10707
Deep Learning

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Restricted Boltzmann Machines

Neural Networks Online Course

• **Disclaimer**: Much of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks:

• Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.

• We will use his material for some of the other lectures.

http://info.usherbrooke.ca/hlarochelle/neural_networks

Click with the mouse or tablet to draw with pen 2

RESTRICTED BOLTZMANN MACHINE

Topics: RBM, visible layer, hidden layer, energy function

$\mathbf{h}$ ← hidden layer (binary units)

b_j bias

$\mathbf{W}$ ← connections

c_k $\mathbf{x}$ ← visible layer (binary units)

Energy function:
$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h}$$
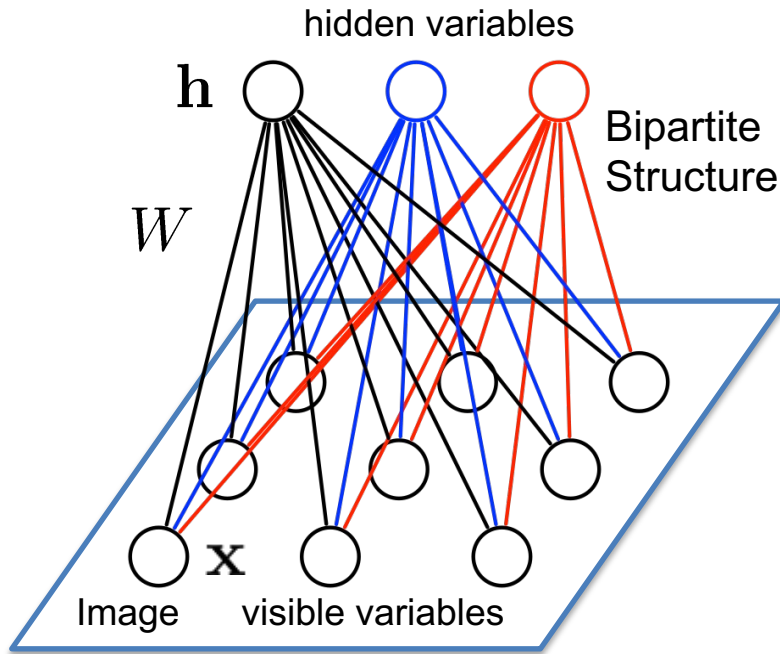$$= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j$$

Distribution: $p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$ ← partition function (intractable)

Unsupervised Learning

- Unsupervised learning: we only use the inputs $\mathbf{x}^{(t)}$ for learning

  - ➢ automatically extract meaningful features for your data

  - ➢ leverage the availability of unlabeled data

  - ➢ add a data-dependent regularizer to training ($-\log p(\mathbf{x}^{(t)})$)

- We will consider models for unsupervised learning that will form the basic building blocks for deeper models:

  - ➢ Restricted Boltzmann Machines

  - ➢ Autoencoders

Restricted Boltzmann Machines

hidden variables

$\mathbf{h}$

W

Bipartite Structure

Image   visible variables

$\mathbf{x}$

- Undirected bipartite graphical model

- Stochastic binary visible variables:

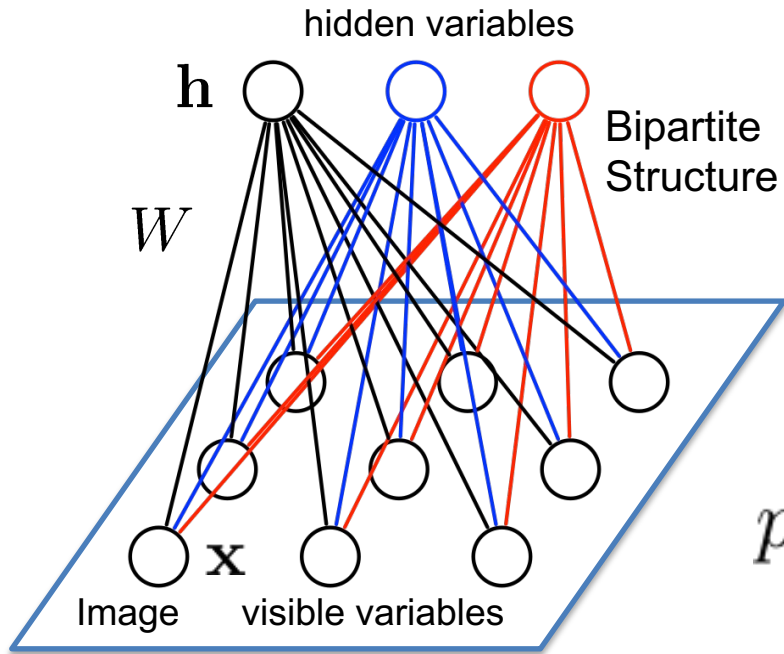$$\mathbf{x} \in \{\mathbf{0}, \mathbf{1}\}^{\mathbf{D}}$$

- Stochastic binary hidden variables:

$$\mathbf{h} \in \{0, 1\}^{F}$$

- The energy of the joint configuration:

$$
\begin{aligned}
E(\mathbf{x}, \mathbf{h}) &= -\mathbf{h}^{\top}\mathbf{W}\mathbf{x} - \mathbf{c}^{\top}\mathbf{x} - \mathbf{b}^{\top}\mathbf{h} \\
&= -\sum_{j}\sum_{k} W_{j,k} h_j x_k - \sum_{k} c_k x_k - \sum_{j} b_j h_j
\end{aligned}
$$

Markov random fields, Boltzmann machines, log-linear models.

Restricted Boltzmann Machines

hidden variables

$\mathbf{h}$

W

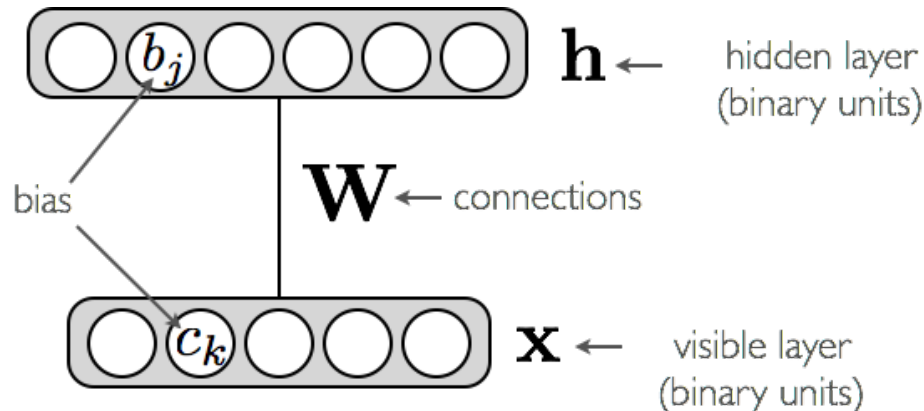Bipartite
Structure

Image   visible variables

$\mathbf{x}$

- Probability of the joint configuration is given by the Boltzmann distribution:

$$p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

Partition function (intractable)

$$Z = \sum_{\mathbf{x}, \mathbf{h}} \exp\left(-E(\mathbf{x}, \mathbf{h})\right)$$

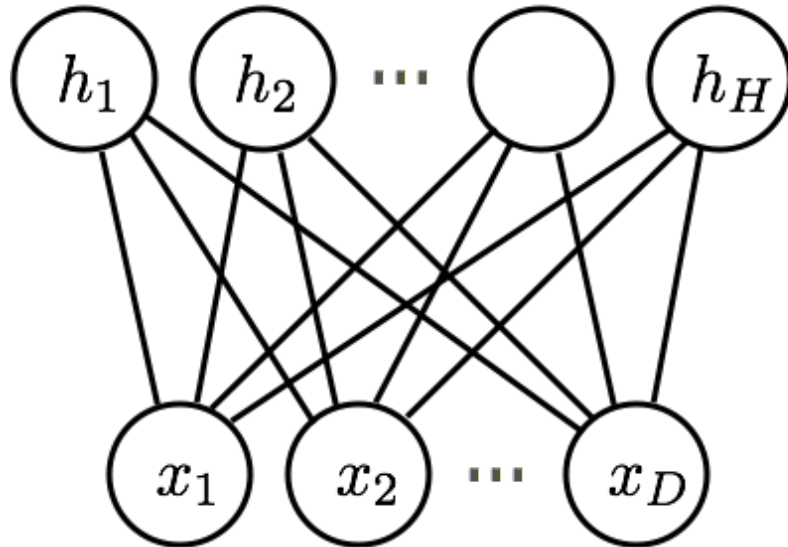Markov random fields, Boltzmann machines, log-linear models.

Restricted Boltzmann Machines

$$
\begin{aligned}
p(\mathbf{x}, \mathbf{h}) &= \exp(-E(\mathbf{x}, \mathbf{h}))/Z \\
&= \exp(\mathbf{h}^\top \mathbf{W} \mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z \\
&= \exp(\mathbf{h}^\top \mathbf{W} \mathbf{x}) \exp(\mathbf{c}^\top \mathbf{x}) \exp(\mathbf{b}^\top \mathbf{h})/Z
\end{aligned}
$$

Factors

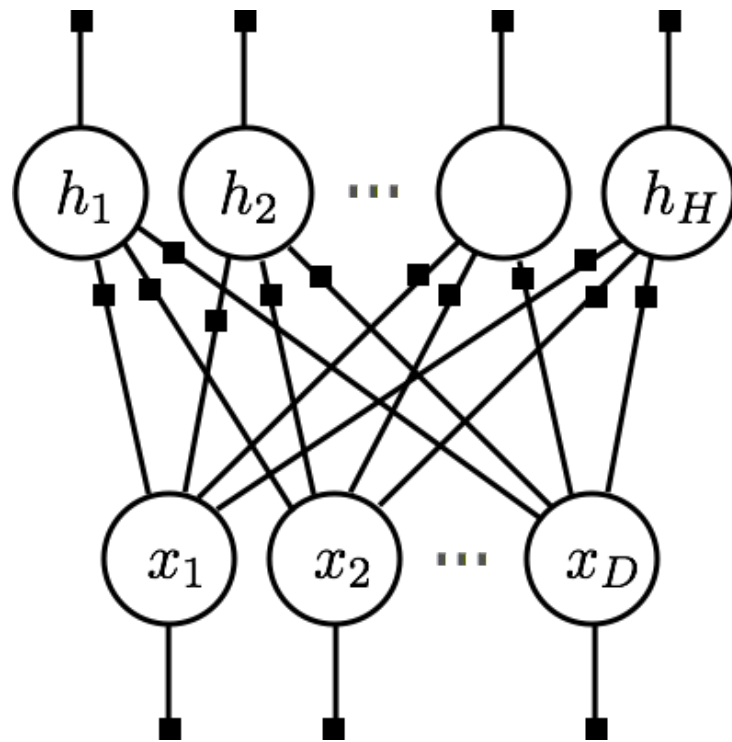• The notation based on an energy function is simply an alternative to the representation as the product of factors

Restricted Boltzmann Machines

Pair-wise factors

$$p(\mathbf{x}, \mathbf{h}) = \frac{1}{Z} \prod_j \prod_k \exp(W_{j,k} h_j x_k)$$

$$\prod_k \exp(c_k x_k)$$

Unary factors

$$\prod_j \exp(b_j h_j)$$

• The scalar visualization is more informative of the structure within the vectors.

Factor Graph View

Pair-wise factors

$$p(\mathbf{x}, \mathbf{h}) \;=\; \frac{1}{Z} \prod_j \prod_k \exp(W_{j,k} h_j x_k)$$

$$\prod_k \exp(c_k x_k)$$

$$\prod_j \exp(b_j h_j)$$

Unary factors

h_1 h_2 $\cdots$ h_H

x_1 x_2 $\cdots$ x_D

Inference

h hidden variables

Bipartite Structure

Image   **x** visible variables
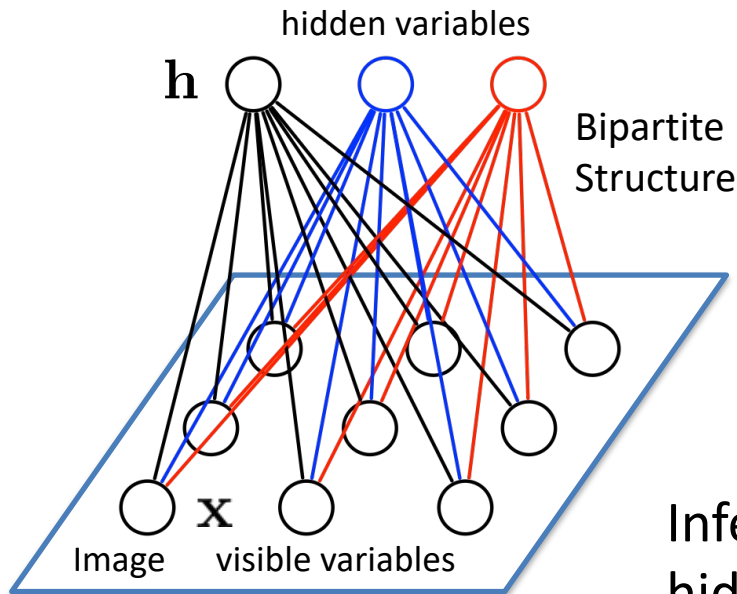
Restricted: No interaction between hidden variables

Inferring the distribution over the hidden variables is easy:

$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$
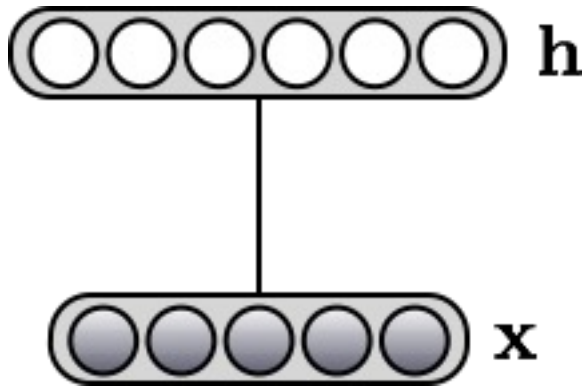
Factorizes: Easy to compute

Similarly:

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

Markov random fields, Boltzmann machines, log-linear models.
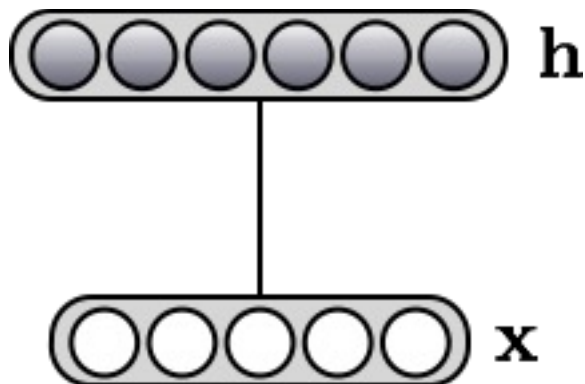
Inference

- Conditional Distributions:

$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

$$p(h_j = 1|\mathbf{x}) = \frac{1}{1 + \exp(-(b_j + \mathbf{W}_{j\cdot}\mathbf{x}))}$$

$$= \mathrm{sigm}(b_j + \mathbf{W}_{j\cdot}\mathbf{x})$$

jth row of W

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

$$p(x_k = 1|\mathbf{h}) = \frac{1}{1 + \exp(-(c_k + \mathbf{h}^\top \mathbf{W}_{\cdot k}))}$$

$$= \mathrm{sigm}(c_k + \mathbf{h}^\top \mathbf{W}_{\cdot k})$$

kth column of W

Local Markov Property

- In general, we have the following property:

$$
\begin{aligned}
p(z_i \mid z_1, \ldots, z_V) &= p(z_i \mid \mathrm{Ne}(z_i)) \\
&= \frac{p(z_i, \mathrm{Ne}(z_i))}{\sum_{z_i'} p(z_i', \mathrm{Ne}(z_i))} \\
&= \frac{\prod_{\substack{f \text{ involving } z_i \\ \text{and any } \mathrm{Ne}(z_i)}} \Psi_f(z_i, \mathrm{Ne}(z_i))}{\sum_{z_i'} \prod_{\substack{f \text{ involving } z_i \\ \text{and any } \mathrm{Ne}(z_i)}} \Psi_f(z_i', \mathrm{Ne}(z_i))}
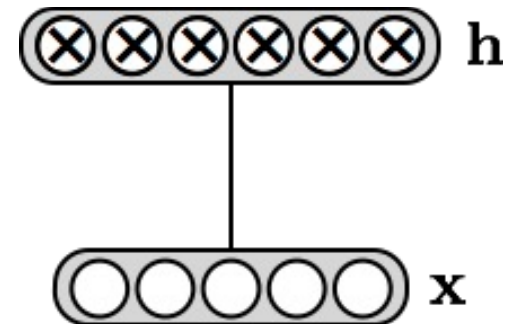\end{aligned}
$$

> z_i is any variable in the Markov network $(x_k$ or h_j in an RBM)
> $\mathrm{Ne}(z_i)$ are the neighbors of z_i in the Markov network

Free Energy

- What about computing marginal $p(\mathbf{x})$?

$$
\begin{aligned}
p(\mathbf{x}) &= \sum_{\mathbf{h} \in \{0,1\}^H} p(\mathbf{x}, \mathbf{h}) = \sum_{\mathbf{h} \in \{0,1\}^H} \exp(-E(\mathbf{x}, \mathbf{h}))/Z \\
&= \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \log(1 + \exp(b_j + \mathbf{W}_{j.}\mathbf{x}))\right)/Z \\
&= \exp(-F(\mathbf{x}))/Z
\end{aligned}
$$

Free Energy

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Free Energy

- What about computing marginal $p(\mathbf{x})$?

$$
\begin{aligned}
p(\mathbf{x}) &= \sum_{\mathbf{h} \in \{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W} \mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \sum_{h_1 \in \{0,1\}} \cdots \sum_{h_H \in \{0,1\}} \exp\left(\sum_j h_j \mathbf{W}_{j.} \mathbf{x} + b_j h_j\right)/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \left(\sum_{h_1 \in \{0,1\}} \exp(h_1 \mathbf{W}_{1.} \mathbf{x} + b_1 h_1)\right) \ldots \left(\sum_{h_H \in \{0,1\}} \exp(h_H \mathbf{W}_{H.} \mathbf{x} + b_H h_H)\right)/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \left(1 + \exp(b_1 + \mathbf{W}_{1.} \mathbf{x})\right) \ldots \left(1 + \exp(b_H + \mathbf{W}_{H.} \mathbf{x})\right)/Z \\
&= \exp(\mathbf{c}^\top \mathbf{x}) \exp(\log(1 + \exp(b_1 + \mathbf{W}_{1.} \mathbf{x}))) \ldots \exp(\log(1 + \exp(b_H + \mathbf{W}_{H.} \mathbf{x})))/Z \\
&= \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^H \log(1 + \exp(b_j + \mathbf{W}_{j.} \mathbf{x}))\right)/Z
\end{aligned}
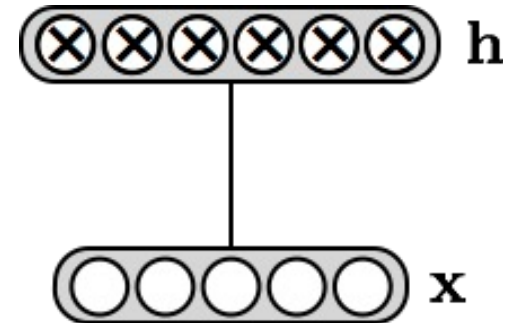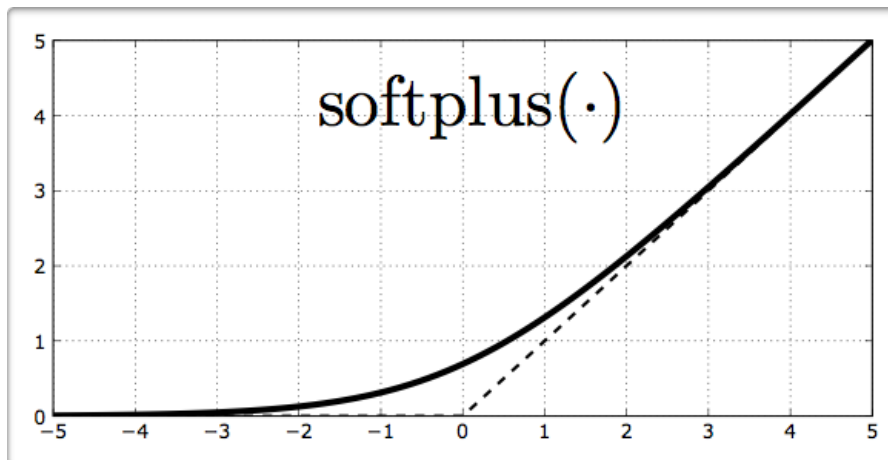$$

- Also known as Product of Experts model.

Free Energy

$$p(\mathbf{x}) \;=\; \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \log(1 + \exp(b_j + \mathbf{W}_{j.}\mathbf{x}))\right) / Z$$

$$\;=\; \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \text{softplus}(b_j + \mathbf{W}_{j.}\mathbf{x})\right) / Z$$
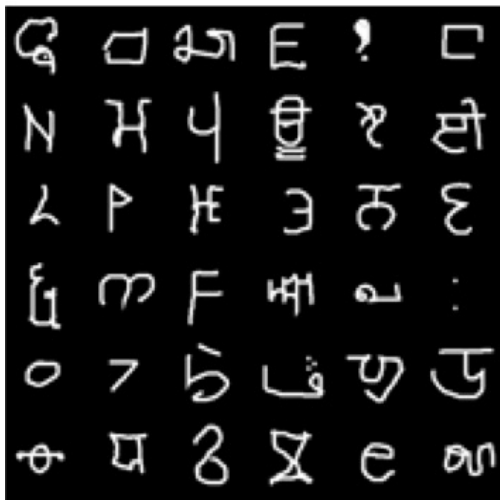
bias the probability
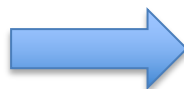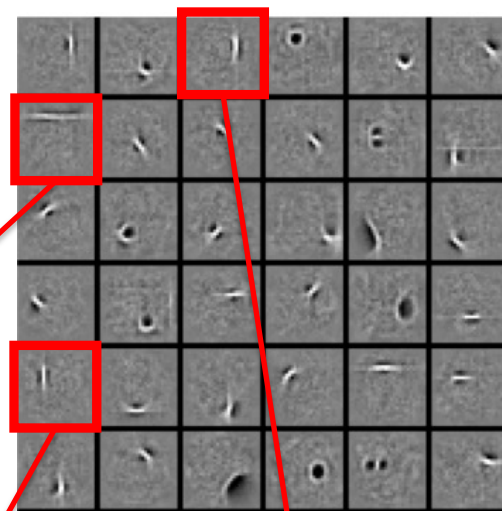of each x_i

bias of each
feature

feature expected
in x

softplus$(\cdot)$

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Learning Features

Observed Data
Subset of 25,000 characters

Learned W: "edges"
Subset of 1000 features

Most hidden variables are off

New Image: $p(h_7 = 1|v)$ $p(h_{29} = 1|v)$

$$= \sigma\left(0.99 \times \quad + \quad 0.97 \times \quad + \quad 0.82 \times \quad \cdots\right)$$
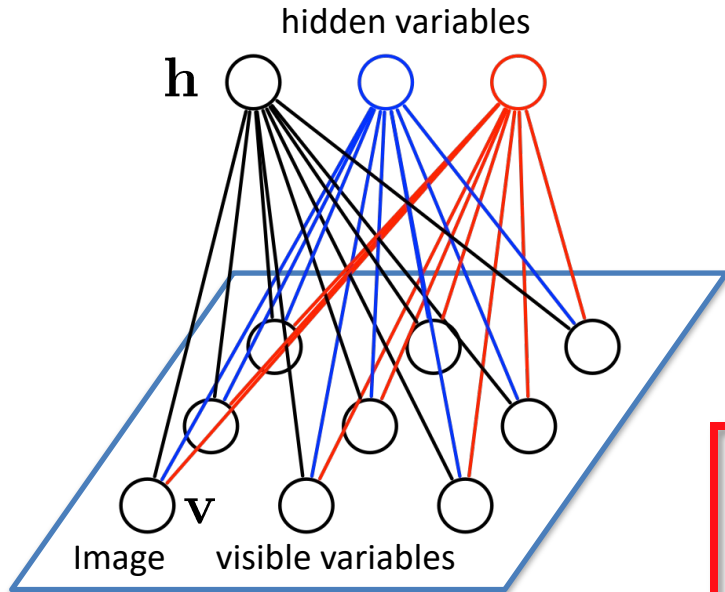
$\sigma(x) = \frac{1}{1 + \exp(-x)}$ Logistic Function: Suitable for modeling binary images
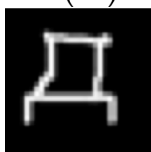
Represent: as $P(\mathbf{h}|\mathbf{v}) = [0, 0, 0.82, 0, 0, 0.99, 0, 0 \dots]$

Model Learning

hidden variables

$\mathbf{h}$

Image   visible variables

$\mathbf{v}$

• Given a set of *i.i.d.* training examples we want to minimize the average negative log-likelihood (NLL):

$$\frac{1}{T} \sum_t l(f(\mathbf{x}^{(t)})) = \frac{1}{T} \sum_t -\log p(\mathbf{x}^{(t)})$$

Remember:

$$p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

• Derivative of the negative log-likelihood objective:

$$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\bigg|\mathbf{x}^{(t)}\right] - \mathrm{E}_{\mathbf{x}, \mathbf{h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right]$$

Positive Phase

Negative Phase
Hard to compute

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Model Learning

hidden variables

$\mathbf{h}$

Image   visible variables

$\mathbf{v}$

$$p(\mathbf{x}, \mathbf{h}) = \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$
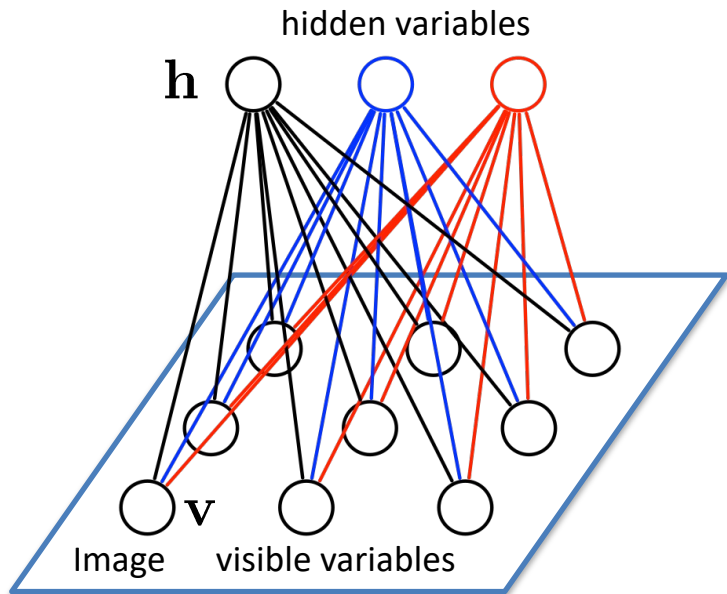
$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

• Derivative of the negative log-likelihood objective:

$$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\bigg|\mathbf{x}^{(t)}\right] - \mathrm{E}_{\mathbf{x}, \mathbf{h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right]$$

Data-Dependent
Expectations w.r.t P(h|x)

Model: Expectation
w.r.t joint P(x,h)

• Second term: intractable due to exponential number of configurations.

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Contrastive Divergence

- Key idea behind Contrastive Divergence:

  - ➢ Replace the expectation by a point estimate at $\tilde{\mathbf{x}}$

  - ➢ Obtain the point $\tilde{\mathbf{x}}$ by Gibbs sampling

  - ➢ Start sampling chain at $\mathbf{x}^{(t)}$

$$\sim p(\mathbf{h}|\mathbf{x}) \quad \sim p(\mathbf{x}|\mathbf{h})$$

$$\mathbf{x}^{(t)} \qquad \mathbf{x}^1 \qquad \mathbf{x}^k = \tilde{\mathbf{x}}$$

negative sample

Hinton, Neural Computation, 2002

Contrastive Divergence

- Intuition: $$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathrm{E}_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \bigg| \mathbf{x}^{(t)} \right] - \mathrm{E}_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right]$$

$$\mathrm{E}_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta} \bigg| \mathbf{x}^{(t)} \right] \approx \frac{\partial E(\mathbf{x}^{(t)}, \tilde{\mathbf{h}}^{(t)})}{\partial \theta} \qquad \mathrm{E}_{\mathbf{x}, \mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \right] \approx \frac{\partial E(\tilde{\mathbf{x}}, \tilde{\mathbf{h}})}{\partial \theta}$$

Contrastive Divergence

- Intuition:
$$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\Big|\mathbf{x}^{(t)}\right] - \mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right]$$

$$\mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\Big|\mathbf{x}^{(t)}\right] \approx \frac{\partial E(\mathbf{x}^{(t)}, \tilde{\mathbf{h}}^{(t)})}{\partial \theta} \qquad \mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right] \approx \frac{\partial E(\tilde{\mathbf{x}}, \tilde{\mathbf{h}})}{\partial \theta}$$
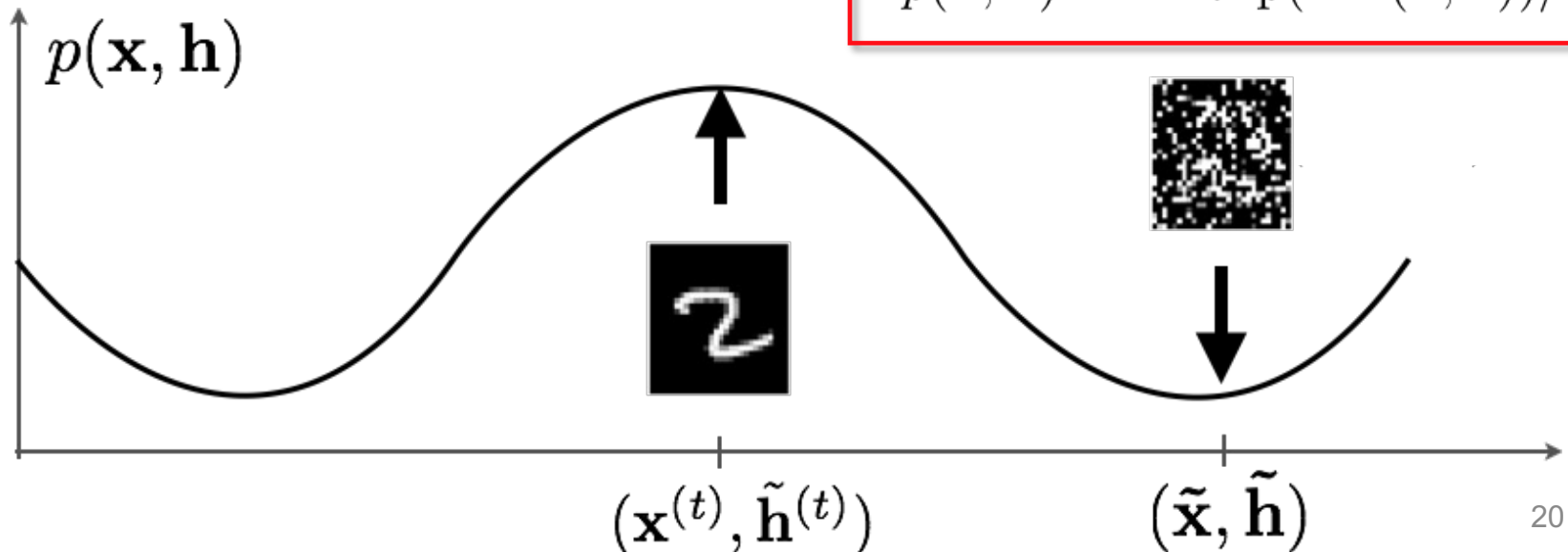
Remember:
$$p(\mathbf{x}, \mathbf{h}) \quad = \quad \exp(-E(\mathbf{x}, \mathbf{h}))/Z$$

$p(\mathbf{x}, \mathbf{h})$

$(\mathbf{x}^{(t)}, \tilde{\mathbf{h}}^{(t)})$ $(\tilde{\mathbf{x}}, \tilde{\mathbf{h}})$

Deriving Learning Rule

- Let us look at derivative of $\dfrac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}$ for $\theta = W_{jk}$

$$\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial W_{jk}} = \frac{\partial}{\partial W_{jk}} \left(-\sum_{jk} W_{jk} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \right)$$

$$= -\frac{\partial}{\partial W_{jk}} \sum_{jk} W_{jk} h_j x_k$$

$$= -h_j x_k$$

Remember:
$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h}$$

- Hence:

$$\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}\,\mathbf{x}^\top$$

Deriving Learning Rule

- Let us now derive $\mathbb{E}_{\mathbf{h}} \left[\dfrac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta} \Big| \mathbf{x} \right]$

$$\mathbb{E}_{\mathbf{h}} \left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial W_{jk}} \Big| \mathbf{x} \right] = \mathbb{E}_{\mathbf{h}} \left[-h_j x_k \Big| \mathbf{x} \right] = \sum_{h_j \in \{0,1\}} -h_j x_k p(h_j | \mathbf{x})$$

$$= -x_k p(h_j = 1 | \mathbf{x})$$

- Hence:

$$\mathbb{E}_{\mathbf{h}} \left[\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) | \mathbf{x} \right] = -\mathbf{h}(\mathbf{x}) \, \mathbf{x}^{\top}$$

$$\mathbf{h}(\mathbf{x}) \stackrel{\text{def}}{=} \begin{pmatrix} p(h_1 = 1 | \mathbf{x}) \\ \cdots \\ p(h_H = 1 | \mathbf{x}) \end{pmatrix}$$

$$= \text{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})$$

Deriving Learning Rule

- Hence:

$$\mathrm{E}_{\mathbf{h}}\left[\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) \,|\, \mathbf{x}\right] = -\mathbf{h}(\mathbf{x})\,\mathbf{x}^{\top}$$

$$\mathbf{h}(\mathbf{x}) \overset{\mathrm{def}}{=} \begin{pmatrix} p(h_1=1|\mathbf{x}) \\ \dots \\ p(h_H=1|\mathbf{x}) \end{pmatrix}$$

$$= \mathrm{sigm}(\mathbf{b} + \mathbf{W}\mathbf{x})$$

$$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\,\bigg|\,\mathbf{x}^{(t)}\right] - \mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right]$$

$$\sum_{\mathbf{x},\mathbf{h}} -\mathbf{h}(\mathbf{x})\mathbf{x}^{\top}\mathbf{P}(\mathbf{x}, \mathbf{h})$$

Easy to
compute exactly

Difficult to compute:
exponentially many
Configurations.

Approximate Learning

- An approximation to the gradient of the log-likelihood objective:

$$\frac{\partial - \log p(\mathbf{x}^{(t)})}{\partial \theta} = \mathbf{E_h}\left[\frac{\partial E(\mathbf{x}^{(t)}, \mathbf{h})}{\partial \theta}\bigg|\mathbf{x}^{(t)}\right] - \mathbf{E_{x,h}}\left[\frac{\partial E(\mathbf{x}, \mathbf{h})}{\partial \theta}\right]$$
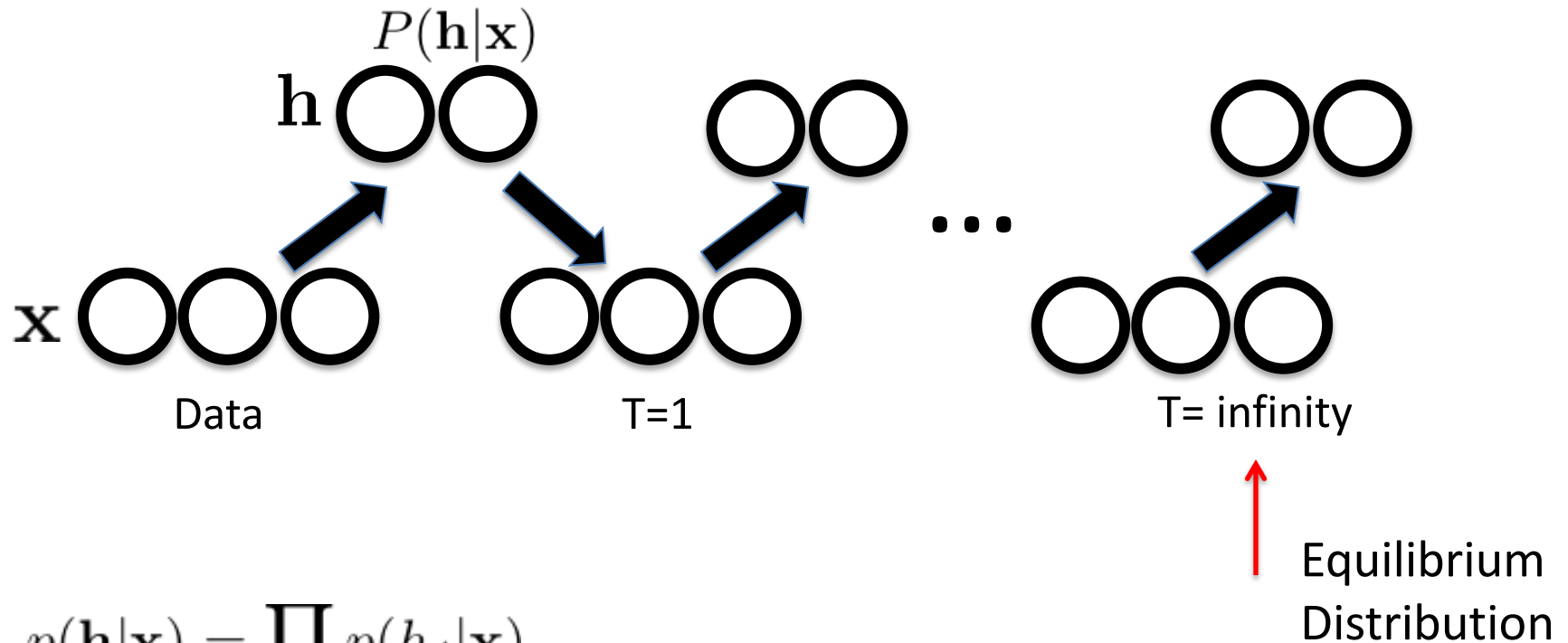
$$\sum_{\mathbf{x,h}} -\mathbf{h}(\mathbf{x})\mathbf{x}^\top \mathbf{P}(\mathbf{x}, \mathbf{h})$$

- Replace the average over all possible input configurations by samples.

- Run MCMC chain (Gibbs sampling) starting from the observed examples.

> - Initialize $x^0 = x$
> - Sample h^0 from $P(h \mid x^0)$
> - For t=1:T
>   - Sample x^t from $P(x \mid h^{t-1})$
>   - Sample h^t from $P(h \mid x^t)$

Approximate ML Learning for RBMs

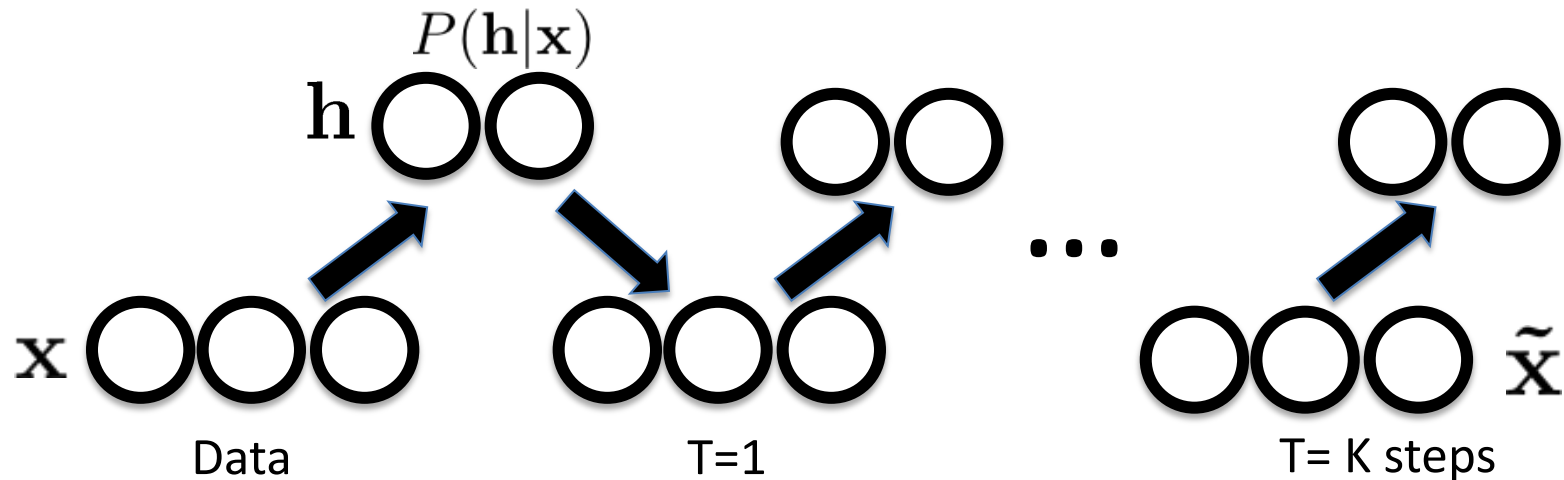Run Markov chain (alternating Gibbs Sampling):

$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

Contrastive Divergence

Run Markov chain (alternating Gibbs Sampling):

$P(\mathbf{h}|\mathbf{x})$

$\mathbf{h}$

$\mathbf{x}$

Data   T=1   T= K steps

$\tilde{\mathbf{x}}$

- K is typically set to 1.

$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

$$p(\mathbf{x}|\mathbf{h}) = \prod_k p(x_k|\mathbf{h})$$

Deriving Learning Rule

$$\mathbf{x}^{(t)} \qquad \tilde{\mathbf{x}} \qquad\qquad\qquad \theta = \mathbf{W}$$

$$
\begin{aligned}
\mathbf{W} \quad &\Longleftarrow \quad \mathbf{W} - \alpha \left(\nabla_{\mathbf{W}} - \log p(\mathbf{x}^{(t)}) \right) \\
&\Longleftarrow \quad \mathbf{W} - \alpha \left(\mathrm{E}_{\mathbf{h}} \left[\nabla_{\mathbf{W}} E(\mathbf{x}^{(t)}, \mathbf{h}) \, \middle| \, \mathbf{x}^{(t)} \right] - \mathrm{E}_{\mathbf{x},\mathbf{h}} \left[\nabla_{\mathbf{W}} E(\mathbf{x}, \mathbf{h}) \right] \right) \\
&\Longleftarrow \quad \mathbf{W} - \alpha \left(\mathrm{E}_{\mathbf{h}} \left[\nabla_{\mathbf{W}} E(\mathbf{x}^{(t)}, \mathbf{h}) \, \middle| \, \mathbf{x}^{(t)} \right] - \mathrm{E}_{\mathbf{h}} \left[\nabla_{\mathbf{W}} E(\tilde{\mathbf{x}}, \mathbf{h}) \, | \, \tilde{\mathbf{x}} \right] \right) \\
&\Longleftarrow \quad \mathbf{W} + \alpha \left(\mathbf{h}(\mathbf{x}^{(t)}) \, {\mathbf{x}^{(t)}}^{\top} - \mathbf{h}(\tilde{\mathbf{x}}) \, \tilde{\mathbf{x}}^{\top} \right)
\end{aligned}
$$

Learning rate

CD-k Algorithm

- For each training example $\mathbf{x}^{(t)}$

  ➢ Generate a negative sample $\tilde{\mathbf{x}}$ using k steps of Gibbs sampling, starting at the data point $\mathbf{x}^{(t)}$

  ➢ Update model parameters:

$$\mathbf{W} \quad \Longleftarrow \mathbf{W} + \alpha \left(\mathbf{h}(\mathbf{x}^{(t)}) \, \mathbf{x}^{(t)^\top} - \mathbf{h}(\tilde{\mathbf{x}}) \, \tilde{\mathbf{x}}^\top \right)$$

$$\mathbf{b} \quad \Longleftarrow \mathbf{b} + \alpha \left(\mathbf{h}(\mathbf{x}^{(t)}) - \mathbf{h}(\tilde{\mathbf{x}}) \right)$$

$$\mathbf{c} \quad \Longleftarrow \mathbf{c} + \alpha \left(\mathbf{x}^{(t)} - \tilde{\mathbf{x}} \right)$$

  ➢ Go back to 1 until stopping criteria

CD-k Algorithm

• CD-k: contrastive divergence with k iterations of Gibbs sampling

• In general, the bigger k is, the less biased the estimate of the gradient will be

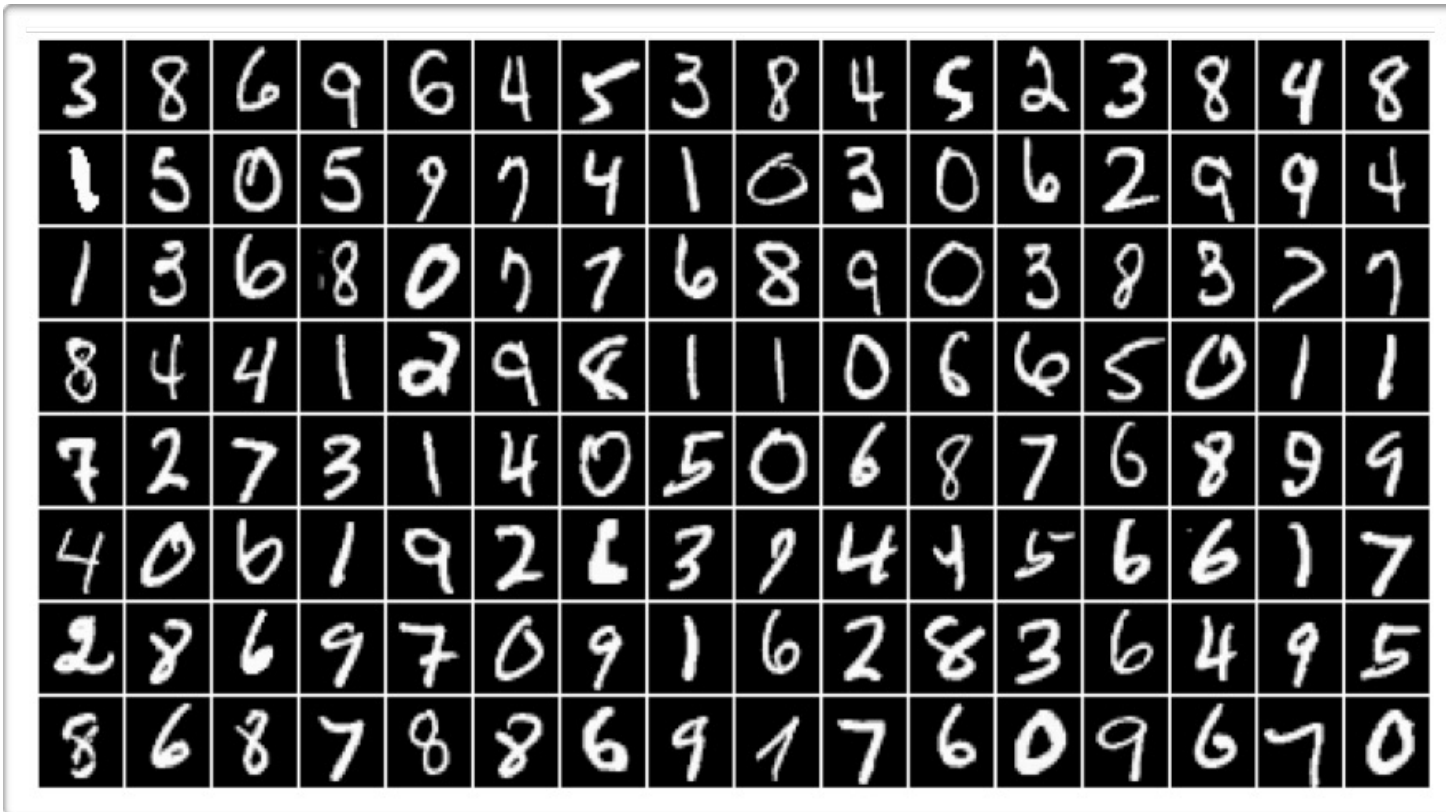• In practice, k=1 works well for learning good features and for pre-training

Persistent CD:
Stochastic ML Estimator

• Idea: instead of initializing the chain to $\mathbf{x}^{(t)}$, initialize the chain to the negative sample of the last iteration
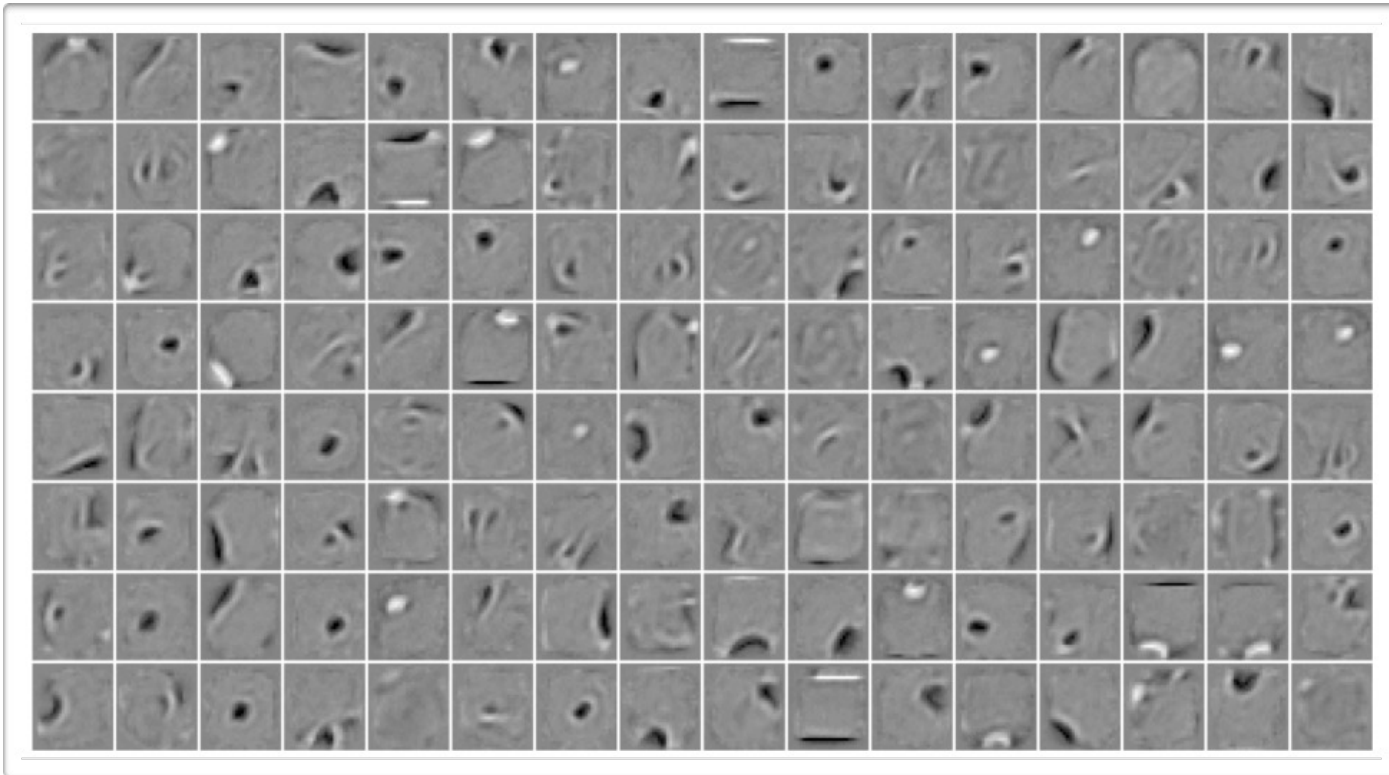
Tieleman, ICML, 2008
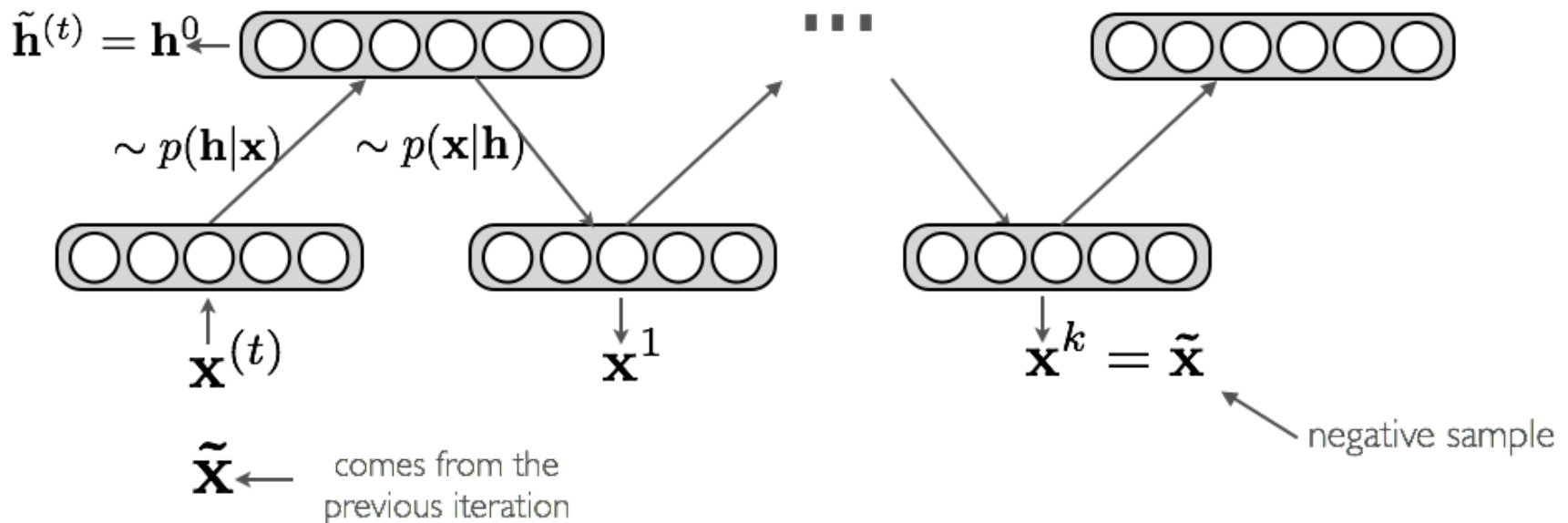
Example: MNIST

- MNIST dataset:

Learned Features

- MNIST dataset:

(Larochelle et al., JMLR 2009)

Tricks and Debugging

• Unfortunately, it is not easy to debug training RBMs (e.g. using gradient checks)

• We instead rely on approximate "tricks"

➢ we plot the average stochastic reconstruction $||\mathbf{x}^{(t)} - \tilde{\mathbf{x}}||^2$ and see if it tends to decrease

➢ for inputs that correspond to image, we visualize the connection coming into each hidden unit as if it was an image

➢ gives an idea of the type of visual feature each hidden unit detects

➢ we can also try to approximate the partition function Z and see whether the (approximated) NLL decreases
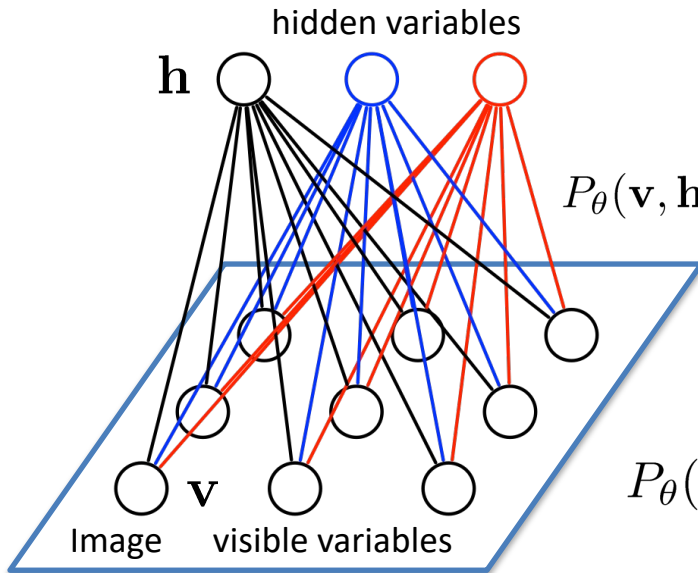
(Salakhutdinov, Murray, ICML 2008)

Gaussian Bernoulli RBMs

• Let x represent a real-valued (unbounded) input.

➢ add a quadratic term to the energy function

$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} + \tfrac{1}{2} \mathbf{x}^\top \mathbf{x}$$

➢ In this case $p(\mathbf{x}|\mathbf{h})$ becomes a Gaussian distribution with mean $\boldsymbol{\mu} = \mathbf{c} + \mathbf{W}^\top \mathbf{h}$ and identity covariance matrix

➢ recommend to normalize the training set by:

 • subtracting the mean of each input

 • dividing each input by the training set standard deviation

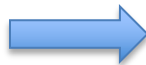➢ should use a smaller learning rate than in the regular RBM

Gaussian Bernoulli RBMs

h   hidden variables

Pair-wise   **Unary**

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{i=1}^{D}\sum_{j=1}^{F} W_{ij} h_j \frac{v_i}{\sigma_i} + \sum_{i=1}^{D} \frac{(v_i - b_i)^2}{2\sigma_i^2} + \sum_{j=1}^{F} a_j h_j \right)$$

$$\theta = \{W, a, b\}$$

Image   visible variables

$$P_\theta(\mathbf{v}|\mathbf{h}) = \prod_{i=1}^{D} P_\theta(v_i|\mathbf{h}) = \prod_{i=1}^{D} \mathcal{N}\left(b_i + \sum_{j=1}^{F} W_{ij} h_j, \sigma_i^2 \right)$$

Learned features (out of 10,000)

4 million **unlabelled** images
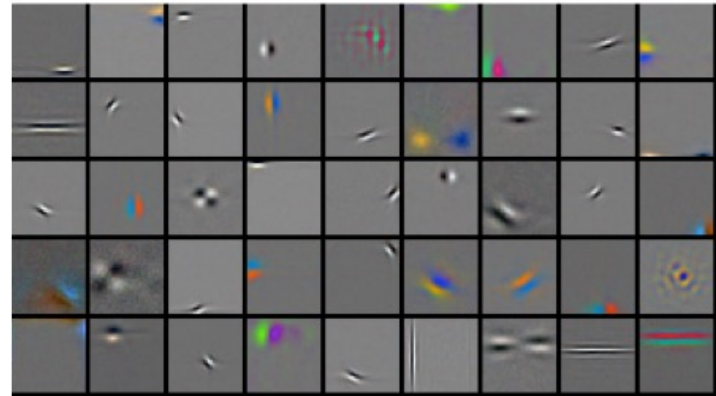

(Notation: vector x is replaced with v).

Gaussian Bernoulli RBMs

4 million unlabelled images

Learned features (out of 10,000)

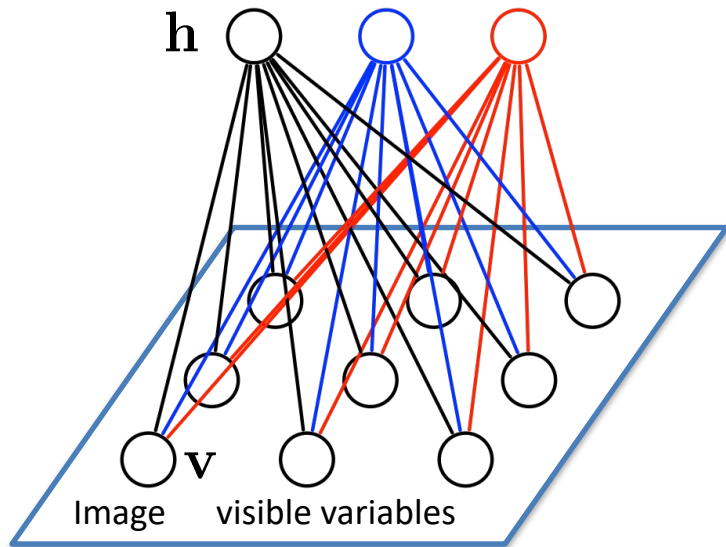$p(h_7 = 1|v)$ $p(h_{29} = 1|v)$

 $= 0.9 *$ $+ 0.8 *$ $+ 0.6 *$ $\ldots$

New Image

RBMs for Images

Gaussian-Bernoulli RBM:

$\mathbf{h}$

$\mathbf{v}$

Image   visible variables
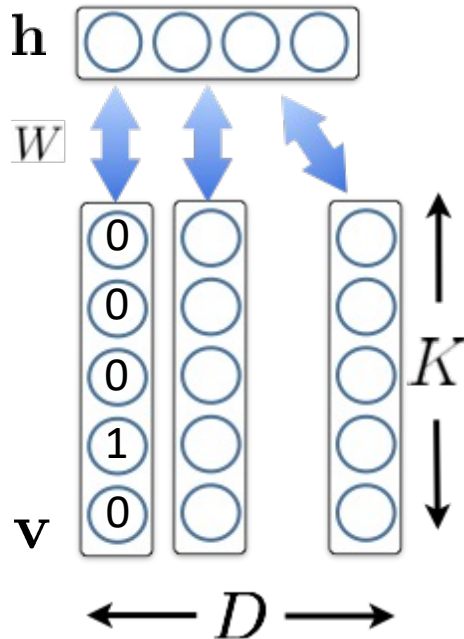
Interpretation: Mixture of exponential number of Gaussians

$$P_\theta(\mathbf{v}) = \sum_{\mathbf{h}} P_\theta(\mathbf{v}|\mathbf{h}) P_\theta(\mathbf{h}),$$

where

$$P_\theta(\mathbf{h}) = \int_{\mathbf{v}} P_\theta(\mathbf{v}, \mathbf{h}) d\mathbf{v} \quad \text{is an implicit prior, and}$$

$$P(v_i = x|\mathbf{h}) = \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left(-\frac{(x - b_i - \sigma_i \sum_j W_{ij}h_j)^2}{2\sigma_i^2}\right) \quad \text{Gaussian}$$

RBMs for Word Counts

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\overbrace{\sum_{i=1}^{D} \sum_{k=1}^{K} \sum_{j=1}^{F} W_{ij}^k v_i^k h_j}^{\text{Pair-wise}} + \overbrace{\sum_{i=1}^{D} \sum_{k=1}^{K} v_i^k b_i^k}^{\text{Unary}} + \overbrace{\sum_{j=1}^{F} h_j a_j}^{} \right)$$
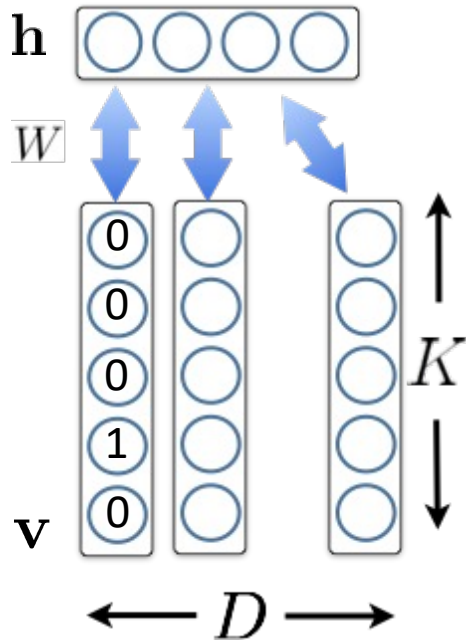
$$\theta = \{W, a, b\}$$

$$P_\theta(v_i^k = 1 | \mathbf{h}) = \frac{\exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k \right)}{\sum_{q=1}^{K} \exp\left(b_i^q + \sum_{j=1}^{F} h_j W_{ij}^q \right)}$$

Replicated Softmax Model: undirected topic model:

- Stochastic 1-of-K visible variables.
- Stochastic binary hidden variables $\mathbf{h} \in \{0, 1\}^F$.
- Bipartite connections.

(Salakhutdinov & Hinton, NIPS 2010, Srivastava & Salakhutdinov, NIPS 2012)

RBMs for Word Counts

Pair-wise   **Unary**

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp \left(\sum_{i=1}^{D} \sum_{k=1}^{K} \sum_{j=1}^{F} W_{ij}^k v_i^k h_j + \sum_{i=1}^{D} \sum_{k=1}^{K} v_i^k b_i^k + \sum_{j=1}^{F} h_j a_j \right)$$
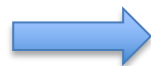
$$\theta = \{W, a, b\}$$

$$P_\theta(v_i^k = 1 | \mathbf{h}) = \frac{\exp\left(b_i^k + \sum_{j=1}^{F} h_j W_{ij}^k\right)}{\sum_{q=1}^{K} \exp\left(b_i^q + \sum_{j=1}^{F} h_j W_{ij}^q\right)}$$

REUTERS

AP Associated Press

WIKIPEDIA
The Free Encyclopedia

Reuters dataset:
804,414 **unlabeled**
newswire stories
Bag-of-Words

Learned features: ``topics''

| russian	clinton	computer	trade	stock
russia	house	system	country	wall
moscow	president	product	import	street
yeltsin	bill	software	world	point
soviet	congress	develop	economy	dow

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RBMs for Word Counts

One-step reconstruction from the Replicated Softmax model.

Input	Reconstruction
chocolate, cake	cake, chocolate, sweets, dessert, cupcake, food, sugar, cream, birthday
nyc	nyc, newyork, brooklyn, queens, gothamist, manhattan, subway, streetart
dog	dog, puppy, perro, dogs, pet, filmshots, tongue, pets, nose, animal
flower, high, 花	flower, 花, high, japan, sakura, 日本, blossom, tokyo, lily, cherry
girl, rain, station, norway	norway, station, rain, girl, oslo, train, umbrella, wet, railway, weather
fun, life, children	children, fun, life, kids, child, playing, boys, kid, play, love
forest, blur	forest, blur, woods, motion, trees, movement, path, trail, green, focus
españa, agua, granada	españa, agua, spain, granada, water, andalucía, naturaleza, galicia, nieve

Collaborative Filtering

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{ijk} W_{ij}^k v_i^k h_j + \sum_{ik} b_i^k v_i^k + \sum_j a_j h_j \right)$$

Binary hidden: user preferences
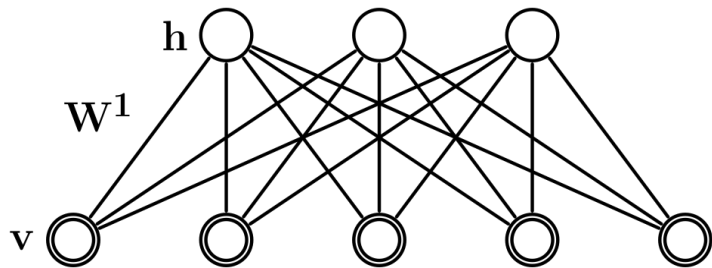
Multinomial visible: user ratings

Netflix dataset:

480,189 users

17,770 movies

Over 100 million ratings

Learned features: ``genre''

Fahrenheit 9/11	Independence Day
Bowling for Columbine	The Day After Tomorrow
The People vs. Larry Flynt	Con Air
Canadian Bacon	Men in Black II
La Dolce Vita	Men in Black

Friday the 13th	Scary Movie
The Texas Chainsaw Massacre	Naked Gun
Children of the Corn	Hot Shots!
Child's Play	American Pie
The Return of Michael Myers	Police Academy

State-of-the-art performance
on the Netflix dataset.

(Salakhutdinov, Mnih, Hinton, ICML 2007)

Different Data Modalities

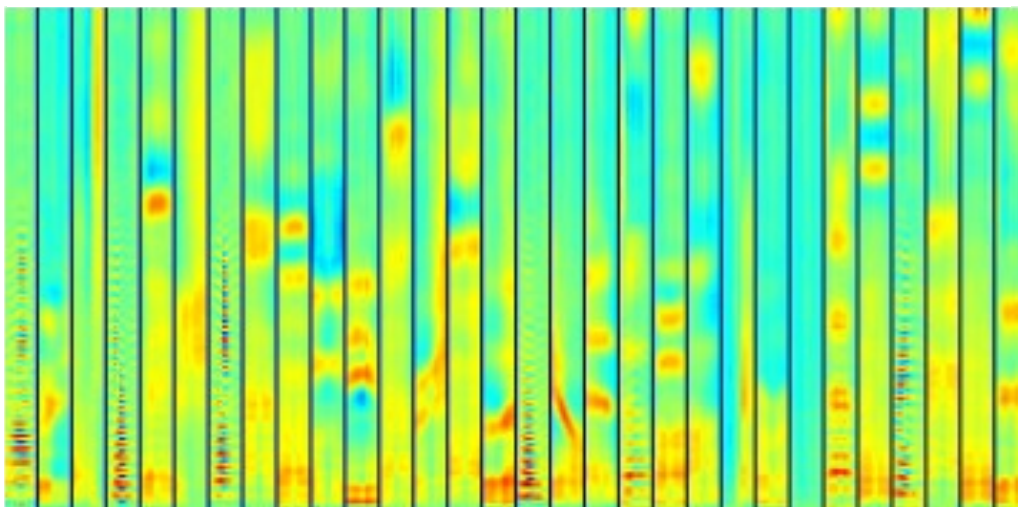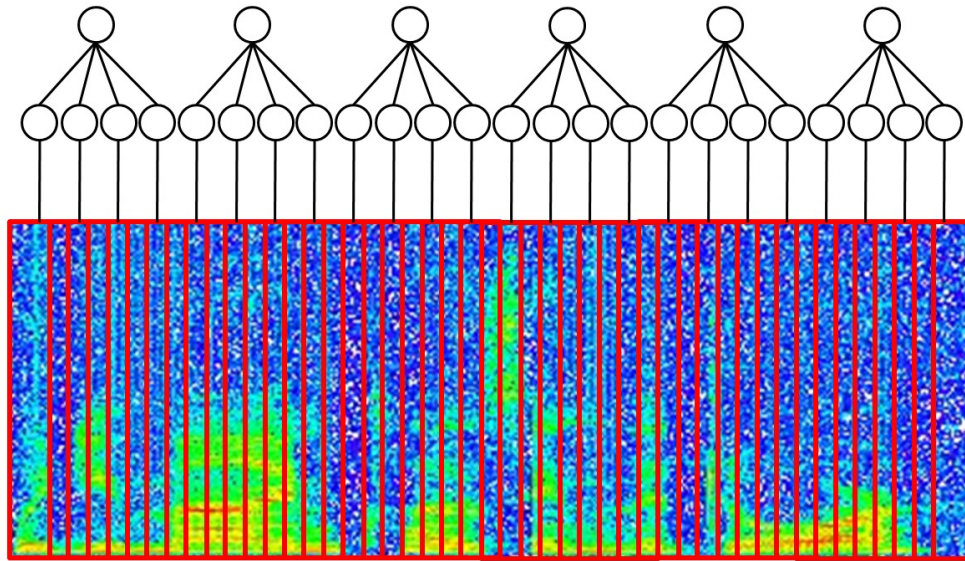• Binary/Gaussian/Softmax RBMs: All have binary hidden variables but use them to model different kinds of data.

Binary

Real-valued

1-of-K
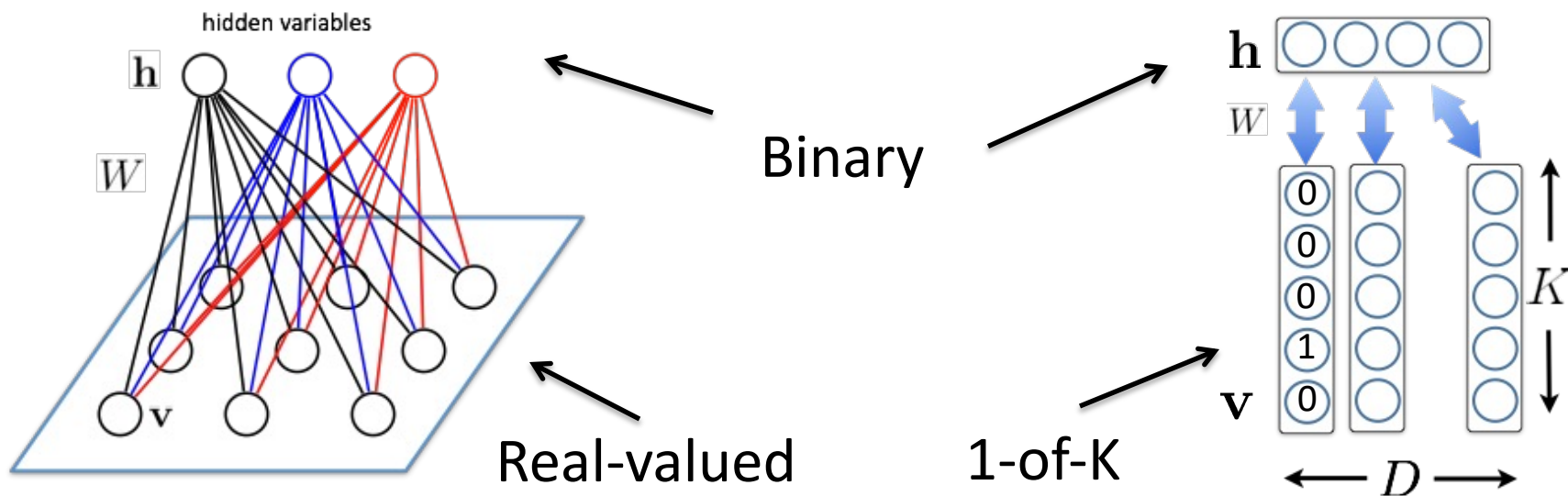
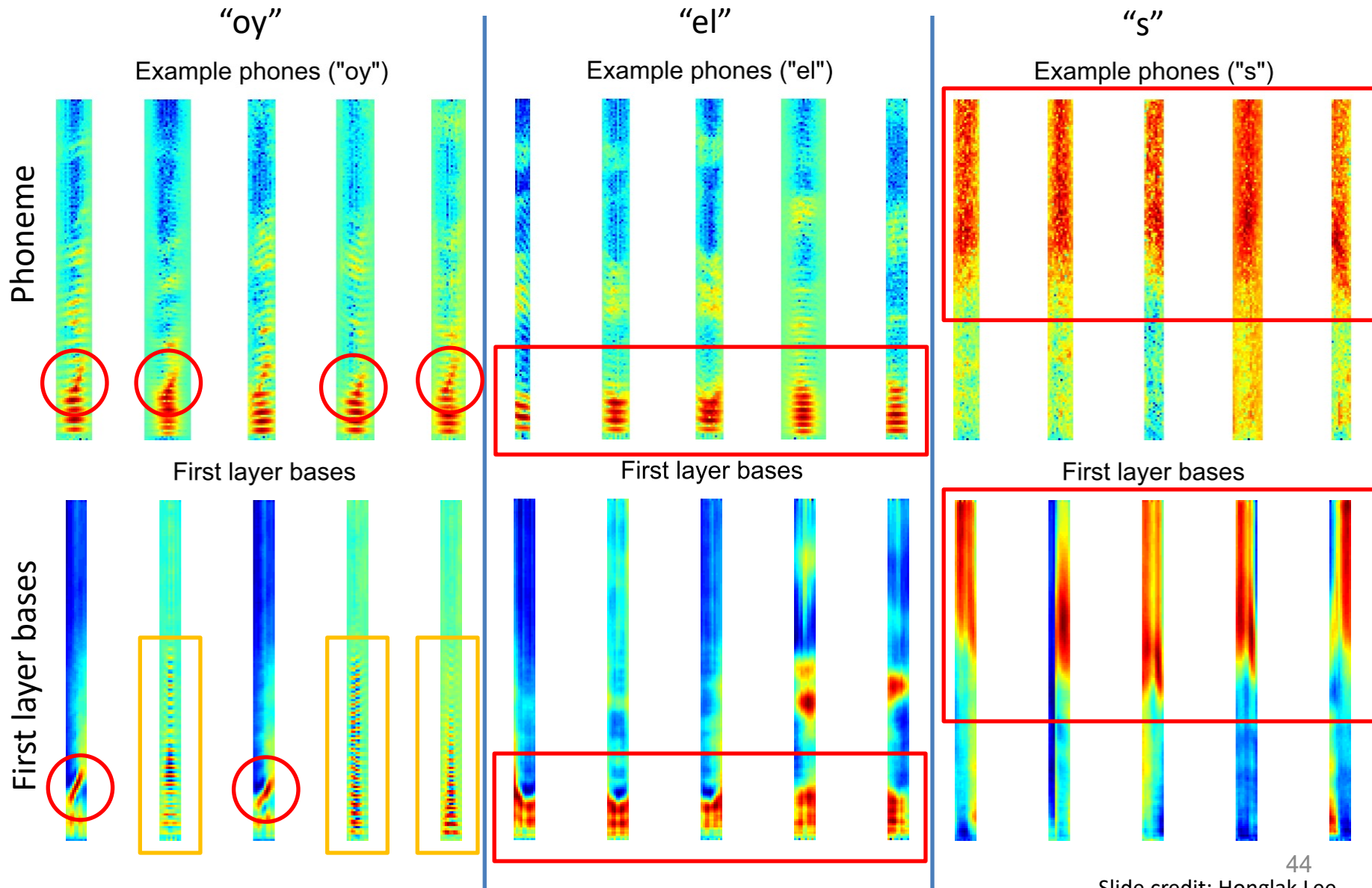• It is easy to infer the states of the hidden variables:

$$P_\theta(\mathbf{h}|\mathbf{v}) = \prod_{j=1}^{F} P_\theta(h_j|\mathbf{v}) = \prod_{j=1}^{F} \frac{1}{1 + \exp(-a_j - \sum_{i=1}^{D} W_{ij} v_i)}$$

Speech

Learned first-layer bases

Lee et.al., NIPS 2009

Comparison of bases to phonemes

Slide credit: Honglak Lee

Product of Experts
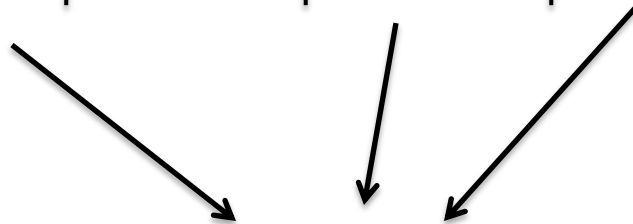
The joint distribution is given by:

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{ij} W_{ij} v_i h_j + \sum_i b_i v_i + \sum_j a_j h_j\right)$$

Marginalizing over hidden variables:

Product of Experts

$$P_\theta(\mathbf{v}) = \sum_{\mathbf{h}} P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \prod_i \exp(b_i v_i) \prod_j \left(1 + \exp(a_j + \sum_i W_{ij} v_i)\right)$$

government	clinton	bribery	mafia	stock	…
authority	house	corruption	business	wall	
power	president	dishonesty	gang	street	
empire	bill	corrupt	mob	point	
federation	congress	fraud	insider	dow	

Silvio Berlusconi

Topics "government", "corruption" and "mafia" can combine to give very high probability to a word "Silvio Berlusconi".

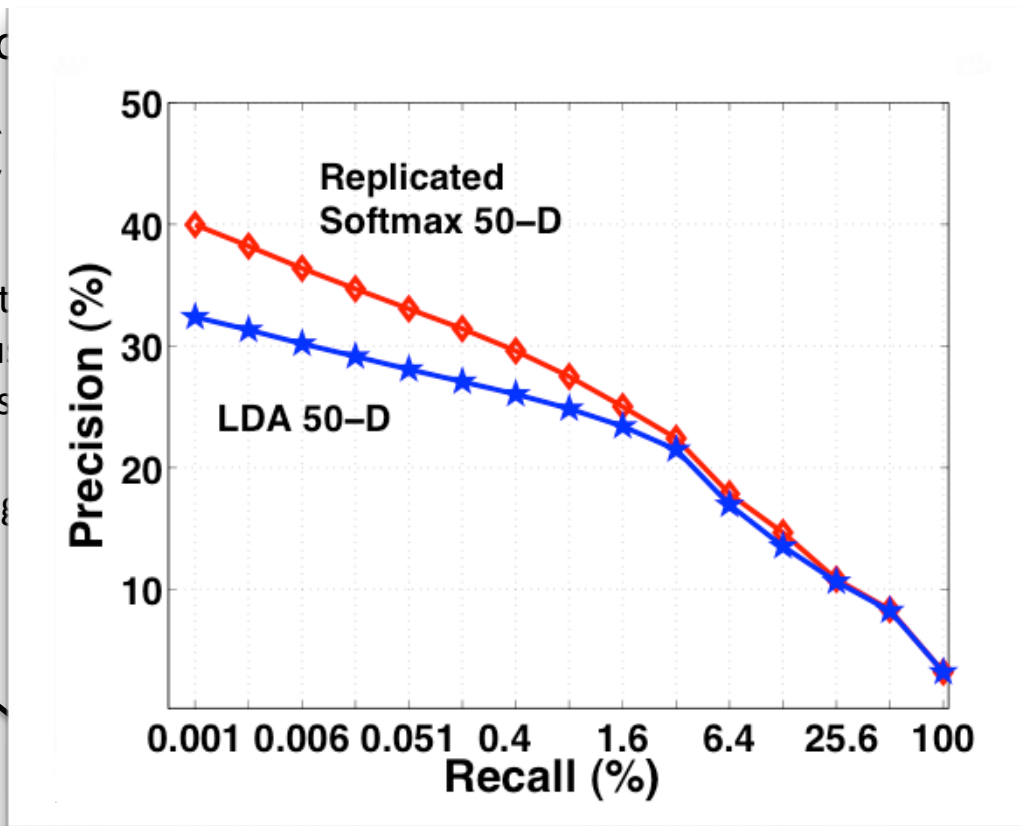# Product of Experts

The joint distribution is given by:

$$P_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{\mathcal{Z}(\theta)} \exp\left(\sum_{ij} W_{ij} v_i h_j + \sum_i b_i v_i + \sum_j a_j h_j\right)$$

Marginalizing **duct of Experts**

$$P_\theta(\mathbf{v}) = \sum_{\mathbf{h}} \qquad \qquad W_{ij} v_i\big)$$

government   clint
authority   hou
power   pres
empire   bill
federation   cong

"corruption" and
to give very high
"Silvio

Berlusconi".

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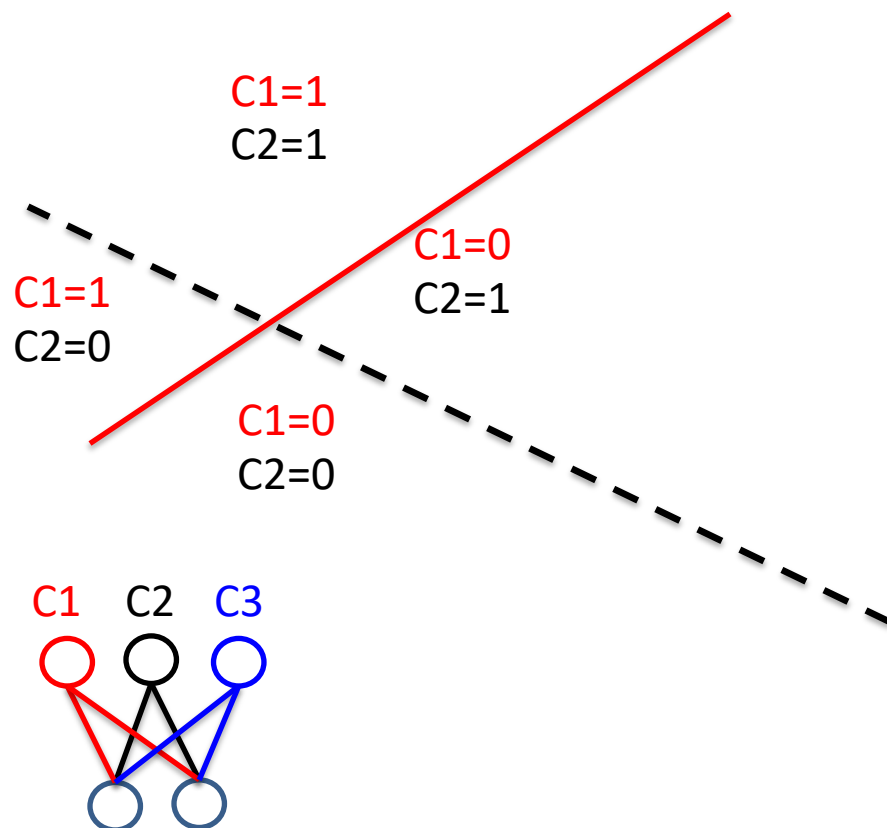# Local vs. Distributed Representations

- Clustering, Nearest Neighbors, RBF SVM, local density estimators

- RBMs, Factor models, PCA, Sparse Coding, Deep models

- Parameters for each region.
- # of regions is linear with # of parameters.

C1=1
C2=1

C1=0
C2=1

C1=1
C2=0

C1=0
C2=0

C1   C2   C3

Learned prototypes

Bengio, 2009, Foundations and Trends in Machine Learning
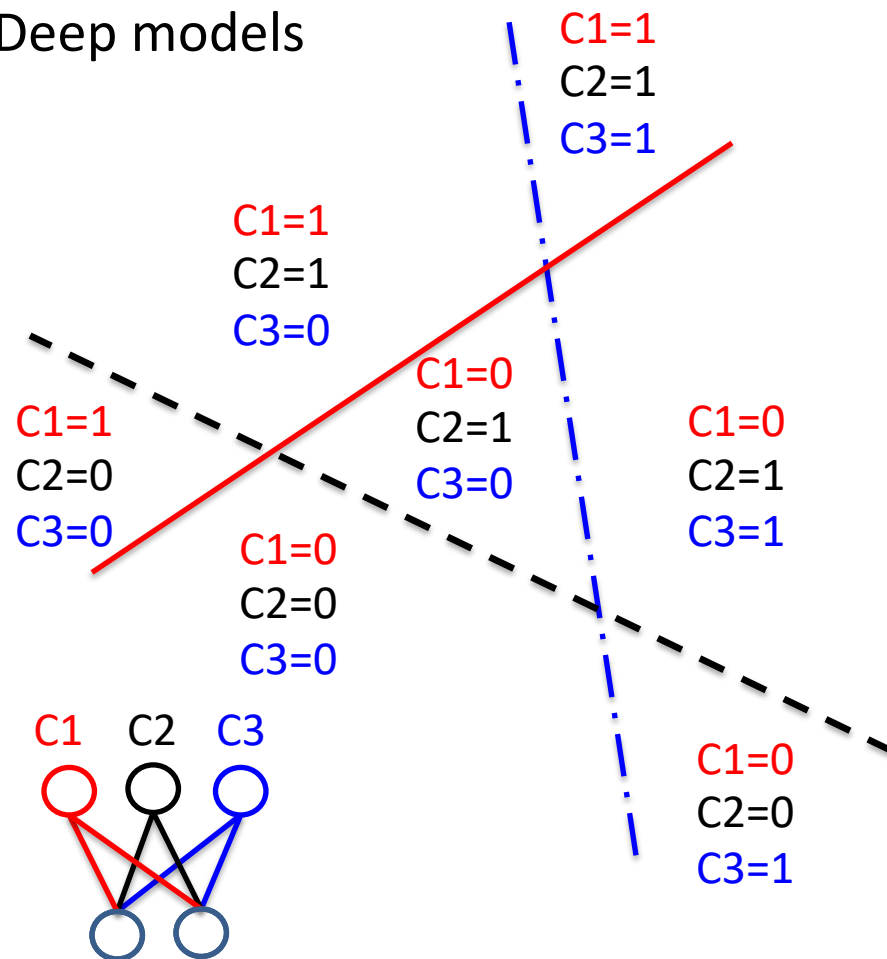
Local vs. Distributed Representations

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Learned prototypes

C1=1
C2=1
C3=1

C1=1
C2=1
C3=0

C1=0
C2=1
C3=0

C1=1
C2=0
C3=0

C1=0
C2=1
C3=1

C1=0
C2=0
C3=0

C1=0
C2=0
C3=1

C1   C2   C3

Bengio, 2009, Foundations and Trends in Machine Learning

Local vs. Distributed Representations

- Clustering, Nearest Neighbors, RBF SVM, local density estimators

- RBMs, Factor models, PCA, Sparse Coding, Deep models

- Parameters for each region.
- # of regions is linear with # of parameters.

- Each parameter affects many regions, not just local.
- # of regions grows (roughly) exponentially in # of parameters.

C1=1
C3=1

C1=1
C2=0
C3=0

C2=1
C3=0

C1=0
C2=1
C3=1

C1=0
C2=0
C3=0

C1   C2   C3

C1=0
C2=0
C3=1

Learned prototypes

Bengio, 2009, Foundations and Trends in Machine Learning
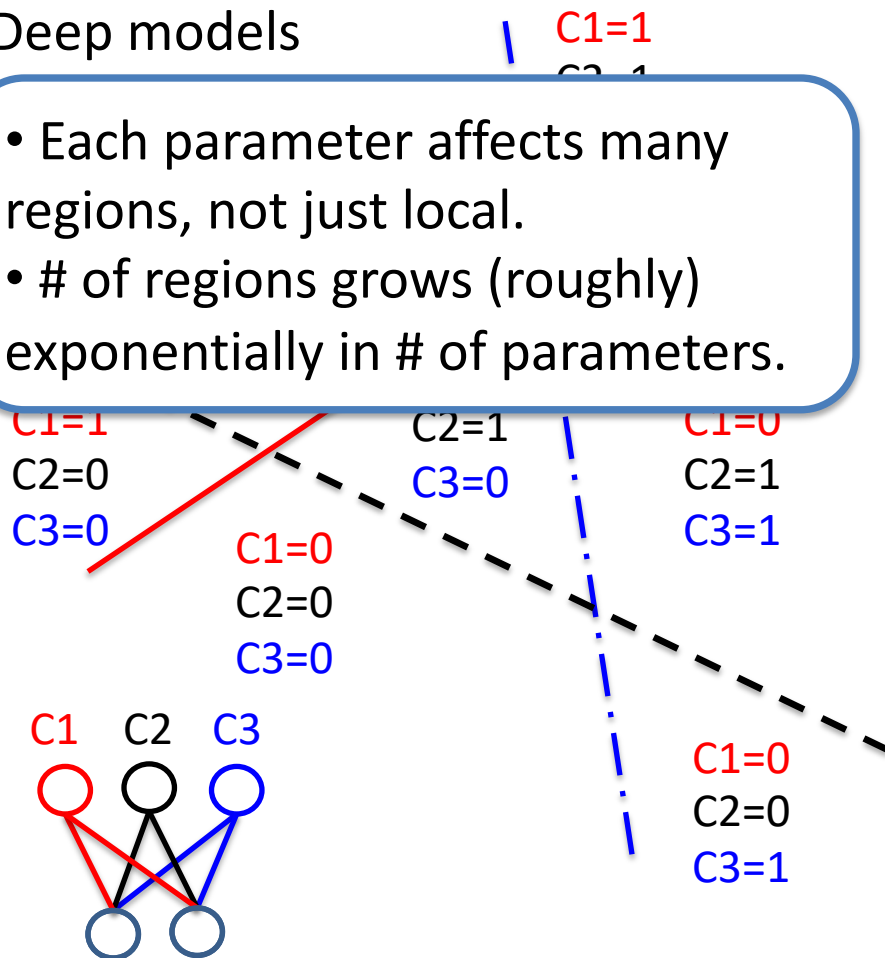
Boltzmann Machines

• The original Boltzmann machine has lateral connections in each layer
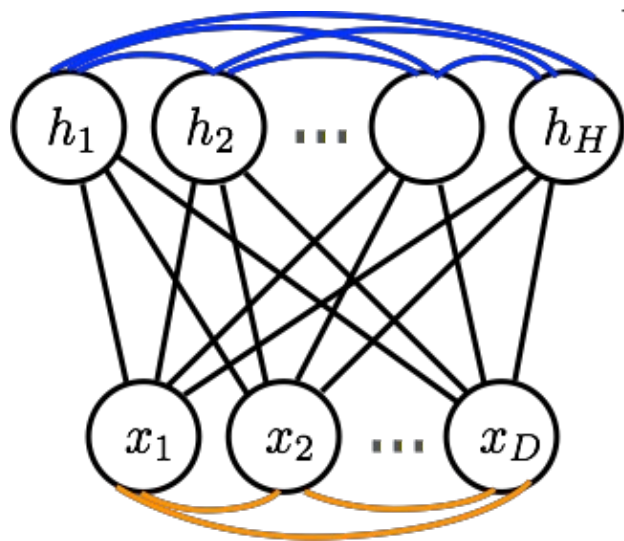
$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h}$$
$$-\frac{1}{2}\mathbf{x}^\top \mathbf{V} \mathbf{x} + \frac{1}{2}\mathbf{h}^\top \mathbf{U} \mathbf{h}$$

➢ when only one layer has lateral connection, the model is called a

semi-restricted Boltzmann machine

Multiple Application Domains

- Natural Images
- Text/Documents
- Collaborative Filtering / Matrix Factorization
- Video (Langford, Salakhutdinov and Zhang, ICML 2009)
- Motion Capture (Taylor et.al. NIPS 2007)
- Speech Perception (Dahl et. al. NIPS 2010, Lee et.al. NIPS 2010)

Same learning algorithm --
multiple input domains.

Limitations on the types of structure that can be represented by a single layer of low-level features!