Lecture 17
Deep Neural Generative Models II

CMSC 35246: Deep Learning

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Recap: Linear Factor Models

- Sample latent factors $\mathbf{h} \sim P(\mathbf{h})$

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- Estimate $W, \mathbf{b}, \sigma^2$ by maximum likelihood estimation or Expectation Maximization (EM)

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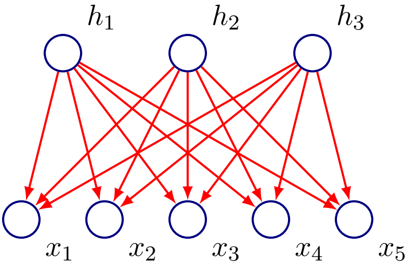
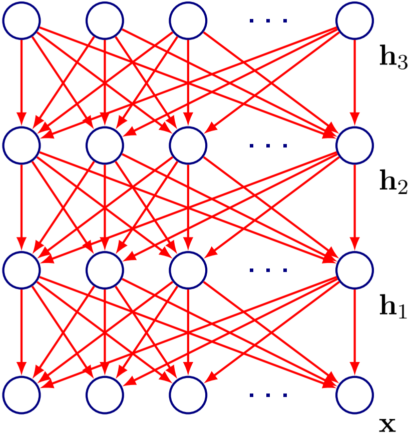
Recap: Linear Factor Models

- $P(\mathbf{h})$ is a factorial distribution



Recap: Sigmoid Belief Networks



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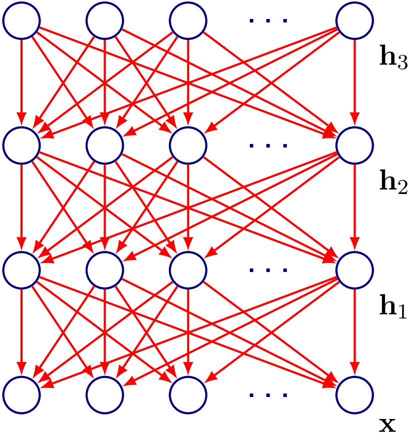

- Just like a feedfoward network, but with arrows reversed
- What if we place a class as a latent variable at the top?

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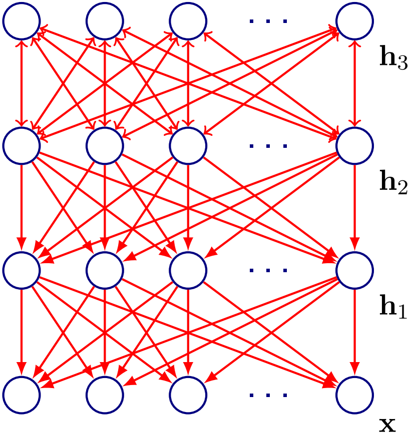
- Marginalization yields $P(\mathbf{x})$

Recap: Deep Belief Networks



- The top two layers are a Restricted Boltzmann Machine

Recap: Deep Belief Networks

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- Z is a normalizing factor called the Partition Function

$$Z = \sum_{\mathbf{x}} \exp(-\text{Energy}(\mathbf{x}))$$

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$$P(\mathbf{x}) \propto \prod_i P_i(\mathbf{x}) \propto \prod_i \exp^{(-f_i(\mathbf{x}))}$$

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- We can write the marginal in terms of free energy:

$$P(\mathbf{x}) = \frac{\exp^{-(\text{FreeEnergy}(\mathbf{x}))}}{Z} \text{ with } Z = \sum_{\mathbf{x}} \exp^{-\text{FreeEnergy}(\mathbf{x})}$$

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$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = -\mathbb{E}_{\tilde{P}}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

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- $\tilde{P}$ is the empirical training distribution
- Easy to compute!

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- Usually very hard to compute!
- Resort to Markov Chain Monte Carlo to get a stochastic estimator of the gradient

End of recap

A Special Case

- Suppose the energy has the following form:

$$\text{Energy}(\mathbf{x}, \mathbf{h}) = -\beta(\mathbf{x}) + \sum_i \gamma_i(\mathbf{x}, \mathbf{h}_i)$$

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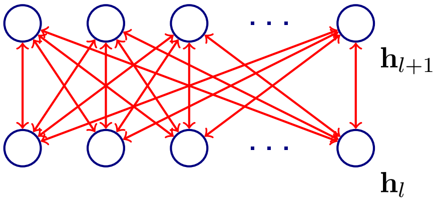
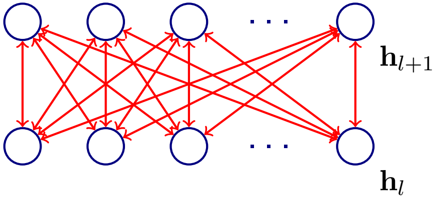
$$\begin{aligned} \text{FreeEnergy}(\mathbf{x}) &= -\log P(\mathbf{x}) - \log Z \\ &= -\beta - \sum_i \log \sum_{\mathbf{h}_i} \exp^{-\gamma_i(\mathbf{x}, \mathbf{h}_i)} \end{aligned}$$

Restricted Boltzmann Machines



- Form of energy:

Restricted Boltzmann Machines



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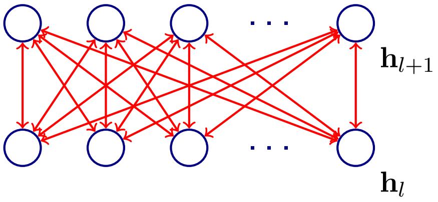

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- Takes the earlier nice form with $\beta(\mathbf{x}) = \mathbf{b}^T\mathbf{x}$ and $\gamma_i(\mathbf{x}, \mathbf{h_i}) = \mathbf{h}_i(\mathbf{c}_i + W_i\mathbf{x})$
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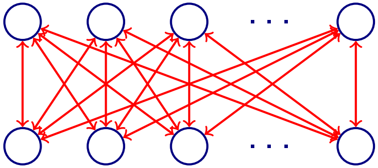

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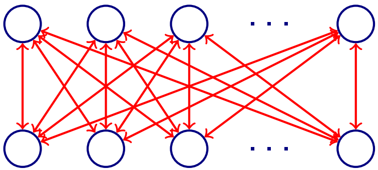

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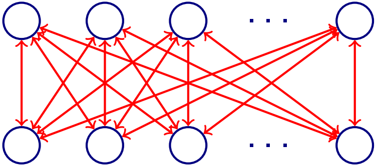

- We have an expression for $P(\mathbf{x})$ and the Free Energy can be computed analytically
- The conditional probability:

$$P(\mathbf{h}|\mathbf{x}) = \frac{\exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\mathbf{h} + \mathbf{h}^T W \mathbf{x}\right)}{\sum_{\tilde{\mathbf{h}}} \exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\tilde{\mathbf{h}} + \tilde{\mathbf{h}}^T W \mathbf{x}\right)} = \prod_i P(\mathbf{h}_i|\mathbf{x})$$

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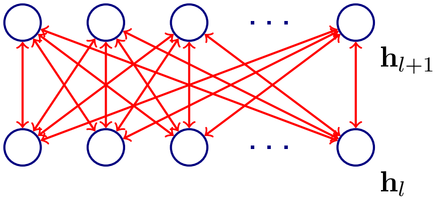

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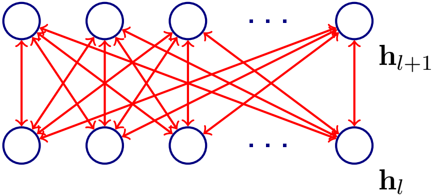

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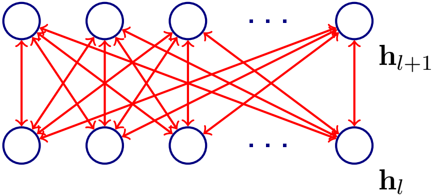

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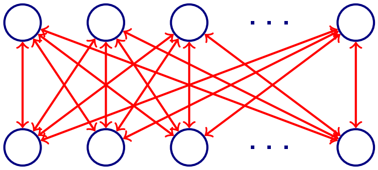

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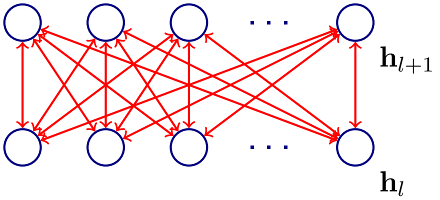

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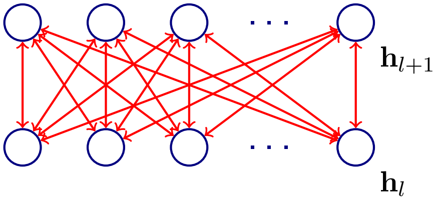

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Approximate Learning and Gibbs Sampling

$$\mathbb{E}_{\tilde{P}}\left[\frac{\partial \log P(\mathbf{x})}{\partial \theta}\right] = -\mathbb{E}_{\tilde{P}}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right] + \mathbb{E}_{P}\left[\frac{\partial \text{FreeEnergy}(\mathbf{x})}{\partial \theta}\right]$$

- We saw the expression for Free Energy for a RBM. But the second term was intractable. How do learn in this case?

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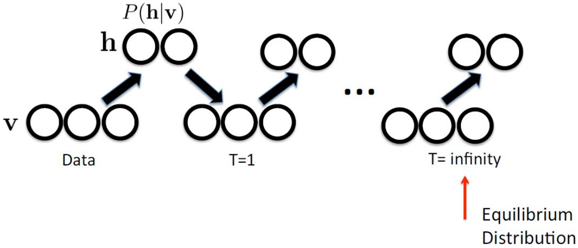
- We saw the expression for Free Energy for a RBM. But the second term was intractable. How do learn in this case?
- Replace the average over all possible input configurations by samples
- Run Markov Chain Monte Carlo (Gibbs Sampling):
- We want $\tilde{P}(\mathbf{x}) \approx P(\mathbf{x})$
- First sample $\mathbf{x}_1 \sim \tilde{P}(\mathbf{x})$, then $\mathbf{h}_1 \sim P(\mathbf{h}|\mathbf{x}_1)$, then $\mathbf{x}_2 \sim P(\mathbf{x}|\mathbf{h}_1)$, then $\mathbf{h}_2 \sim P(\mathbf{h}|\mathbf{x}_2)$ till $\mathbf{x}_{k+1}$

Approximate Learning, Alternating Gibbs Sampling



- We have already seen: $P(\mathbf{x}|\mathbf{h}) = \prod_i P(\mathbf{x}_i|\mathbf{h})$ and

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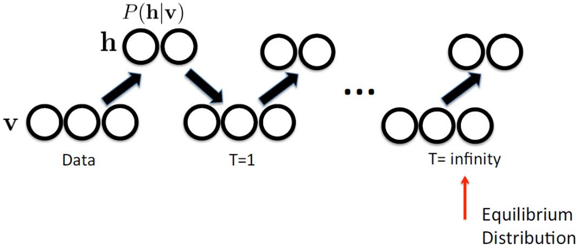

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- With: $P(\mathbf{h}_i = 1|\mathbf{x}) = \sigma(\mathbf{c_i} + W_i\mathbf{x})$ and $P(\mathbf{x}_j = 1|\mathbf{h}) = \sigma(\mathbf{b_j} + W_{:,j}^T\mathbf{h})$

Training a RBM: The Contrastive Divergence Algorithm

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- Aside: Easy to extend RBM (and contrastive divergence) to the continuous case

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$$\text{Energy}(\mathbf{x}, \mathbf{h}) = -\mathbf{b}^T\mathbf{x} - \mathbf{c}^T\mathbf{h} - \mathbf{h}^T W\mathbf{x} - \mathbf{x}^T U\mathbf{x} - \mathbf{h}^T V\mathbf{h}$$

Boltzmann Machines

- A model in which the energy has the form:

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- Originally proposed by Hinton and Sejnowski (1983)
- Important historically. But very difficult to train (why?)

Gradient of Log-Likelihood Revisited

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After basic manipulations and substitution:

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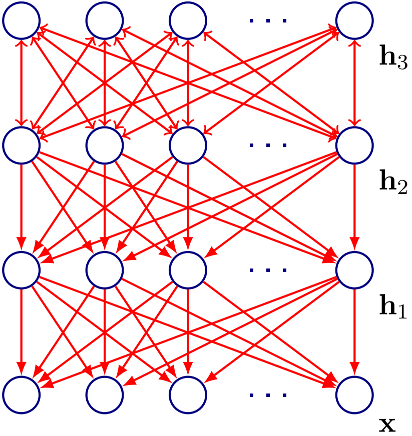
Back to Deep Belief Networks



$$P(\mathbf{x}, \mathbf{h}^1, \ldots, \mathbf{h}^l) = P(\mathbf{h}^l, \mathbf{h}^{l-1}) \Big(\prod_{k=1}^{l-2} P(\mathbf{h}^k | \mathbf{h}^{k+1}) \Big) P(\mathbf{x} | \mathbf{h}^1)$$

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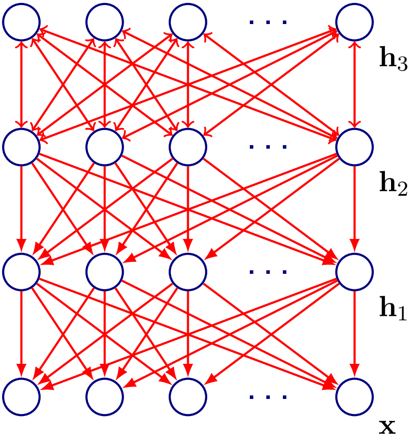

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Greedy Layer-wise Training of DBNs

- Reference: G. E. Hinton, S. Osindero and Y-W Teh: A Fast Learning Algorithm for Deep Belief Networks, In **Neural Computation**, 2006.

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- Can then be discriminatively fine-tuned using backpropagation

Deep Autoencoders (2006)

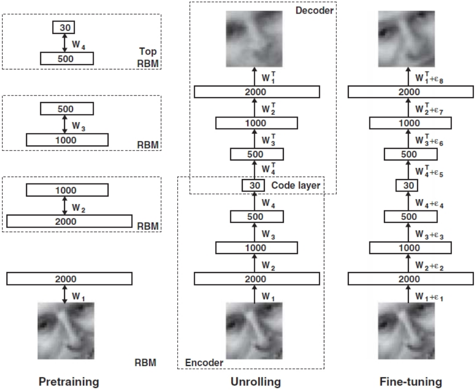
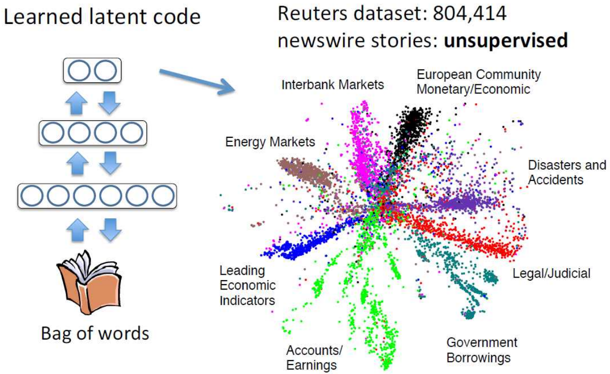


Fig. 1. Pretraining consists of learning a stack of restricted Boltzmann machines (RBMs), each having only one layer of feature detectors. The learned feature activations of one RBM are used as the "data" for training the next RBM in the stack. After the pretraining, the RBMs are "unrolled" to create a deep autoencoder, which is then fine-tuned using backpropagation of error derivatives.

G. E. Hinton, R. R. Salakhutdinov, Reducing the dimensionality of data with neural networks, Science, 2006

From last time: Was hard to train deep networks from scratch in 2006!

Semantic Hashing



G. Hinton and R. Salakhutdinov, "Semantic Hashing", 2006

Why does Unsupervised Pre-training work?

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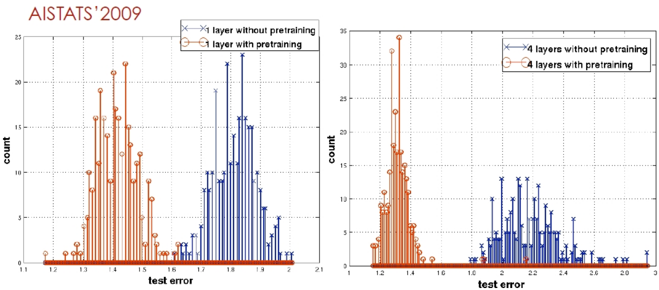
- Optimization: Unsupervised pre-training leads to better regions of the space i.e. better than random initialization

Effect of Unsupervised Pre-training



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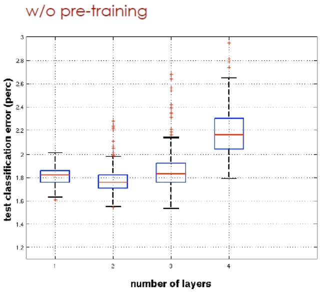

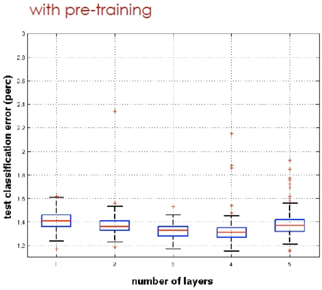

- Important topics we didn't talk about in detail/at all:
  - Joint unsupervised training of all layers (Wake-Sleep algorithm)
  - Deep Boltzmann Machines
  - Variational bounds justifying greedy layerwise training
  - Conditional RBMs, Multimodal RBMs, Temporal RBMs etc

Generative Adversarial Networks

Representations

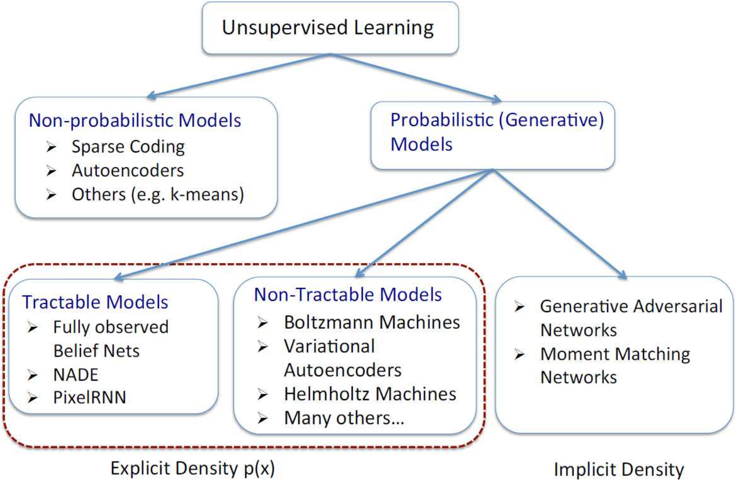

Figure: Ruslan Salakhutdinov

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- By playing an adversarial game!

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Goal

- Assume we have training samples $\mathcal{D} = \{X | X \sim P_{\text{data}}, X \in \mathcal{X}\}$
- We want a generative model P_{model} from which we can draw new samples $X \sim P_{\text{model}}$
- Such that $P_{\text{model}} \approx P_{\text{data}}$

$\mathbf{x} \sim p_{\text{data}}$

$\longrightarrow$

$\mathbf{x} \sim p_{\text{model}}$

Figure by Gilles Louppe

Generative Adversarial Networks (Goodfellow et al. 2014)

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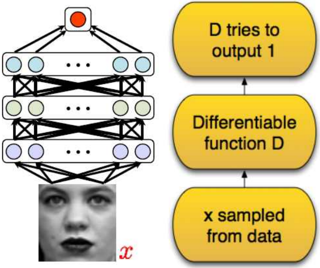
- Setup a two-player game between:
  - A Generator G
  - A Discriminator D
- The discriminator D tries to distinguish between a sample from P_{model} and a sample from G
- The generator G tries to *fool* D by producing samples that are hard to discriminate from the real data

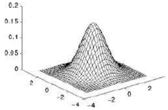
Catch me if you can

Leo is G Tom is D

Slide adapted from Gilles Louppe

Generative Adversarial Networks





Slide adapted from Ian Goodfellow

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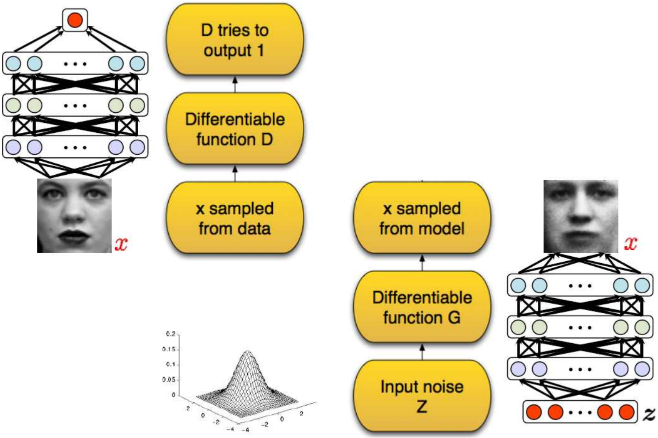

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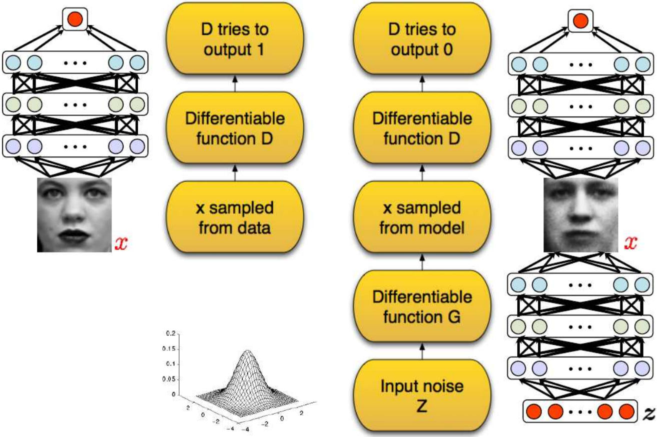

Slide adapted from Ian Goodfellow

Generative Adversarial Networks

- Minimax value function

Generator: generate samples that D would classify as real

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

Discriminator: Pushes up

Discriminator: Classify data as being real

Discriminator: Classify generator samples as being fake

Generator: Pushes down

- Optimal strategy for Discriminator is:

$$D(x) = \frac{p_{\text{data}}(x)}{p_{\text{data}}(x) + p_{\text{model}}(x)}$$

Slide adapted from Ian Goodfellow

Generative Adversarial Networks

- The value function:

$$V(D,G) = \mathbb{E}_{X\sim P_{\text{data}}}[\log(D(X))] + \mathbb{E}_{Z\sim P_{\text{noise}}}[\log(1 - D(G(X)))]$$

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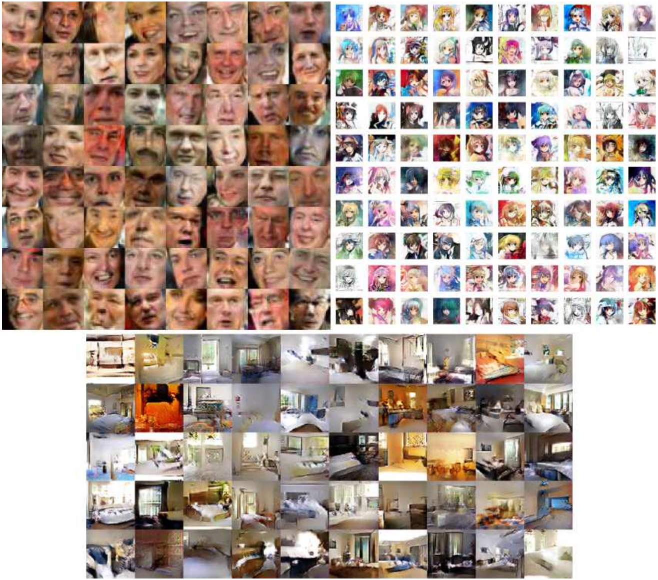
  - Fix D, find G which **minimizes** $V(D,G)$
- Alternate till convergence
- This is good since we can use the machinery for neural networks

Samples



Samples

- Open Question: How do you evaluate goodness of generated samples?

Next Time

- GANs wrap-up
- Quiz