Neural networks

Restricted Boltzmann machine - definition

UNSUPERVISED LEARNING

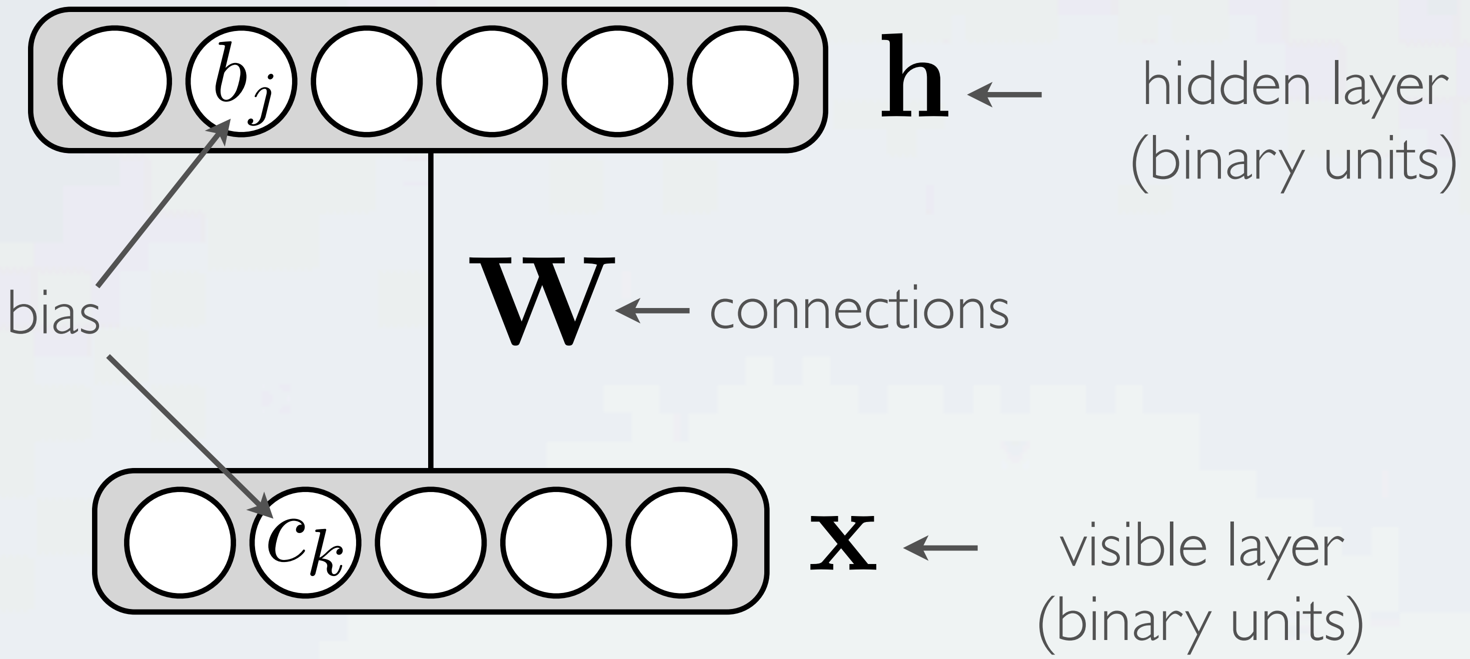
Topics: unsupervised learning

- Unsupervised learning: 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 see 3 neural networks for unsupervised learning
    - **restricted Boltzmann machines**
    - autoencoders
    - sparse coding model

RESTRICTED BOLTZMANN MACHINE

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



Energy function:

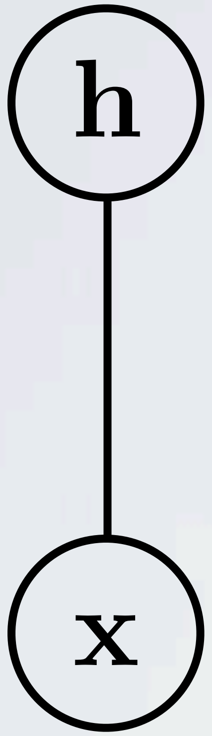
$$\begin{aligned} E(\mathbf{x},\mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\ &= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \end{aligned}$$

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

partition function
(intractable)

MARKOV NETWORK VIEW

Topics: Markov network (with vector nodes)

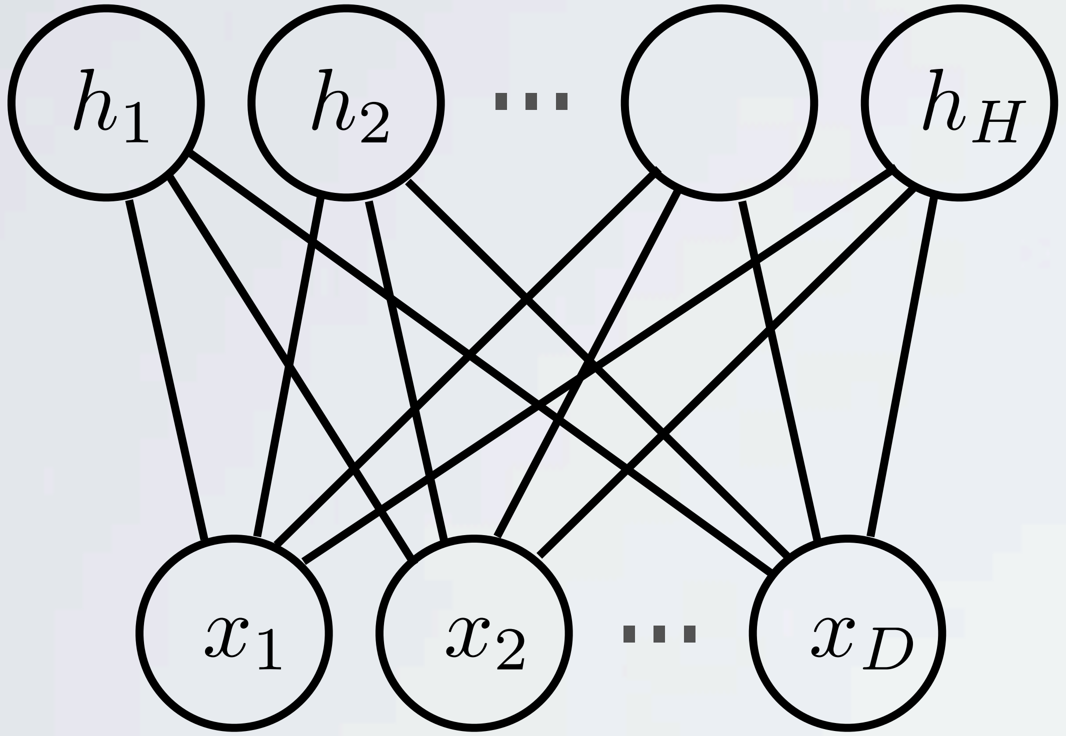


$$
\begin{aligned}
p(\mathbf{x},\mathbf{h}) &= \exp(-E(\mathbf{x},\mathbf{h}))/Z \\
&= \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z \\
&= \underbrace{\exp(\mathbf{h}^\top \mathbf{W}\mathbf{x})\exp(\mathbf{c}^\top \mathbf{x})\exp(\mathbf{b}^\top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

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

MARKOV NETWORK VIEW

Topics: Markov network (with scalar nodes)

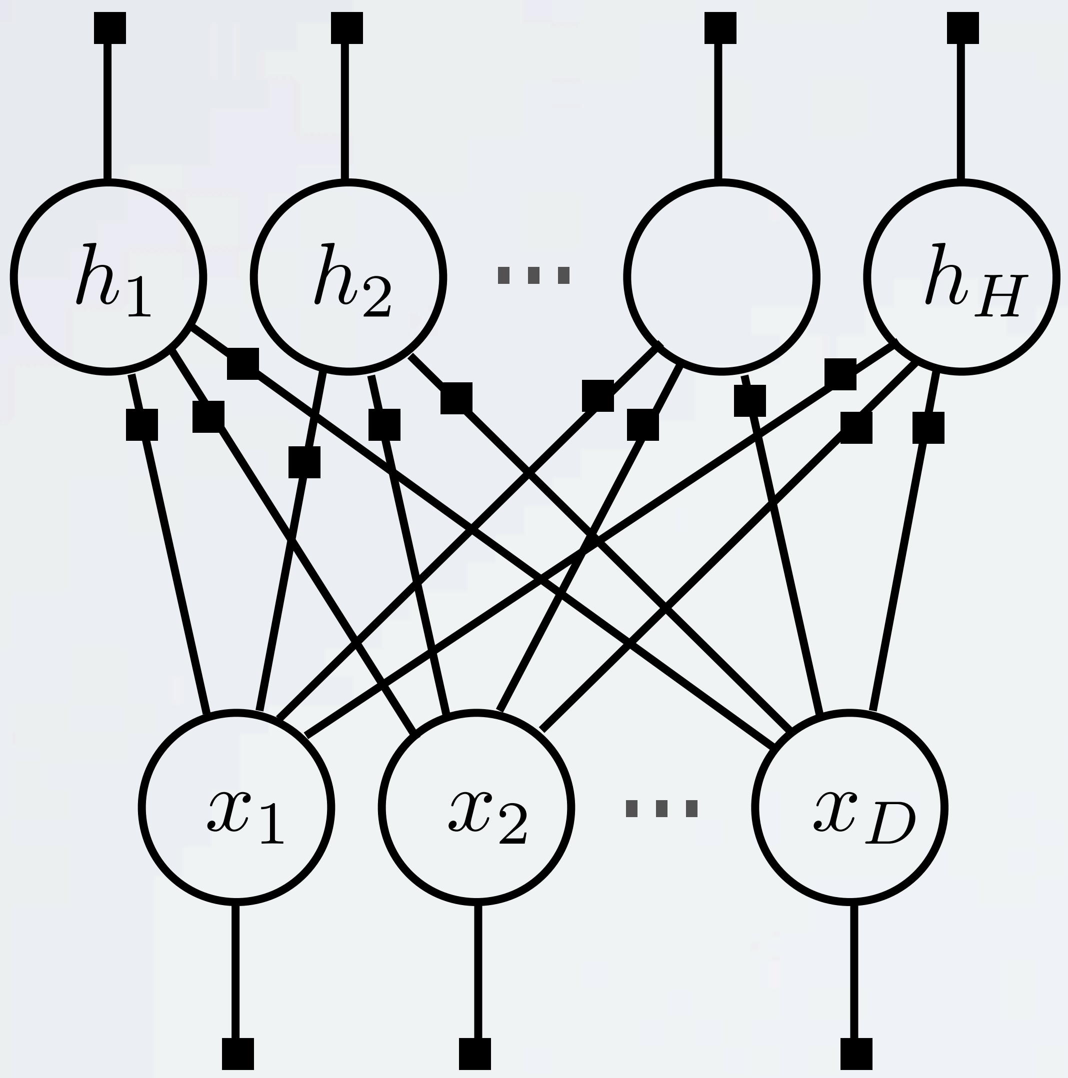


$$p(\mathbf{x},\mathbf{h}) \;=\; \frac{1}{Z}\overbrace{\prod_j\prod_k \exp(W_{j,k}h_jx_k)}^{\text{pair-wise factors}}\left.\begin{array}{l}\displaystyle\prod_k \exp(c_kx_k)\\ \displaystyle\prod_j \exp(b_jh_j)\end{array}\right\}\text{unary factors}$$

- The scalar visualization is more informative of the structure within the vectors

FACTOR GRAPH VIEW

Topics: factor graph of an RBM

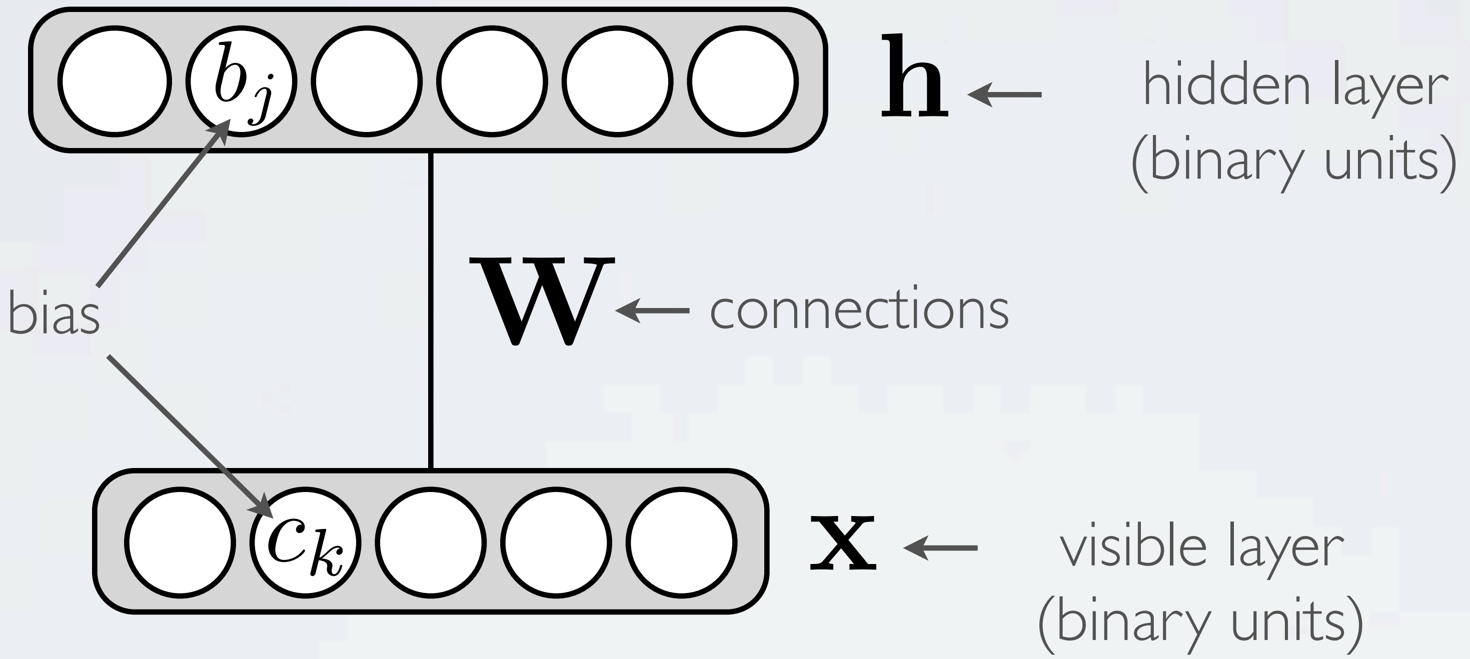


Neural networks

Restricted Boltzmann machine - inference

RESTRICTED BOLTZMANN MACHINE

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



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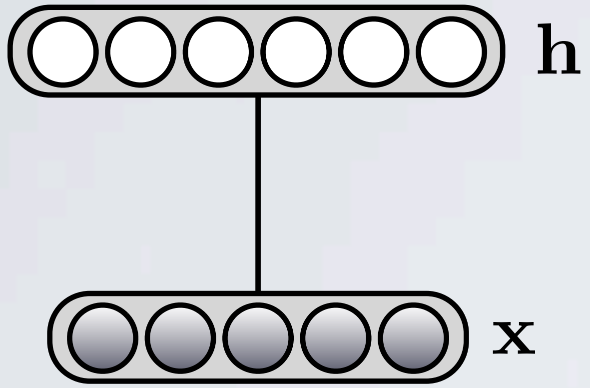
Distribution: $p(\mathbf{x},\mathbf{h}) = \exp(-E(\mathbf{x},\mathbf{h}))/Z$

partition function
(intractable)

INFERENCE

Topics: conditional distributions

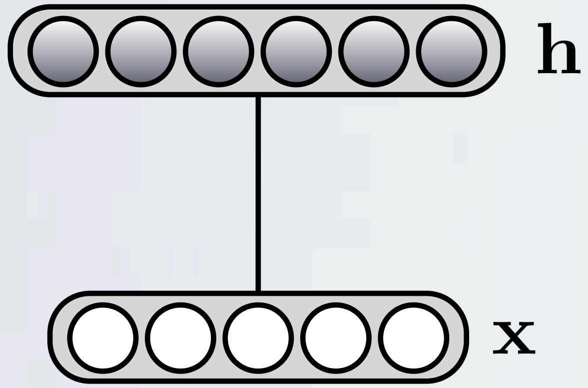


$$p(\mathbf{h}|\mathbf{x}) = \prod_j p(h_j|\mathbf{x})$$

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

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

j th row of $\mathbf{W}$



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

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

k th column of $\mathbf{W}$

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

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

$$p(\mathbf{h}|\mathbf{x}) \quad = \quad p(\mathbf{x},\mathbf{h}) / \sum_{\mathbf{h}'} p(\mathbf{x},\mathbf{h}')$$

$$
\begin{aligned}
p(\mathbf{h}|\mathbf{x}) &= p(\mathbf{x},\mathbf{h}) / \sum_{\mathbf{h}'} p(\mathbf{x},\mathbf{h}') \\
&= \frac{\exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z}{\sum_{\mathbf{h}' \in \{0,1\}^H} \exp(\mathbf{h}'^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h}')/Z}
\end{aligned}
$$

$$
\begin{aligned}
p(\mathbf{h}|\mathbf{x}) &= p(\mathbf{x},\mathbf{h}) / \sum_{\mathbf{h}'} p(\mathbf{x},\mathbf{h}') \\
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\end{aligned}
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&= \frac{\exp(\sum_j h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \exp(\sum_j h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)}
\end{aligned}
$$

$$
\begin{aligned}
p(\mathbf{h}|\mathbf{x}) &= p(\mathbf{x},\mathbf{h}) \Big/ \sum_{\mathbf{h}'} p(\mathbf{x},\mathbf{h}') \\
&= \frac{\exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \cancel{\mathbf{c}^\top \mathbf{x}} + \mathbf{b}^\top \mathbf{h}) / \cancel{Z}}{\sum_{\mathbf{h}' \in \{0,1\}^H} \exp(\mathbf{h}'^\top \mathbf{W}\mathbf{x} + \cancel{\mathbf{c}^\top \mathbf{x}} + \mathbf{b}^\top \mathbf{h}') / \cancel{Z}} \\
&= \frac{\exp(\sum_j h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \exp(\sum_j h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \prod_j \exp(h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)}
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p(\mathbf{h}|\mathbf{x}) &= p(\mathbf{x},\mathbf{h}) / \sum_{\mathbf{h}'} p(\mathbf{x},\mathbf{h}') \\
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&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \prod_j \exp(h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\left(\sum_{h'_1 \in \{0,1\}} \exp(h'_1 \mathbf{W}_{1\cdot}\mathbf{x} + b_1 h'_1)\right) \cdots \left(\sum_{h'_H \in \{0,1\}} \exp(h'_H \mathbf{W}_{H\cdot}\mathbf{x} + b_H h'_H)\right)}
\end{aligned}
$$

$$
\begin{aligned}
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&= \frac{\exp(\sum_j h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \exp(\sum_j h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \prod_j \exp(h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\left(\sum_{h'_1 \in \{0,1\}} \exp(h'_1 \mathbf{W}_{1\cdot}\mathbf{x} + b_1 h'_1)\right) \dots \left(\sum_{h'_H \in \{0,1\}} \exp(h'_H \mathbf{W}_{H\cdot}\mathbf{x} + b_H h'_H)\right)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\prod_j \left(\sum_{h'_j \in \{0,1\}} \exp(h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)\right)}
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&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\prod_j (1 + \exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x}))}
\end{aligned}
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$$
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&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\sum_{h'_1 \in \{0,1\}} \cdots \sum_{h'_H \in \{0,1\}} \prod_j \exp(h'_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h'_j)} \\
&= \frac{\prod_j \exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{\left(\sum_{h'_1 \in \{0,1\}} \exp(h'_1 \mathbf{W}_{1\cdot}\mathbf{x} + b_1 h'_1)\right) \ldots \left(\sum_{h'_H \in \{0,1\}} \exp(h'_H \mathbf{W}_{H\cdot}\mathbf{x} + b_H h'_H)\right)} \\
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&= \prod_j \frac{\exp(h_j \mathbf{W}_{j\cdot}\mathbf{x} + b_j h_j)}{1 + \exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x})}
\end{aligned}
$$

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

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

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

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

$$\begin{aligned} p(h_j = 1|\mathbf{x}) &= \frac{\exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x})}{1 + \exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x})} \\ &= \frac{1}{1 + \exp(-b_j - \mathbf{W}_{j\cdot}\mathbf{x})} \\ &= \mathrm{sigm}(b_j + \mathbf{W}_{j\cdot}\mathbf{x}) \end{aligned}$$

LOCAL MARKOV PROPERTY

Topics: local Markov property

- In general, we have the following property:

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

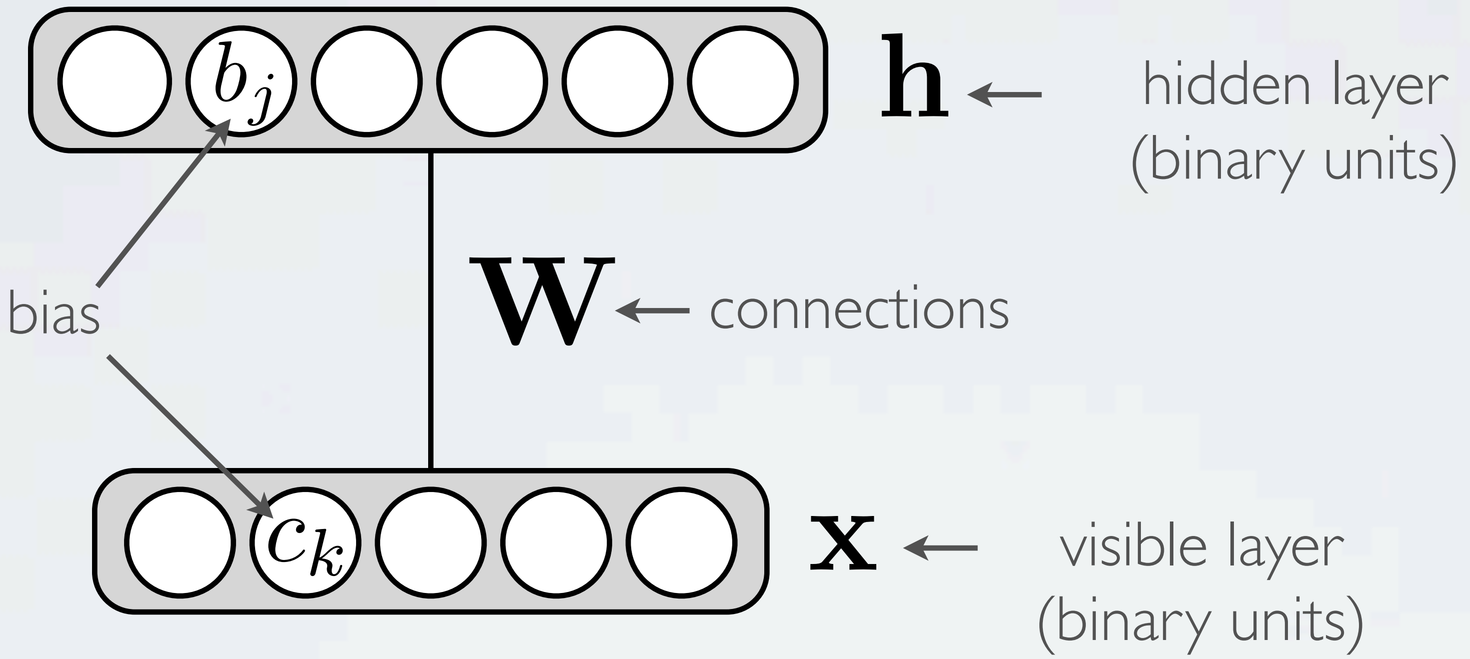
  - z_i is any variable in the Markov network (x_k or h_j in an RBM)
  - $\mathrm{Ne}(z_i)$ are the neighbors of z_i in the Markov network

Neural networks

Restricted Boltzmann machine - free energy

RESTRICTED BOLTZMANN MACHINE

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



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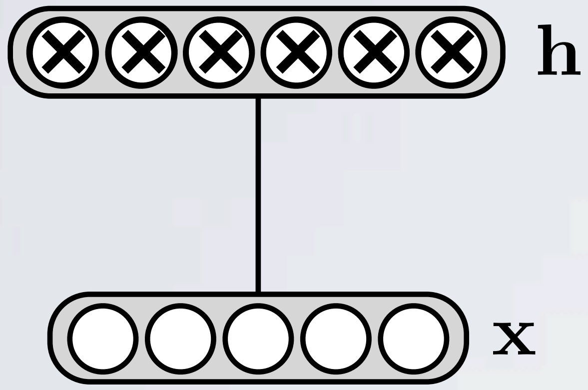
Distribution: $p(\mathbf{x},\mathbf{h}) = \exp(-E(\mathbf{x},\mathbf{h}))/Z$

partition function
(intractable)

FREE ENERGY

Topics: free energy

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



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

free energy

$p(\mathbf{x})$

$$p(\mathbf{x}) \quad = \quad \sum_{\mathbf{h}\in\{0,1\}^H} \exp(\mathbf{h}^\top \mathbf{W}\mathbf{x} + \mathbf{c}^\top \mathbf{x} + \mathbf{b}^\top \mathbf{h})/Z$$

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

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

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

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

$$
\begin{aligned}
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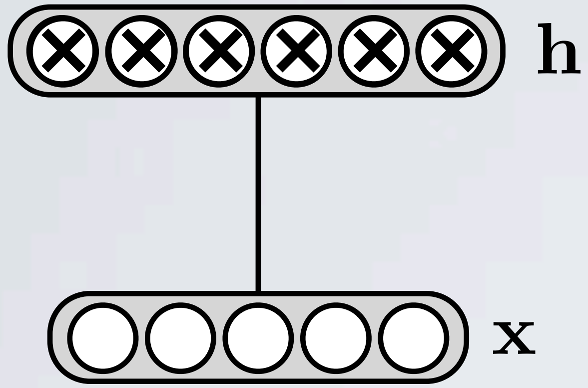
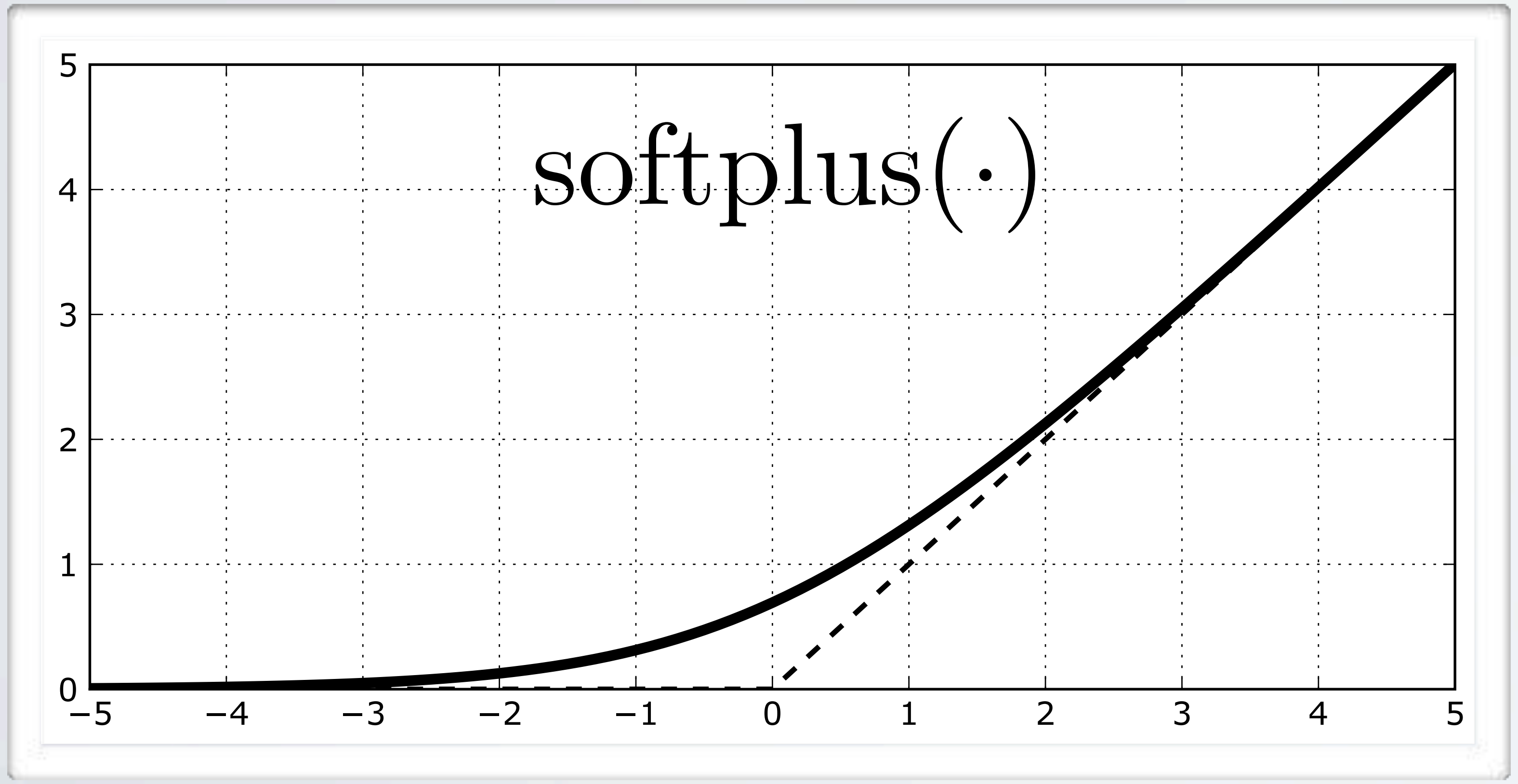
&= \exp(\mathbf{c}^\top \mathbf{x}) \exp(\log(1 + \exp(b_1 + \mathbf{W}_{1\cdot}\mathbf{x}))) \dots \exp(\log(1 + \exp(b_H + \mathbf{W}_{H\cdot}\mathbf{x})))/Z \\
&= \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \log(1 + \exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x}))\right)/Z
\end{aligned}
$$

RESTRICTED BOLTZMANN MACHINE

Topics: free energy

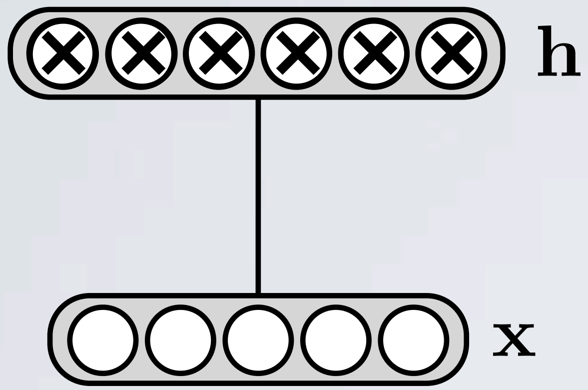


$$
\begin{aligned}
p(\mathbf{x}) &= \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \log(1 + \exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x}))\right) / Z \\
&= \exp\left(\mathbf{c}^\top \mathbf{x} + \sum_{j=1}^{H} \operatorname{softplus}(b_j + \mathbf{W}_{j\cdot}\mathbf{x})\right) / Z
\end{aligned}
$$



RESTRICTED BOLTZMANN MACHINE

Topics: free energy



$$
\begin{aligned}
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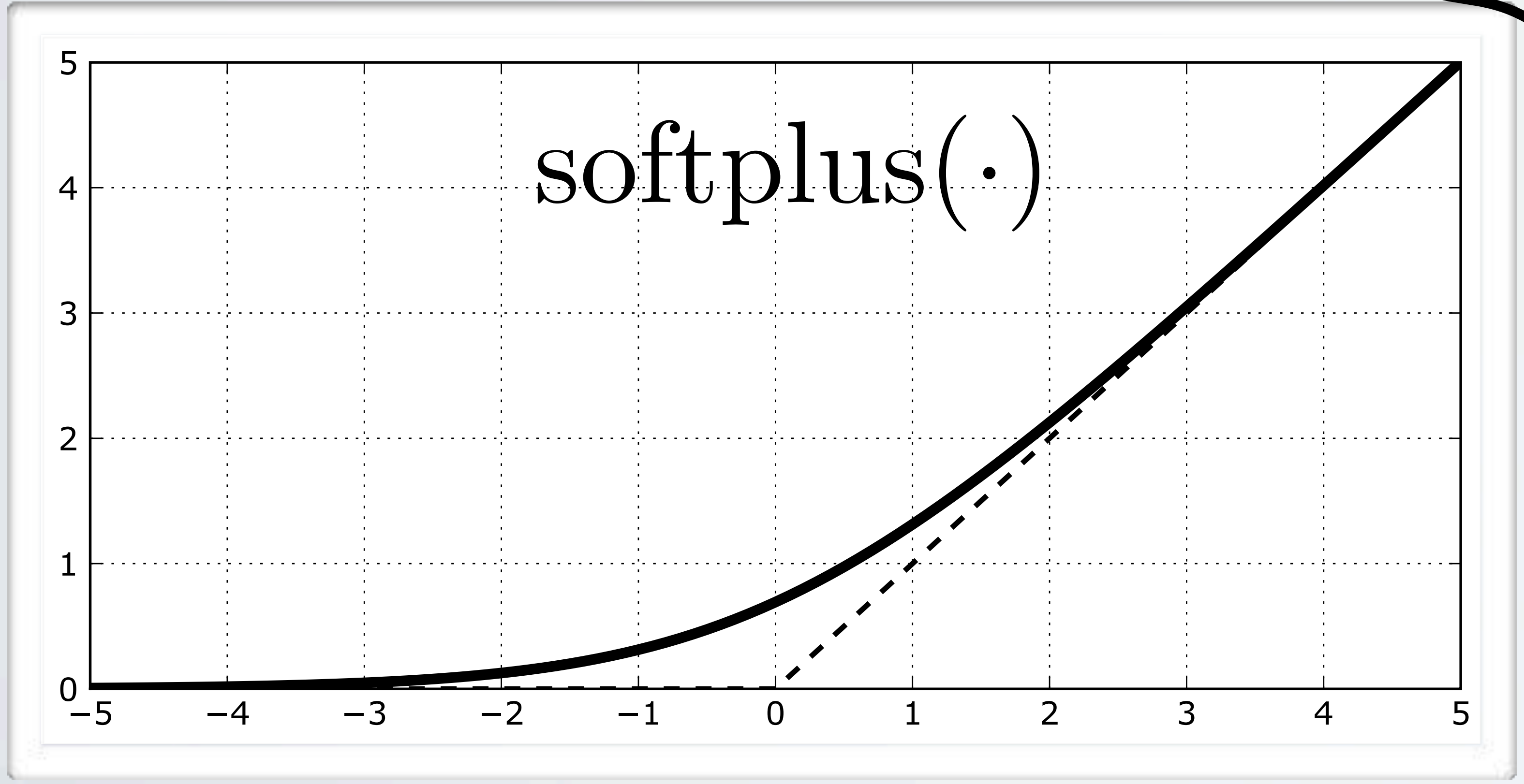
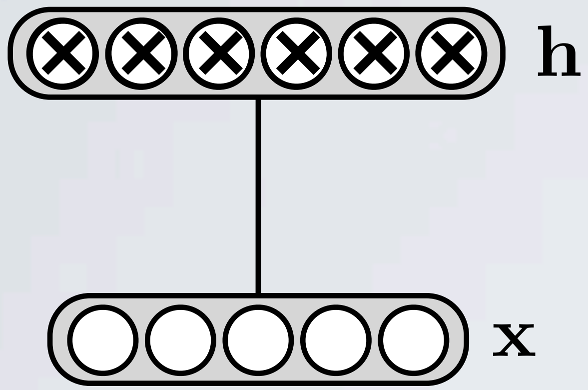


bias the prob of each x_i

RESTRICTED BOLTZMANN MACHINE

Topics: free energy



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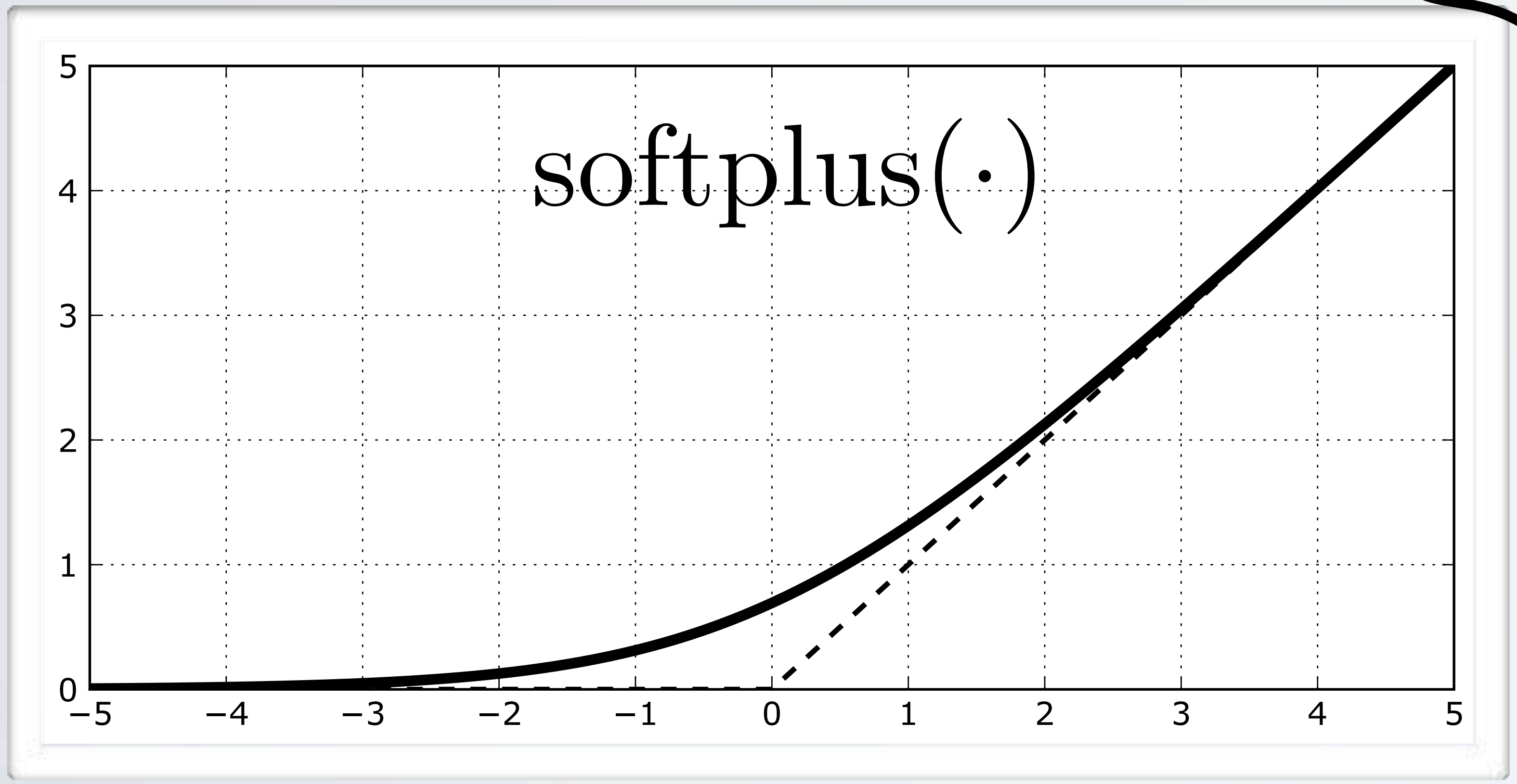
&= \exp\left(\mathbf{c}^\top\mathbf{x} + \sum_{j=1}^{H} \mathrm{softplus}(b_j + \mathbf{W}_{j\cdot}\mathbf{x})\right) / Z
\end{aligned}
$$

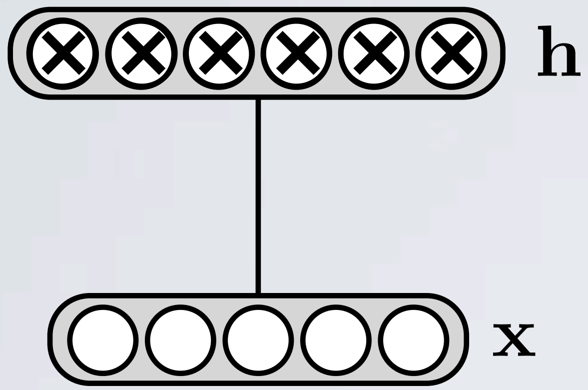
“feature” expected in $\mathbf{X}$

bias the prob of each x_i



RESTRICTED BOLTZMANN MACHINE

Topics: free energy



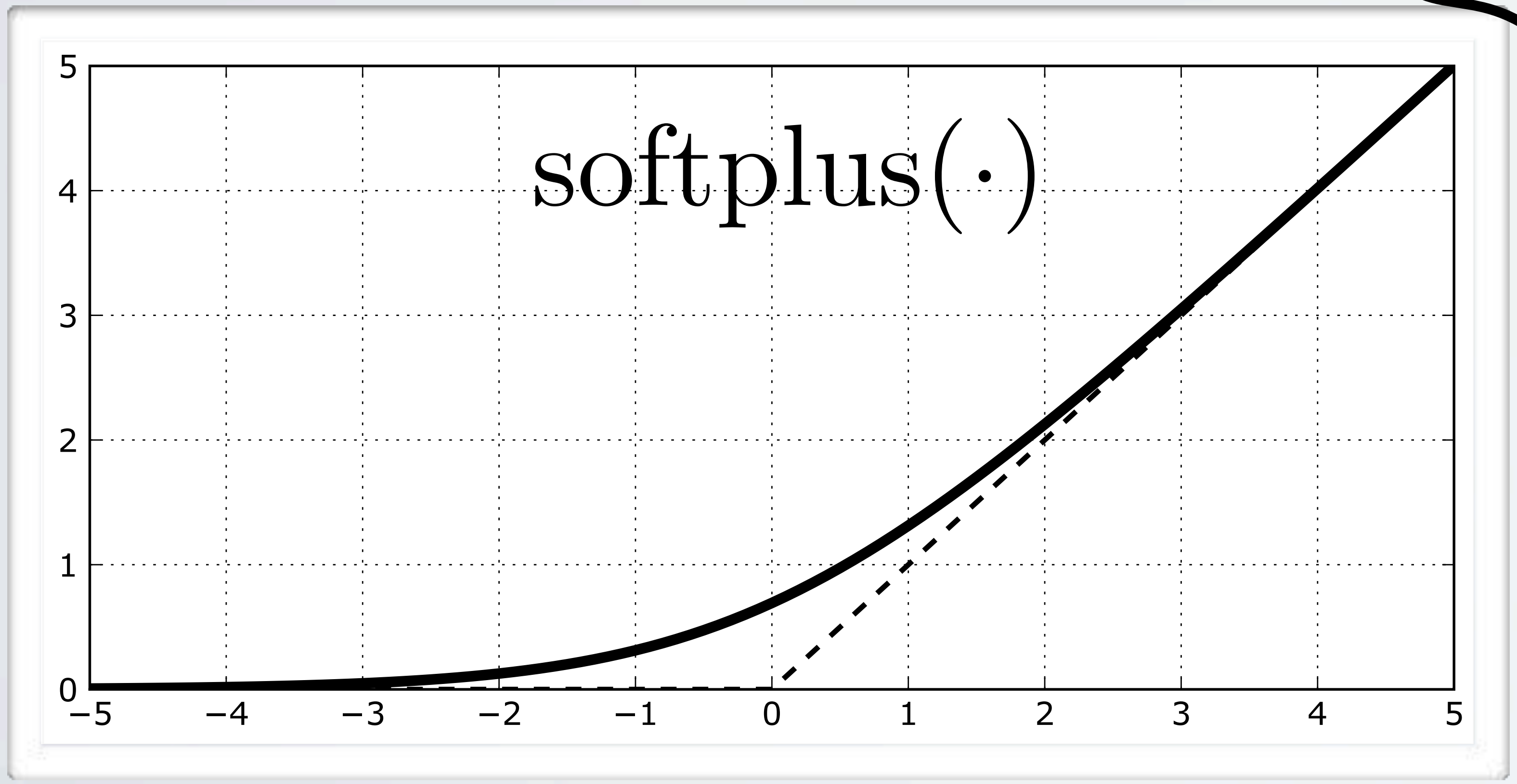
$$p(\mathbf{x}) = \exp\left(\mathbf{c}^\top\mathbf{x} + \sum_{j=1}^{H}\log(1+\exp(b_j + \mathbf{W}_{j\cdot}\mathbf{x}))\right)/Z$$

$$= \exp\left(\mathbf{c}^\top\mathbf{x} + \sum_{j=1}^{H}\mathrm{softplus}(b_j + \mathbf{W}_{j\cdot}\mathbf{x})\right)/Z$$

"feature" expected in $\mathbf{x}$

bias of each feature

bias the prob of each x_i

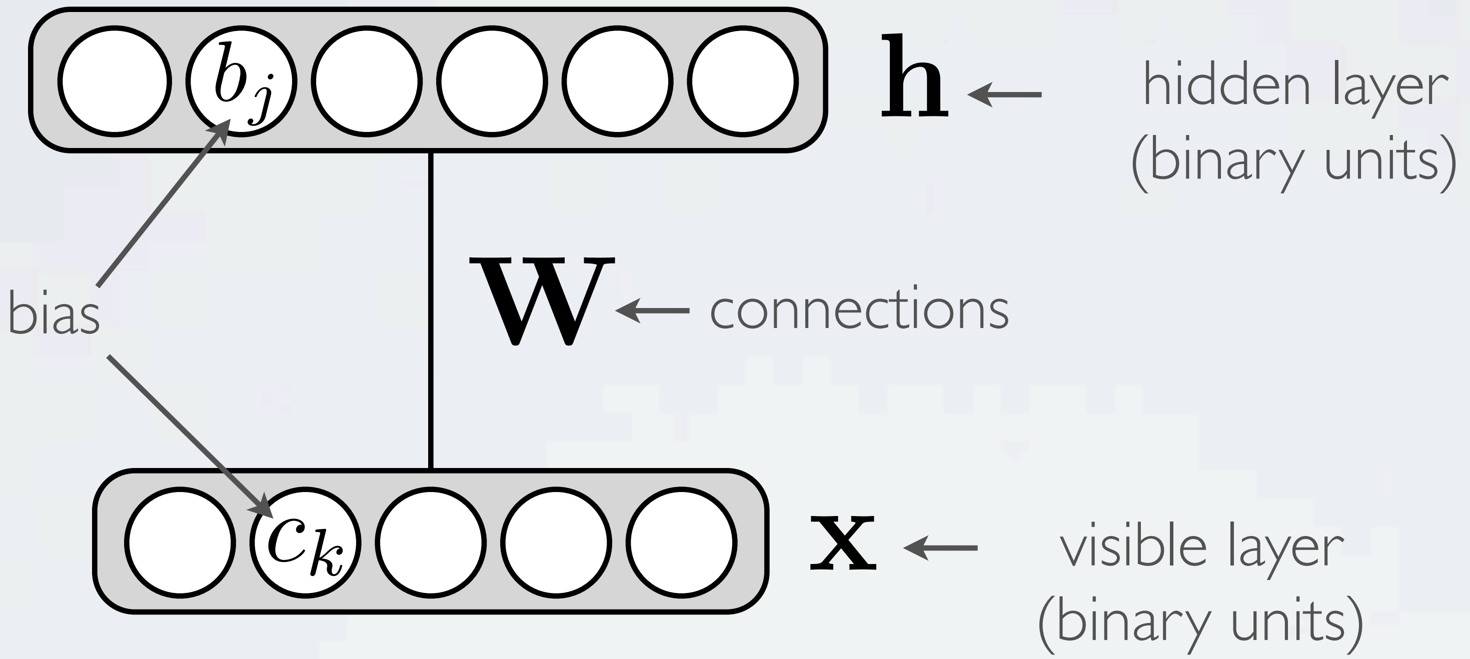


Neural networks

Restricted Boltzmann machine - contrastive divergence

RESTRICTED BOLTZMANN MACHINE

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



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

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

partition function
(intractable)

TRAINING

Topics: training objective

- To train an RBM, we'd like to minimize the average negative log-likelihood (NLL)

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

- We'd like to proceed by stochastic gradient descent

$$\frac{\partial -\log p(\mathbf{x}^{(t)})}{\partial \theta} = \underbrace{\mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)},\mathbf{h})}{\partial \theta}\,\middle|\,\mathbf{x}^{(t)}\right]}_{\text{positive phase}} - \underbrace{\mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x},\mathbf{h})}{\partial \theta}\right]}_{\text{negative phase}}$$

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hard to compute

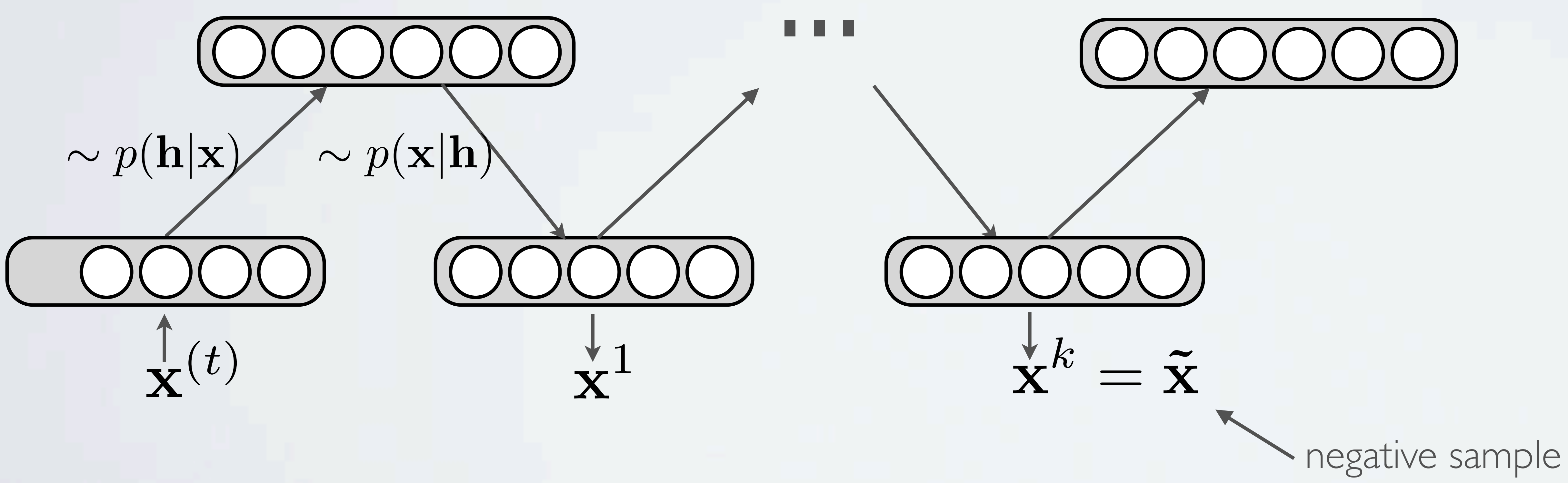
$$\frac{\partial -\log p(\mathbf{x}^{(t)})}{\partial\theta} = \underbrace{\mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)},\mathbf{h})}{\partial\theta}\,\middle|\,\mathbf{x}^{(t)}\right]}_{\text{positive phase}} - \underbrace{\boxed{\mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x},\mathbf{h})}{\partial\theta}\right]}}_{\text{negative phase}}$$

CONTRASTIVE DIVERGENCE (CD)

(HINTON, NEURAL COMPUTATION, 2002)

Topics: contrastive divergence, negative sample

- Idea:
  1. replace the expectation by a point estimate at $\tilde{\mathbf{x}}$
  2. obtain the point $\tilde{\mathbf{x}}$ by Gibbs sampling
  3. start sampling chain at $\mathbf{x}^{(t)}$

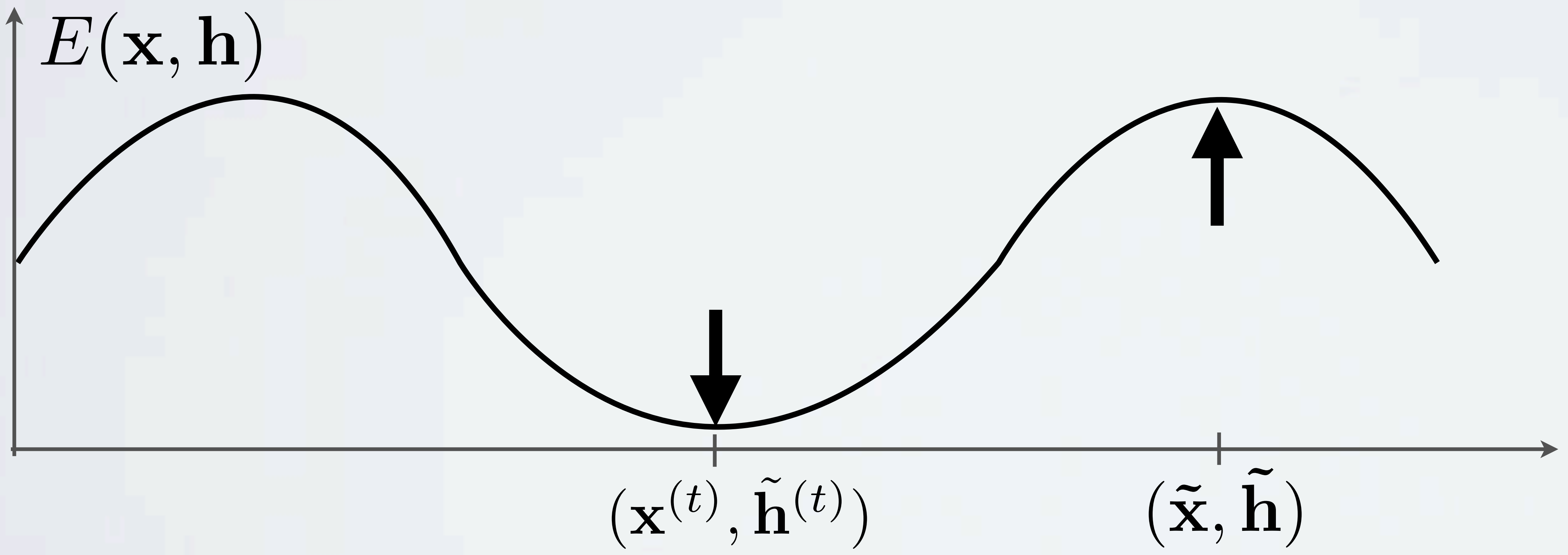


CONTRASTIVE DIVERGENCE (CD)

(HINTON, NEURAL COMPUTATION, 2002)

Topics: contrastive divergence, negative sample

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



CONTRASTIVE DIVERGENCE (CD)

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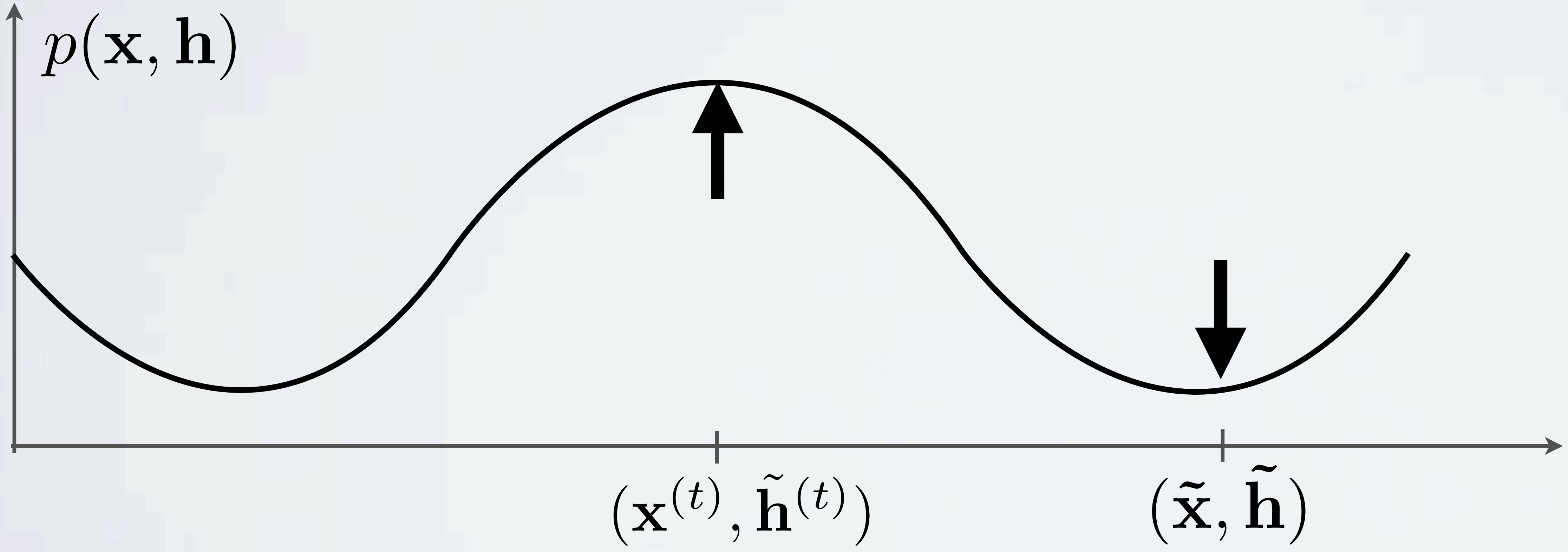

CONTRASTIVE DIVERGENCE (CD)

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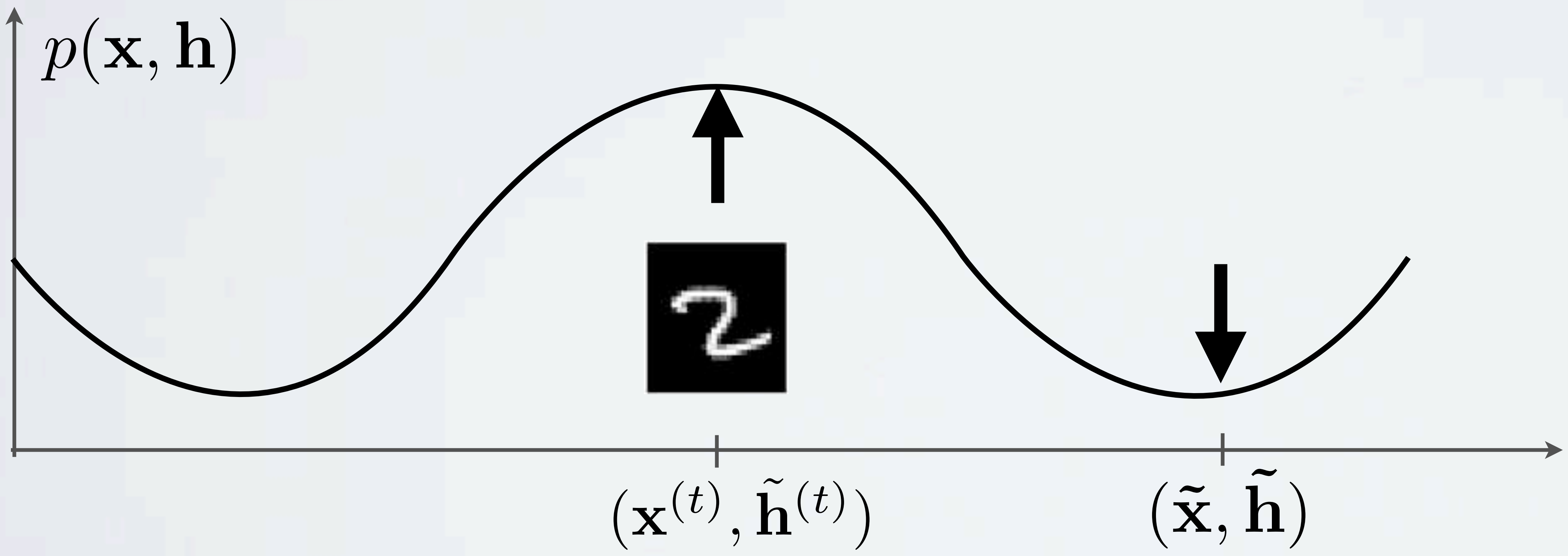

CONTRASTIVE DIVERGENCE (CD)

(HINTON, NEURAL COMPUTATION, 2002)

Topics: contrastive divergence, negative sample

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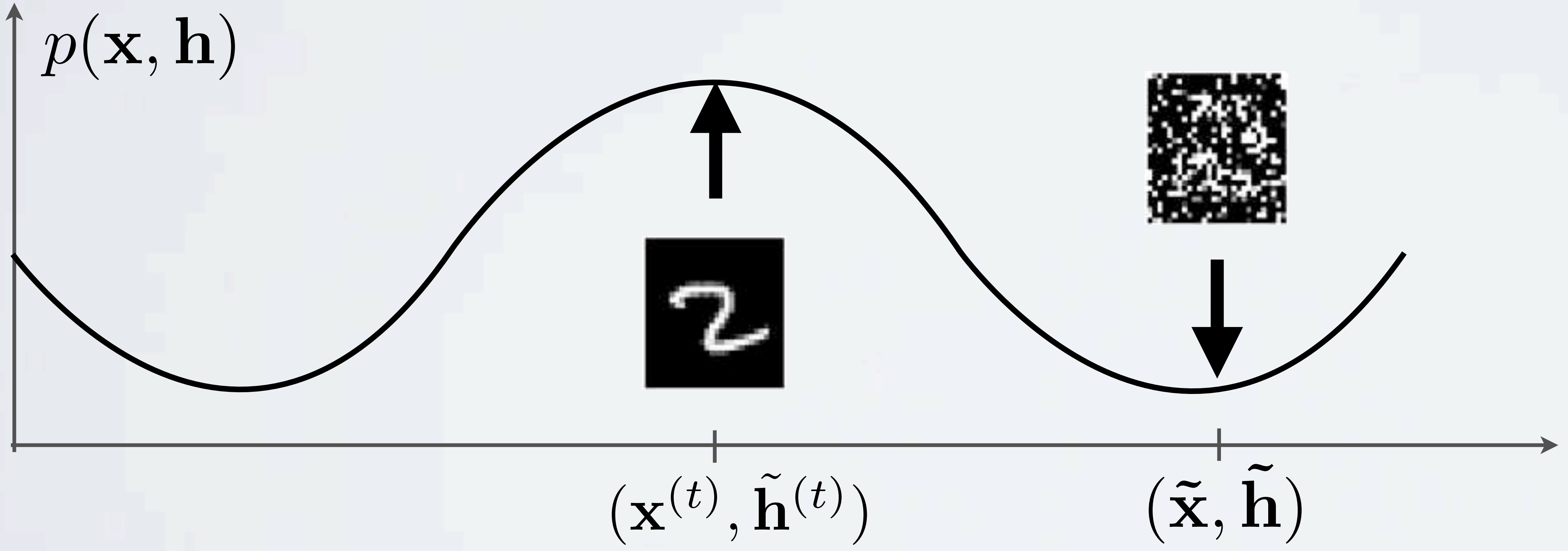

Neural networks

Restricted Boltzmann machine - contrastive divergence (parameter update)

TRAINING

Topics: training objective

- To train an RBM, we'd like to minimize the average negative log-likelihood (NLL)

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

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TRAINING

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

- We'd like to proceed by stochastic gradient descent

hard to compute

$$\frac{\partial -\log p(\mathbf{x}^{(t)})}{\partial \theta} = \underbrace{\mathrm{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x}^{(t)},\mathbf{h})}{\partial \theta}\,\middle|\,\mathbf{x}^{(t)}\right]}_{\text{positive phase}} - \underbrace{\boxed{\mathrm{E}_{\mathbf{x},\mathbf{h}}\left[\frac{\partial E(\mathbf{x},\mathbf{h})}{\partial \theta}\right]}}_{\text{negative phase}}$$

DERIVATION OF THE LEARNING RULE

Topics: contrastive divergence

- Derivation of $\frac{\partial E(\mathbf{x},\mathbf{h})}{\partial \theta}$ for $\theta = W_{jk}$

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

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

$$= -h_j x_k$$

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

DERIVATION OF THE LEARNING RULE

Topics: contrastive divergence

- Derivation of $\mathbb{E}_{\mathbf{h}}\left[\frac{\partial E(\mathbf{x},\mathbf{h})}{\partial \theta}\middle|\mathbf{x}\right]$ for $\theta = W_{jk}$

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

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

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

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

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

DERIVATION OF THE LEARNING RULE

Topics: contrastive divergence

- Given $\mathbf{x}^{(t)}$ and $\tilde{\mathbf{x}}$ the learning rule for $\theta = \mathbf{W}$ becomes

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

CD-K: PSEUDOCODE

Topics: contrastive divergence

1. For each training example $\mathbf{x}^{(t)}$
   i. generate a negative sample $\tilde{\mathbf{x}}$ using k steps of Gibbs sampling, starting at $\mathbf{x}^{(t)}$
   ii. update parameters

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

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

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

2. Go back to 1 until stopping criteria

CONTRASTIVE DIVERGENCE (CD)

(HINTON, NEURAL COMPUTATION, 2002)

Topics: contrastive divergence

- 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 pre-training

Neural networks

Restricted Boltzmann machine - persistent CD

CD-K: PSEUDOCODE

Topics: contrastive divergence

1. For each training example $\mathbf{x}^{(t)}$
   i. generate a negative sample $\tilde{\mathbf{x}}$ using
      k steps of Gibbs sampling, starting at $\mathbf{x}^{(t)}$
   ii. update parameters

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

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

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

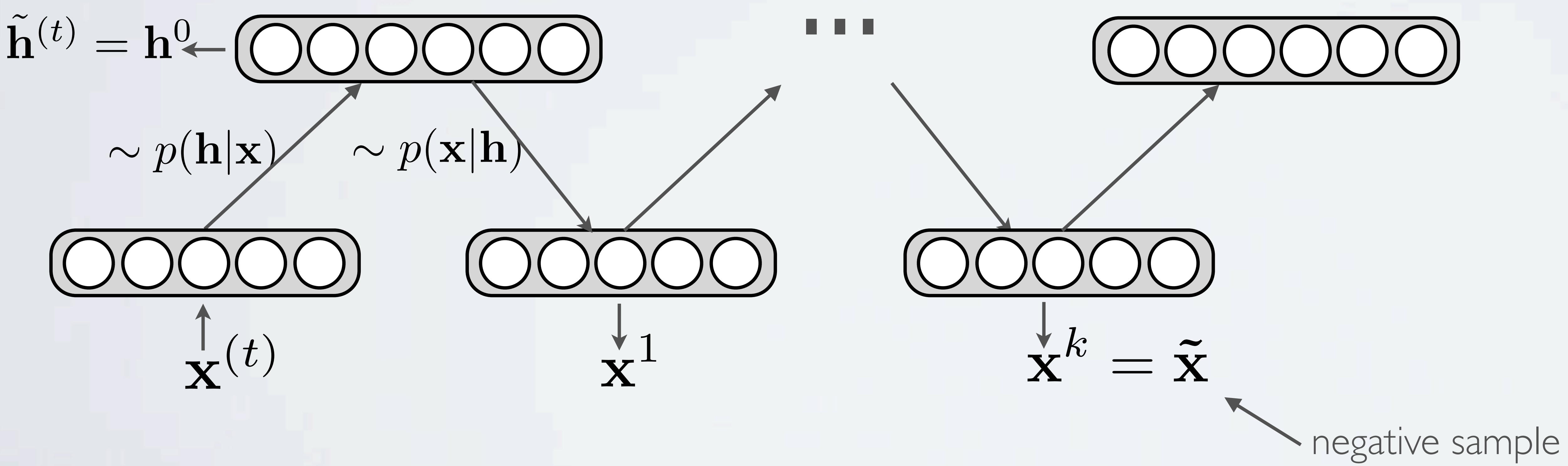
2. Go back to 1 until stopping criteria

PERSISTENT CD (PCD)

(TIELEMAN, ICML 2008)

Topics: persistent contrastive divergence

- Idea: instead of initializing the chain to $\mathbf{x}^{(t)}$, initialize the chain to the negative sample of the last iteration

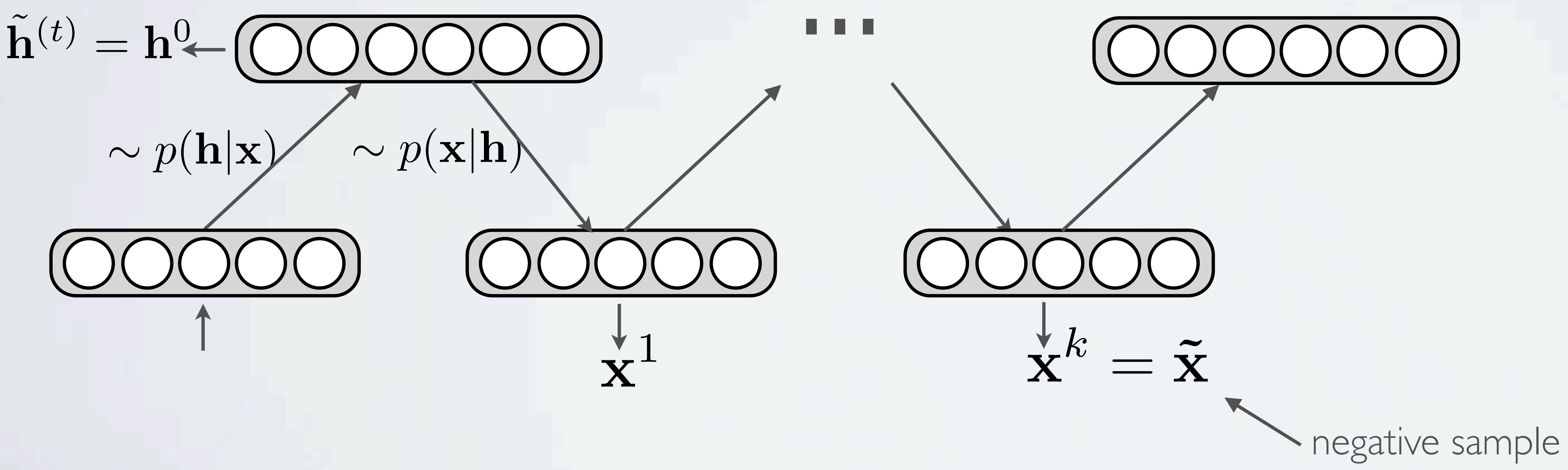


PERSISTENT CD (PCD)

(TIELEMAN, ICML 2008)

Topics: persistent contrastive divergence

- Idea: instead of initializing the chain to $\mathbf{x}^{(t)}$, initialize the chain to the negative sample of the last iteration



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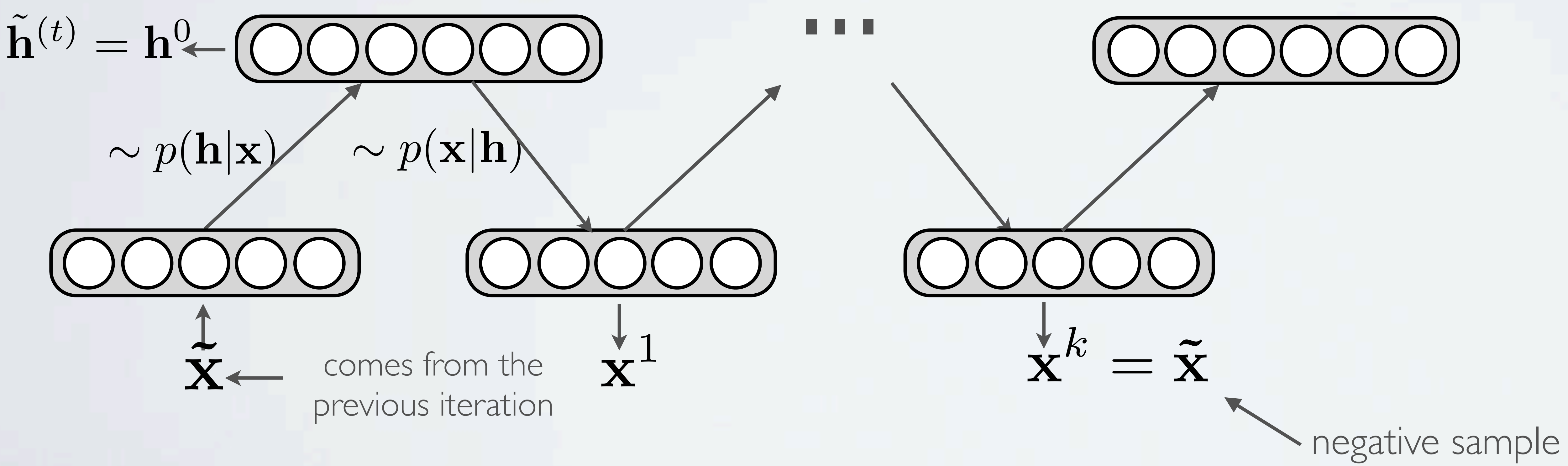
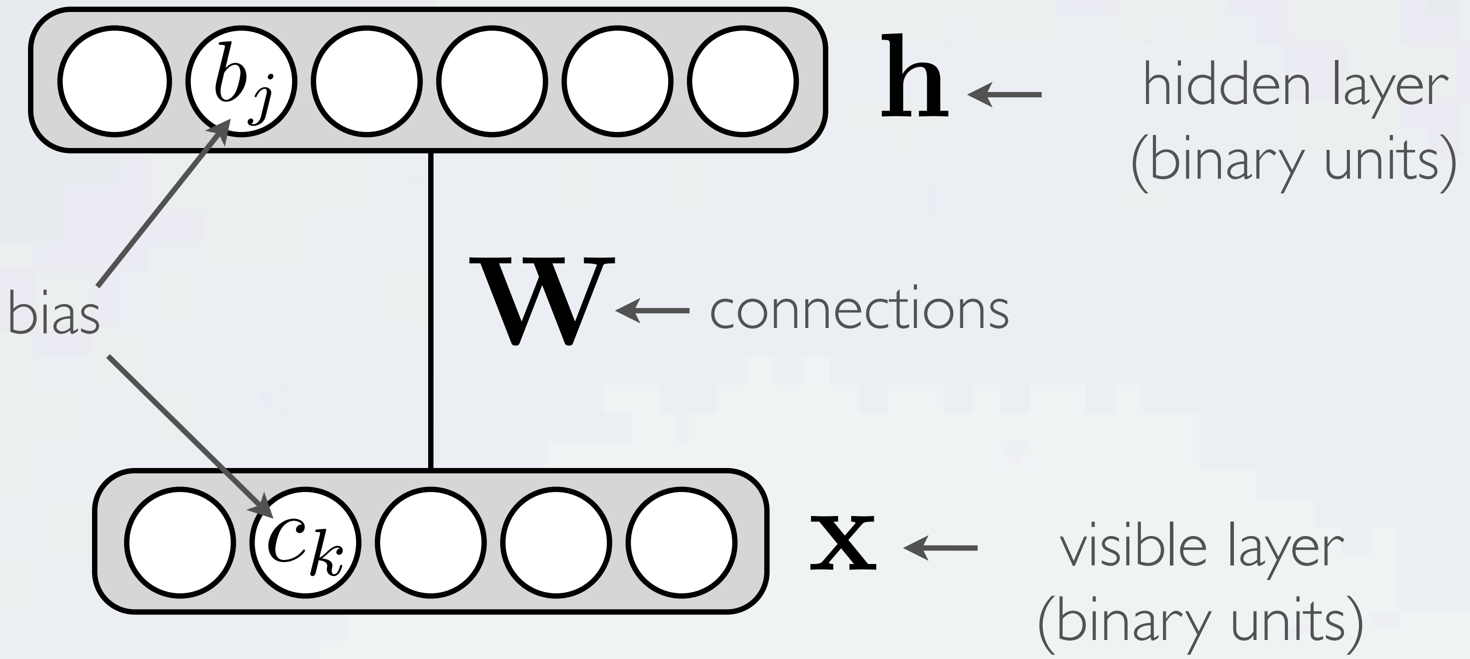


Neural networks

Restricted Boltzmann machine - example

RESTRICTED BOLTZMANN MACHINE

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

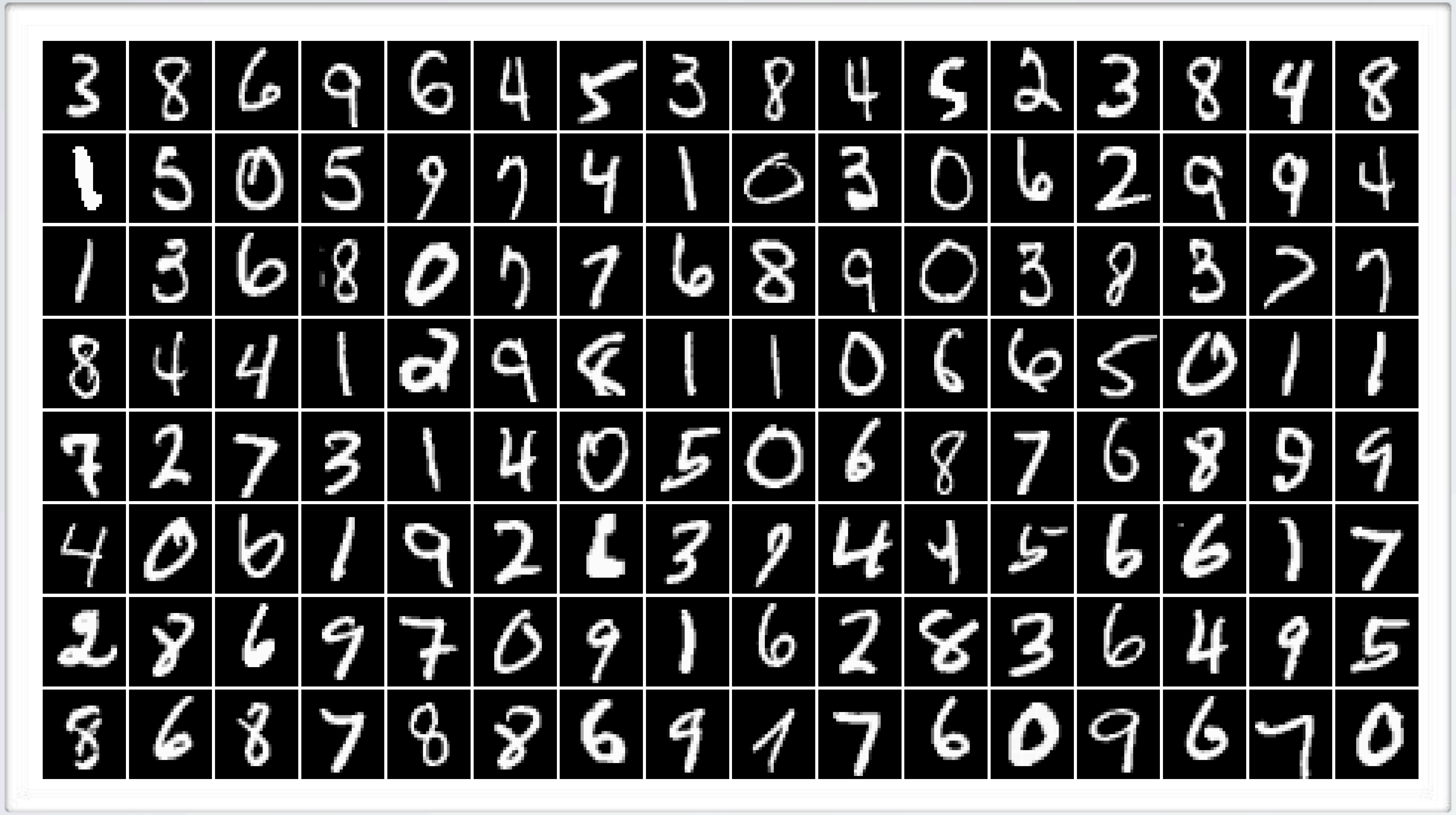


Energy function:
$$\begin{aligned} E(\mathbf{x},\mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\ &= -\sum_j \sum_k W_{j,k} h_j x_k - \sum_k c_k x_k - \sum_j b_j h_j \end{aligned}$$

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

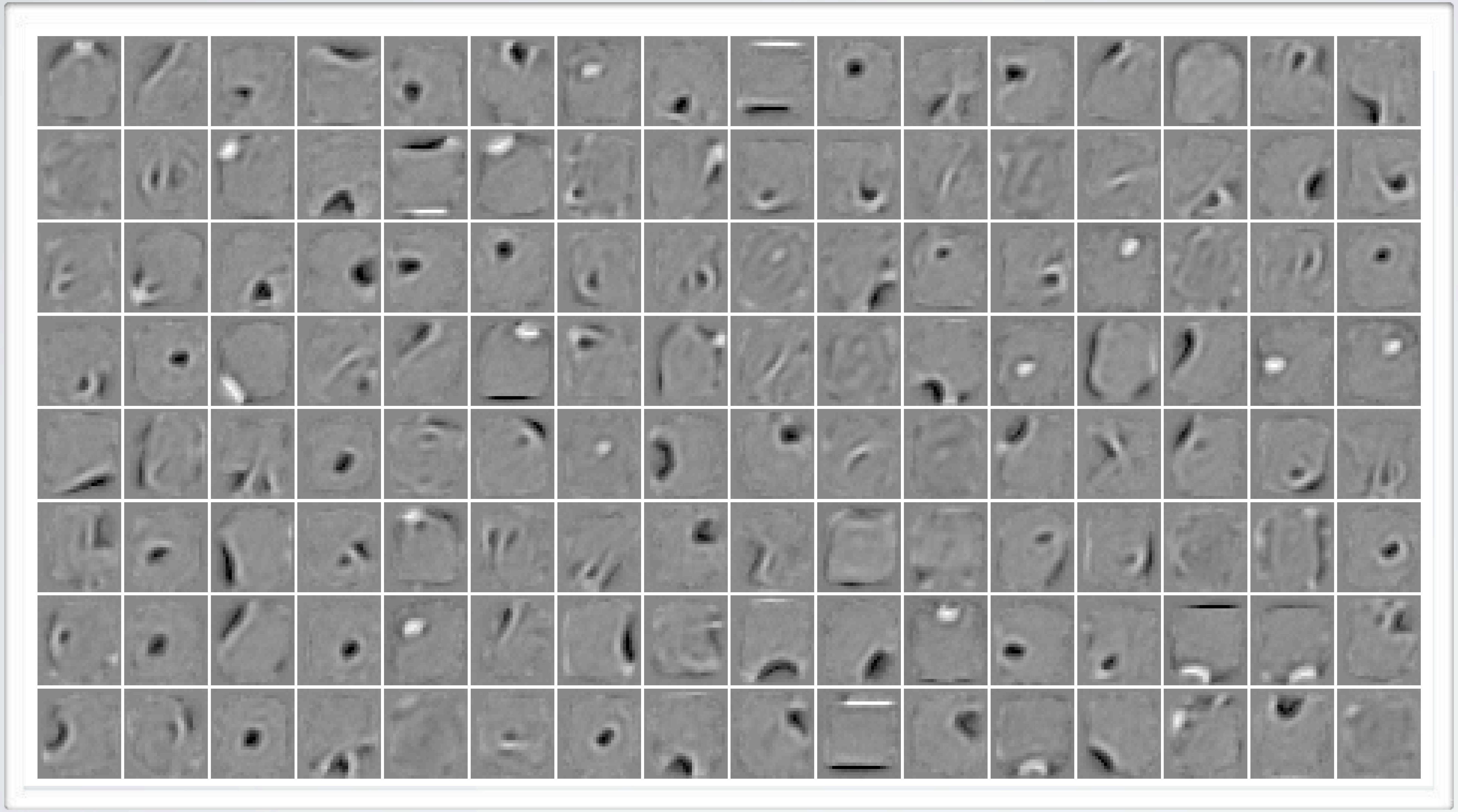
partition function
(intractable)

EXAMPLE OF DATA SET: MNIST



FILTERS

(LAROCHELLE ET AL., JMLR2009)



DEBUGGING

Topics: stochastic reconstruction, filters

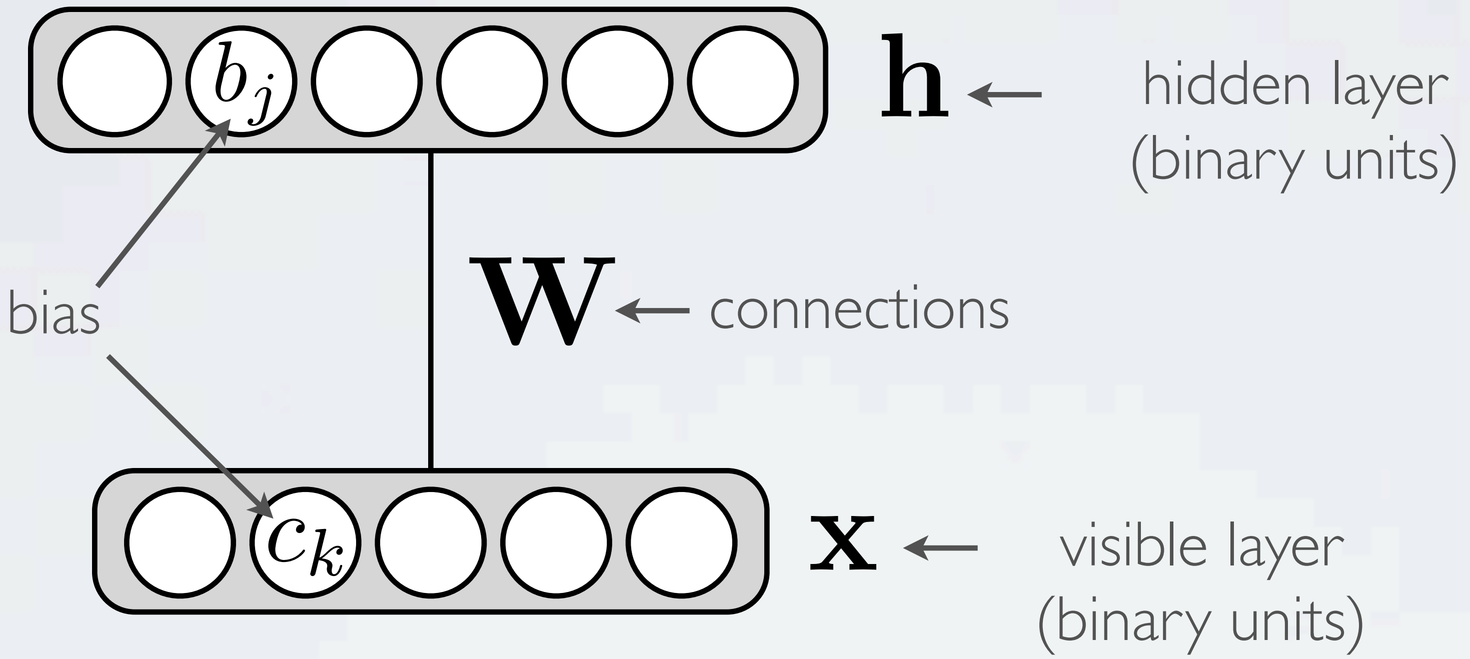
- Unfortunately, we can't debug with a comparison with finite difference
- We instead rely on approximate "tricks"
  - we plot the average stochastic reconstruction $||\mathbf{x}^{(t)} - \tilde{\mathbf{x}}||^2$ and see if it tends to decrease:
  - for inputs that correspond to image, we visualize the 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
    - On the Quantitative Analysis of Deep Belief Networks.
      Ruslan Salakhutdinov and Iain Murray, 2008

Neural networks

Restricted Boltzmann machine - extensions

RESTRICTED BOLTZMANN MACHINE

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



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

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

partition function
(intractable)

GAUSSIAN-BERNOULLI RBM

Topics: Gaussian-Bernoulli RBM

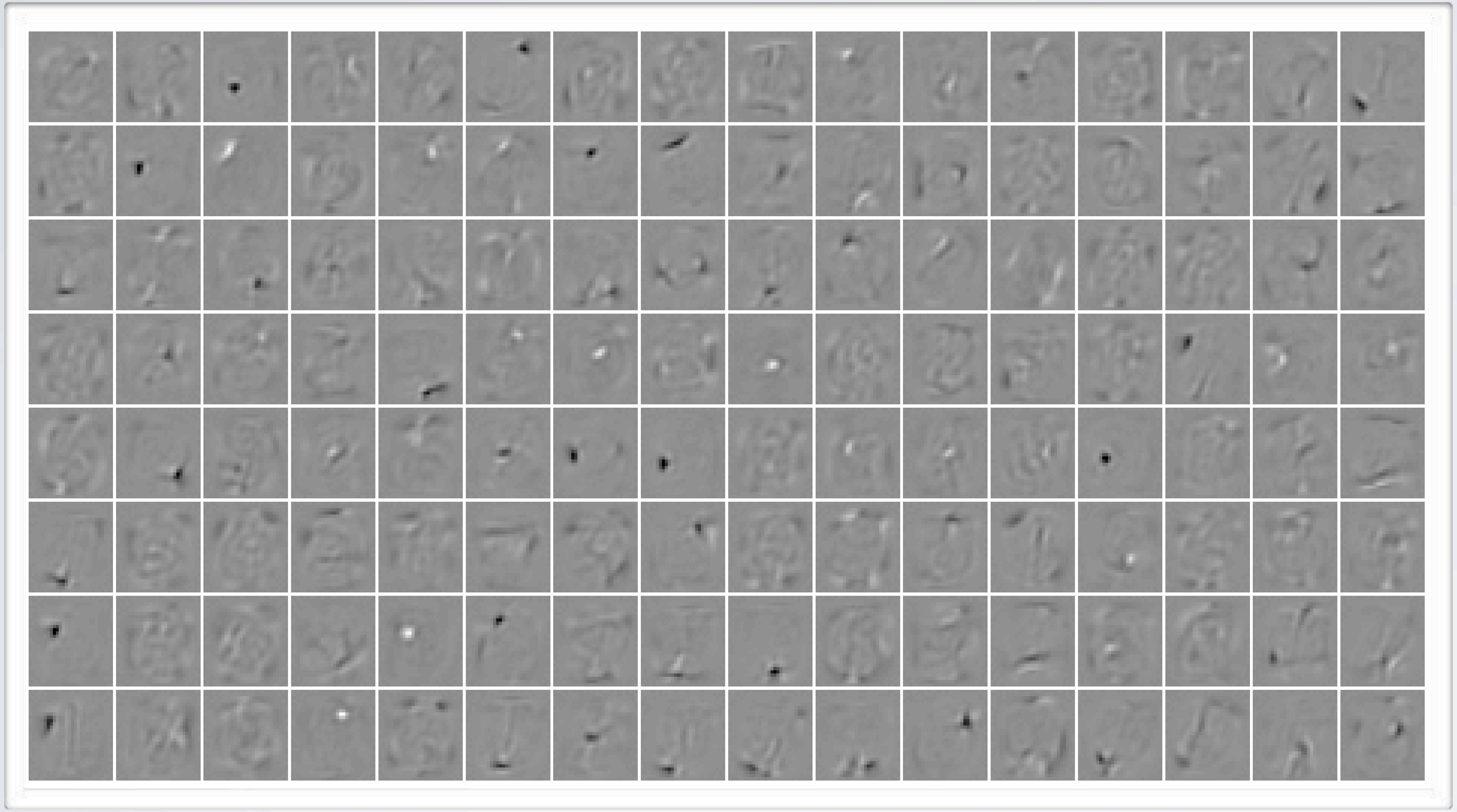
- Inputs $\mathbf{x}$ are unbounded reals
  - add a quadratic term to the energy function

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

  - only thing that changes is that $p(\mathbf{x}|\mathbf{h})$ is now a Gaussian distribution with mean $\boldsymbol{\mu} = \mathbf{c} + \mathbf{W}^\top \mathbf{h}$ and identity covariance matrix
  - recommended to normalize the training set by
    - subtracting the mean of each input
    - dividing each input x_k by the training set standard deviation
  - should use a smaller learning rate than in the regular RBM

FILTERS

(LAROCHELLE ET AL., JMLR2009)



OTHER TYPES OF OBSERVATIONS

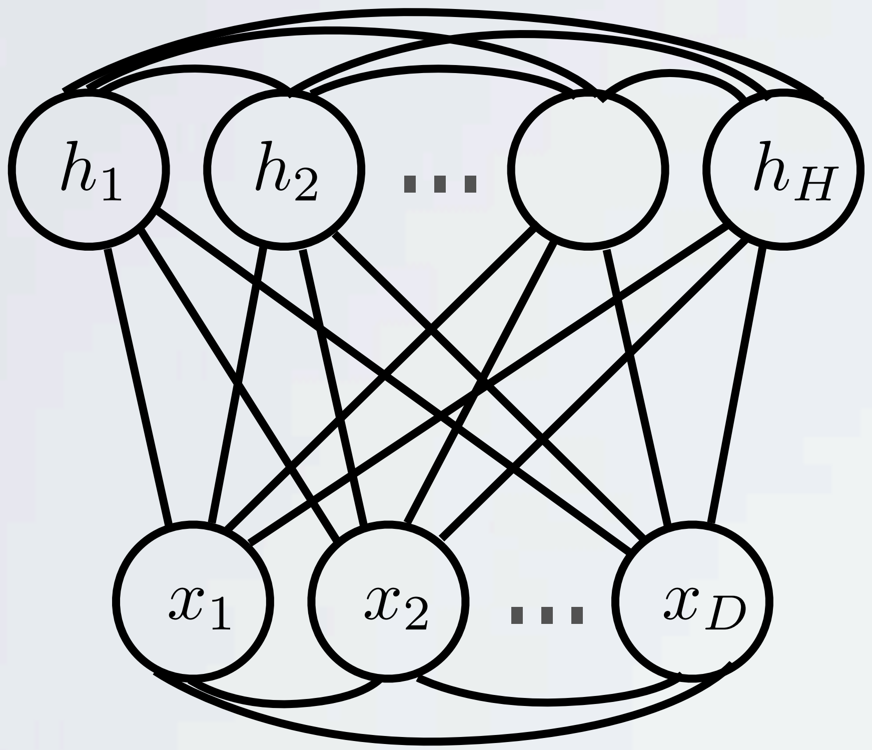
Topics: extensions to other observations

- Extensions support other types:
  - real-valued: Gaussian-Bernoulli RBM
  - Binomial observations:
    - Rate-coded Restricted Boltzmann Machines for Face Recognition.
      Yee Whye Teh and Geoffrey Hinton, 2001
  - Multinomial observations:
    - Replicated Softmax: an Undirected Topic Model.
      Ruslan Salakhutdinov and Geoffrey Hinton, 2009
    - Training Restricted Boltzmann Machines on Word Observations.
      George Dahl, Ryan Adam and Hugo Larochelle, 2012
  - and more (see course website)

BOLTZMANN MACHINE

Topics: Boltzmann machine

- The original Boltzmann machine has lateral connections in each layer



$$\begin{aligned} E(\mathbf{x},\mathbf{h}) &= -\mathbf{h}^\top \mathbf{W}\mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \\ &\quad -\frac{1}{2}\mathbf{x}^\top \mathbf{V}\mathbf{x} - \frac{1}{2}\mathbf{h}^\top \mathbf{U}\mathbf{h} \end{aligned}$$

  - when only one layer has lateral connection, it's a semi-restricted Boltmann machine

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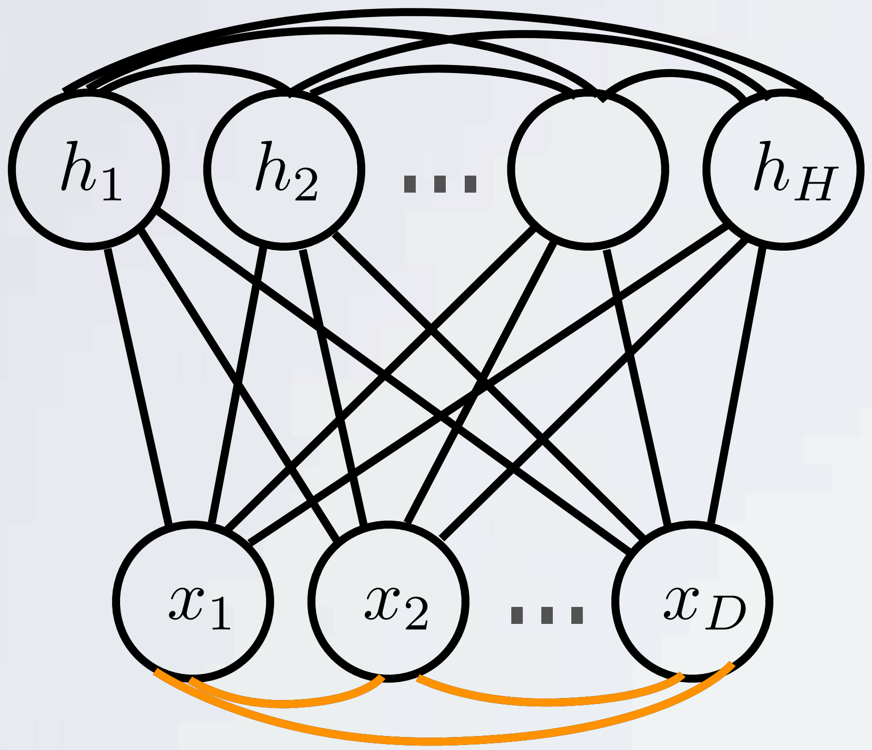

$$E(\mathbf{x}, \mathbf{h}) = -\mathbf{h}^\top \mathbf{W} \mathbf{x} - \mathbf{c}^\top \mathbf{x} - \mathbf{b}^\top \mathbf{h} \boxed{-\frac{1}{2}\mathbf{x}^\top \mathbf{V} \mathbf{x}} - \frac{1}{2}\mathbf{h}^\top \mathbf{U} \mathbf{h}$$

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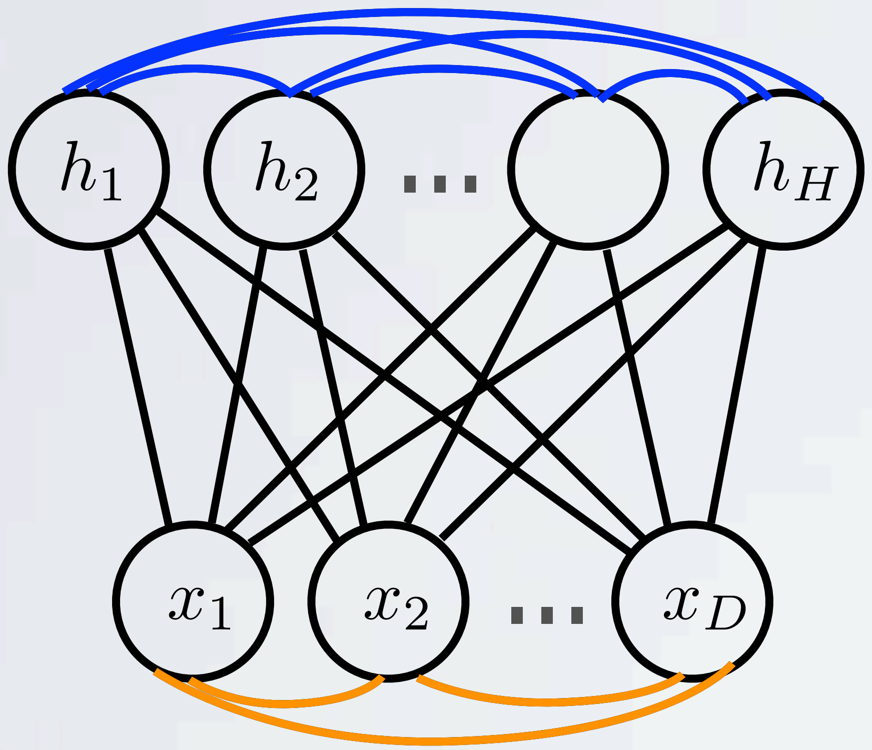

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