DD2437 – Artificial Neural Networks and Deep Architectures (annda)

Lecture 8b: **Boltzmann machines and RBMs, autoencoders**

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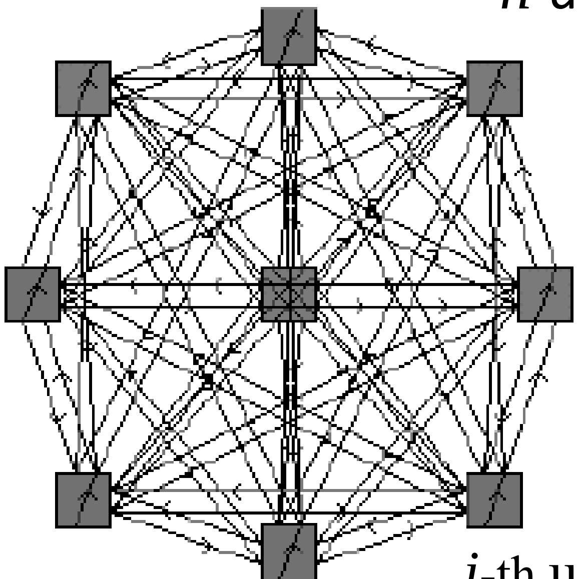
September 2019

Lecture overview

- Boltzmann machine
- Restricted Boltzmann machine, RBM

Hopfield network



$$\forall_i \, w_{i,i} = 0$$ no self-connections

$$\vec{x}' = \mathrm{sgn}(\mathbf{W}\vec{x} + \vec{\theta})$$

$$E(state = \vec{x}) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j} x_i x_j + \sum_{i=1}^{n} \theta_i x_i$$

From Hopfield networks to Boltzmann machines

- Continuous Hopfield network

$$x_i = \frac{1}{1+e^{-a}} \quad \text{instead of} \quad x_i = \operatorname{sgn}(a)$$

- Stochastic component

$$x_i = \begin{cases} 1 & \text{with probability } p_i \\ -1, & \text{with probability } 1\text{-}p_i \end{cases} \qquad p_i = \frac{1}{1+e^{-\frac{1}{T}\sum_j w_{i,j}x_j}}$$

T is a positive temperature const.

From Hopfield networks to Boltzmann machines

- Stochastic component

$$x_i = \begin{cases} 1 & \text{with probability } p_i \\ -1, & \text{with probability } 1\text{-}p_i \end{cases}$$

$$p_i = \frac{1}{1 + e^{-\frac{1}{T}\sum_j w_{i,j} x_j}}$$

$$p(v) = \frac{1}{1 + e^{-v}} \quad \text{where} \quad v = \frac{1}{T}\sum_j w_{i,j} x_j$$

T controls the level of randomness

From Hopfield networks to Boltzmann machines

- Stochastic component

$$x_i = \begin{cases} 1 & \text{with probability } p_i \\ -1, & \text{with probability } 1\text{-}p_i \end{cases}$$

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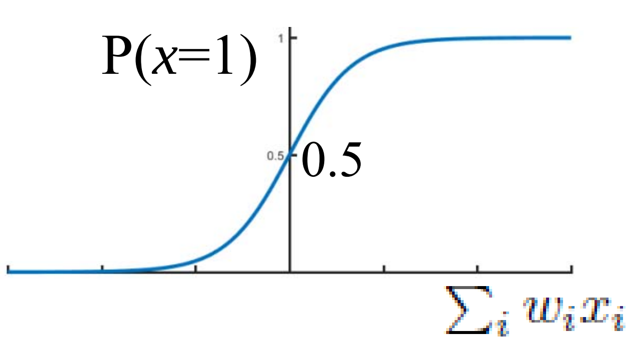
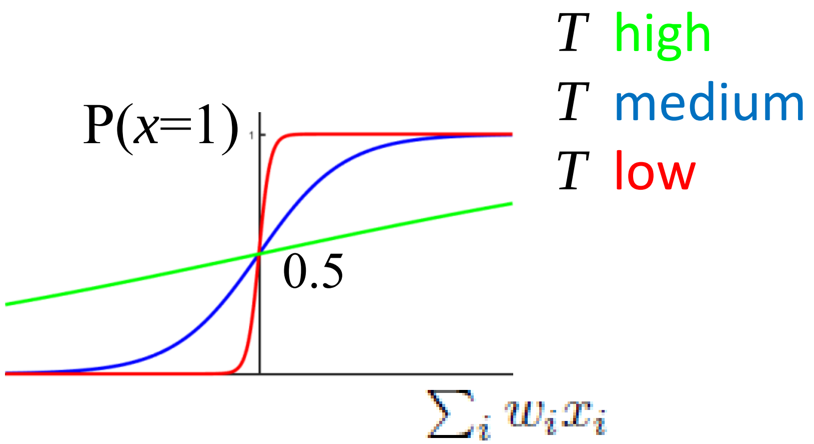




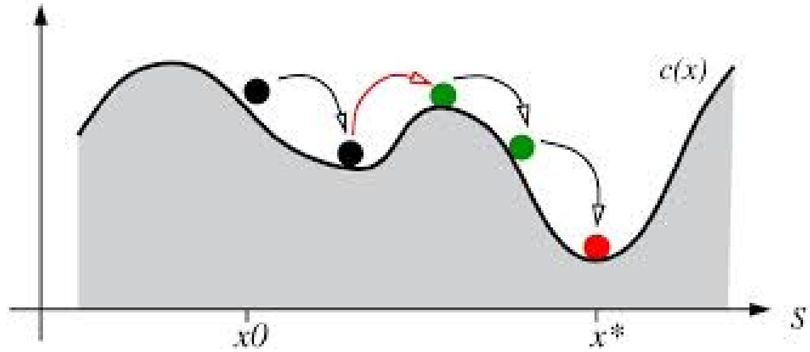
From Hopfield networks to Boltzmann machines

- Stochastic component

$$x_i = \begin{cases} 1 & \text{with probability } p_i \\ -1, & \text{with probability } 1\text{-}p_i \end{cases}$$

$$\boxed{p_i = \frac{1}{1 + e^{-\frac{1}{T}\sum_j w_{i,j} x_j}}}$$

Analogy to simulated annealing (relaxation technique common in metallurgy)

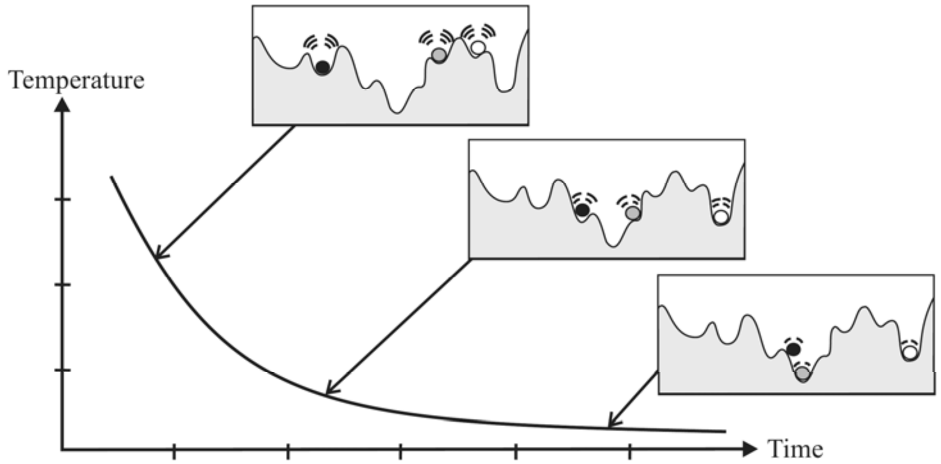


$$p_{\Delta E} = \frac{1}{1 + e^{\Delta E / T}}$$

"When optimising a large complex system with many degrees of freedom, instead of always going downhill, try to go downhill most of the time"

Simulated annealing to reach the global energy min

The critical role of temperature T.

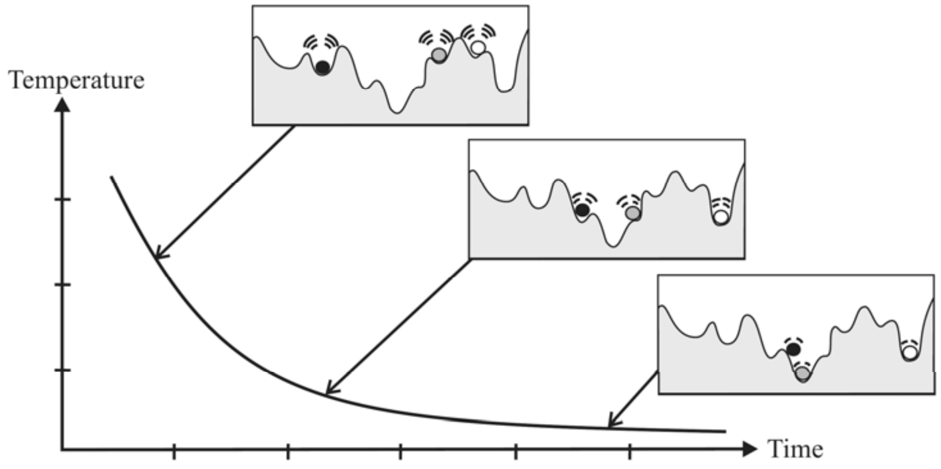


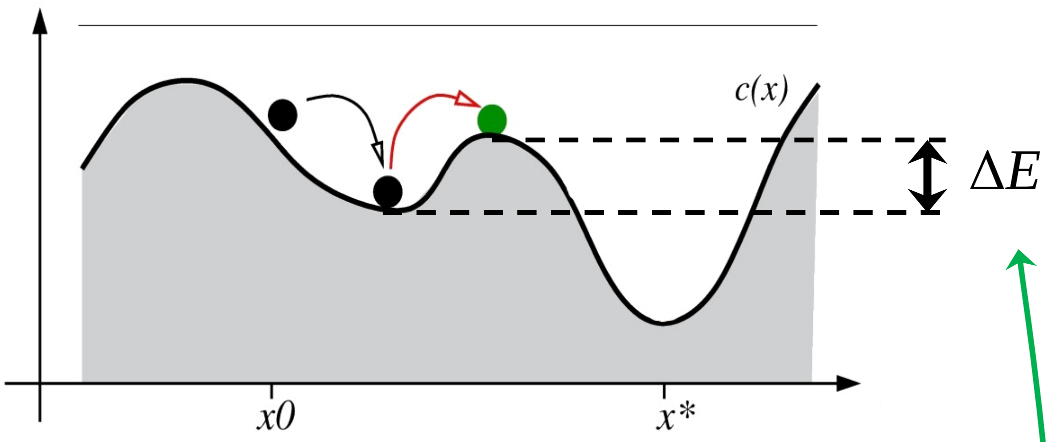
T decreases over time

$$p_{\Delta E} = \frac{1}{1 + e^{\Delta E / T}}$$

Simulated annealing to reach the global energy min

The critical role of temperature T.





$$p_{\Delta E} = \frac{1}{1 + e^{\Delta E / T}}$$

From Hopfield networks to Boltzmann machines

- Energy of this stochastic network is the same as before

$$E = -\frac{1}{2}\vec{x}^{\mathrm{T}}\mathbf{W}\vec{x} = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}x_i x_j$$

- The key difference is a stochastic nature of transitions

from state $s1$ to $s2$:

$$p_{s1\to s2} = \frac{1}{1+e^{(E_2-E_1)/T}} = \frac{1}{1+e^{\Delta E/T}}$$

From Hopfield networks to Boltzmann machines

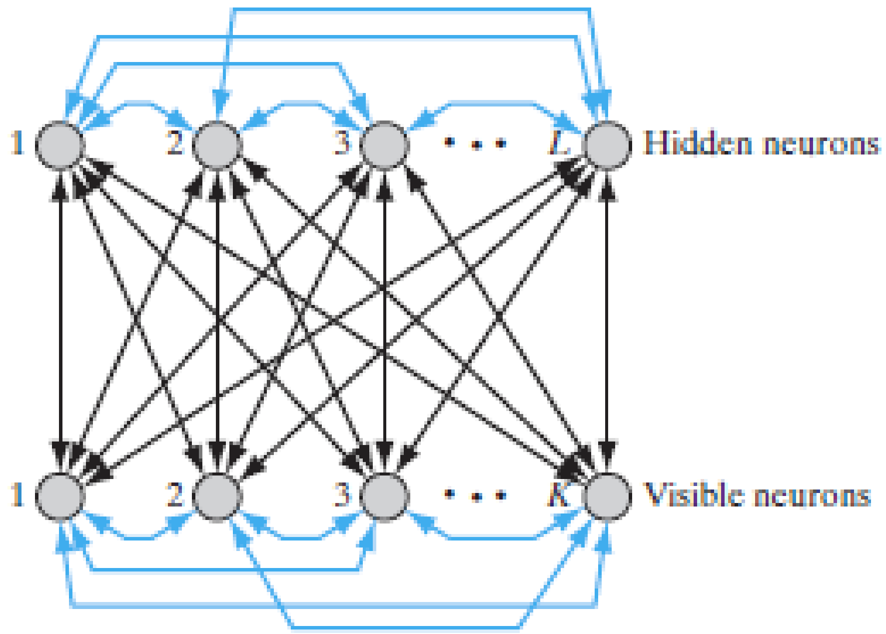
- Energy of this stochastic network is the same as before

$$E = -\frac{1}{2}\vec{x}^{\mathrm{T}}\mathbf{W}\vec{x} = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j} x_i x_j$$

- Given a set of examples $\{\vec{x}_i\}_1^m$ the idea is to adjust $\mathbf{W}$ to describe data distribution (well matched to these examples)

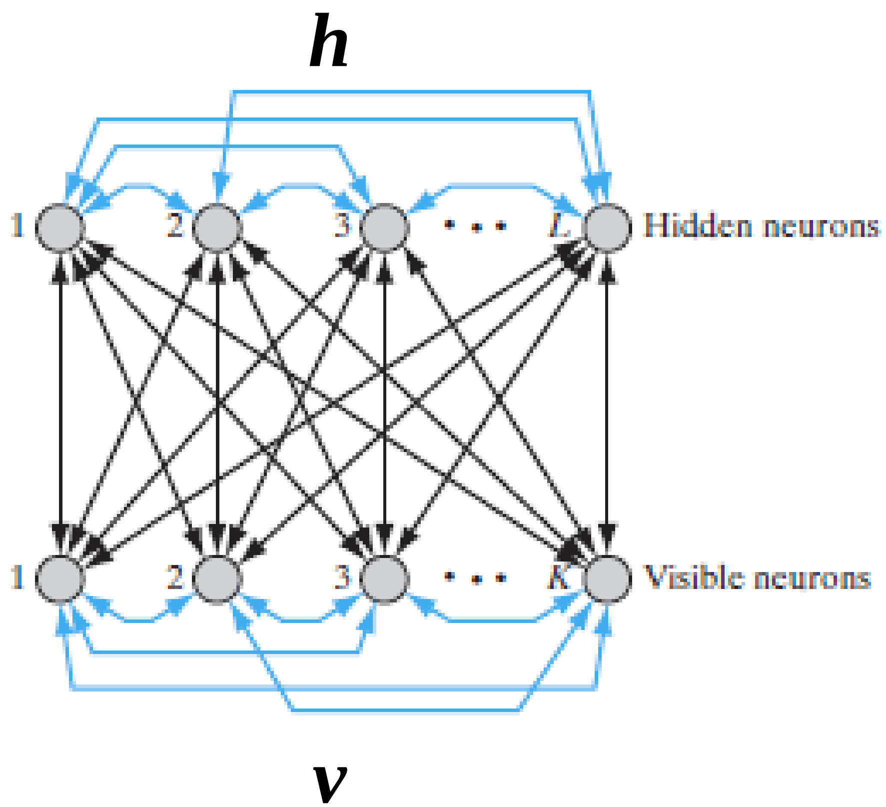
$$P(\vec{x} \mid \mathbf{W}) = \frac{e^{-E}}{Z} = \frac{1}{Z(\mathbf{W})}\exp\left(\frac{1}{2}\vec{x}^{\mathrm{T}}\mathbf{W}\vec{x}\right)$$

Hidden and visible units



- Symmetric connections between visible, $\boldsymbol{v}$, and hidden neurons, $\boldsymbol{h}$
- Hidden neurons help account for higher-order correlations in the input vectors (data)
- Visible units provide interface to the external world – environment (data, $\boldsymbol{v}=\boldsymbol{x}$)
- Hidden units operate freely and are used to explain environmental input vectors

Hidden and visible units



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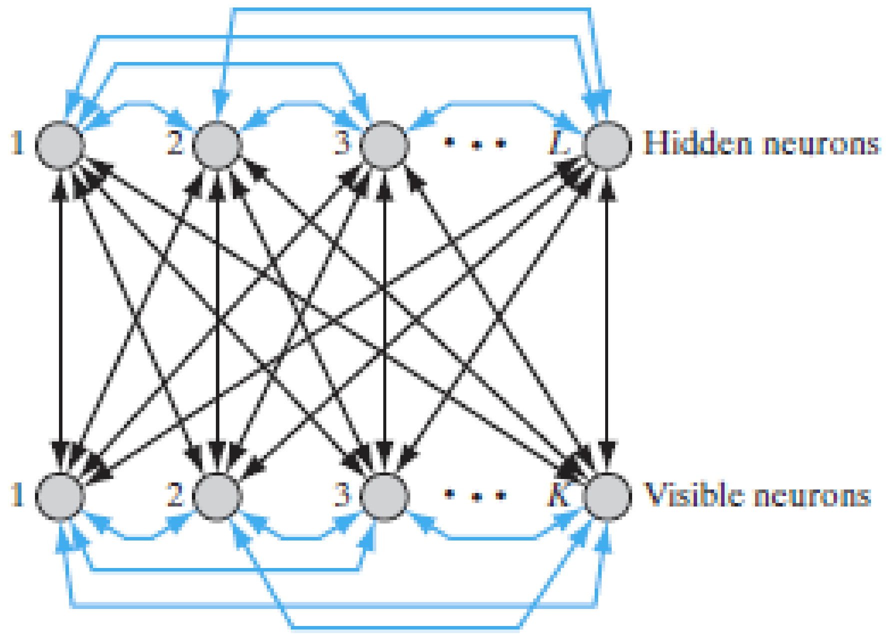
Hidden and visible units

$\boldsymbol{h}$



$\boldsymbol{v}$

$$\boldsymbol{v}^{(p)} = \boldsymbol{x}^{(p)}$$

$$\Downarrow$$

$$\boldsymbol{y}^{(p)} = [\boldsymbol{x}^{(p)}, \boldsymbol{h}]$$

- Symmetric connections between visible, $\boldsymbol{v}$, and hidden neurons, $\boldsymbol{h}$
- Hidden neurons help account for higher-order correlations in the input vectors (data)
- Visible units provide interface to the external world – environment (data, $\boldsymbol{v}$=$\boldsymbol{x}$)
- Hidden units operate freely and are used to explain environmental input vectors
- Modelling a probability distribution (and hidden representation) by clamping patterns onto the visible units $\boldsymbol{v}^{(p_i)} = \boldsymbol{x}^{(p_i)}$

Boltzmann learning

- The primary goal is to correctly model input patterns according to Boltzmann distribution
  - each input pattern is assumed to last long enough (it might have to be clamped for long) for the network to reach thermal equilibrium (converge) at temperature T
  - to reduce this time, simulated annealing is used with a sequence decreasing temperatures (from “hot” to “cold”)
- Essentially, hidden units learn probabilistically representation of data (seen through visible units)

Boltzmann learning

- The idea is to maximise log-likelihood, $L(\mathbf{W})=\log\,(P(\mathbf{X})|\mathbf{W})$

$$\Delta w_{ji} = \varepsilon \frac{\partial L(\mathbf{W})}{\partial w_{ji}} = \eta(\rho_{j,i}^{+} - \rho_{j,i}^{-}), \qquad \eta = \varepsilon / T$$

Boltzmann learning

- The idea is to maximise log-likelihood, $L(\mathbf{W})=\log\left(P(\mathbf{X})|\mathbf{W}\right)$

$$\Delta w_{ji} = \varepsilon \frac{\partial L(\mathbf{W})}{\partial w_{ji}} = \eta(\rho_{j,i}^{+} - \rho_{j,i}^{-}), \qquad \eta = \varepsilon / T$$

$$\frac{\partial L(\mathbf{W})}{\partial w_{i,j}} = \frac{\partial}{\partial w_{i,j}} \log P\left(\{\mathbf{x}^{(p)}\}_1^M \mid \mathbf{W}\right) = \sum_p \left\{ \underbrace{\left\langle y_i y_j \right\rangle_{P(\mathbf{h}|\mathbf{v}=\mathbf{x}^{(p)},\mathbf{W})}} - \underbrace{\left\langle y_i y_j \right\rangle_{P(\mathbf{v},\mathbf{h}|\mathbf{W})}} \right\}$$

positive phase (awake), with clamping, $\mathbf{v}^{(p)}=\mathbf{x}^{(p)}$

negative phase (sleep) free running

$$\left\langle y_i y_j \right\rangle_{P(\mathbf{h}|\mathbf{v}=\mathbf{x}^{(p)},\mathbf{W})} = \sum_p \sum_h P\left(\mathbf{h} \mid \mathbf{v} = \mathbf{x}^{(p)}\right) y_i y_j$$

$$\left\langle y_i y_j \right\rangle_{P(\mathbf{v},\mathbf{h}|\mathbf{W})} = \sum_p \sum_y P(\mathbf{y})\, y_i y_j$$

Boltzmann learning – two phases

$$\frac{\partial L(\mathbf{W})}{\partial w_{i,j}} = \frac{\partial}{\partial w_{i,j}} \log P\left(\{\boldsymbol{x}^{(p)}\}_1^M \mid \mathbf{W}\right) = \sum_p \left\{ \boxed{\left\langle y_i y_j \right\rangle_{P(\boldsymbol{h}|\boldsymbol{v}=\boldsymbol{x}^{(p)},\mathbf{W})}} - \boxed{\left\langle y_i y_j \right\rangle_{P(\boldsymbol{v},\boldsymbol{h}|\mathbf{W})}} \right\}$$

$$\Delta w_{i,j} \propto \left\langle y_i, y_j \right\rangle_{\text{data}} - \left\langle y_i, y_j \right\rangle_{\text{model}}$$

Boltzmann learning – two phases

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- **Positive** phase implies clamping the inputs (relative fast)

$$\left\langle y_i, y_j \right\rangle_{data} \leftarrow$$

Expected value at thermal equilibrium

- **Negative** phase involves updating all the units (can be very slow)

$$\left\langle y_i, y_j \right\rangle_{\text{model}}$$

Boltzmann learning – two phases

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Thermal equilibrium <u>does not</u> imply only that the system settles down into the lowest energy state.

It is about the convergence of probability distribution over different configurations.

Expected value at thermal equilibrium

- **Nega**

Boltzmann learning – two phases

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- **Positive** phase implies clamping the inputs (relative fast)

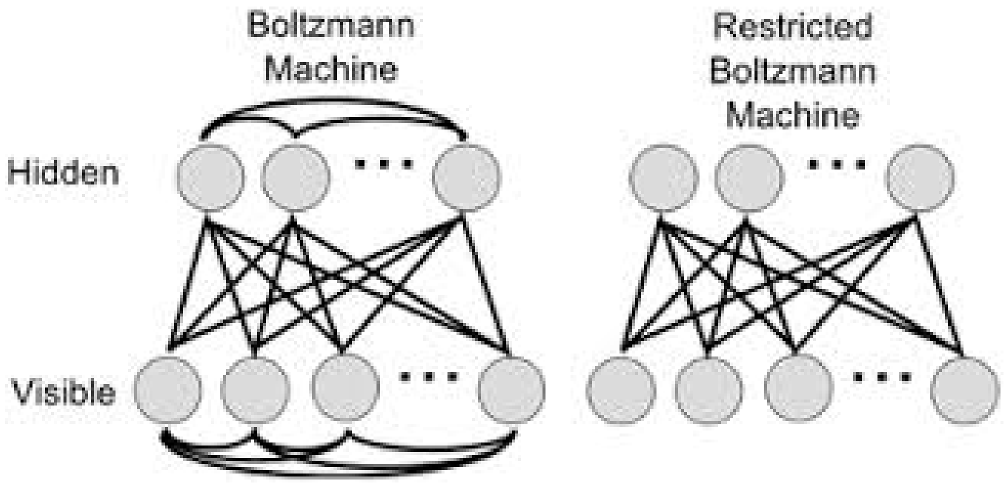
"Hebbian learning" $\left\langle y_i, y_j \right\rangle_{data}$

- **Negative** phase involves updating all the units (can be very slow)

"Hebbian forgetting" $\left\langle y_i, y_j \right\rangle_{\mathrm{model}}$

prevent from learning false, spontaneously generated states

Restricted Boltzmann machine (RBM)

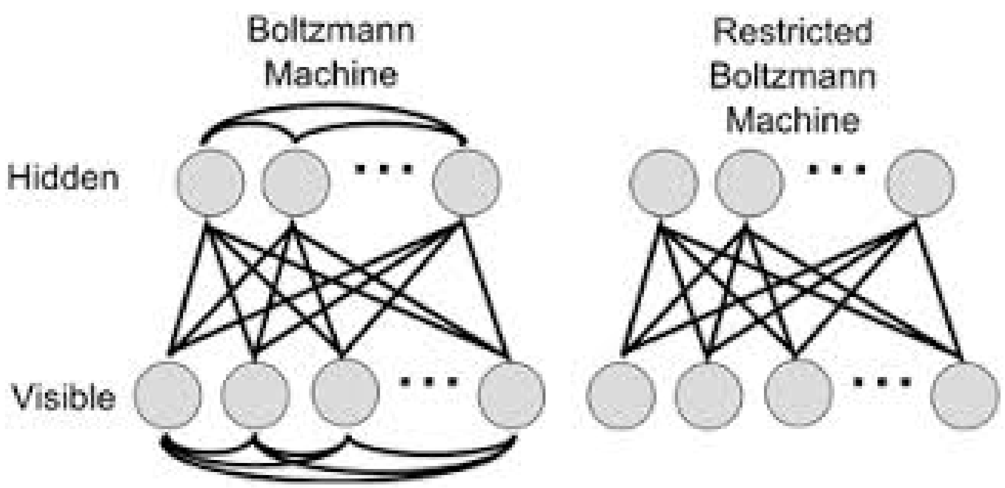


Visible and hidden units are conditionally independent given one another

$$p(\boldsymbol{h} \mid \boldsymbol{v}) = \prod_i p(h_i \mid \boldsymbol{v})$$

$$p(\boldsymbol{v} \mid \boldsymbol{h}) = \prod_j p(v_j \mid \boldsymbol{h})$$

Restricted Boltzmann machine (RBM)



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Following the same principle of maximising log likelihood by means of gradient ascent, one obtains:

$$\Delta w_{ji} = \varepsilon \frac{\partial L(\mathbf{W})}{\partial w_{ji}} = \varepsilon \left(\left\langle v_j h_i \right\rangle_{\text{data}} - \left\langle v_j h_i \right\rangle_{\text{model}} \right)$$

Restricted Boltzmann machine (RBM)

$$P(h_i = 1 \mid \boldsymbol{v}) = \frac{1}{1 + \exp\left(-bias_{h_i} - \boldsymbol{v}^{\mathrm{T}} \mathbf{W}_{:,i}\right)}$$

$$P(v_j = 1 \mid \boldsymbol{h}) = \frac{1}{1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:}\,\boldsymbol{h}\right)}$$

$\Leftarrow$

Visible and hidden units are conditionally independent given one another

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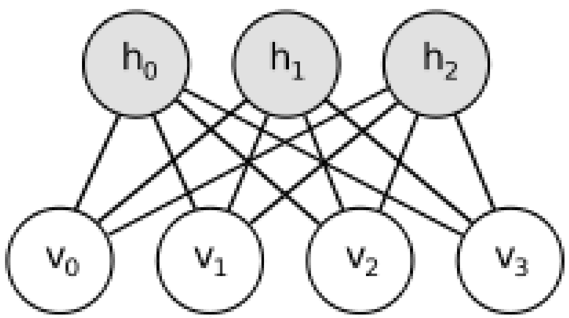
RBM learning with Contrastive Divergence (CD)



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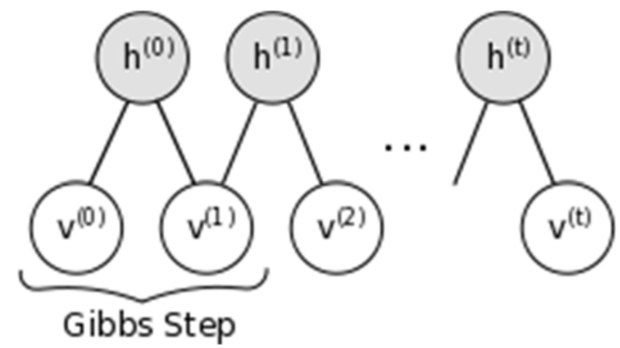
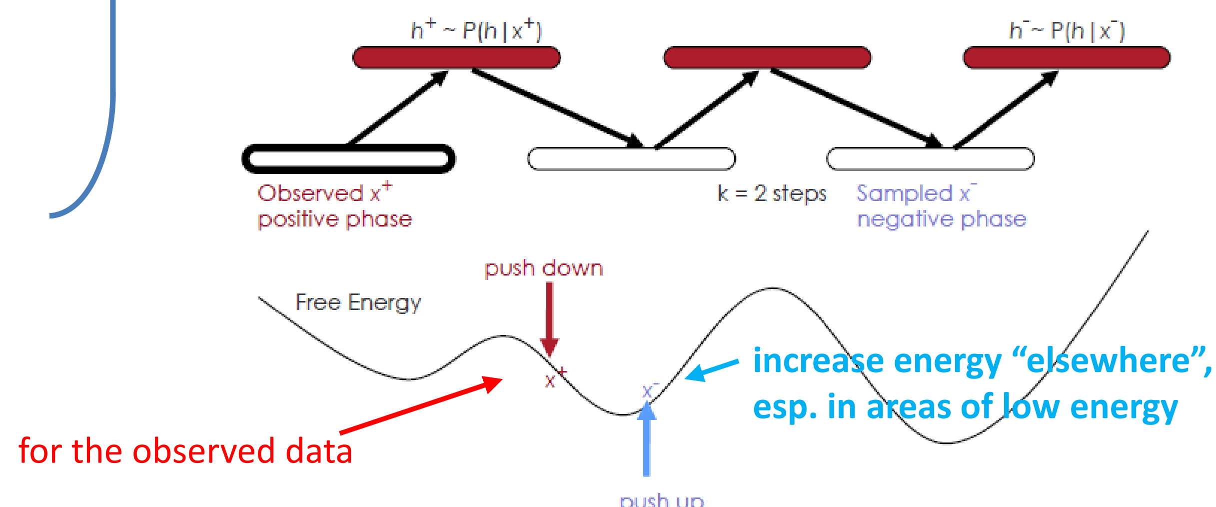
$$P(v_j = 1 \mid \boldsymbol{h}) = \frac{1}{1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:}\boldsymbol{h}\right)}$$

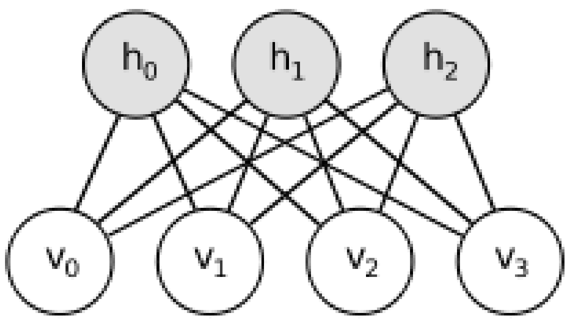
Gibbs sampling





Hinton, 2003

RBM learning with Contrastive Divergence (CD)



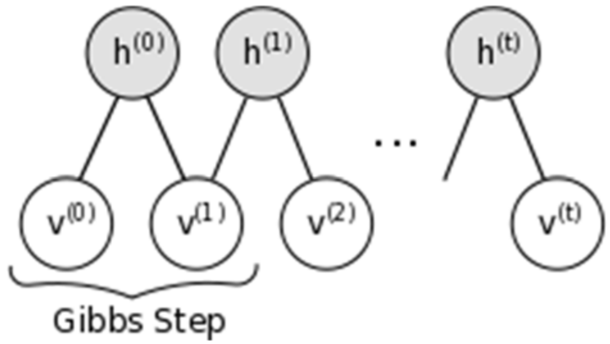
$$P(h_i = 1 \mid \boldsymbol{v}) = \frac{1}{1 + \exp\left(-bias_{h_i} - \boldsymbol{v}^{\mathrm{T}} \mathbf{W}_{:,i}\right)}$$

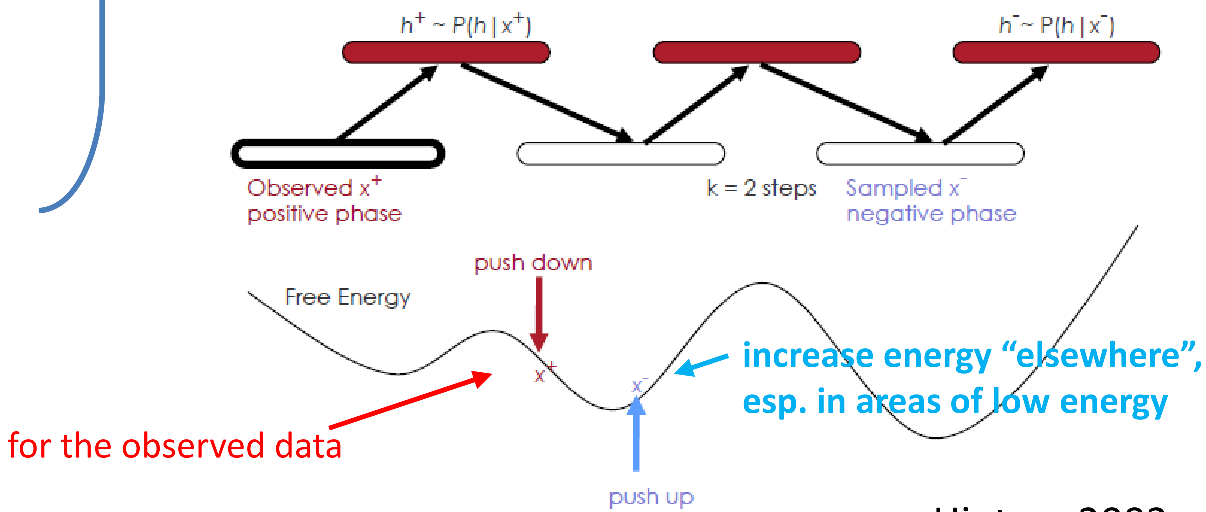
$$P(v_j = 1 \mid \boldsymbol{h}) = \frac{1}{1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:} \boldsymbol{h}\right)}$$

GOOD TO KNOW:

Contrastive Divergence does not optimise the likelihood but it works effectively!

Gibbs sampling

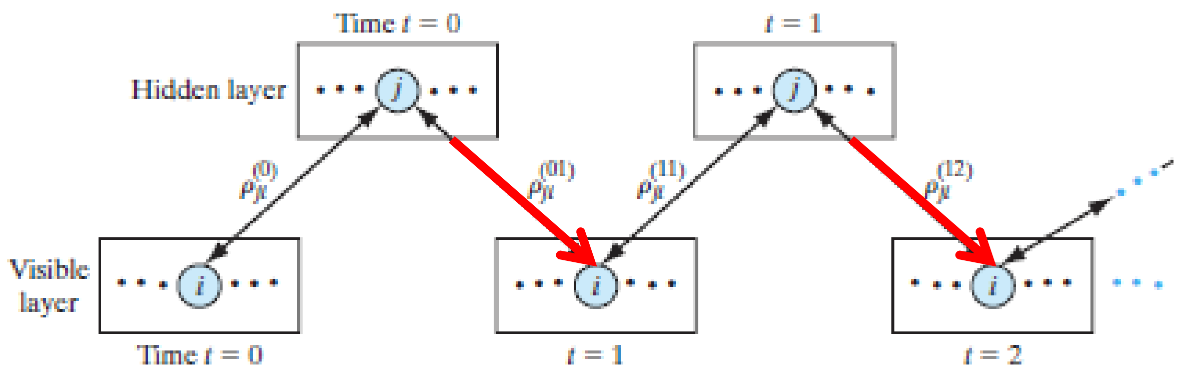




Hinton, 2003

CD_k recipe for training RBM

Gibbs sampling



1) Clamp the visible units with an input vector and update hidden units.

$$P(h_i = 1 \mid \boldsymbol{v}) = \left(1 + \exp\left(-bias_{h_i} - \boldsymbol{v}^{\mathrm{T}} \mathbf{W}_{:,i}\right)\right)^{-1}$$

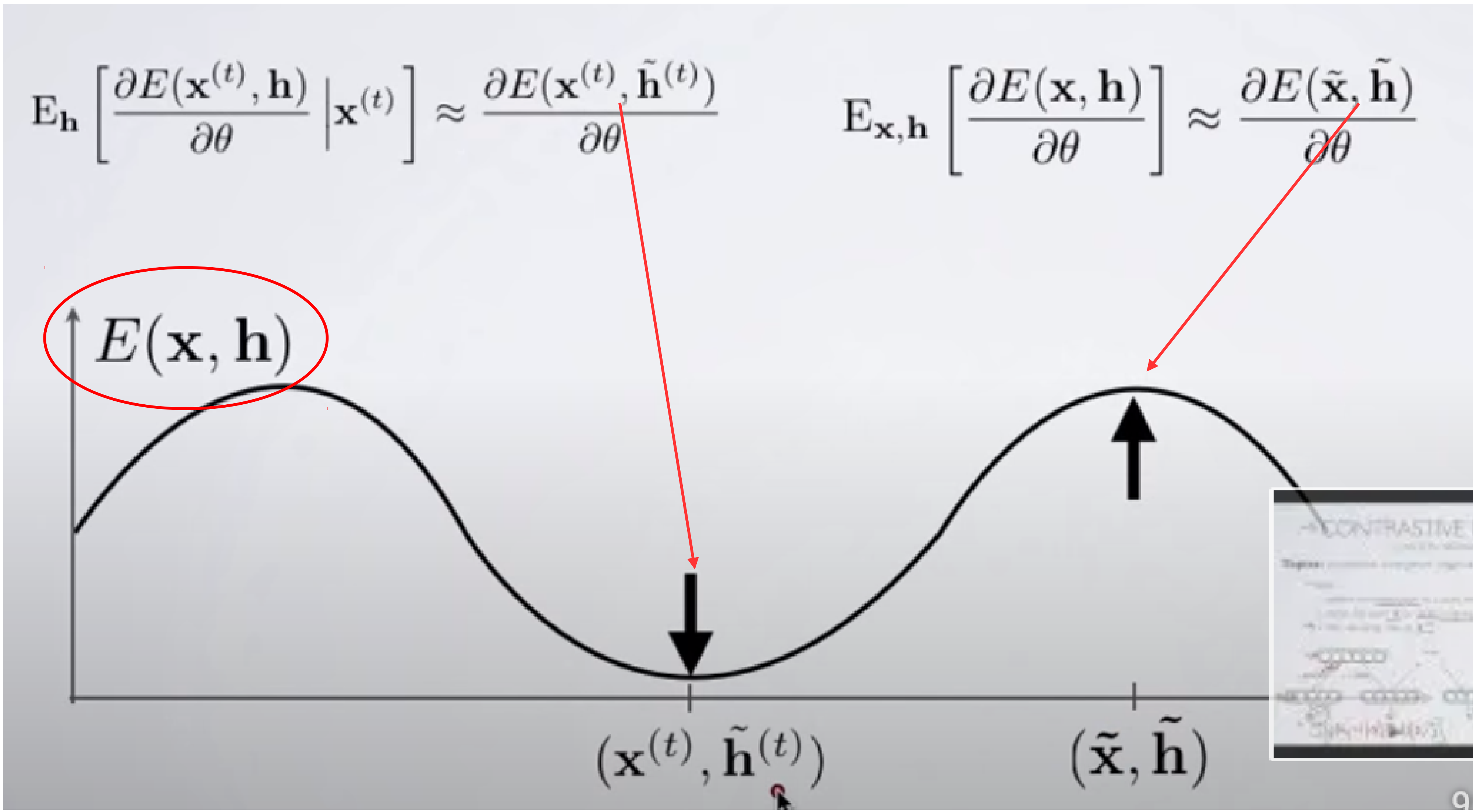
2) Update all the visible units in parallel to get a **reconstruction**.

$$P(v_j = 1 \mid \boldsymbol{h}) = \left(1 + \exp\left(-bias_{v_j} - \mathbf{W}_{j,:} \boldsymbol{h}\right)\right)^{-1}$$

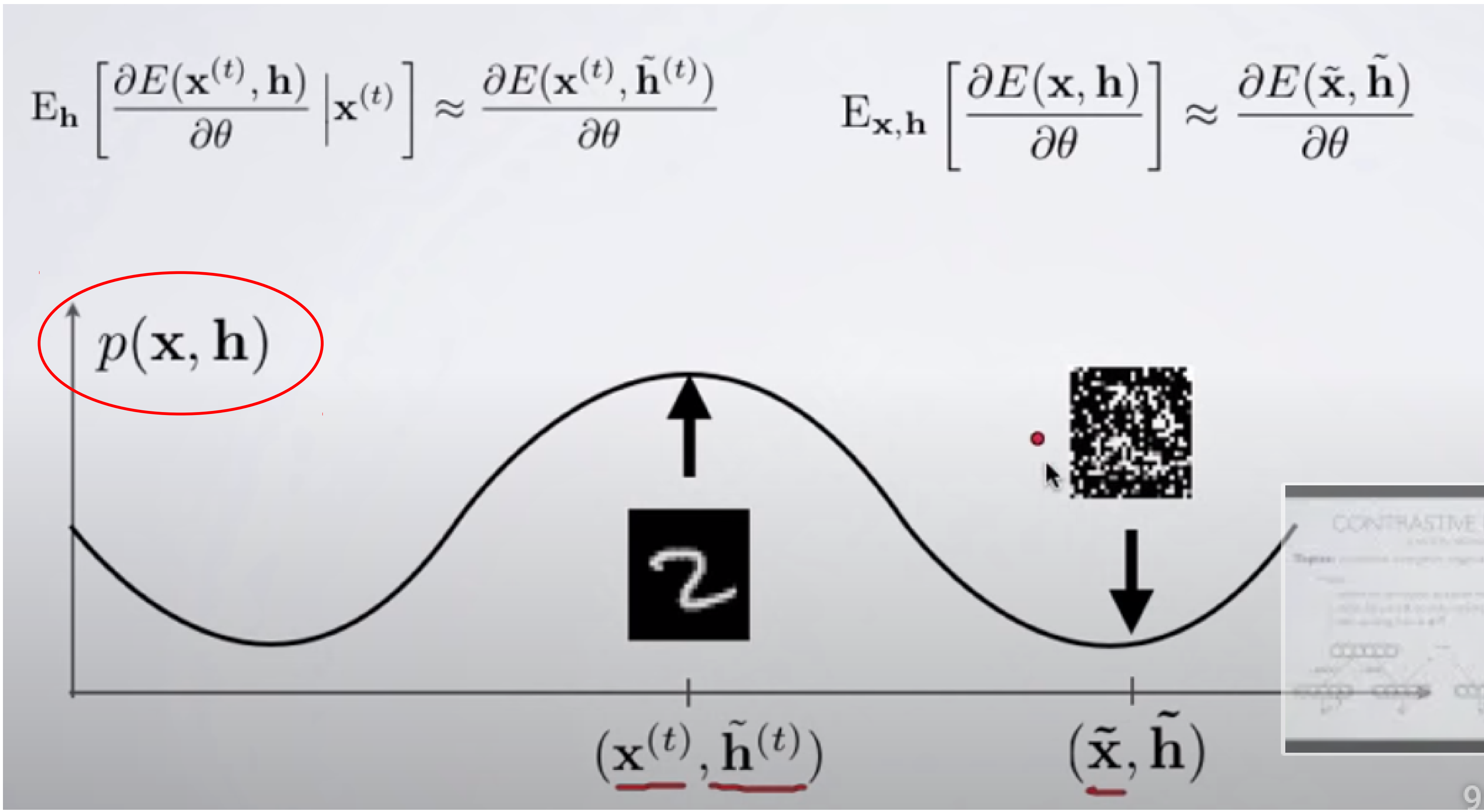
3) Collect the statistics for correlations after *k* steps using mini-batches and update weights:

$$\Delta w_{j,i} = \frac{1}{N} \sum_{n=1}^{N} \left(v_j^{(n)} h_i^{(n)} - \hat{v}_j^{(n)} \hat{h}_i^{(n)} \right)$$

Illustration of pos. and neg. phase



Example if patterns are digits



More in-depth lectures

Videos by Hugo Larochelle

RBM
https://www.youtube.com/watch?v=MD8qXWucJBY

Contrastive divergence, by Hugo Larochelle
https://www.youtube.com/watch?v=MD8qXWucJBY

persistent CD (just beginning which is explaining CD)
https://www.youtube.com/watch?v=S0kFFiHzR8M

From RBM to Gaussian-Bernoulli RBM

Bernoulli-Bernoulli (binary-binary)

$$p(v_i = 1|\mathbf{h}) = g\left(\sum_j W_{ij} h_j + b_i\right)$$

$$p(h_j = 1|\mathbf{v}) = g\left(\sum_i W_{ij} v_i + a_j\right)$$

Gaussian-Bernoulli (real/cont.-binary)

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

$$p(h_j = 1|\mathbf{v}) = g\left(b_j + \sum_i W_{ij} \frac{v_i}{\sigma_i}\right),$$

Visible units are real-valued whereas hidden units remain binary.

Salakhutdinov, 2015

From RBM to Gaussian-Bernoulli RBM

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Gaussian-Bernoulli (real/cont.-binary)

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$$p(h_j = 1|\mathbf{v}) = g\left(b_j + \sum_i W_{ij} \frac{v_i}{\sigma_i}\right),$$

Visible units are real-valued whereas hidden units remain binary.

The derivative of the log-likelihood:

$$\frac{\partial \log P(\mathbf{v};\theta)}{\partial W_{ij}} = \mathbb{E}_{P_{\text{data}}}\left[\frac{1}{\sigma_i} v_i h_j\right] - \mathbb{E}_{P_{\text{model}}}\left[\frac{1}{\sigma_i} v_i h_j\right]$$

Salakhutdinov, 2015