Lecture 16
Deep Neural Generative Models

CMSC 35246: Deep Learning

Shubhendu Trivedi
&
Risi Kondor

University of Chicago

May 22, 2017

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- We don't construct a probabilistic model of the data
- Can't sample from the model

Representations

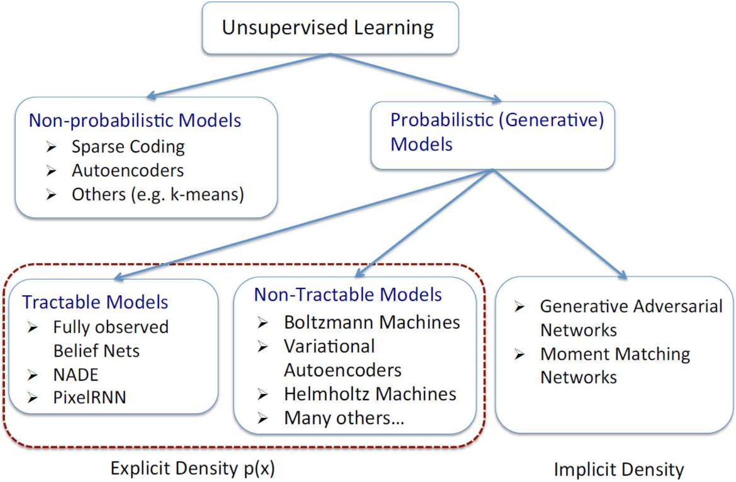

Figure: Ruslan Salakhutdinov

- To motivate Deep Neural Generative models, like before, let's seek inspiration from simple linear models first

Linear Factor Model

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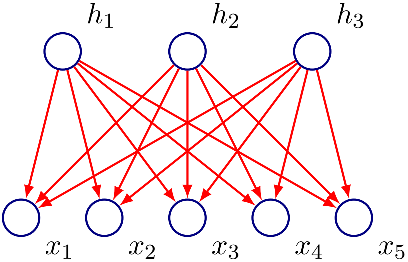
- Formally: Suppose we sample the latent factors from a distribution $\mathbf{h} \sim P(\mathbf{h})$
- Then: $\mathbf{x} = W\mathbf{h} + \mathbf{b} + \epsilon$

Linear Factor Model

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



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- How do learn in such a model?
- Let's look at a simple example

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- We care about the marginal $P(\mathbf{x})$ (predictive distribution):

$$P(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mathbf{b}, WW^T + \sigma^2 I)$$

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- Let $C = WW^T + \sigma^2 I$
- We want to maximize $\ell(\theta; X) = \sum_i \log P(\mathbf{x}_i|\theta)$

Probabilistic PCA: ML Estimation

$$\ell(\theta; X) = \sum_i \log P(\mathbf{x}_i|\theta)$$

$$= -\frac{N}{2}\log|C| - \frac{1}{2}\sum_i (\mathbf{x}_i - \mathbf{b})C^{-1}(\mathbf{x}_i - \mathbf{b})^T$$

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- Now fit the parameters $\theta = W, \mathbf{b}, \sigma$ to maximize log-likelihood
- Can also use EM

Factor Analysis

- Fix the latent factor prior to be the unit Gaussian as before:

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- Still consider linear relationship between inputs and observed variables: Marginal $P(\mathbf{x}) \sim \mathcal{N}(\mathbf{x}; b, WW^T + \Psi)$

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- Parameters are coupled, makes ML estimation difficult
- Need to employ EM (or non-linear optimization)

More General Models

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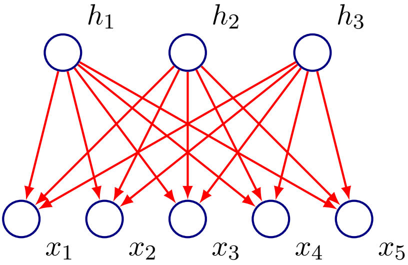
- The decoding of the input from the latent states can be a complicated non-linear function
- Estimation and inference can get complicated!

Earlier we had:



Quick Review

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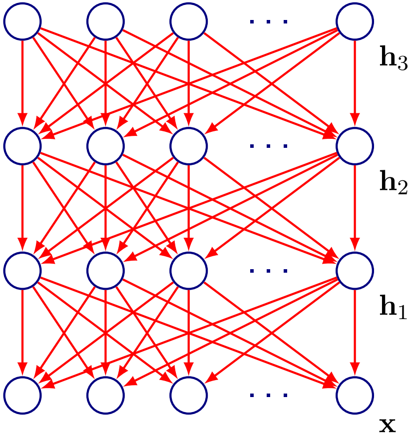
- The nodes represent random variables and arcs indicate dependency
- Some of the random variables are observed, others are hidden

Sigmoid Belief Networks



- Just like a feedfoward network, but with arrows reversed.

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- Marginalization yields $P(\mathbf{x})$, intractable in practice except for very small models

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- Deep Belief Networks are like Sigmoid Belief Networks except for the top two layers

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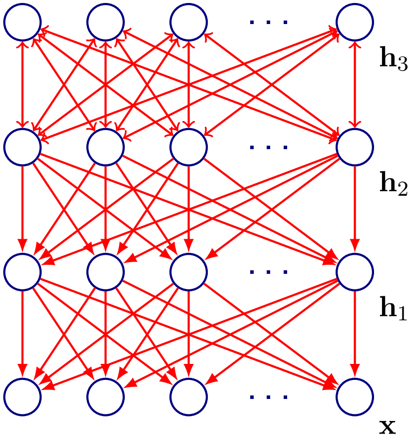
Deep Belief Networks



- The top two layers now have undirected edges

Deep Belief Networks

- The joint probability changes as:

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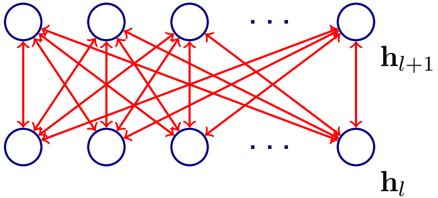

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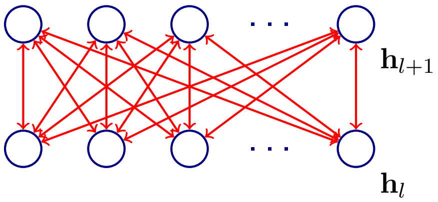

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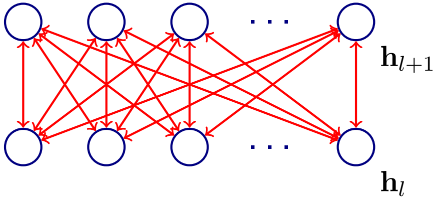

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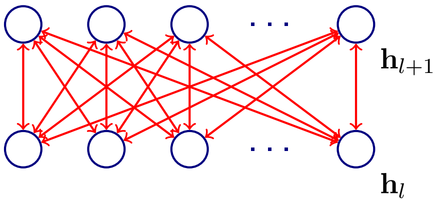

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- We will return to RBMs and training procedures in a while, but first we look at the mathematical machinery that will make our task easier

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- Energies are in the log-probability domain:

$$\text{Energy}(\mathbf{x}) = \log \frac{1}{(ZP(\mathbf{x}))}$$

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- How do we specify the energy function?

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- In this formulation, the energy function is:

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- We have the product of experts:

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

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- Contrast this with mixture models

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- Free Energy is just a marginalization of energies in the log-domain:

$$\text{FreeEnergy}(\mathbf{x}) = -\log \sum_{\mathbf{h}} \exp^{-(\text{Energy}(\mathbf{x},\mathbf{h}))}$$

Latent Variables

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- We have an expression for $P(\mathbf{x})$ (and hence for the data log-likelihood). Let us see how the gradient looks like

Data Log-Likelihood Gradient

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- Note that $P(\tilde{\mathbf{x}}) = \exp^{-(\text{FreeEnergy}(\tilde{\mathbf{x}}))}$

Data Log-Likelihood Gradient

- The expected log-likelihood gradient over the training set has the following form:

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

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

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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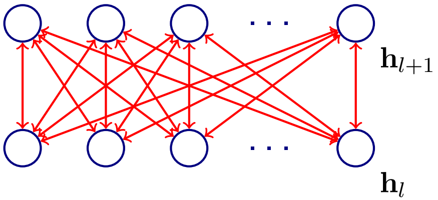
$$= -\beta - \sum_i \log \sum_{\mathbf{h}_i} \exp^{-\gamma_i(\mathbf{x},\mathbf{h}_i)}$$

Restricted Boltzmann Machines



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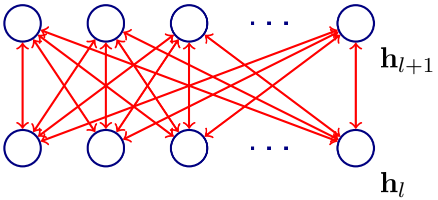

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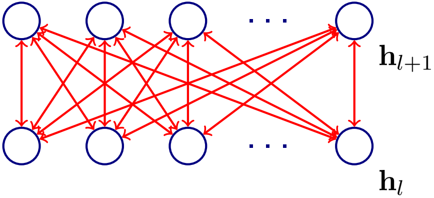

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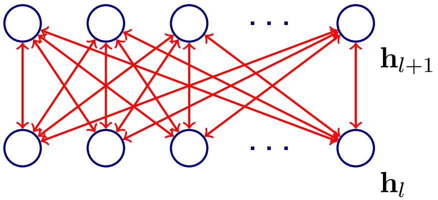

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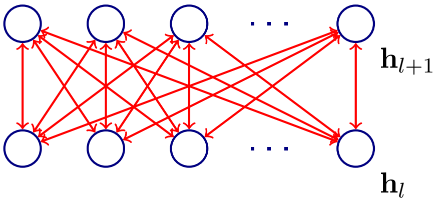

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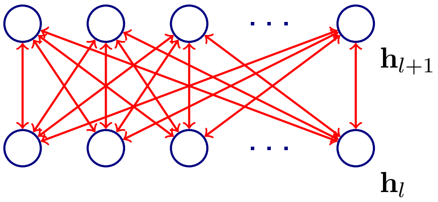

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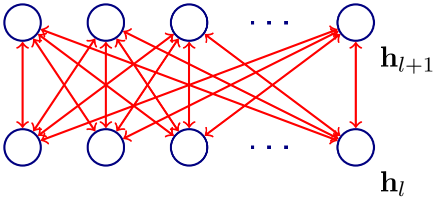
- The conditional probability:

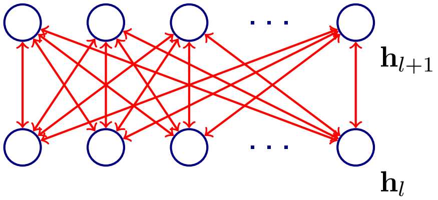
$$P(\mathbf{h}|\mathbf{x}) = \frac{\exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\mathbf{h} + \mathbf{h}^T W\mathbf{x}\right)}{\sum_{\tilde{\mathbf{h}}} \exp\left(\mathbf{b}^T\mathbf{x} + \mathbf{c}^T\tilde{\mathbf{h}} + \tilde{\mathbf{h}}^T W\mathbf{x}\right)} = \prod_i P(\mathbf{h}_i|\mathbf{x})$$

Restricted Boltzmann Machines



- $\mathbf{x}$ and $\mathbf{h}$ play symmetric roles:

Restricted Boltzmann Machines



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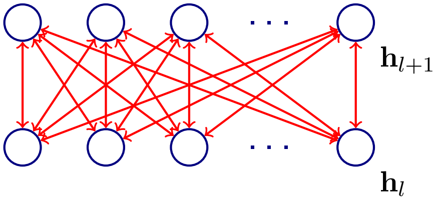

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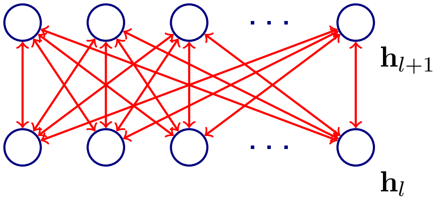

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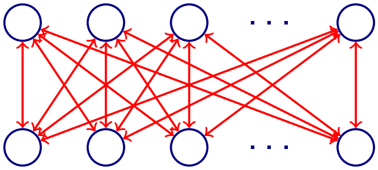

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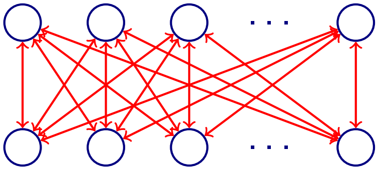

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Approximate Learning and Gibbs Sampling

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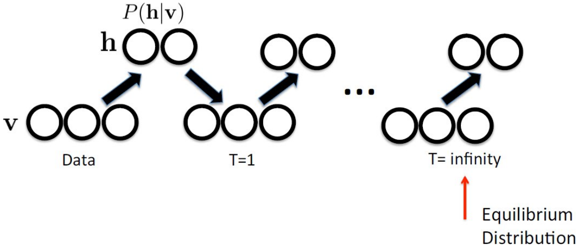
Approximate Learning, Alternating Gibbs Sampling



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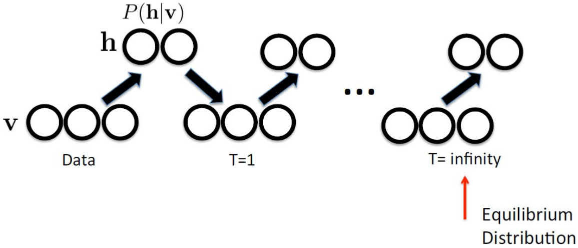

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Training a RBM: The Contrastive Divergence Algorithm

- Start with a training example on the visible units

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

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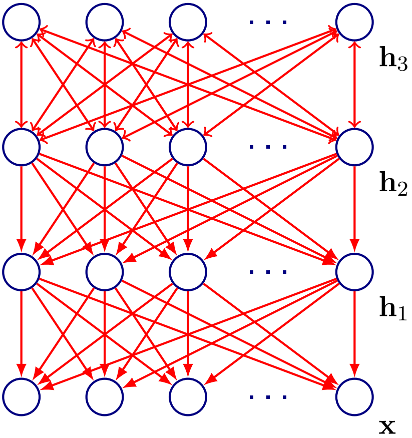
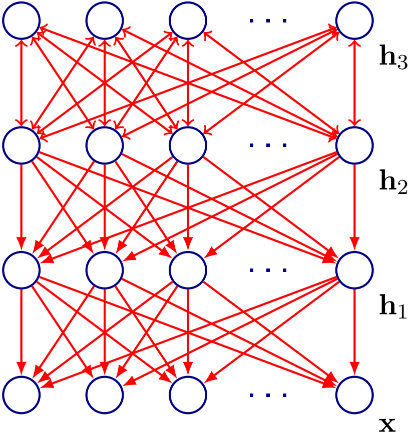
- Originally proposed by Hinton and Sejnowski (1983)
- Important historically. But very difficult to train (why?)

Back to Deep Belief Networks



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

Back to Deep Belief Networks



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- Can then be discriminatively fine-tuned using backpropagation

Deep Autoencoders (2006)

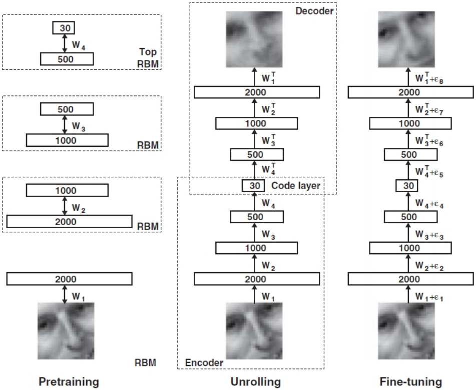
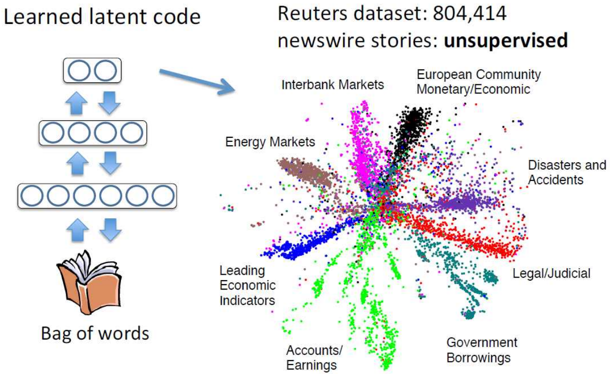


Fig. 1. Pretraining consists of learning a stack of restricted Boltzmann machines (RBMs), each having only one layer of feature detectors. The learned feature activations of one RBM are used as the "data" for training the next RBM in the stack. After the pretraining, the RBMs are "unrolled" to create 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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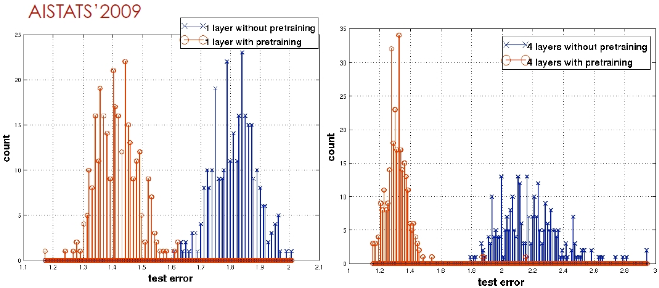
- Optimization: Unsupervised pre-training leads to better regions of the space i.e. better than random initialization

Effect of Unsupervised Pre-training



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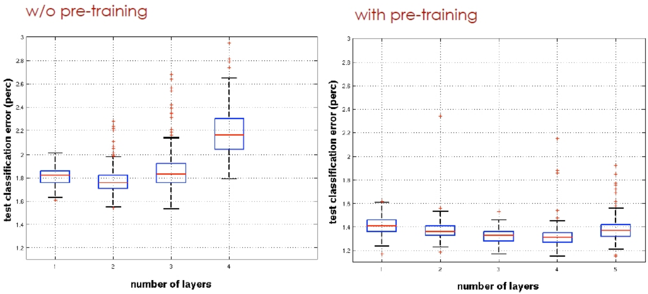

- Important topics we didn't talk about in detail/at all:
  - Joint unsupervised training of all layers (Wake-Sleep algorithm)
  - Deep Boltzmann Machines
  - Variational bounds justifying greedy layerwise training
  - Conditional RBMs, Multimodal RBMs, Temporal RBMs etc

Next Time

- Some Applications of methods we just considered

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