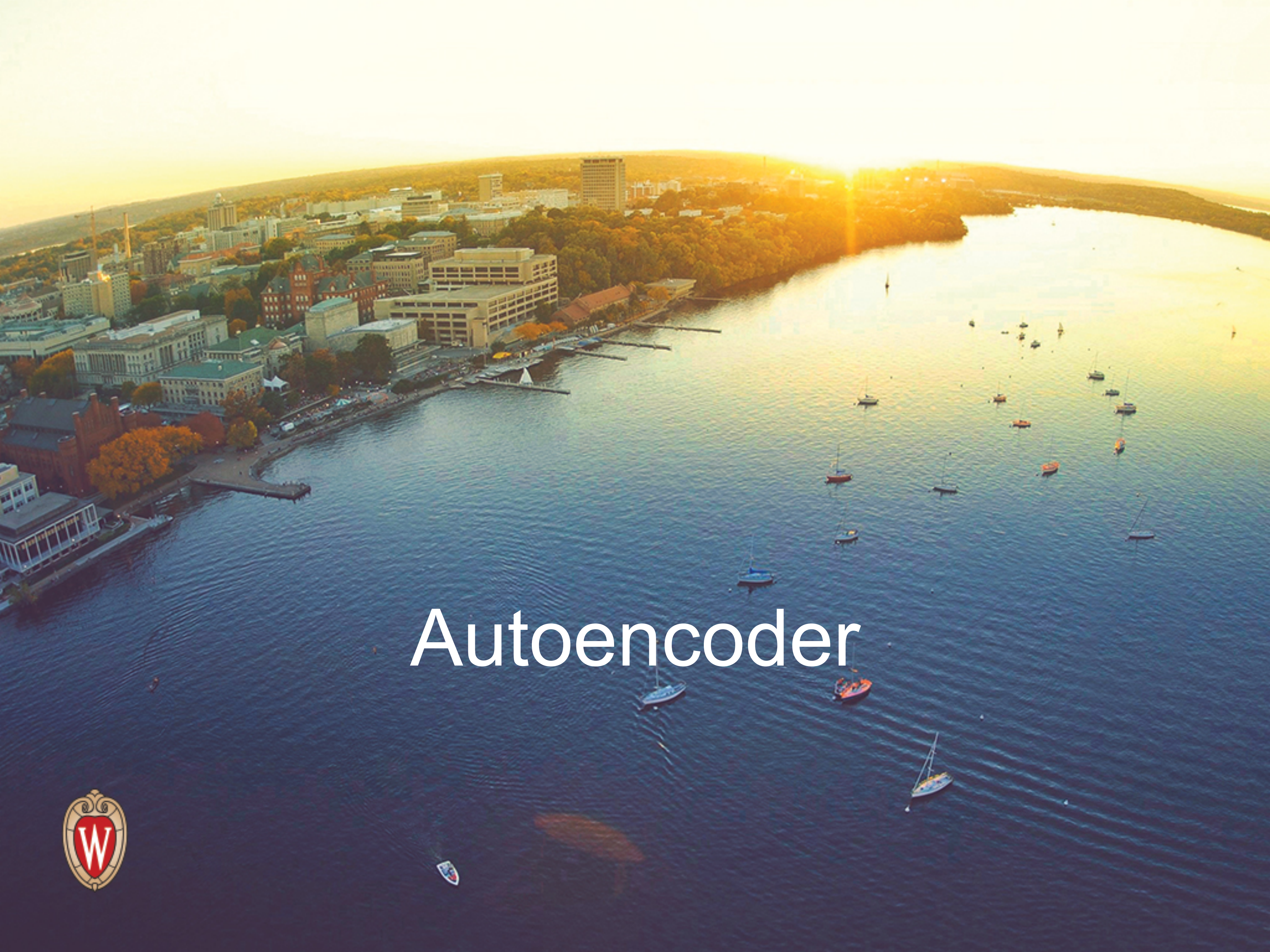
Neural Network Part 5: Unsupervised Models

CS 760@UW-Madison

Goals for the lecture

you should understand the following concepts

- autoencoder
- restricted Boltzmann machine (RBM)
- Nash equilibrium
- minimax game
- generative adversarial network (GAN)



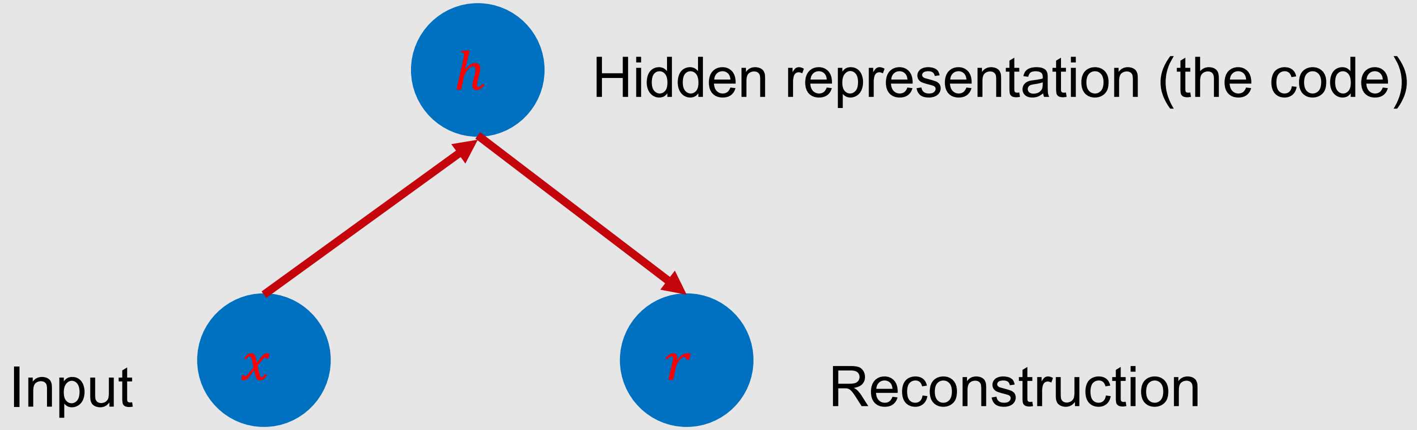
Autoencoder

Autoencoder

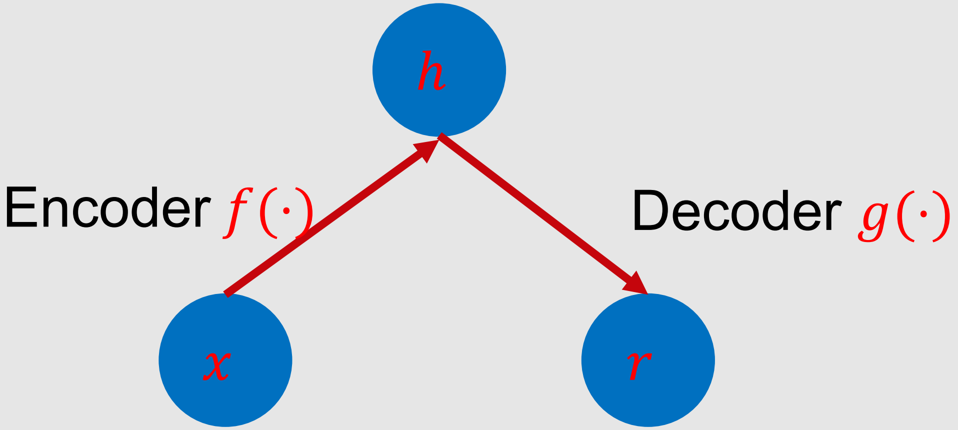
- Neural networks trained to attempt to copy its input to its output

- Contain two parts:
  - Encoder: map the input to a hidden representation
  - Decoder: map the hidden representation to the output

Autoencoder



Autoencoder



$$h = f(x), r = g(h) = g(f(x))$$

Why want to copy input to output

- Not really care about copying

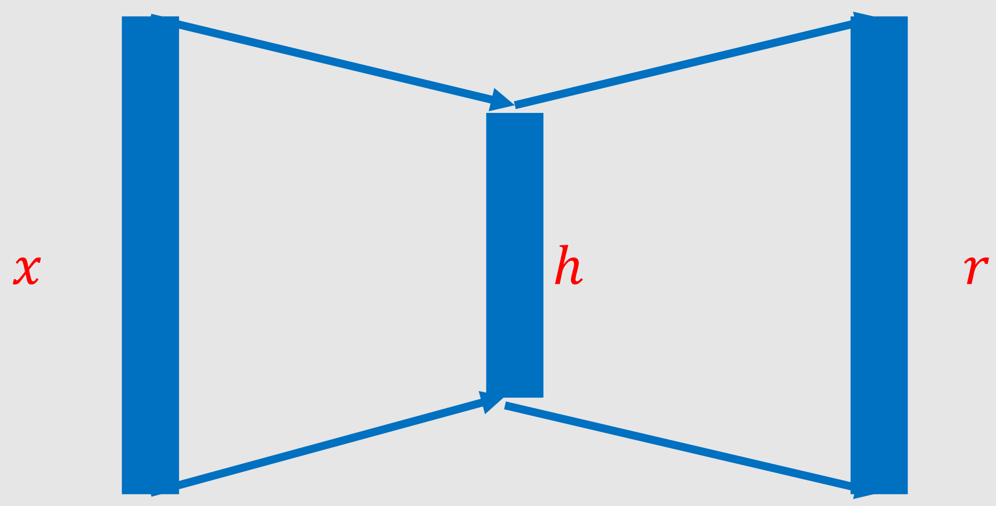
- Interesting case: NOT able to copy exactly but strive to do so
- Autoencoder forced to select which aspects to preserve and thus hopefully can learn useful properties of the data

- Historical note: goes back to (LeCun, 1987; Bourlard and Kamp, 1988; Hinton and Zemel, 1994).

Undercomplete autoencoder

- Constrain the code to have smaller dimension than the input
- Training: minimize a loss function

$$L(x, r) = L(x, g(f(x)))$$



Undercomplete autoencoder

- Constrain the code to have smaller dimension than the input
- Training: minimize a loss function

$$L(x, r) = L(x, g(f(x)))$$

- Special case: f, g linear, L mean square error
- Reduces to Principal Component Analysis

Undercomplete autoencoder

- What about nonlinear encoder and decoder?

- Capacity should not be too large
- Suppose given data $x_1, x_2, \ldots, x_n$
  - Encoder maps x_i to i
  - Decoder maps i to x_i
- One dim h suffices for perfect reconstruction

Regularization

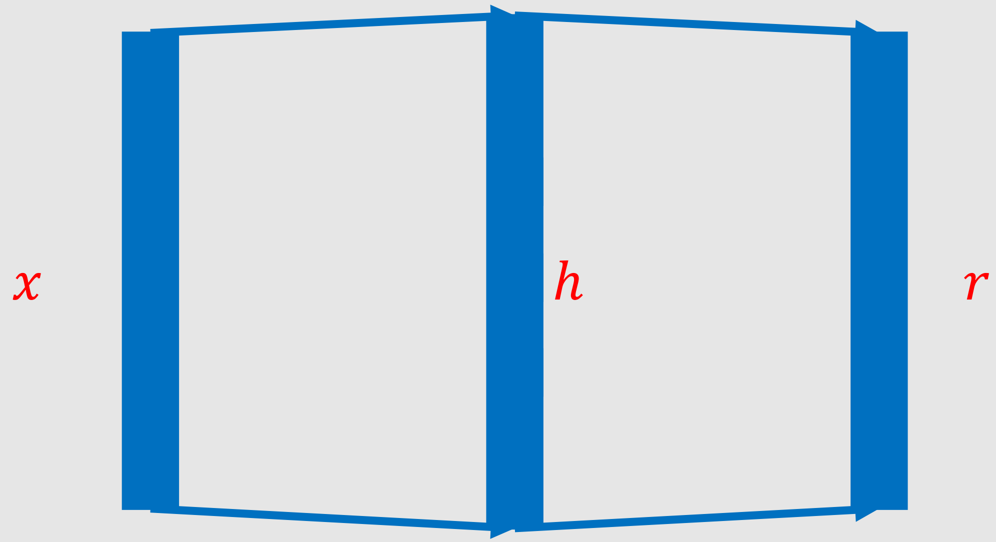
- Typically NOT
  - Keeping the encoder/decoder shallow or
  - Using small code size

- Regularized autoencoders: add regularization term that encourages the model to have other properties
  - Sparsity of the representation (sparse autoencoder)
  - Robustness to noise or to missing inputs (denoising autoencoder)

Sparse autoencoder

- Constrain the code to have sparsity
- Training: minimize a loss function

$$L_R = L(x, g(f(x))) + R(h)$$



Probabilistic view of regularizing h

- Suppose we have a probabilistic model $p(h, x)$
- MLE on x

$$\log p(x) = \log \sum_{h'} p(h', x)$$

- ☹ Hard to sum over h'

Probabilistic view of regularizing h

- Suppose we have a probabilistic model $p(h, x)$
- MLE on x

$$\max \log p(x) = \max \log \sum_{h'} p(h', x)$$

- Approximation: suppose $h = f(x)$ gives the most likely hidden representation, and $\sum_{h'} p(h', x)$ can be approximated by $p(h, x)$

Probabilistic view of regularizing h

- Suppose we have a probabilistic model $p(h, x)$
- Approximate MLE on $x, h = f(x)$

$$\max \log p(h, x) = \max \log p(x|h) + \log p(h)$$

Loss

Regularization

Sparse autoencoder

- Constrain the code to have sparsity
- Laplacian prior: $p(h) = \frac{\lambda}{2} \exp(-\frac{\lambda}{2} |h|_1)$

- Training: minimize a loss function

$$L_R = L(x, g(f(x))) + \lambda |h|_1$$

Denoising autoencoder

- Traditional autoencoder: encourage to learn $g\left(f(\cdot)\right)$ to be identity

- Denoising : minimize a loss function

$$L(x, r) = L(x, g\left(f(\tilde{x})\right))$$

where $\tilde{x}$ is $x + noise$

Boltzmann Machine

Boltzmann machine

- Introduced by Ackley *et al.* (1985)

- General "connectionist" approach to learning arbitrary probability distributions over binary vectors
- Special case of energy model: $p(x) = \frac{\exp(-E(x))}{Z}$

Boltzmann machine

- Energy model:

$$p(x) = \frac{\exp(-E(x))}{Z}$$

- Boltzmann machine: special case of energy model with

$$E(x) = -x^T U x - b^T x$$

where U is the weight matrix and b is the bias parameter

Boltzmann machine with latent variables

- Some variables are not observed

$$x = (x_v, x_h), \qquad x_v \text{ visible, } x_h \text{ hidden}$$

$$E(x) = -x_v^T R x_v - x_v^T W x_h - x_h^T S x_h - b^T x_v - c^T x_h$$

- Universal approximator of probability mass functions

Maximum likelihood

- Suppose we are given data $X = (x_v^1, x_v^2, \dots, x_v^n)$
- Maximum likelihood is to maximize

$$\log p(X) = \sum_i \log p(x_v^i)$$

where

$$p(x_v) = \sum_{x_h} p(x_v, x_h) = \sum_{x_h} \frac{1}{Z} \exp(-E(x_v, x_h))$$

- $Z = \sum \exp(-E(x_v, x_h))$: partition function, difficult to compute

Restricted Boltzmann machine

- Invented under the name *harmonium* (Smolensky, 1986)
- Popularized by Hinton and collaborators to *Restricted Boltzmann machine*

Restricted Boltzmann machine

- Special case of Boltzmann machine with latent variables:

$$p(v, h) = \frac{\exp(-E(v, h))}{Z}$$

  where the energy function is

$$E(v, h) = -v^T W h - b^T v - c^T h$$

  with the weight matrix W and the bias b, c

- Partition function

$$Z = \sum_v \sum_h \exp(-E(v, h))$$

Restricted Boltzmann machine

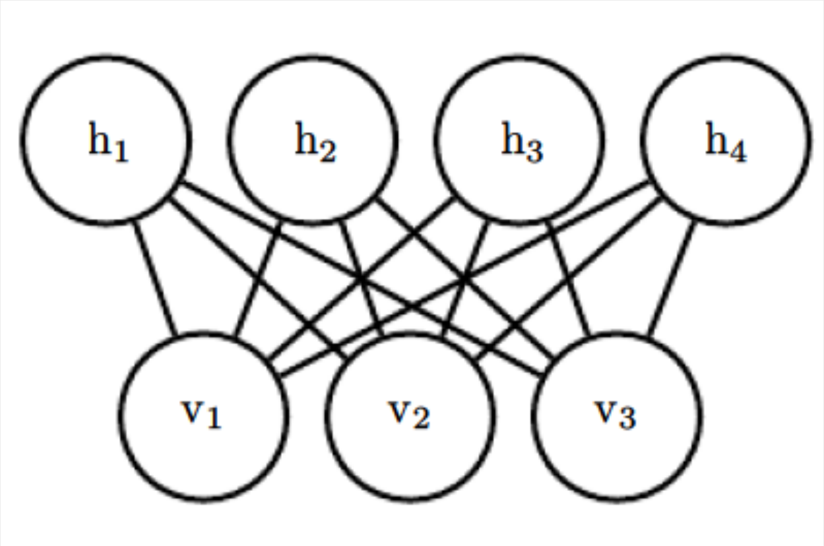


Figure from *Deep Learning*,
Goodfellow, Bengio and Courville

Restricted Boltzmann machine

- Conditional distribution is factorial

$$p(h|v) = \frac{p(v,h)}{p(v)} = \prod_j p(h_j|v)$$

and

$$p\left(h_j = 1|v\right) = \sigma\left(c_j + v^T W_{:,j}\right)$$

is logistic function

Restricted Boltzmann machine

- Similarly,

$$p(v|h) = \frac{p(v,h)}{p(h)} = \prod_i p(v_i|h)$$

and

$$p(v_i = 1|h) = \sigma\left(b_i + W_{i,:}h\right)$$

is logistic function

Generative Adversarial Networks (GAN)

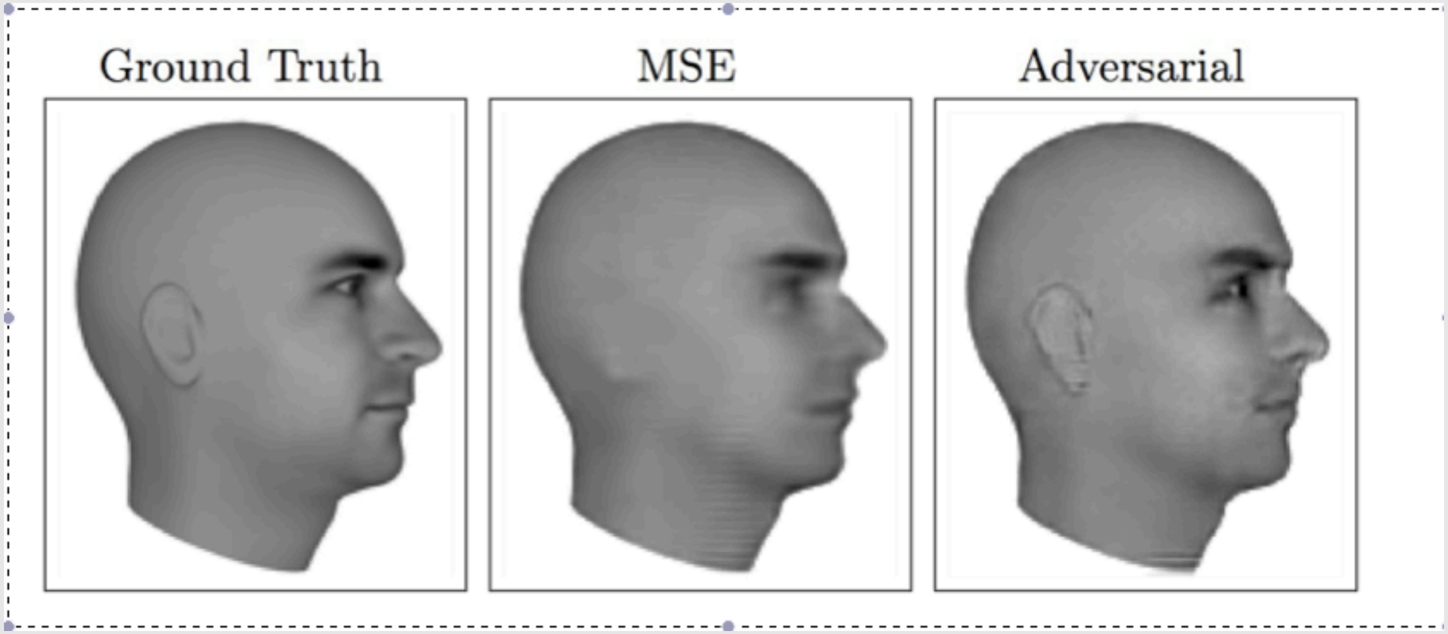
See Ian Goodfellow's tutorial slides:
http://www.iangoodfellow.com/slides/2018-06-22-gan_tutorial.pdf

Generative Adversarial Networks

- **Approach:** Set up zero-sum game between deep nets to
  - **Generator:** Generate data that looks like training set
  - **Discriminator:** Distinguish between real and synthetic data

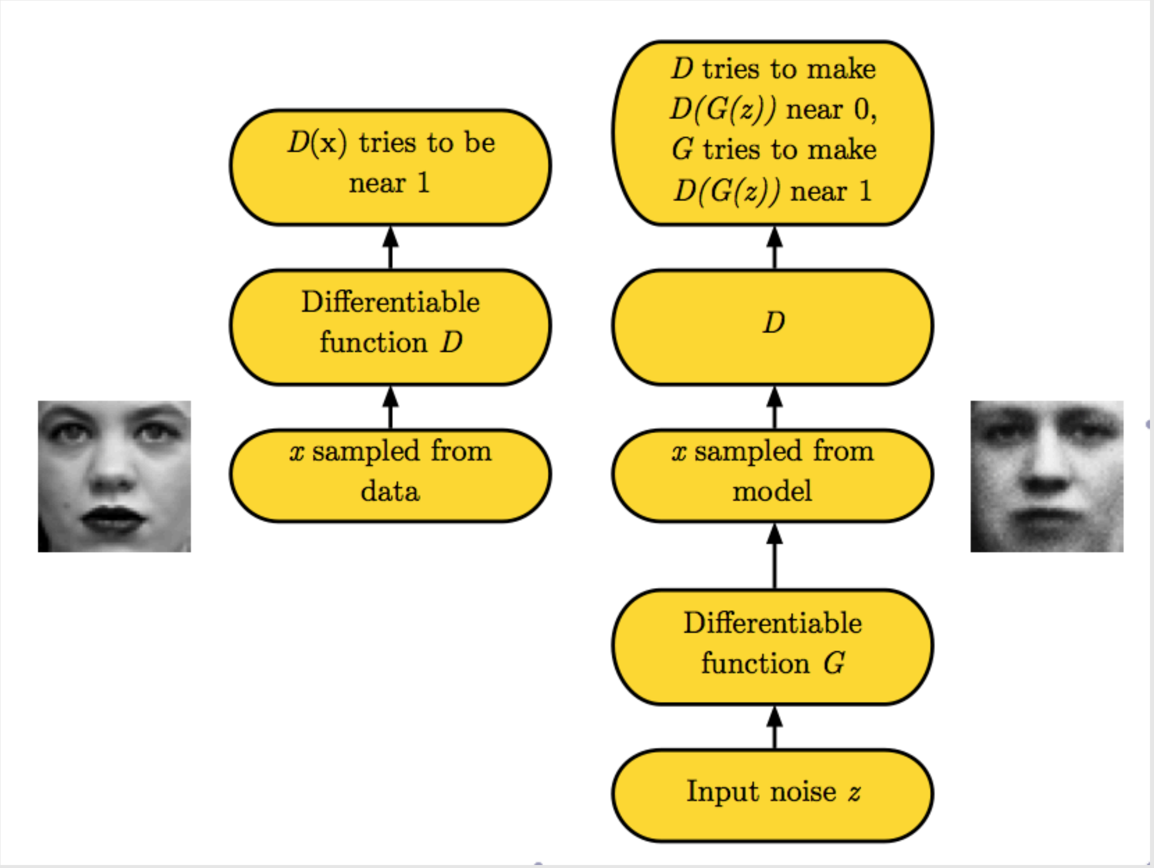
- **Motivation:**
  - Building accurate generative models is hard (e.g., *learning* ***and*** *sampling* from Markov net or Bayes net)
  - Want to use all our great progress on *supervised learners* to do this *unsupervised* learning task better
  - Deep nets may be our favorite supervised learner, especially for image data, if nets are convolutional (use tricks of sliding windows with parameter tying, cross-entropy transfer function, batch normalization)

Does It Work?



Thanks, Ian Goodfellow, NIPS 2016 Tutorial on GANS, for this and most of what follows…

A Bit More on GAN Algorithm



The Rest of the Details

- Use deep convolutional neural networks for Discriminator D and Generator G

- Let **x** denote trainset and **z** denote random, uniform input

- Set up zero-sum game by giving D the following objective, and G the negation of it:

$$-\frac{1}{2}\mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}}\log D(\boldsymbol{x}) - \frac{1}{2}\mathbb{E}_{\boldsymbol{z}}\log\left(1 - D\left(G(\boldsymbol{z})\right)\right)$$

- Let D and G compute their gradients simultaneously, each make one step in direction of the gradient, and repeat until neither can make progress… Minimax

More Math on GAN

- Real data distribution $q(x)$
- Fake data distribution $p_\theta(x) \coloneqq [x = G_\theta(z), z \sim p(z)]$
- Discriminator $D(x) \coloneqq \sigma(f_\beta(x))$
- GAN: $min_\theta max_\beta E_{q(x)} \log \sigma(f_\beta(x))$ +$E_{p_\theta(x)} \log(1 - \sigma\left(f_\beta(x)\right))$
- Given θ, the optimal $f_{\beta^*}(x) = \log \frac{q(x)}{p_\theta(x)}$ (not necessarily realizable by the discriminator neural network)
- Plug $f_{\beta^*}(x)$ back in GAN: $\min_\theta JS(p_\theta, q)$
- Recall
  - Jensen-Shannon divergence $JS(p,q) = KL\left(p || \frac{p+q}{2}\right) + KL(q || \frac{p+q}{2})$
  - Kullback-Leibler divergence $KL(p||q) = \sum_x p(x) \log \frac{p(x)}{q(x)}$
  - Maximum Likelihood Estimate $\min_\theta KL(q||p_\theta)$

THANK YOU

Some of the slides in these lectures have been adapted/borrowed from materials developed by Yingyu Liang, Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Matt Gormley, Elad Hazan, Tom Dietterich, Pedro Domingos, Geoffrey Hinton, and Ian Goodfellow.