training for High Fidelity Natural Image Synthesis*

# Example Generated Images - BigGAN

(a) 128×128 (b) 256×256 (c) 512×512 (d)

Figure 4: Samples from our model with truncation threshold 0.5 (a-c) and an example of class leakage in a partially trained model (d).

*Brock et al., Large Scale GAN Training for High Fidelity Natural Image Synthesis*

# Failure Examples - BigGAN


https://www.youtube.com/watch?v=PCBTZh41Ris

# Video Generation

- A few other examples:
  - Deep nostalgia: https://www.myheritage.com/deep-nostalgia
  - High-resolution outputs: https://compvis.github.io/taming-transformers/

# 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!

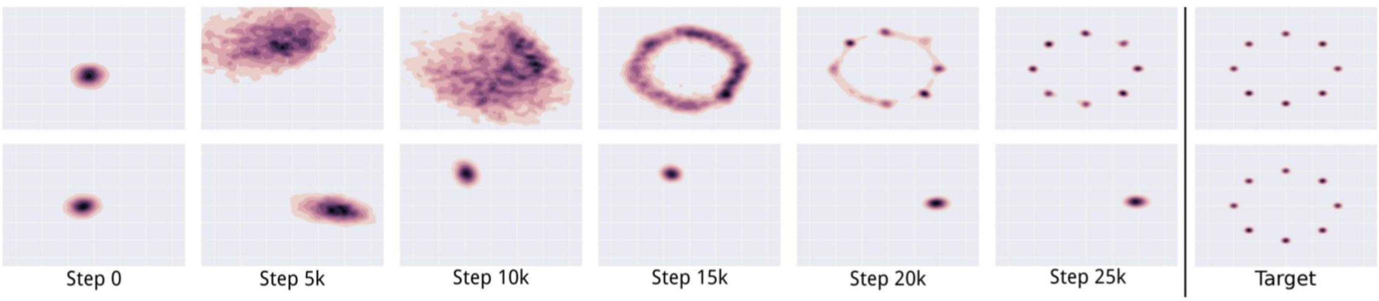
Cons:
- Trickier / more unstable to train
- Can’t solve inference queries such as p(x), p(z|x)

Active areas of research:
- Better loss functions, more stable training (Wasserstein GAN, LSGAN, many others)
- Conditional GANs, GANs for all kinds of applications

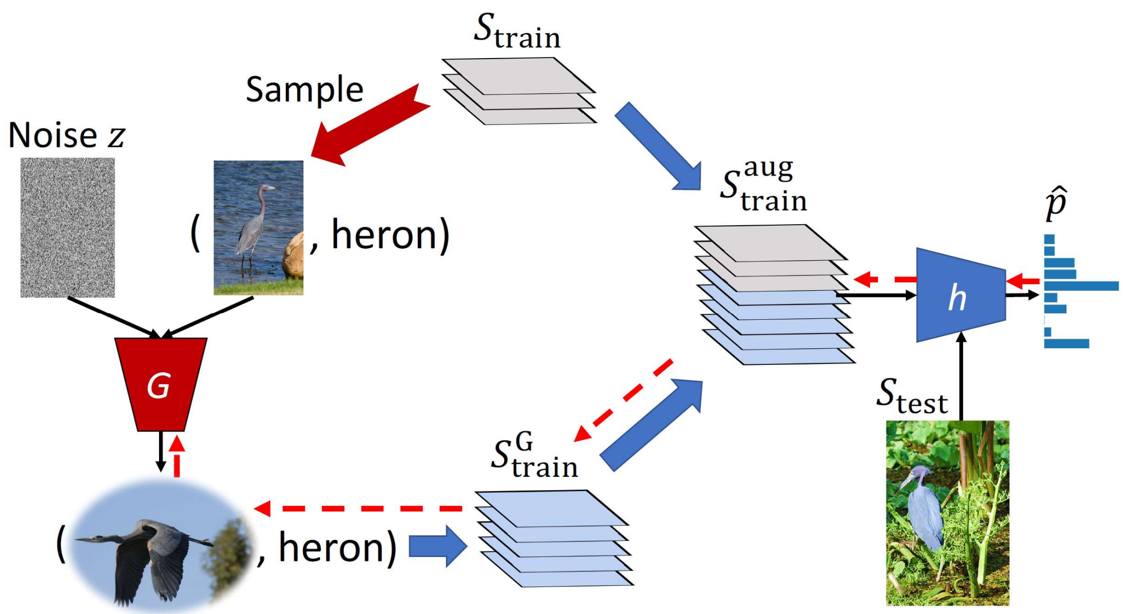
# Mode Collapse

- Optimization of GANs is tricky
  - Not guaranteed to find Nash equilibrium

- Large number of methods to combat:
  - Use history of discriminators
  - Regularization
  - Different divergence measures

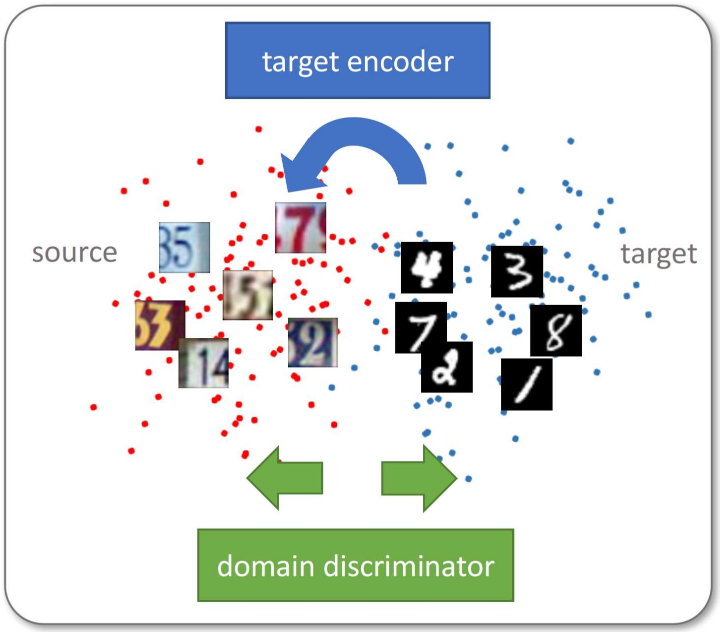


# Application: Data Augmentation

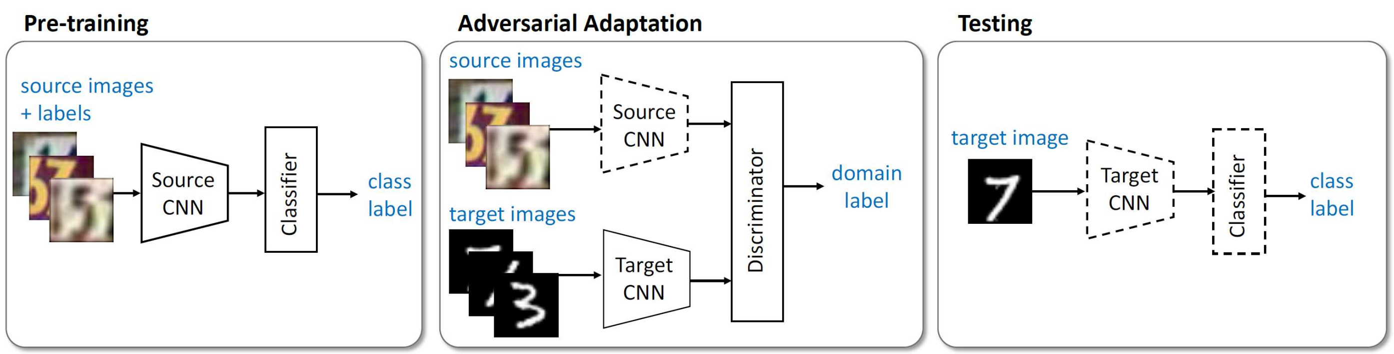


# Application: Domain Adaptation

- **Idea:** Train a model on *source* data and adapt to *target* data using unlabeled examples from target



# Approach

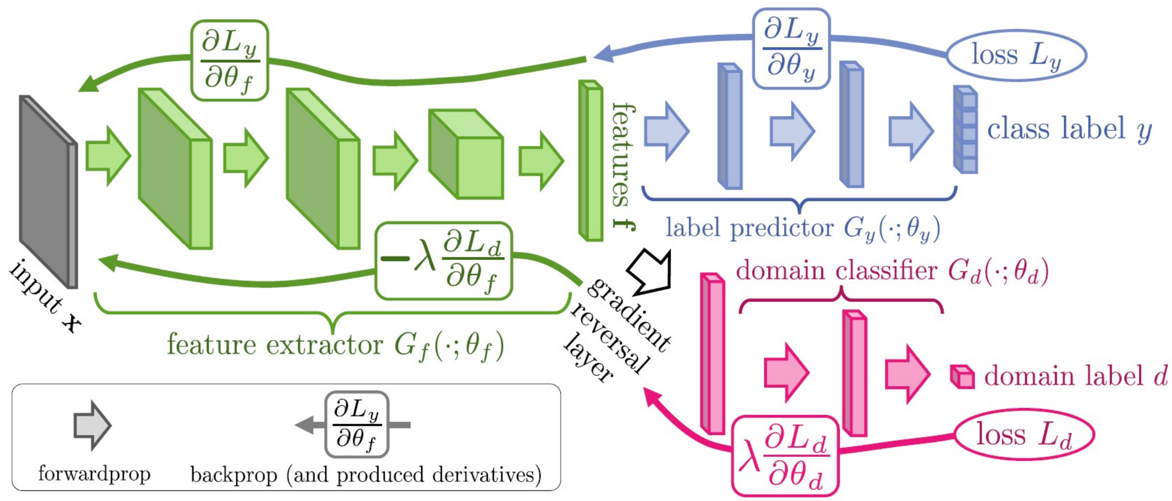



| Method | MNIST → USPS | USPS → MNIST | SVHN → MNIST |
|---|---|---|---|
| Source only | 0.752 ± 0.016 | 0.571 ± 0.017 | 0.601 ± 0.011 |
| Gradient reversal | 0.771 ± 0.018 | 0.730 ± 0.020 | 0.739 [16] |
| Domain confusion | 0.791 ± 0.005 | 0.665 ± 0.033 | 0.681 ± 0.003 |
| CoGAN | 0.912 ± 0.008 | 0.891 ± 0.008 | did not converge |
| ADDA (Ours) | 0.894 ± 0.002 | 0.901 ± 0.008 | 0.760 ± 0.018 |

Table 2: Experimental results on unsupervised adaptation among MNIST, USPS, and SVHN.

# Aside: Other ways to Align

digital SLR camera | low-cost camera, flash




[Ganin et al. , JMLR 2016]

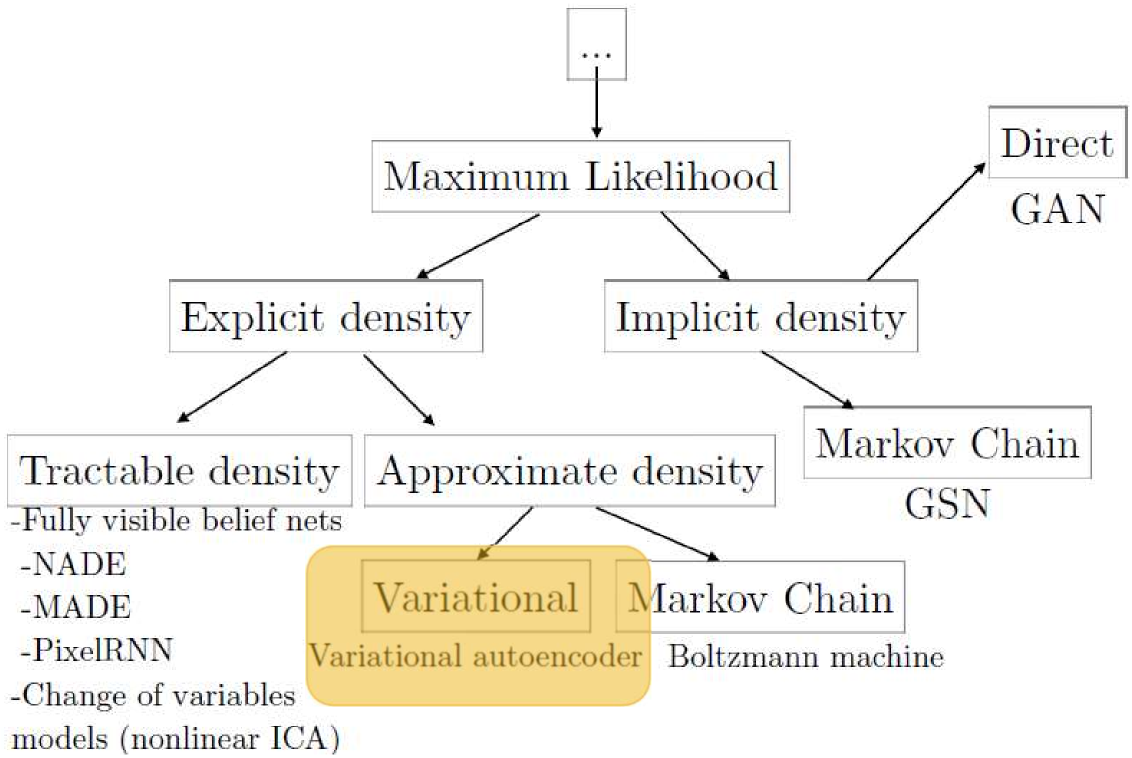
- Generative Adversarial Networks (GANs) can produce amazing images!

- Several drawbacks
  - High-fidelity generation heavy to train
  - Training can be unstable
  - No explicit model for distribution

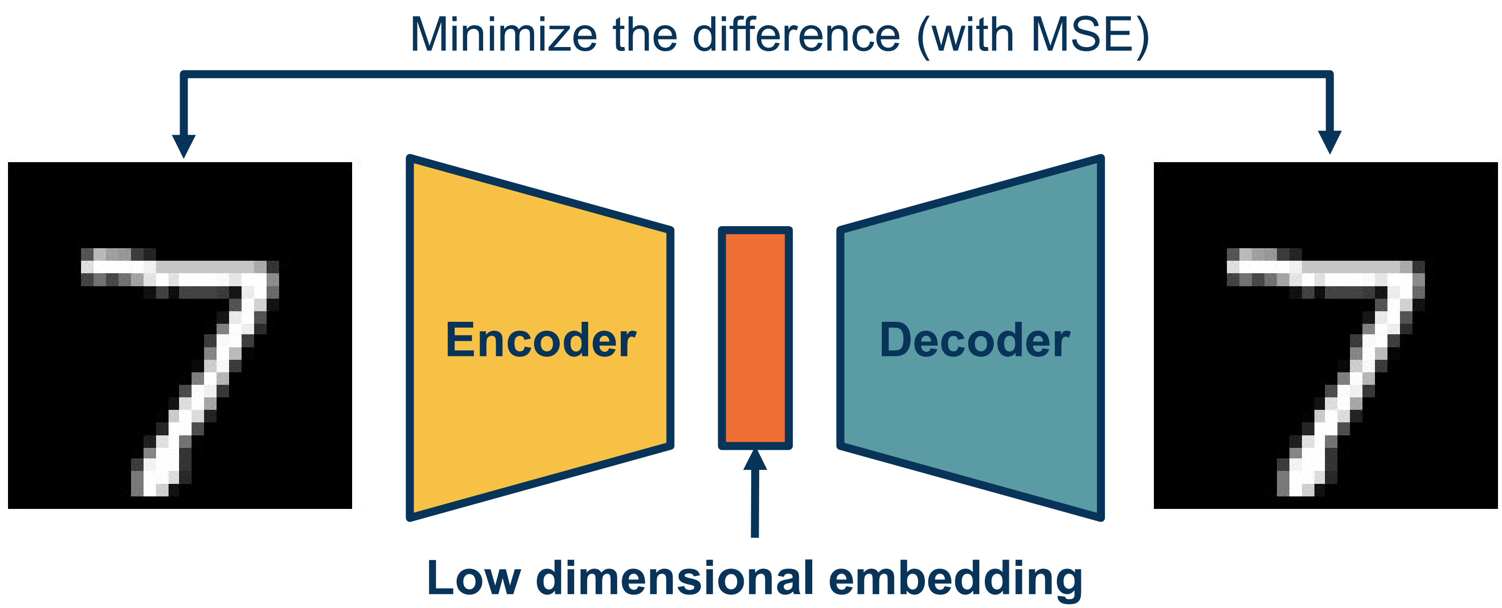
- Larger number of extensions:
  - GANs conditioned on labels or other information
  - Adversarial losses for other applications

# Summary

# Variational Autoencoders (VAEs)



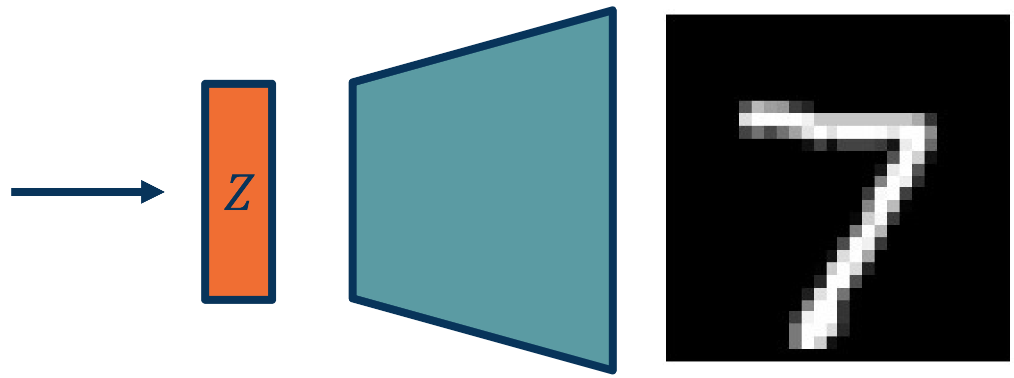

*Goodfellow, NeurIPS 2016 Tutorial: Generative Adversarial Networks*




Linear layers with reduced dimension or Conv-2d layers with stride

Linear layers with increasing dimension or Conv-2d layers with bilinear upsampling

**What is this?**
**Hidden/Latent variables**
**Factors of variation that produce an image:**
**(digit, orientation, scale, etc.)**



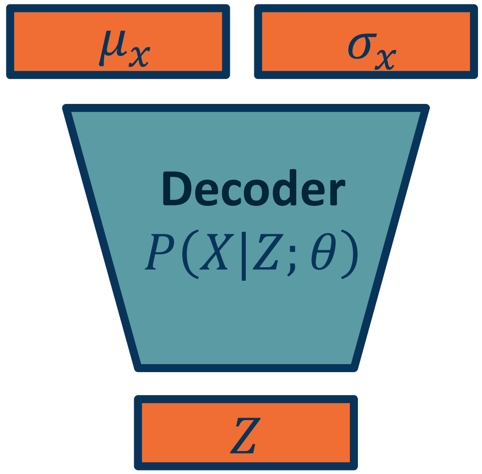

$$P(X) = \int P(X|Z;\theta)P(Z)dZ$$

- We cannot maximize this likelihood due to the integral
- Instead we maximize a variational *lower bound* (VLB) that we *can* compute

*Kingma & Welling, Auto-Encoding Variational Bayes*

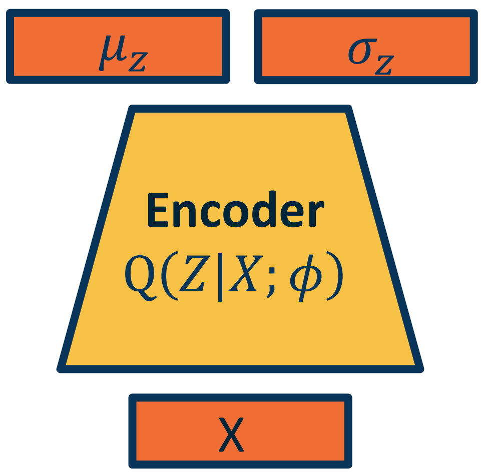
# Formalizing the Generative Model

- We can combine the probabilistic view, sampling, autoencoders, and approximate optimization
- Just as before, sample $Z$ from simpler distribution
- We can also output parameters of a probability distribution!
  - **Example**: $\mu, \sigma$ of Gaussian distribution
  - For multi-dimensional version output diagonal covariance
- How can we maximize $P(X) = \int P(X|Z;\theta)P(Z)dZ$




# Variational Autoencoder: Decoder

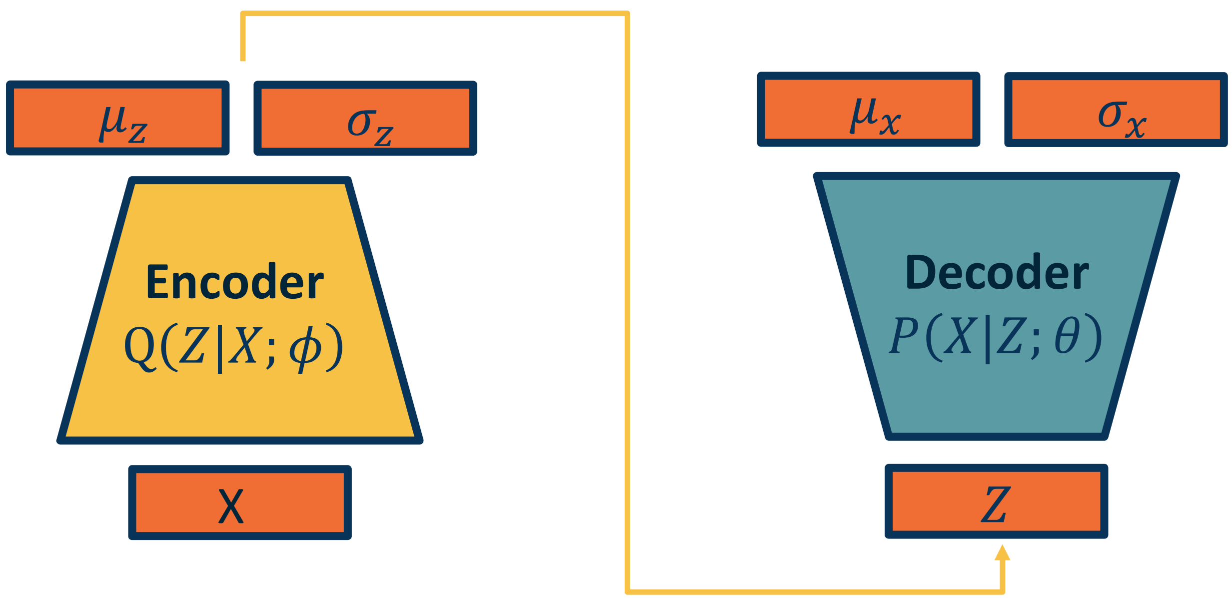
- We can combine the probabilistic view, sampling, autoencoders, and approximate optimization




- Given an image, estimate $Z$
- Again, output *parameters of a distribution*

# Variational Autoencoder: Encoder

- We can tie the encoder and decoder together into a probabilistic autoencoder
  - Given data (X), estimate $\mu_z, \sigma_z$ and sample from $N(\mu_z, \sigma_z)$
  - Given $Z$, estimate $\mu_x, \sigma_x$ and sample from $N(\mu_x, \sigma_x)$




# Putting Them Together

- How can we optimize the parameters of the two networks?

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

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

*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

# Maximizing Likelihood

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

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

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

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

*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

## Maximizing Likelihood

Aside: KL Divergence (distance measure for distributions), always >= 0

$$KL(p||q) = H_c(p,q) - H(p) = \sum p\,(x) \log p(x) - \sum p(x) \log q(x)$$

Definition of Expectation

$$\mathbb{E}[f] = \mathbb{E}_{x\sim q}[f(x)] = \sum_{x\in\Omega} q(x) f(x)$$

$$\mathrm{KL}\,(q(\mathbf{z})||p(\mathbf{z}\,|\,\mathbf{x})) = \mathbb{E}\,[\log q(\mathbf{z})] - \mathbb{E}\,[\log p(\mathbf{z}\,|\,\mathbf{x})]$$

## KL-Divergence

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

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

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

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

*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

## Maximizing Likelihood

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

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

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

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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.

*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

# Maximizing Likelihood

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

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

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

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

Variational lower bound ("ELBO")

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

Training: Maximize lower bound

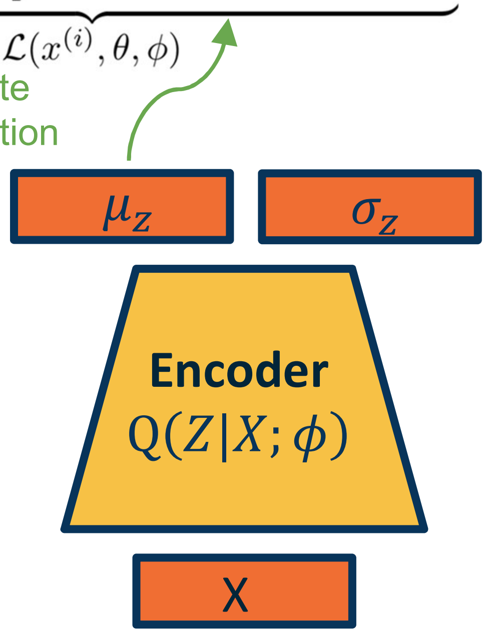
*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

# Maximizing Likelihood

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

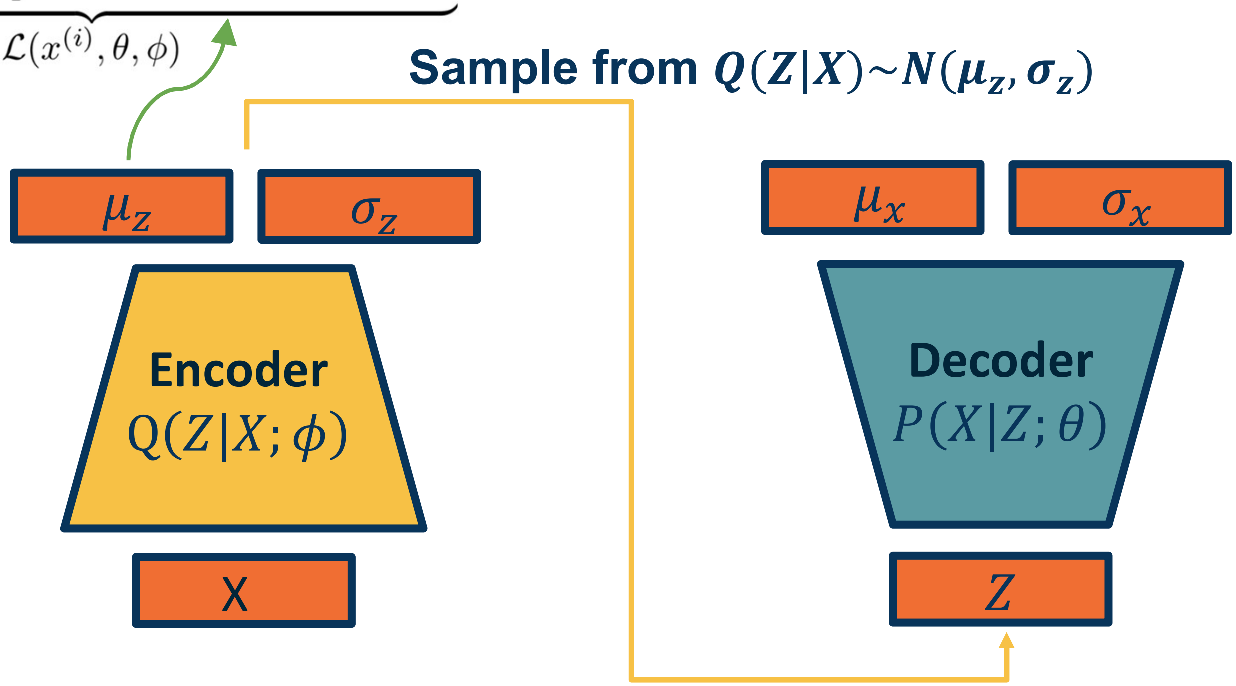



*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

# Forward and Backward Passes

Putting it all together: maximizing the likelihood lower bound

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

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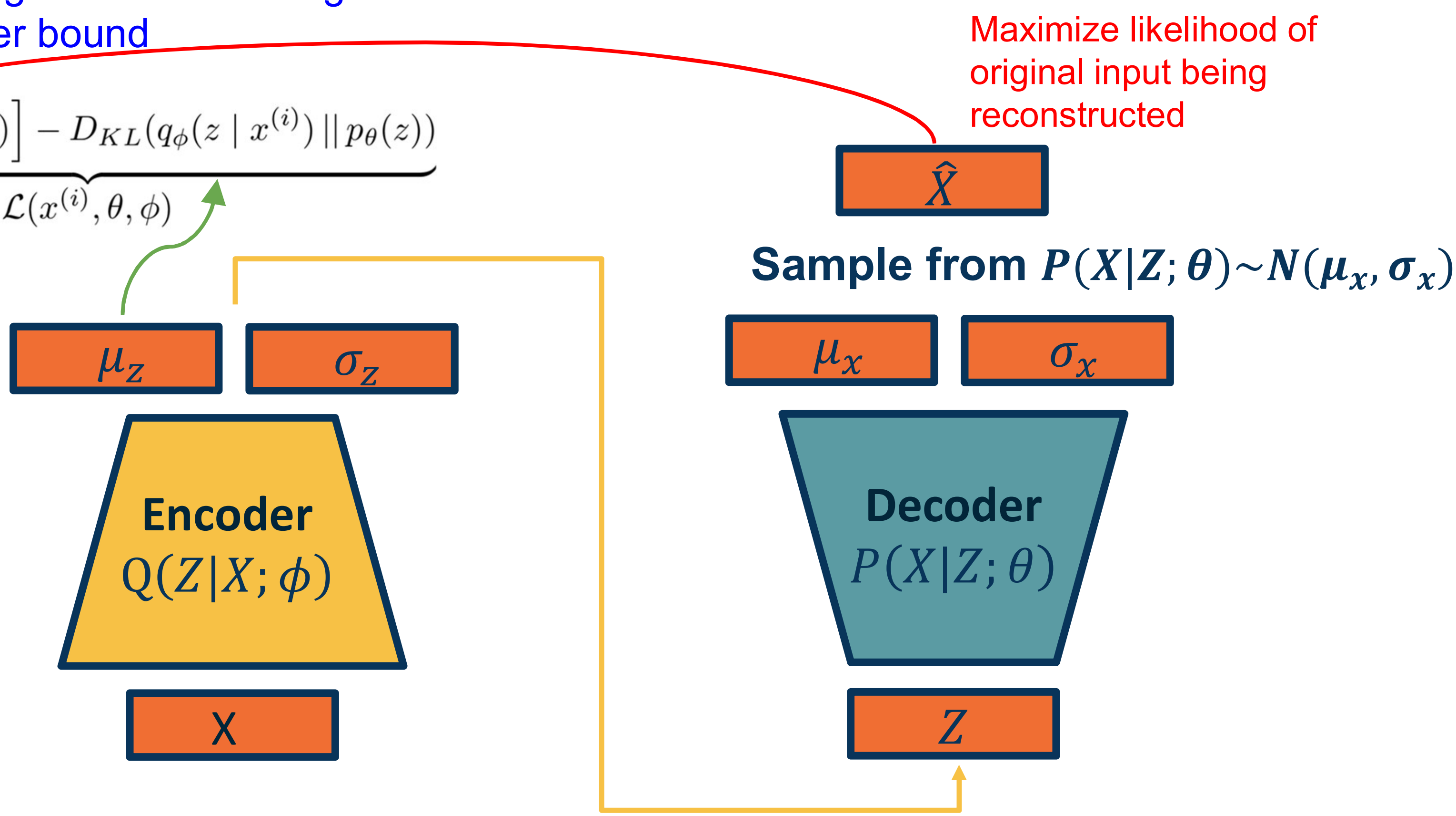
# Forward and Backward Passes

Putting it all together: maximizing the likelihood lower bound

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



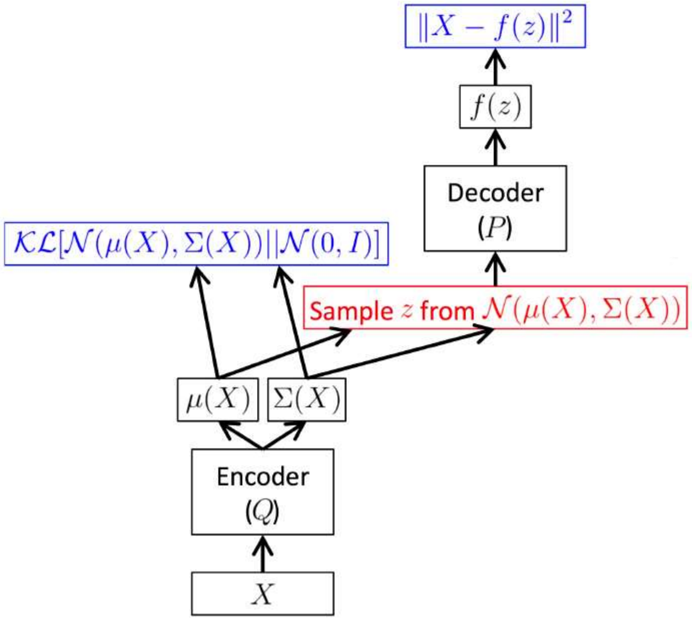

*From CS231n, Fei-Fei Li, Justin Johnson, Serena Yeung*

# Forward and Backward Passes

- Problem with respect to the VLB: updating $\phi$

$$\mathcal{L}_{\text{VAE}} = \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\left[\log \frac{p_\theta(\boldsymbol{z},\boldsymbol{x})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})}\right]$$
$$= -D_{\text{KL}}(q_\phi(\boldsymbol{z}|\boldsymbol{x})||p_\theta(\boldsymbol{z})) + \mathbb{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z}$$

- $Z \sim Q(Z|X;\phi)$ : need to differentiate through the sampling process w.r.t $\phi$ (encoder is probabilistic)

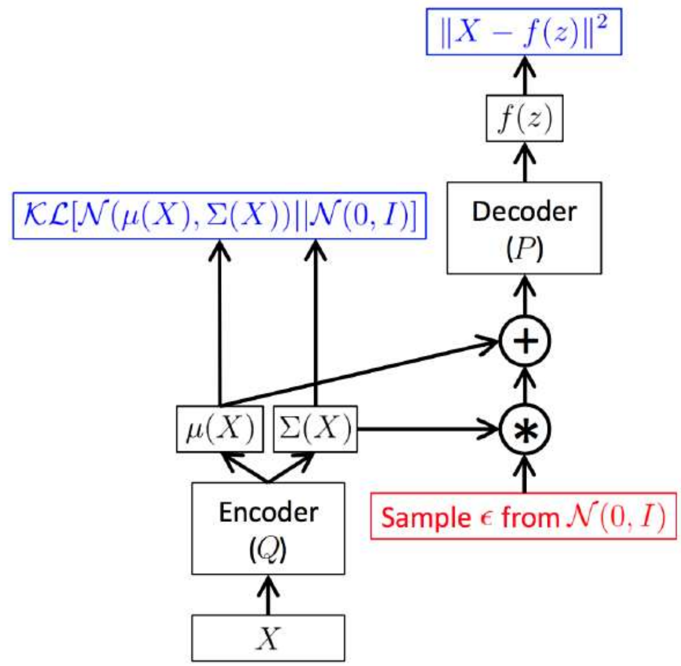



*From: Tutorial on Variational Autoencoders*
*https://arxiv.org/abs/1606.05908*

*From: http://gokererdogan.github.io/2016/07/01/reparameterization-trick/*

## Reparameterization Trick: Problem

- Solution: make the randomness independent of encoder output, making the encoder deterministic
- Gaussian distribution example:
  - Previously: encoder output = random variable $z \sim N(\mu, \sigma)$
  - Now encoder output = distribution parameter $[\mu, \sigma]$
  - $z = \mu + \epsilon * \sigma, \epsilon \sim N(0,1)$




*From: Tutorial on Variational Autoencoders*
*https://arxiv.org/abs/1606.05908*

*From:* *http://gokererdogan.github.io/2016/07/01/reparameterization-trick/*

# Reparameterization Trick: Solution

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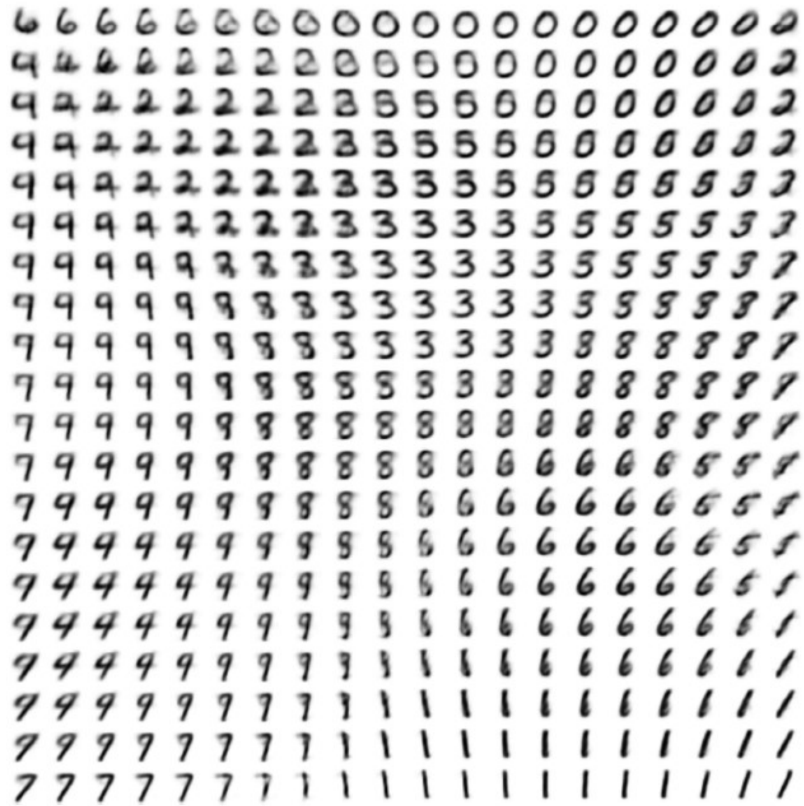
$z_1$

$z_2$



*Kingma & Welling, Auto-Encoding Variational Bayes*

# Interpretability of Latent Vector

- Variational Autoencoders (VAEs) provide a principled way to perform approximate maximum likelihood optimization
  - Requires some assumptions (e.g. Gaussian distributions)
- Samples are often not as competitive as GANs
- Latent features (learned in an unsupervised way!) often good for downstream tasks:
  - Example: World models for reinforcement learning (Ha et al., 2018)

*Ha & Schmidhuber, World Models, 2018*

# Summary

- Several ways to learn *generative* models via deep learning

- **PixelRNN/CNN:**
  - Simple tractable densities we can model via a NN and optimize
  - Slow generation – limited scaling to large complex images
- **Generative Adversarial Networks (GANs):**
  - Pro: Amazing results across many image modalities
  - Con: Unstable/difficult training process, computationally heavy for good results
  - Con: Limited success for discrete distributions (language)
  - Con: Hard to evaluate (implicit model)
- **Variational Autoencoders:**
  - Pro: Principled mathematical formulation
  - Pro: Results in disentangled latent representations
  - Con: Approximation inference, results in somewhat lower quality reconstructions

*Ha & Schmidhuber, World Models, 2018*

# Overall Summary