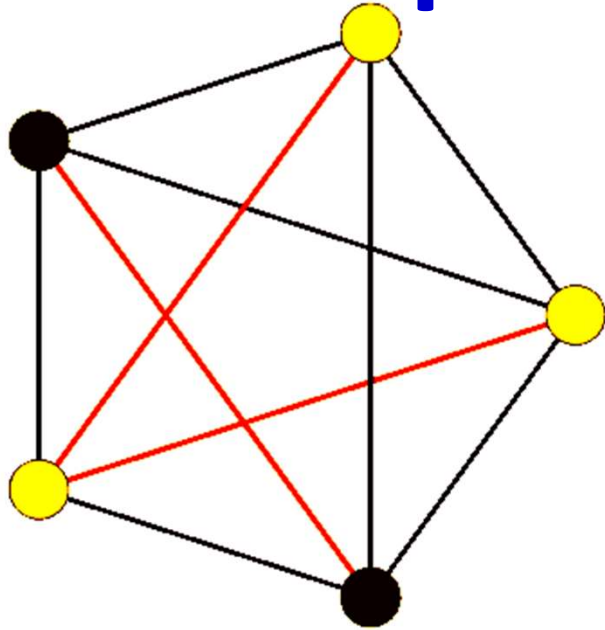


Neural Networks

Hopfield Nets and Boltzmann Machines

Recap: Hopfield network

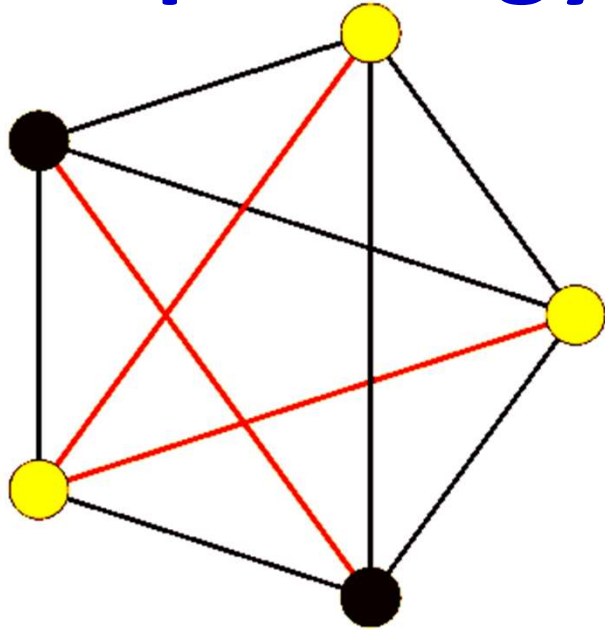


$$y_i = \Theta \left(\sum_{j \neq i} w_{ji} y_j + b_i \right)$$

$$\Theta(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

- At each time each neuron receives a “field” $\sum_{j \neq i} w_{ji} y_j + b_i$
- If the sign of the field matches its own sign, it does not respond
- If the sign of the field opposes its own sign, it “flips” to match the sign of the field

Recap: Energy of a Hopfield Network



$$y_i = \Theta \left(\sum_{j \neq i} w_{ji} y_j + b_i \right)$$

$$\Theta(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

$$E = - \sum_{i,j < i} w_{ij} y_i y_j - \sum_i b_i y_i$$

- The system will evolve until the energy hits a local minimum
- In vector form
 - Bias term may be viewed as an extra input pegged to 1.0

$$E = -\frac{1}{2} \mathbf{y}^T \mathbf{W} \mathbf{y} - \mathbf{b}^T \mathbf{y}$$

Recap: Hopfield net computation

1. Initialize network with initial pattern

$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. Iterate until convergence

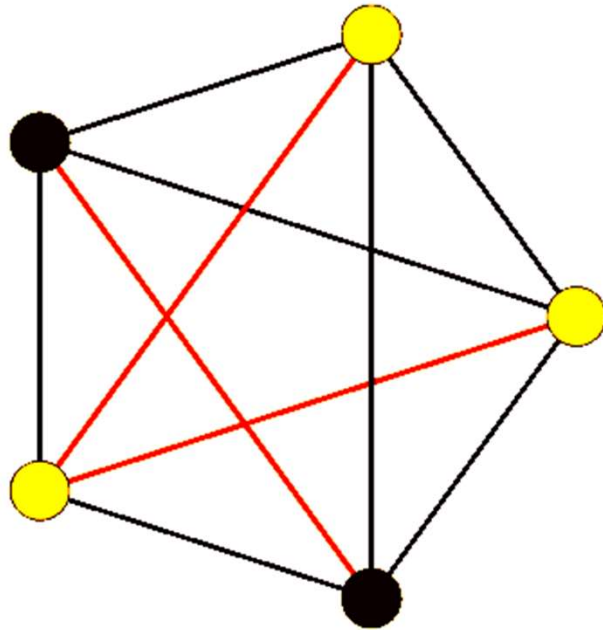
$$y_i(t + 1) = \Theta \left(\sum_{j \neq i} w_{ji} y_j \right), \quad 0 \leq i \leq N - 1$$

- Very simple
- Updates can be done sequentially, or all at once
- Convergence

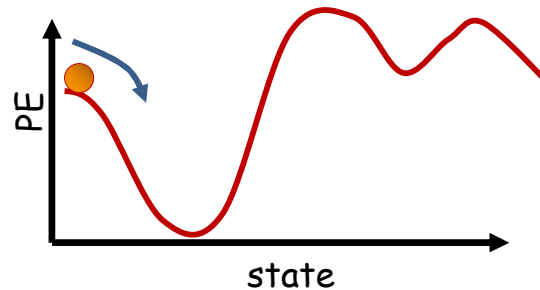
$$E = - \sum_i \sum_{j > i} w_{ji} y_j y_i$$

does not change significantly any more

Recap: Evolution

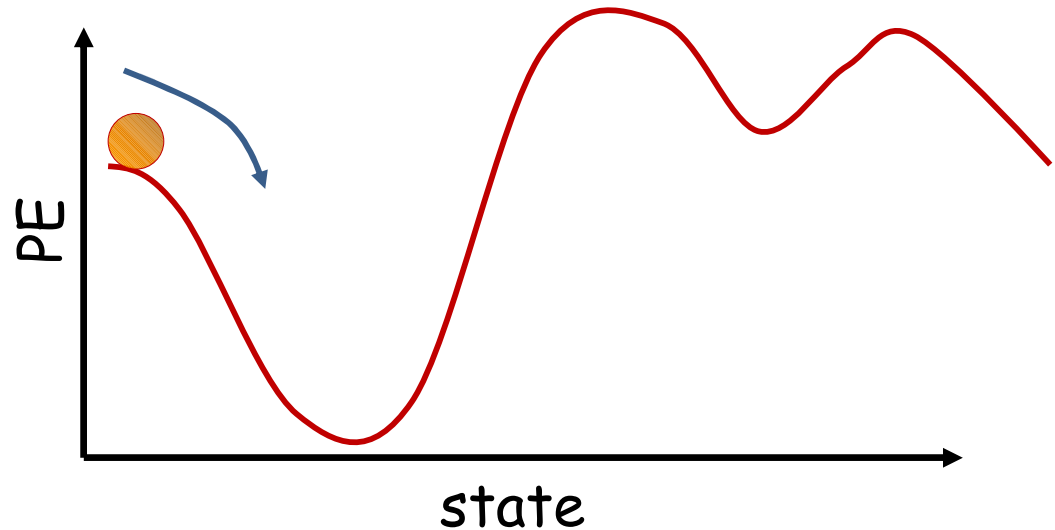
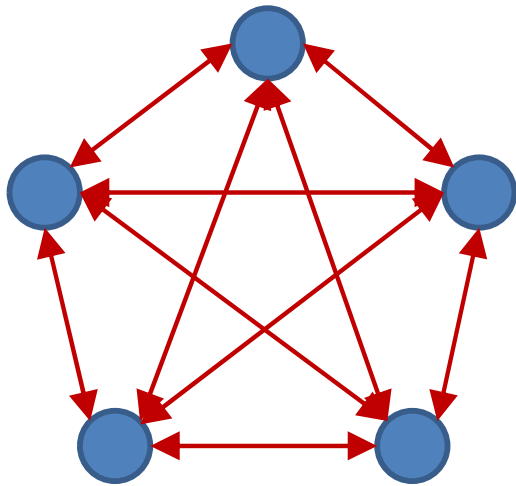


$$E = -\frac{1}{2} \mathbf{y}^T \mathbf{W} \mathbf{y}$$



- The network will evolve until it arrives at a local minimum in the energy contour

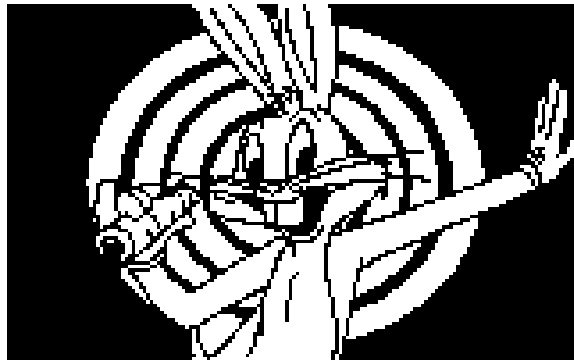
Recap: Content-addressable memory



- Each of the minima is a “stored” pattern
 - If the network is initialized close to a stored pattern, it will inevitably evolve to the pattern
- **This is a *content addressable memory***
 - Recall memory content from partial or corrupt values
- Also called ***associative memory***

Examples: Content addressable memory

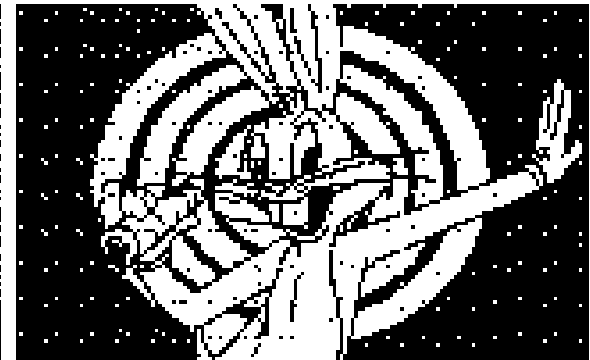
Original



Degraded



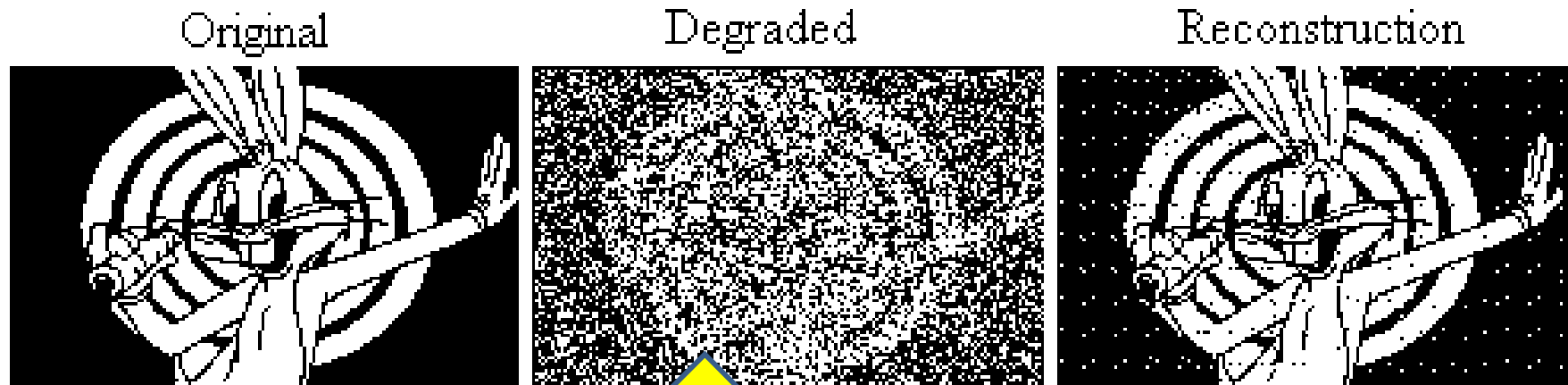
Reconstruction



Hopfield network reconstructing degraded images
from noisy (top) or partial (bottom) cues.

- <http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/> ₇

Examples: Content addressable memory



Noisy pattern completion: Initialize the entire network and let the entire network evolve

Hopfield network reconstructing degraded images
from noisy (top) or partial (bottom) cues.

- <http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/> ₈

Examples: Content addressable memory

Original

Degraded

Reconstruction



Pattern completion: Fix the “seen” bits and only let the “unseen” bits evolve



Hopfield network reconstructing degraded images
from noisy (top) or partial (bottom) cues.

- <http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/> ₉

Training a Hopfield Net to “Memorize” target patterns

- The Hopfield network can be *trained* to remember specific “target” patterns
 - E.g. the pictures in the previous example
- This can be done by setting the weights \mathbf{W} appropriately

Random Question:

Can you use *backprop* to train Hopfield nets?

Hint: Think unwrapping...

Training a Hopfield Net to “Memorize” target patterns

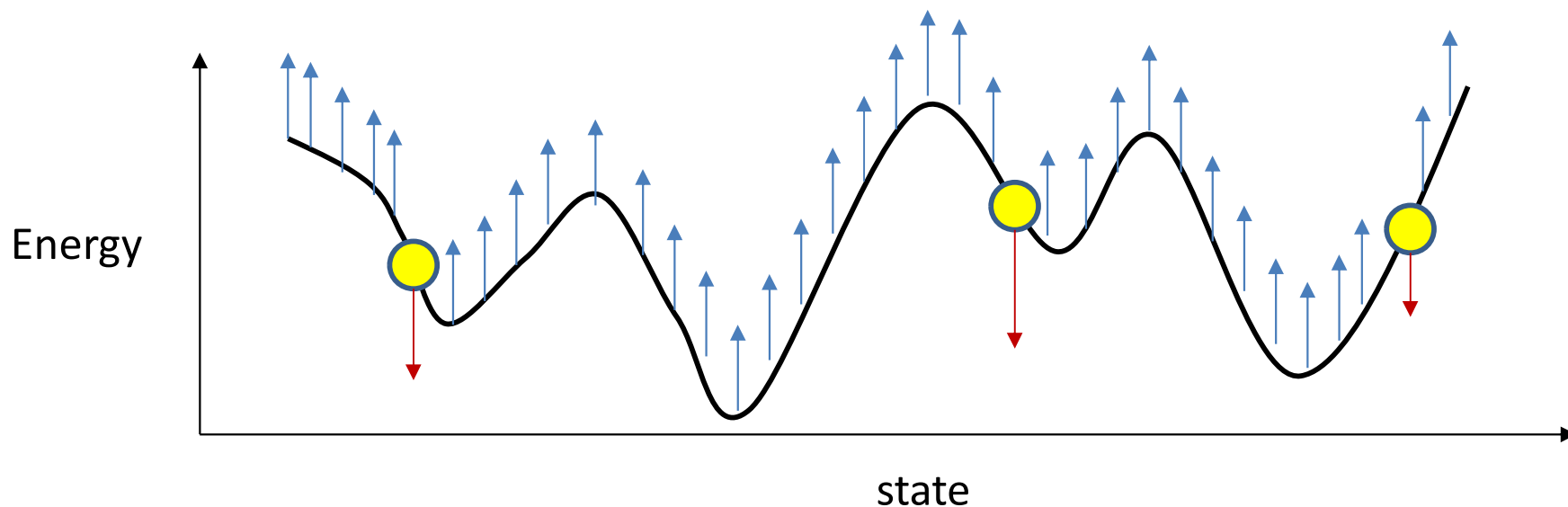
- The Hopfield network can be *trained* to remember specific “target” patterns
 - E.g. the pictures in the previous example
- A Hopfield net with N neurons can be designed to store up to N target N -bit memories
 - But can store an exponential number of unwanted “parasitic” memories along with the target patterns
- **Training the network:** Design weights matrix \mathbf{W} such that the energy of ...
 - Target patterns is minimized, so that they are in energy wells
 - *Other untargeted* potentially parasitic patterns is maximized so that they don't become parasitic

Training the network

$$\hat{\mathbf{W}} = \operatorname{argmin}_{\mathbf{W}} \underbrace{\sum_{\mathbf{y} \in Y_P} E(\mathbf{y})}_{\text{Minimize energy of target patterns}} - \underbrace{\sum_{\mathbf{y} \notin Y_P} E(\mathbf{y})}_{\text{Maximize energy of all other patterns}}$$

Minimize energy of target patterns

Maximize energy of all other patterns



Optimizing \mathbf{W}

$$E(\mathbf{y}) = -\frac{1}{2}\mathbf{y}^T\mathbf{W}\mathbf{y} \quad \hat{\mathbf{W}} = \operatorname{argmin}_{\mathbf{W}} \sum_{\mathbf{y} \in \mathbf{Y}_P} E(\mathbf{y}) - \sum_{\mathbf{y} \notin \mathbf{Y}_P} E(\mathbf{y})$$

- Simple gradient descent:

$$\mathbf{W} = \mathbf{W} + \eta \left(\underbrace{\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T}_{\text{Minimize energy of target patterns}} - \underbrace{\sum_{\mathbf{y} \notin \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T}_{\text{Maximize energy of all other patterns}} \right)$$

Minimize energy of
target patterns

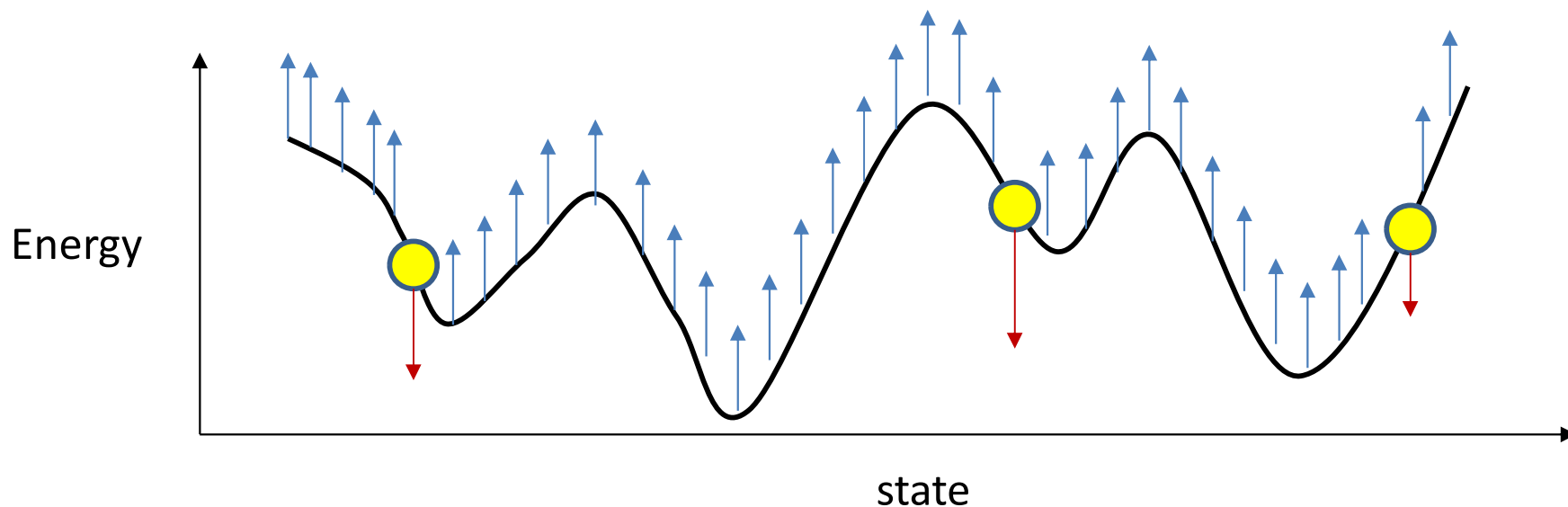
Maximize energy of
all other patterns

Training the network

$$\mathbf{W} = \mathbf{W} + \eta \left(\underbrace{\sum_{\mathbf{y} \in Y_P} \mathbf{y}\mathbf{y}^T}_{\text{Minimize energy of target patterns}} - \underbrace{\sum_{\mathbf{y} \notin Y_P} \mathbf{y}\mathbf{y}^T}_{\text{Maximize energy of all other patterns}} \right)$$

Minimize energy of target patterns

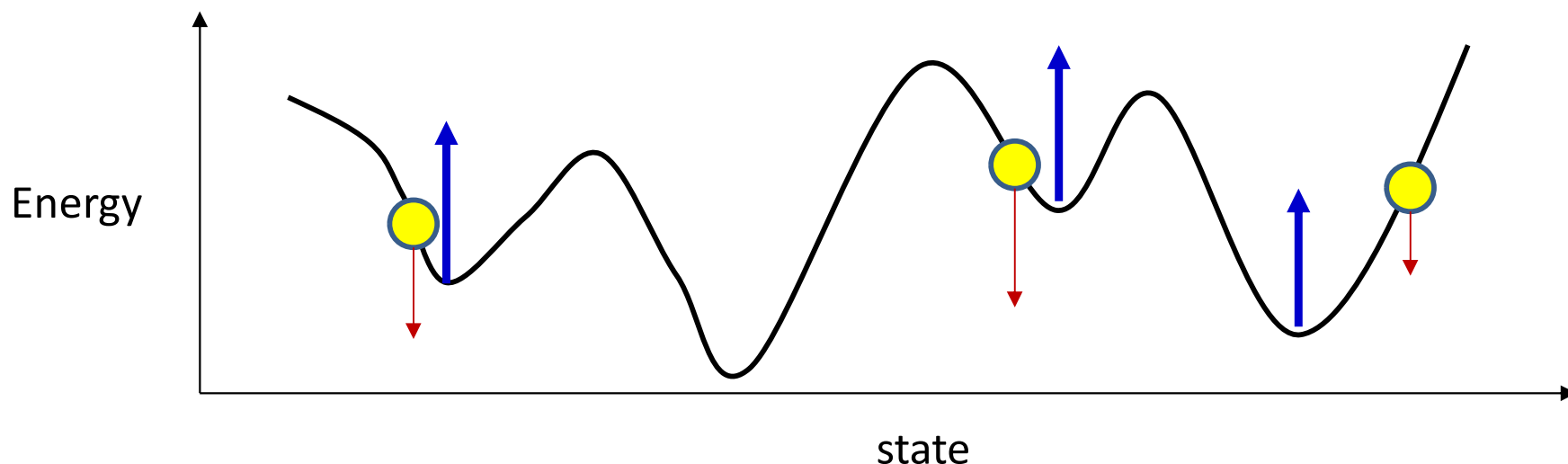
Maximize energy of all other patterns



Simpler: Focus on confusing parasites

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = \text{valley}} \mathbf{y}\mathbf{y}^T \right)$$

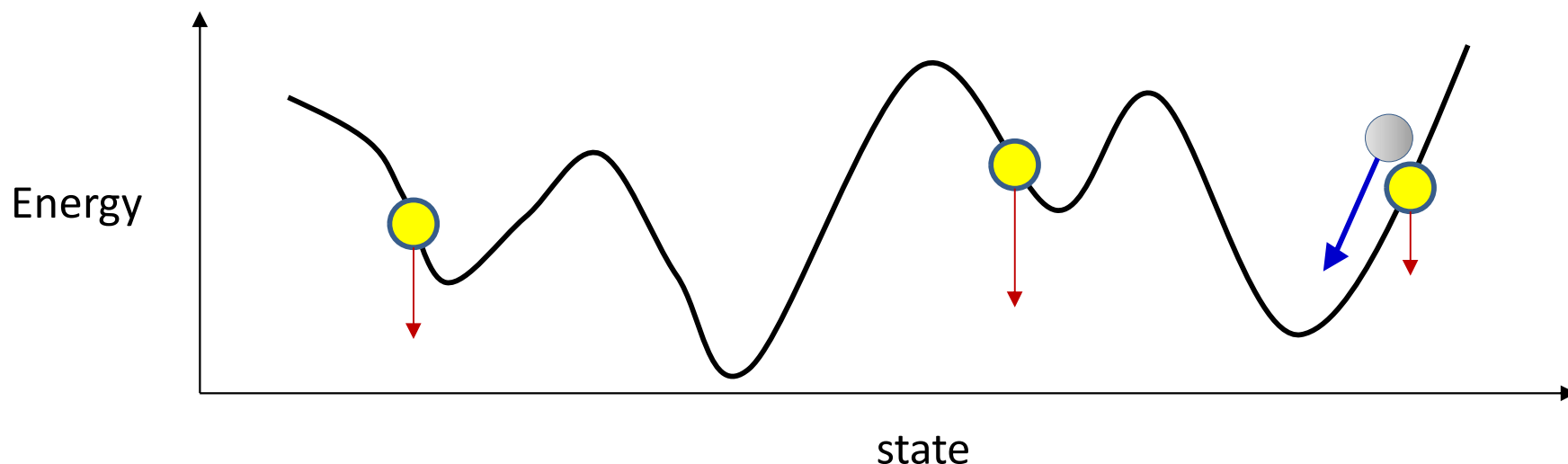
- Focus on minimizing parasites that can prevent the net from remembering target patterns
 - Energy valleys in the neighborhood of target patterns



Simpler: Focus on confusing patterns

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = \text{valley}} \mathbf{y}\mathbf{y}^T \right)$$

- Lower energy at valid memories
- Initialize the network at valid memories and let it evolve
 - It will settle in a valley. If this is not the target pattern, raise it



Training the Hopfield network

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = \text{valley}} \mathbf{y}\mathbf{y}^T \right)$$

- Initialize \mathbf{W}
- Compute the total outer product of all target patterns
 - More important patterns presented more frequently
- Initialize the network with each target pattern and let it evolve
 - And settle at a valley
- Compute the total outer product of valley patterns
- Update weights

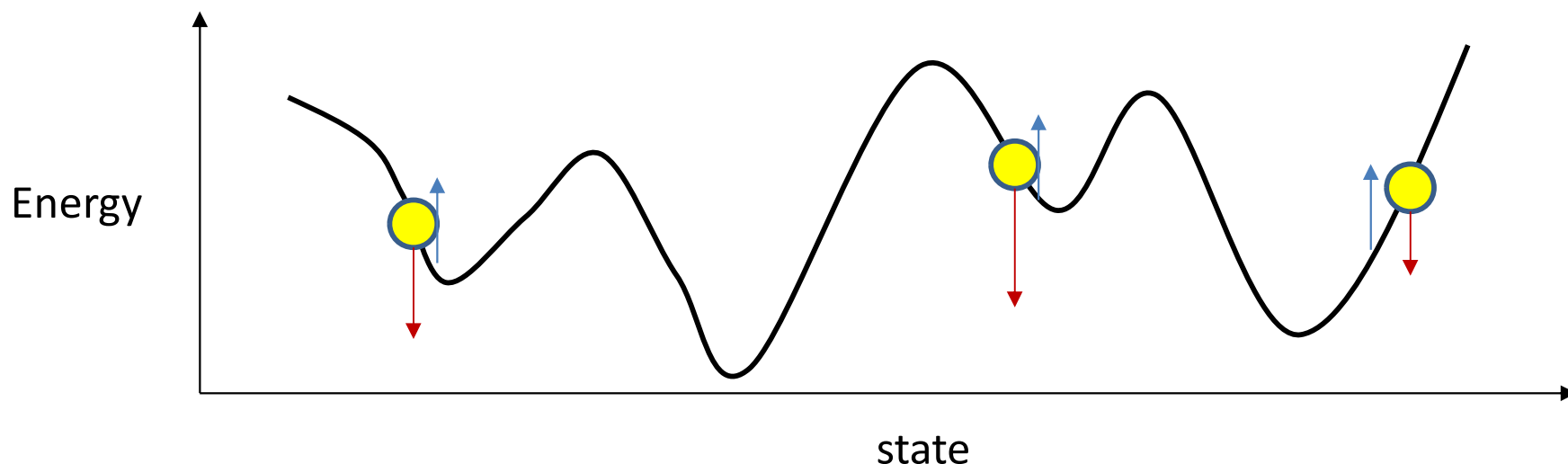
Training the Hopfield network: SGD version

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = \text{valley}} \mathbf{y}\mathbf{y}^T \right)$$

- Initialize \mathbf{W}
- Do until convergence, satisfaction, or death from boredom:
 - Sample a target pattern \mathbf{y}_p
 - Sampling frequency of pattern must reflect importance of pattern
 - Initialize the network at \mathbf{y}_p and let it evolve
 - And settle at a valley \mathbf{y}_v
 - Update weights
 - $\mathbf{W} = \mathbf{W} + \eta(\mathbf{y}_p\mathbf{y}_p^T - \mathbf{y}_v\mathbf{y}_v^T)$

More efficient training

- Really no need to raise the entire surface, or even every valley
- Raise the *neighborhood* of each target memory
 - Sufficient to make the memory a valley
 - The broader the neighborhood considered, the broader the valley

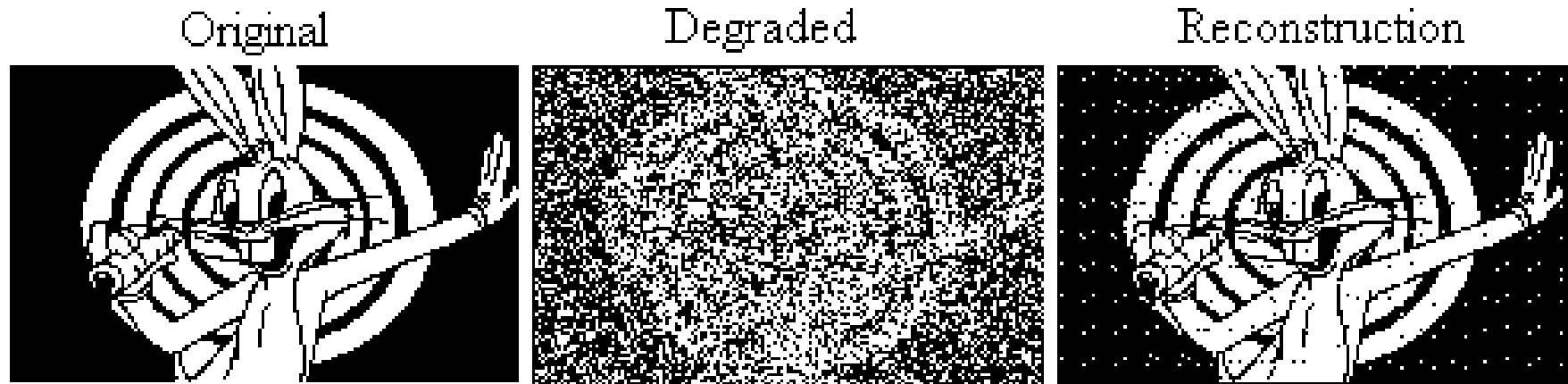


Training the Hopfield network: SGD version

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y}\mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = \text{valley}} \mathbf{y}\mathbf{y}^T \right)$$

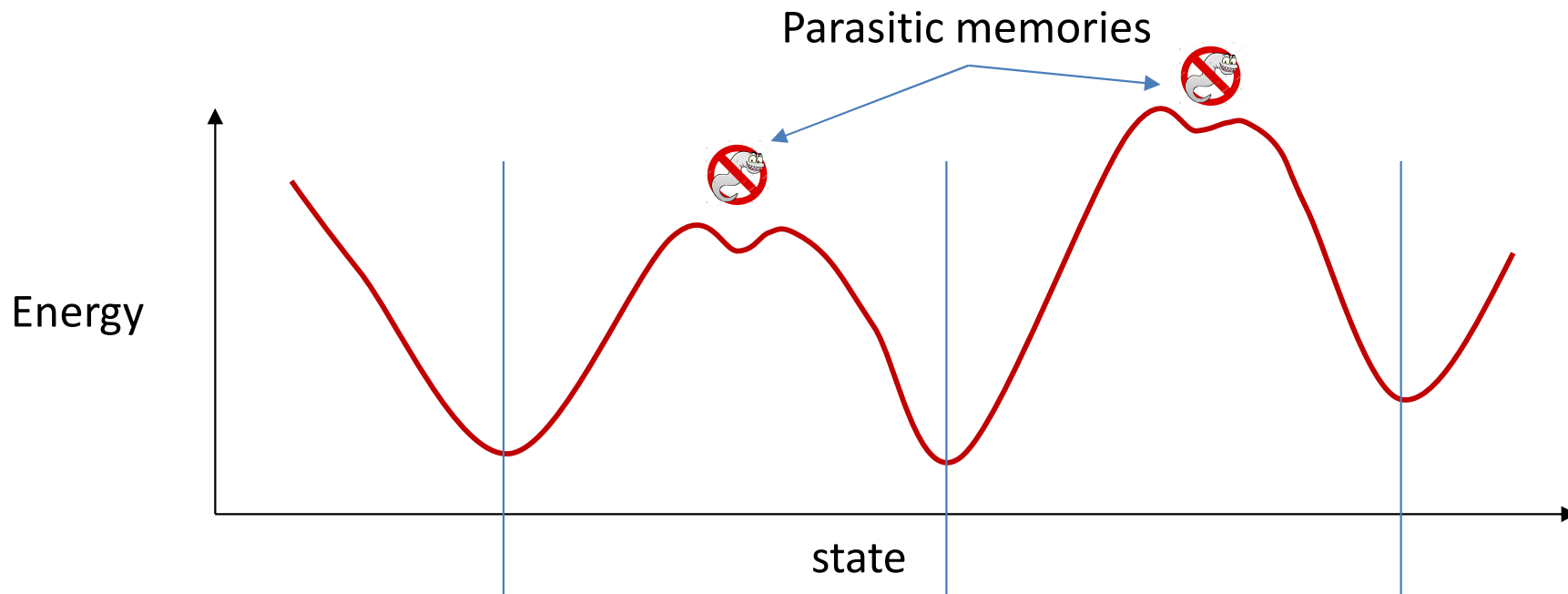
- Initialize \mathbf{W}
- Do until convergence, satisfaction, or death from boredom:
 - Sample a target pattern \mathbf{y}_p
 - Sampling frequency of pattern must reflect importance of pattern
 - Initialize the network at \mathbf{y}_p and let it evolve *a few steps (2-4)*
 - And arrive at a down-valley position \mathbf{y}_d
 - Update weights
 - $\mathbf{W} = \mathbf{W} + \eta(\mathbf{y}_p\mathbf{y}_p^T - \mathbf{y}_d\mathbf{y}_d^T)$

Problem with Hopfield net



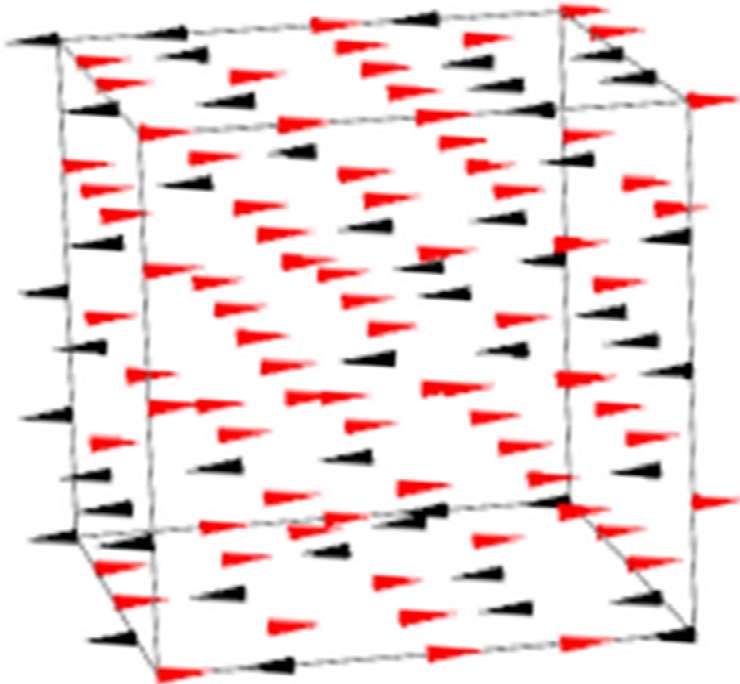
- Why is the recalled pattern not perfect?

A Problem with Hopfield Nets



- Many local minima
 - Parasitic memories
- May be escaped by adding some *noise* during evolution
 - Permit changes in state even if energy increases..
 - Particularly if the increase in energy is small

Recap – Analogy: Spin Glasses



Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} J_{ij} x_j + b_i$$

Response of current dipole

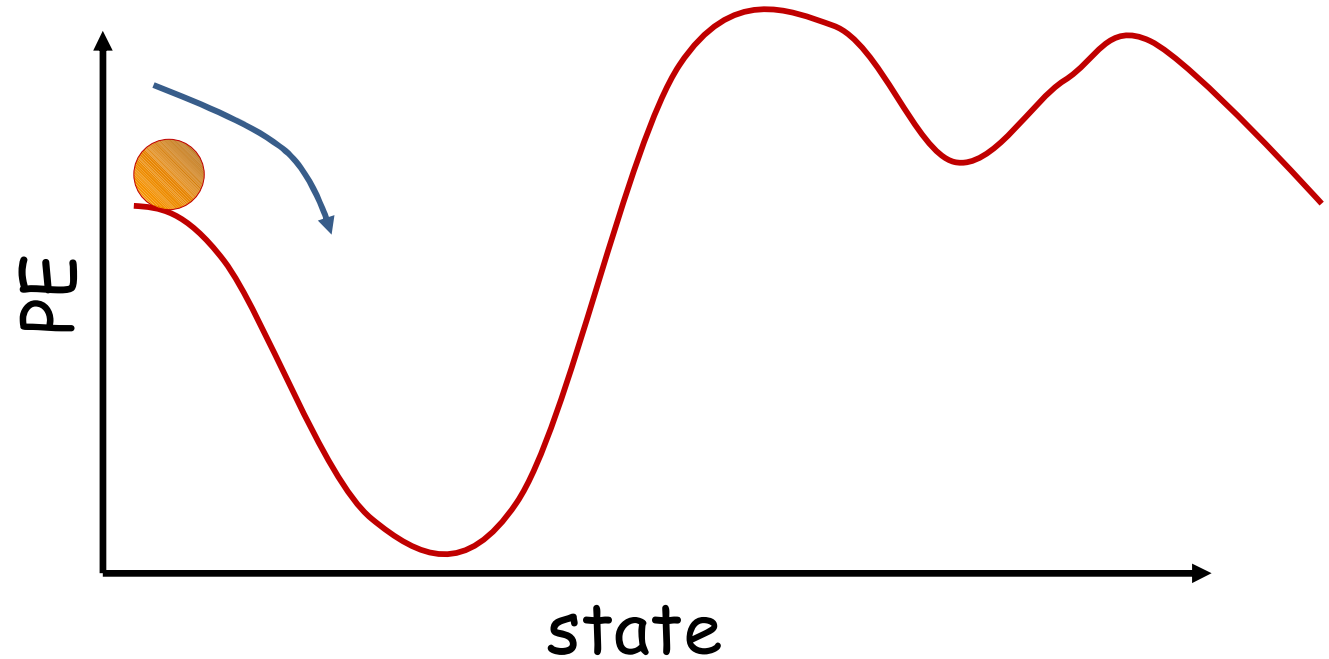
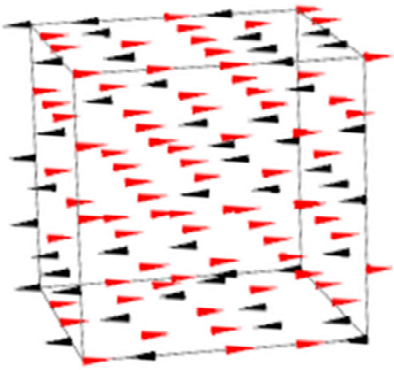
$$x_i = \begin{cases} x_i & \text{if } \text{sign}(x_i f(p_i)) = 1 \\ -x_i & \text{otherwise} \end{cases}$$

- The total energy of the system

$$E(s) = C - \frac{1}{2} \sum_i x_i f(p_i) = - \sum_i \sum_{j > i} J_{ij} x_i x_j - \sum_i b_i x_i$$

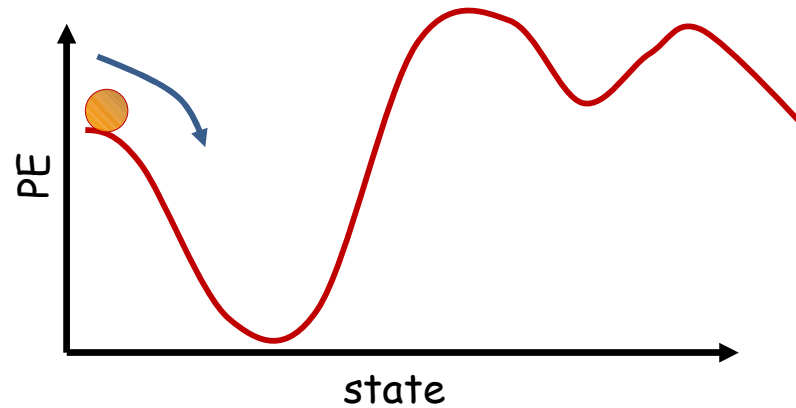
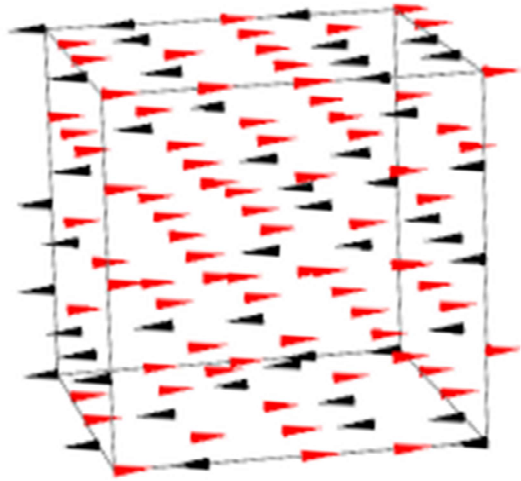
- The system *evolves* to minimize the energy
 - Dipoles stop flipping if flips result in increase of energy

Recap : Spin Glasses



- The system stops at one of its *stable* configurations
 - Where energy is a local minimum

Revisiting Thermodynamic Phenomena



- Is the system actually in a specific state at any time?
- No – the state is actually continuously changing
 - Based on the temperature of the system
 - At higher temperatures, state changes more rapidly
- What is actually being characterized is the *probability* of the state at equilibrium
 - The system “prefers” low energy states
 - Evolution of the system favors transitions towards lower-energy states

The Helmholtz Free Energy of a System

- A thermodynamic system at temperature T can exist in one of many states
 - Potentially infinite states
 - At any time, the probability of finding the system in state s at temperature T is $P_T(s)$
- At each state s it has a potential energy E_s
- The *internal energy* of the system, representing its capacity to do work, is the average:

$$U_T = \sum_s P_T(s) E_s$$

The Helmholtz Free Energy of a System

- The capacity to do work is counteracted by the internal disorder of the system, i.e. its entropy

$$H_T = - \sum_s P_T(s) \log P_T(s)$$

- The *Helmholtz* free energy of the system measures the *useful* work derivable from it and combines the two terms

$$F_T = U_T - kTH_T$$

$$= \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s)$$

The Helmholtz Free Energy of a System

$$F_T = \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s)$$

- A system held at a specific temperature *anneals* by varying the rate at which it visits the various states, to reduce the free energy in the system, until a minimum free-energy state is achieved
- The probability distribution of the states at steady state is known as the *Boltzmann distribution*

The Helmholtz Free Energy of a System

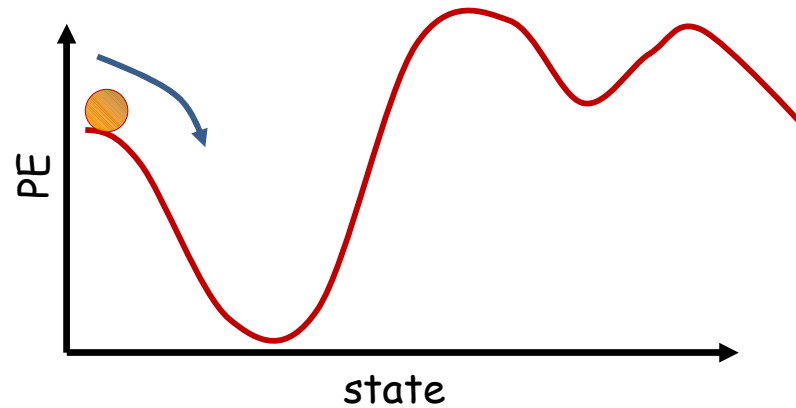
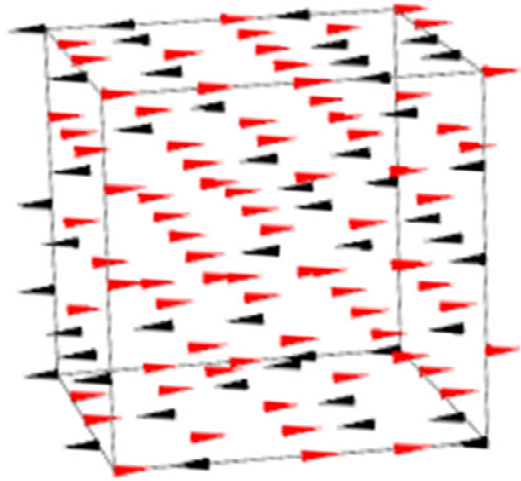
$$F_T = \sum_s P_T(s) E_s + kT \sum_s P_T(s) \log P_T(s)$$

- Minimizing this w.r.t $P_T(s)$, we get

$$P_T(s) = \frac{1}{Z} \exp\left(\frac{-E_s}{kT}\right)$$

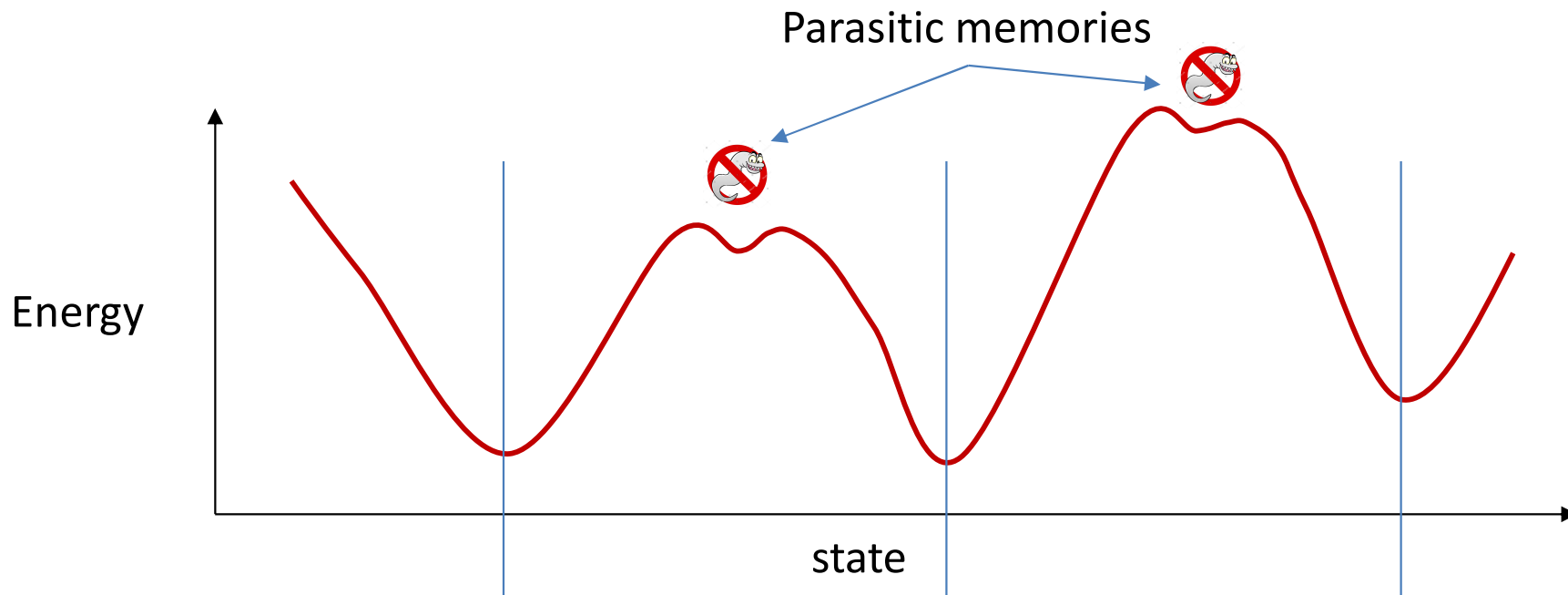
- Also known as the *Gibbs* distribution
- Z is a normalizing constant
- Note the dependence on T
- As $T \rightarrow 0$, the system will always remain at the lowest-energy configuration with prob = 1.

Revisiting Thermodynamic Phenomena



- The evolution of the system is actually *stochastic*
- At equilibrium the system visits various states according to the Boltzmann distribution
 - The probability of any state is inversely related to its energy
 - and also temperatures: $P(s) \propto \exp\left(\frac{-E_s}{kT}\right)$
- The most likely state is the lowest energy state

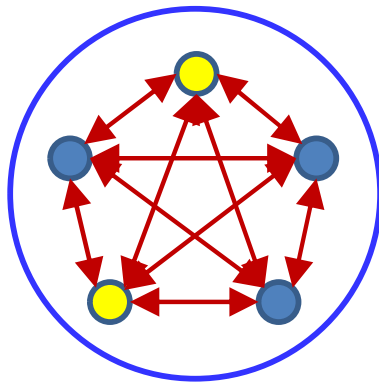
Returning to the problem with Hopfield Nets



- Many local minima
 - Parasitic memories
- May be escaped by adding some *noise* during evolution
 - Permit changes in state even if energy increases..
 - Particularly if the increase in energy is small

The Hopfield net as a distribution

Visible
Neurons



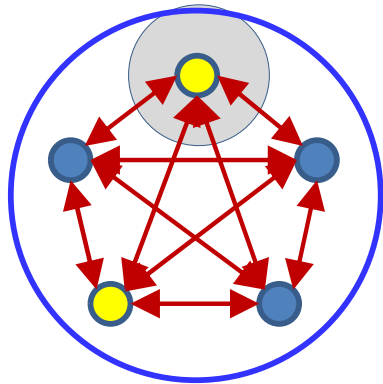
$$E(S) = - \sum_{i < j} w_{ij} s_i s_j - b_i s_i$$

$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

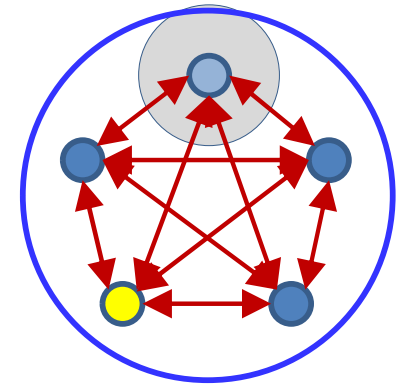
- Mimics the Spin glass system
- The stochastic Hopfield network models a ***probability distribution*** over states
 - Where a state is a binary string
 - Specifically, it models a *Boltzmann distribution*
 - **The parameters of the model are the weights of the network**
- The probability that (at equilibrium) the network will be in any state is $P(S)$
 - It is a *generative* model: generates states according to $P(S)$

The field at a single node

- Let S and S' be otherwise identical states that only differ in the i -th bit
 - S has i -th bit = $+1$ and S' has i -th bit = -1



$$P(S) = P(s_i = 1 | s_{j \neq i}) P(s_{j \neq i})$$
$$P(S') = P(s_i = -1 | s_{j \neq i}) P(s_{j \neq i})$$

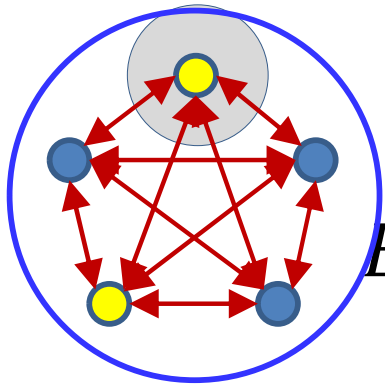


$$\log P(S) - \log P(S') = \log P(s_i = 1 | s_{j \neq i}) - \log P(s_i = -1 | s_{j \neq i})$$

$$\log P(S) - \log P(S') = \log \frac{P(s_i = 1 | s_{j \neq i})}{1 - P(s_i = 1 | s_{j \neq i})}$$

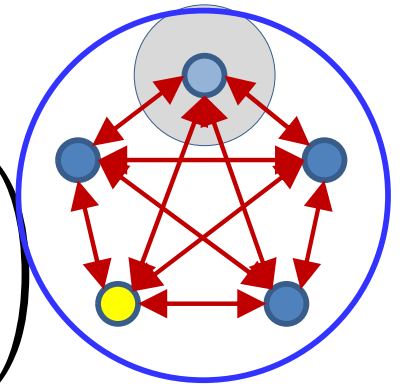
The field at a single node

- Let S and S' be the states with the i th bit in the $+1$ and -1 states



$$\log P(S) = -E(S) + C$$

$$E(S) = -\frac{1}{2} \left(E_{not\ i} + \sum_{j \neq i} w_{ij} S_j + b_i \right)$$



$$E(S') = -\frac{1}{2} \left(E_{not\ i} - \sum_{j \neq i} w_{ij} S_j - b_i \right)$$

- $\log P(S) - \log P(S') = E(S') - E(S) = \sum_{j \neq i} w_{ij} S_j + b_i$

The field at a single node

$$\log \left(\frac{P(s_i = 1 | s_{j \neq i})}{1 - P(s_i = 1 | s_{j \neq i})} \right) = \sum_{j \neq i} w_{ij} s_j + b_i$$

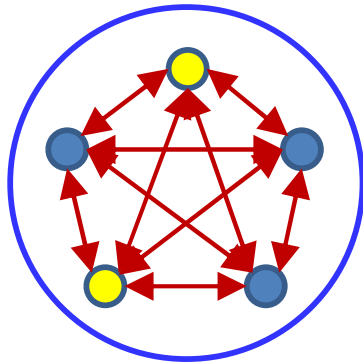
- Giving us

$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-\left(\sum_{j \neq i} w_{ij} s_j + b_i\right)}}$$

- The probability of any node taking value 1 given other node values is a logistic

Redefining the network

Visible
Neurons



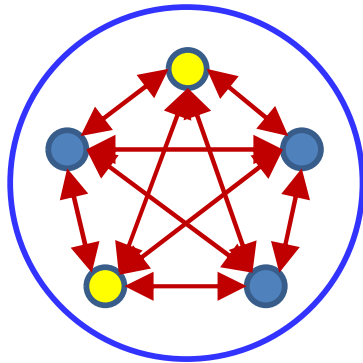
$$z_i = \sum_j w_{ij} s_j + b_i$$

$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}$$

- First try: Redefine a regular Hopfield net as a stochastic system
- Each neuron is *now a stochastic unit* with a binary state s_i , which can take value 0 or 1 with a probability that depends on the local field
 - Note the slight change from Hopfield nets
 - Not actually necessary; only a matter of convenience

The Hopfield net is a distribution

Visible
Neurons



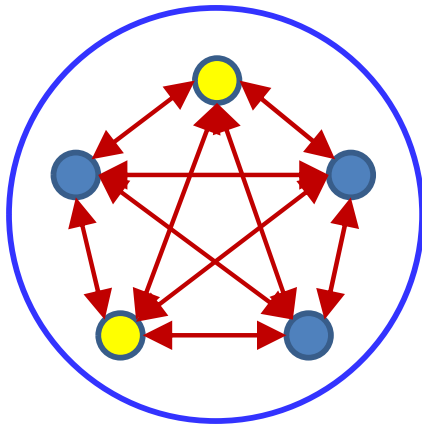
$$z_i = \sum_j w_{ij} s_j + b_i$$

$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}$$

- The Hopfield net is a probability distribution over binary sequences
 - The Boltzmann distribution
- The *conditional* distribution of individual bits in the sequence is a logistic

Running the network

Visible
Neurons



$$z_i = \sum_j w_{ij} s_j + b_i$$

$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}$$

- Initialize the neurons
- Cycle through the neurons and randomly set the neuron to 1 or 0 according to the probability given above
 - Gibbs sampling: Fix N-1 variables and sample the remaining variable
 - As opposed to energy-based update (mean field approximation): run the test $z_i > 0$?
- After many many iterations (until “convergence”), *sample* the individual neurons

Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

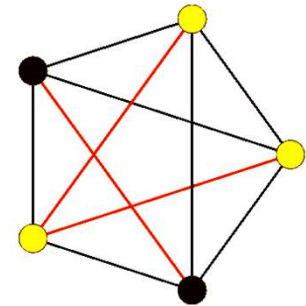
$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. Iterate $0 \leq i \leq N - 1$

$$P = \sigma \left(\sum_{j \neq i} w_{ji} y_j \right)$$

$$y_i(t + 1) \sim \text{Binomial}(P)$$

Assuming $T = 1$



Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

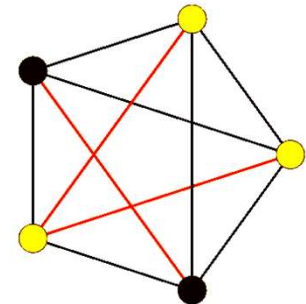
$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. Iterate $0 \leq i \leq N - 1$

$$P = \sigma \left(\sum_{j \neq i} w_{ji} y_j \right)$$

$$y_i(t + 1) \sim \text{Binomial}(P)$$

Assuming $T = 1$



- When do we stop?
- What is the final state of the system
 - How do we “recall” a memory?

Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

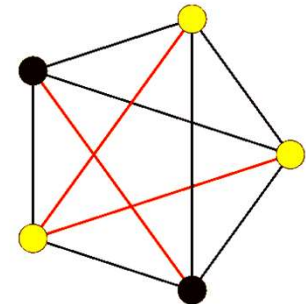
$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. Iterate $0 \leq i \leq N - 1$

$$P = \sigma \left(\sum_{j \neq i} w_{ji} y_j \right)$$

$$y_i(t + 1) \sim \text{Binomial}(P)$$

Assuming $T = 1$



- When do we stop?
- What is the final state of the system
 - How do we “recall” a memory?

Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

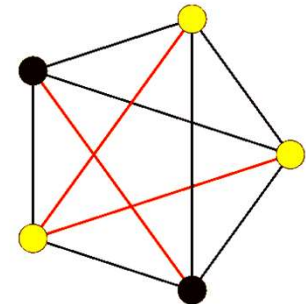
$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. Iterate $0 \leq i \leq N - 1$

$$P = \sigma \left(\sum_{j \neq i} w_{ji} y_j \right)$$

$$y_i(t + 1) \sim \text{Binomial}(P)$$

Assuming $T = 1$



- Let the system evolve to “equilibrium”
- Let $\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_L$ be the sequence of values (L large)
- Final predicted configuration: from the average of the final few iterations

$$\mathbf{y} = \left(\frac{1}{M} \sum_{t=L-M+1}^L \mathbf{y}_t \right) > 0?$$

- Estimates the probability that the bit is 1.0.
- If it is greater than 0.5, sets it to 1.0

Evolution of the stochastic network

1. Initialize network with initial pattern

$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. For $T = T_0$ down to T_{min}

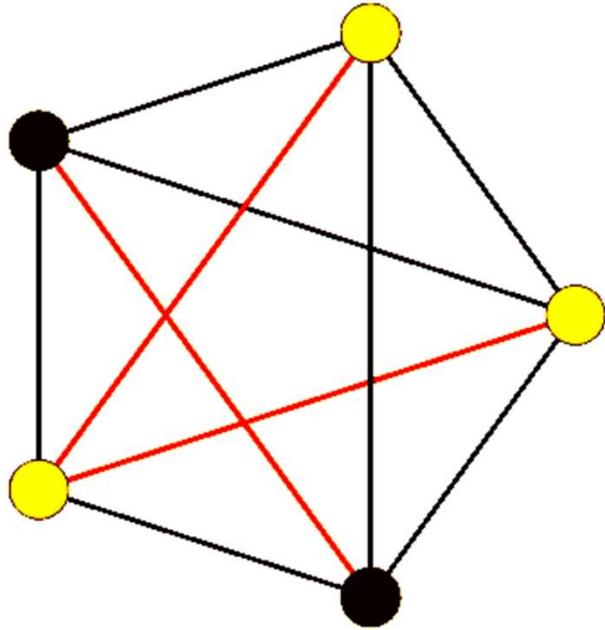
Noisy pattern completion: Initialize the entire network and let the entire network evolve

Pattern completion: Fix the “seen” bits and only let the “unseen” bits evolve

- Let the system evolve to “equilibrium”
- Let $\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_L$ be the sequence of values (L large)
- Final predicted configuration: from the average of the final few iterations

$$\mathbf{y} = \left(\frac{1}{M} \sum_{t=L-M+1}^L \mathbf{y}_t \right) > 0?$$

Including a “Temperature” term



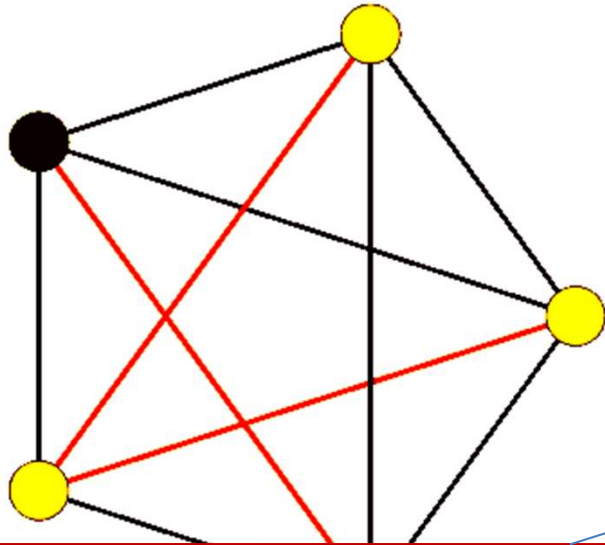
$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ij} y_j$$

$$P(y_i = 1) = \sigma(z_i)$$

$$P(y_i = 0) = 1 - \sigma(z_i)$$

- Including a temperature term in computing the local field
 - This is much more in accord with Thermodynamic models
- At $T = \infty$ the energy “surface” will be flat. At $T = 1$ the surface will be the usual energy surface
 - This can be used to improve the likelihood of finding good (or optimal) minimum-energy states

Recap: Stochastic Hopfield Nets



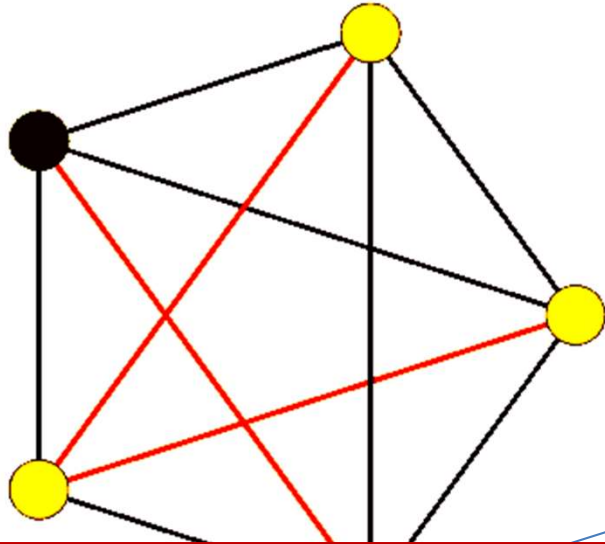
$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j$$

$$P(y_i = 1) = \sigma(z_i)$$

The field quantifies the energy difference obtained by flipping the current unit

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Recap: Stochastic Hopfield Nets



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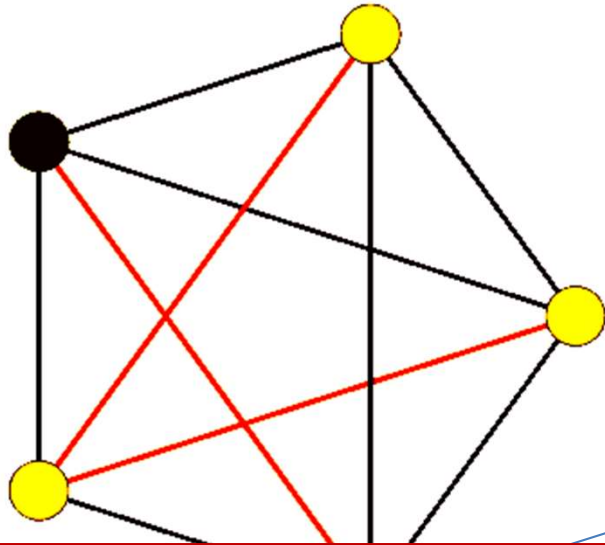
$$P(y_i = 1) = \sigma(z_i)$$

The field quantifies the energy difference obtained by flipping the current unit

- Including a temperature term in computing the local field
- If the difference is not large, the probability of flipping approaches 0.5
- This is much more in accord with thermodynamic models

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 - This can be used to improve the likelihood of finding good (or optimal) minimum-energy states

Recap: Stochastic Hopfield Nets



$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j$$

$$P(y_i = 1) = \sigma(z_i)$$

The field quantifies the energy difference obtained by flipping the current unit

- Including a temperature term in computing the local field

If the difference is not large, the probability of flipping approaches 0.5

– This is much more in accord with thermodynamic models

T is a "temperature" parameter: increasing it moves the probability of the bits towards 0.5

At $T=1.0$ we get the traditional definition of field and energy

At $T=0$, we get deterministic Hopfield behavior

- This can be used to improve the likelihood of finding good (or optimal) minimum-energy states

Annealing

1. Initialize network with initial pattern

$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. For $T = T_0$ down to T_{min}

i. For iter 1.. L

a) For $0 \leq i \leq N - 1$

$$P = \sigma \left(\frac{1}{T} \sum_{j \neq i} w_{ji} y_j \right)$$

$$y_i(t + 1) \sim \text{Binomial}(P)$$

- Let the system evolve to “equilibrium”
- Let $\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_L$ be the sequence of values (L large)
- Final predicted configuration: from the average of the final few iterations

$$\mathbf{y} = \left(\frac{1}{M} \sum_{t=L-M+1}^L \mathbf{y}_t \right) > 0?$$

Evolution of a stochastic Hopfield net

1. Initialize network with initial pattern

$$y_i(0) = x_i, \quad 0 \leq i \leq N - 1$$

2. For $T = T_0$ down to T_{min}

i. For iter $1..L$

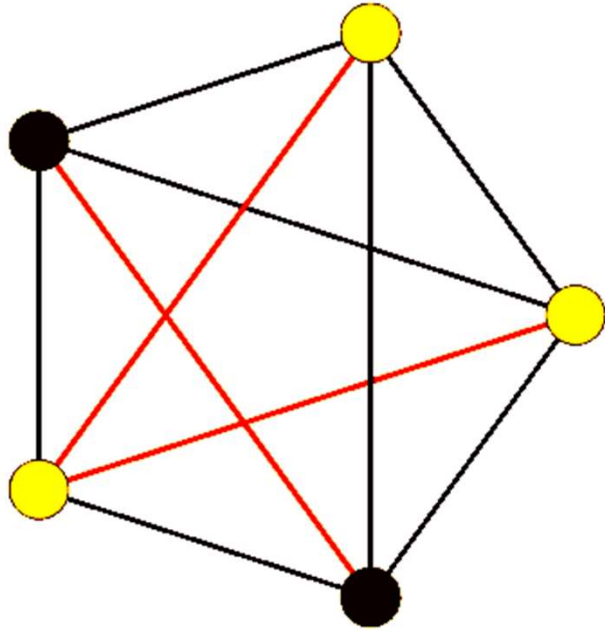
a) For $0 \leq i \leq N - 1$

$$P = \sigma \left(\frac{1}{T} \sum_{j \neq i} w_{ji} y_j \right)$$

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- When do we stop?
- What is the final state of the system
 - How do we “recall” a memory?

Recap: Stochastic Hopfield Nets

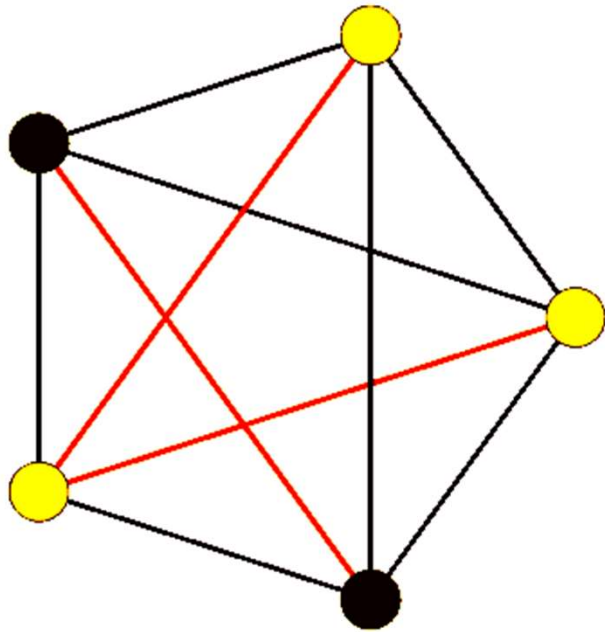


$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j$$

$$P(y_i = 1 | y_{j \neq i}) = \sigma(z_i)$$

- The probability of each neuron is given by a *conditional* distribution
- What is the overall probability of *the entire set of neurons* taking any configuration \mathbf{y}

The overall probability



$$z_i = \frac{1}{T} \sum_{j \neq i} w_{ji} y_j$$

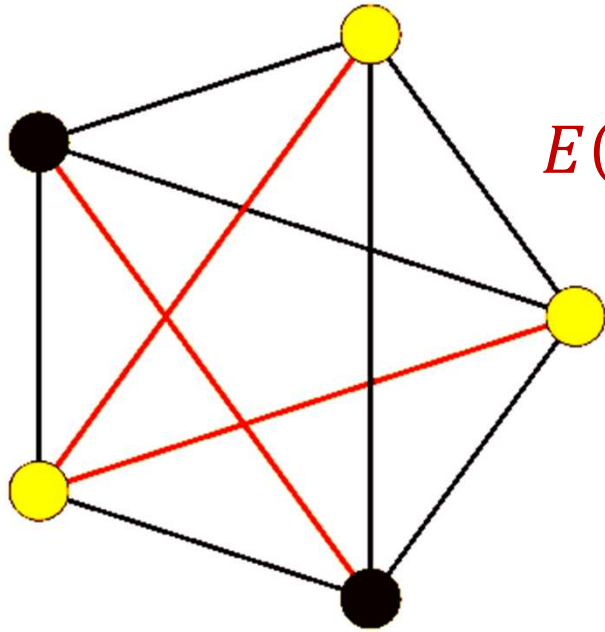
$$P(y_i = 1 | y_{j \neq i}) = \sigma(z_i)$$

- The probability of any state \mathbf{y} can be shown to be given by the *Boltzmann distribution*

$$E(\mathbf{y}) = -\frac{1}{2} \mathbf{y}^T \mathbf{W} \mathbf{y} \quad P(\mathbf{y}) = C \exp \left(\frac{-E(\mathbf{y})}{T} \right)$$

- Minimizing energy maximizes log likelihood

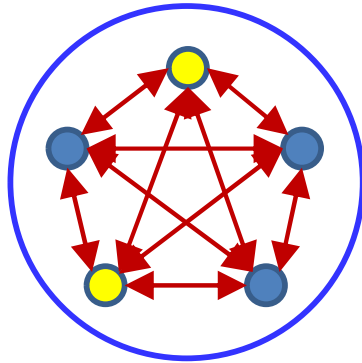
The overall probability



$$E(\mathbf{y}) = -\frac{1}{2}\mathbf{y}^T \mathbf{W} \mathbf{y} \quad P(\mathbf{y}) = C \exp\left(\frac{-E(\mathbf{y})}{T}\right)$$

- Stop when the running average of the log probability of patterns stops increasing
 - I.e. when the (running average) of the energy of the patterns stops decreasing

The Hopfield net is a distribution



$$z_i = \frac{1}{T} \sum_j w_{ji} s_j$$

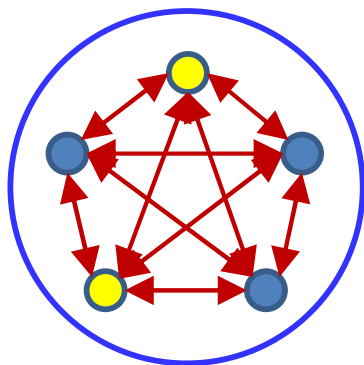
$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}$$

- The Hopfield net is a probability distribution over binary sequences
 - The Boltzmann distribution

$$E(\mathbf{y}) = -\frac{1}{2} \mathbf{y}^T \mathbf{W} \mathbf{y}$$
$$P(\mathbf{y}) = C \exp\left(-\frac{E(\mathbf{y})}{T}\right)$$

- The parameter of the distribution is the weights matrix \mathbf{W}
- The *conditional* distribution of individual bits in the sequence is a logistic
- We will call this a Boltzmann machine

The Boltzmann Machine



$$z_i = \frac{1}{T} \sum_j w_{ji} s_j$$

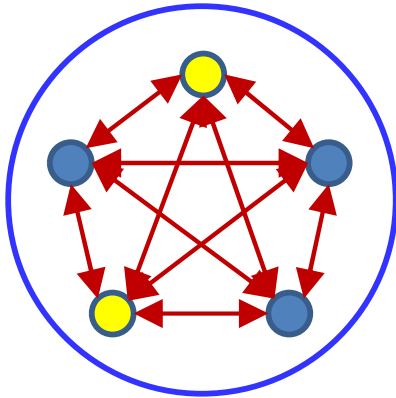
$$P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}$$

- The entire model can be viewed as a *generative model*
- Has a probability of producing any binary vector **y**:

$$E(\mathbf{y}) = -\frac{1}{2} \mathbf{y}^T \mathbf{W} \mathbf{y}$$

$$P(\mathbf{y}) = C \exp \left(-\frac{E(\mathbf{y})}{T} \right)$$

Training the network



$$E(S) = - \sum_{i < j} w_{ij} s_i s_j$$

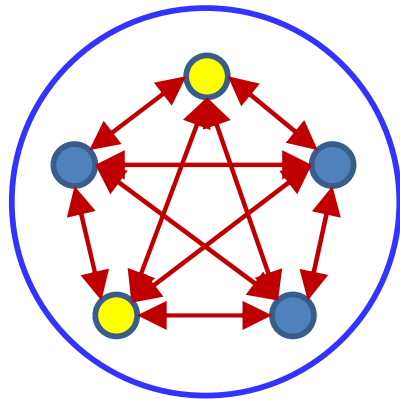
$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

$$P(S) = \frac{\exp(\sum_{i < j} w_{ij} s_i s_j)}{\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}$$

- Training a Hopfield net: Must learn weights to “remember” target states and “dislike” other states
 - **“State” == binary pattern of all the neurons**
- Training Boltzmann machine: Must learn weights to assign a desired probability distribution to states
 - (vectors y , which we will now call S because I’m too lazy to normalize the notation)
 - This should assign more probability to patterns we “like” (or try to memorize) and less to other patterns

Training the network

Visible
Neurons



$$E(S) = - \sum_{i < j} w_{ij} s_i s_j$$

$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

$$P(S) = \frac{\exp(\sum_{i < j} w_{ij} s_i s_j)}{\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}$$

- Must train the network to assign a desired probability distribution to states
- Given a set of “training” inputs S_1, \dots, S_N
 - Assign higher probability to patterns seen more frequently
 - Assign lower probability to patterns that are not seen at all
- Alternately viewed: *maximize likelihood of stored states*

Maximum Likelihood Training

$$\log(P(S)) = \left(\sum_{i < j} w_{ij} s_i s_j \right) - \log \left(\sum_{S'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

$$\mathcal{L} = \frac{1}{N} \sum_{S \in \mathbf{S}} \log(P(S))$$

Average log likelihood of training vectors
(to be maximized)

$$= \frac{1}{N} \sum_S \left(\sum_{i < j} w_{ij} s_i s_j \right) - \log \left(\sum_{S'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

- Maximize the average log likelihood of all “training” vectors $\mathbf{S} = \{S_1, S_2, \dots, S_N\}$
 - In the first summation, s_i and s_j are bits of S
 - In the second, s'_i and s'_j are bits of S'

Maximum Likelihood Training

$$\mathcal{L} = \frac{1}{N} \sum_s \left(\sum_{i < j} w_{ij} s_i s_j \right) - \log \left(\sum_{s'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

$$\frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_s s_i s_j - ???$$

- We will use gradient ascent, but we run into a problem..
- The first term is just the average $s_i s_j$ over all training patterns
- But the second term is summed over *all* states
 - Of which there can be an exponential number!

The second term

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \frac{1}{\sum_{S''} \exp(\sum_{i < j} w_{ij} s''_i s''_j)} \frac{d \sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}{dw_{ij}}$$

$$= \frac{1}{\sum_{S''} \exp(\sum_{i < j} w_{ij} s''_i s''_j)} \sum_{S'} \exp\left(\sum_{i < j} w_{ij} s'_i s'_j\right) s'_i s'_j$$

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \sum_{S'} \frac{\exp(\sum_{i < j} w_{ij} s'_i s'_j)}{\sum_{S''} \exp(\sum_{i < j} w_{ij} s''_i s''_j)} s'_i s'_j$$

The second term

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$P(S')$

The second term

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \frac{1}{\sum_{S''} \exp(\sum_{i < j} w_{ij} s''_i s''_j)} \frac{d \sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}{dw_{ij}}$$

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$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j$$

The second term

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j$$

- The second term is simply the *expected value* of $s_i s_j$, over all possible values of the state
- We cannot compute it exhaustively, but we can compute it by sampling!

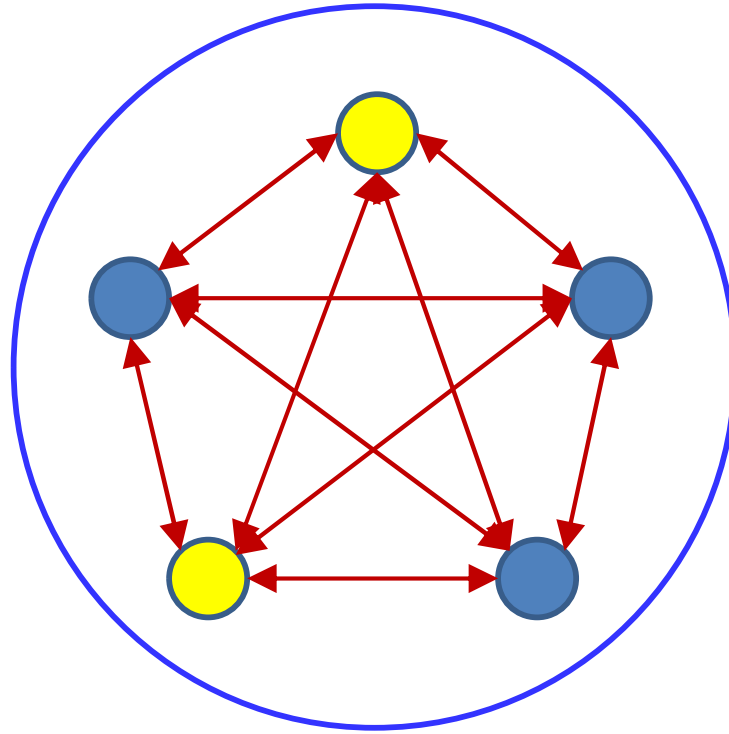
Estimating the second term

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j$$

$$\sum_{S'} P(S') s'_i s'_j \approx \frac{1}{M} \sum_{S' \in \mathbf{S}_{samples}} s'_i s'_j$$

- The expectation can be estimated as the average of samples drawn from the distribution
- Question: How do we draw samples from the Boltzmann distribution?
 - How do we draw samples from the network?

The simulation solution



- Initialize the network randomly and let it “evolve”
 - By probabilistically selecting state values according to our model
- After many many epochs, take a snapshot of the state
- Repeat this many many times
- Let the collection of states be

$$\mathbf{S}_{simul} = \{S_{simul,1}, S_{simul,1=2}, \dots, S_{simul,M}\}$$

The simulation solution for the second term

$$\frac{d \log(\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j))}{dw_{ij}} = \sum_{S'} P(S') s'_i s'_j$$

$$\sum_{S'} P(S') s'_i s'_j \approx \frac{1}{M} \sum_{S' \in \mathcal{S}_{simul}} s'_i s'_j$$

- The second term in the derivative is computed as the average of sampled states when the network is running “freely”

Maximum Likelihood Training

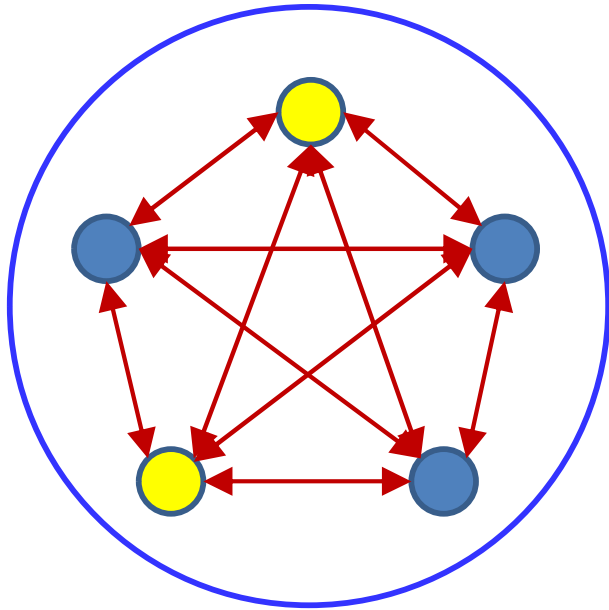
Sampled estimate

$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{N} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{\text{simul}}} s'_i s'_j$$

$$w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}}$$

- The overall gradient ascent rule

Overall Training

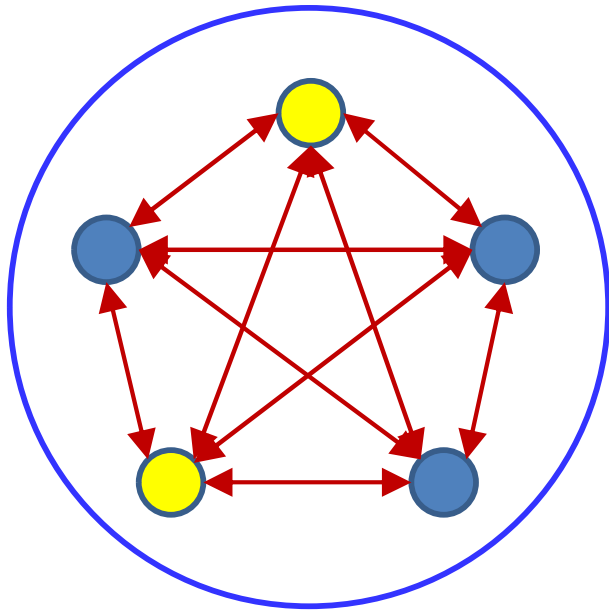


$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{N} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{simul}} s'_i s'_j$$

$$w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}}$$

- Initialize weights
- Let the network run to obtain simulated state samples
- Compute gradient and update weights
- Iterate

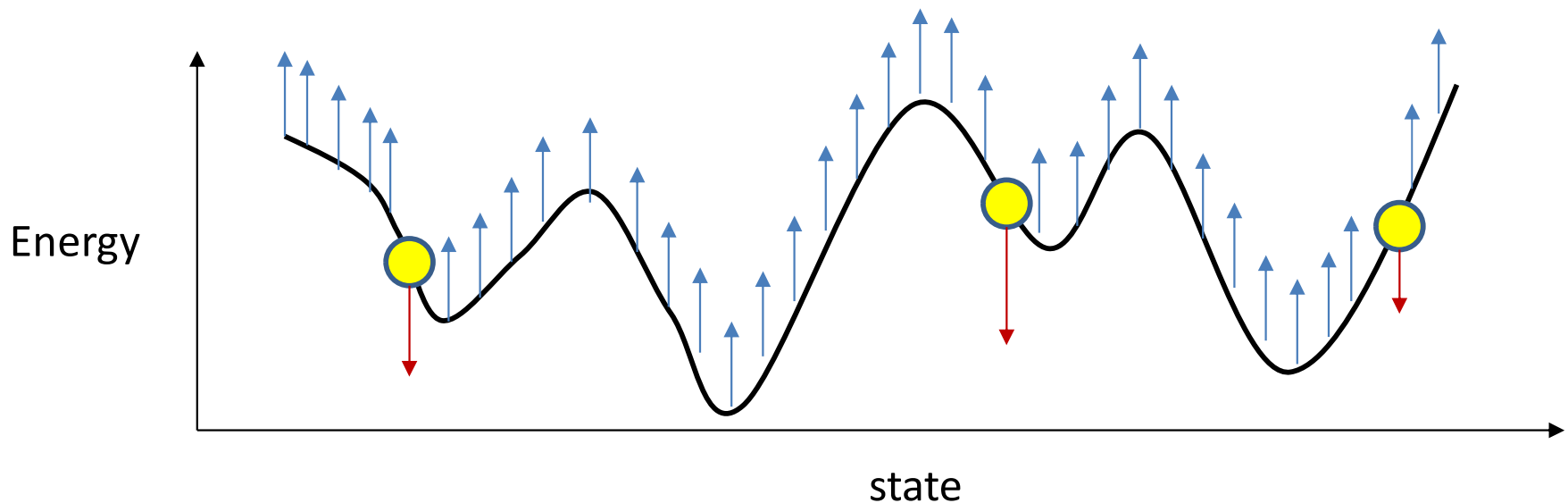
Overall Training



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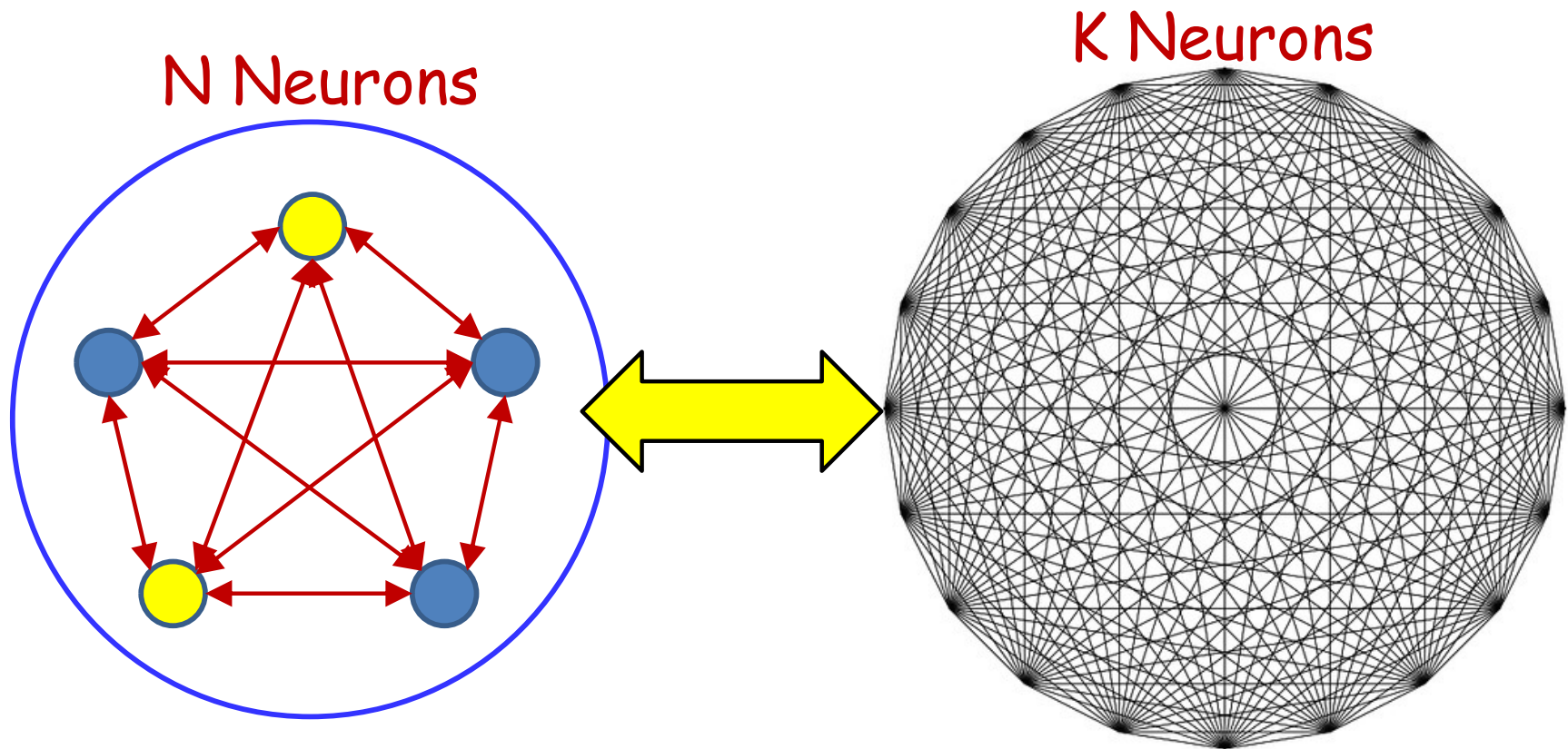
Note the similarity to the update rule for the Hopfield network



Adding Capacity to the Hopfield Network / Boltzmann Machine

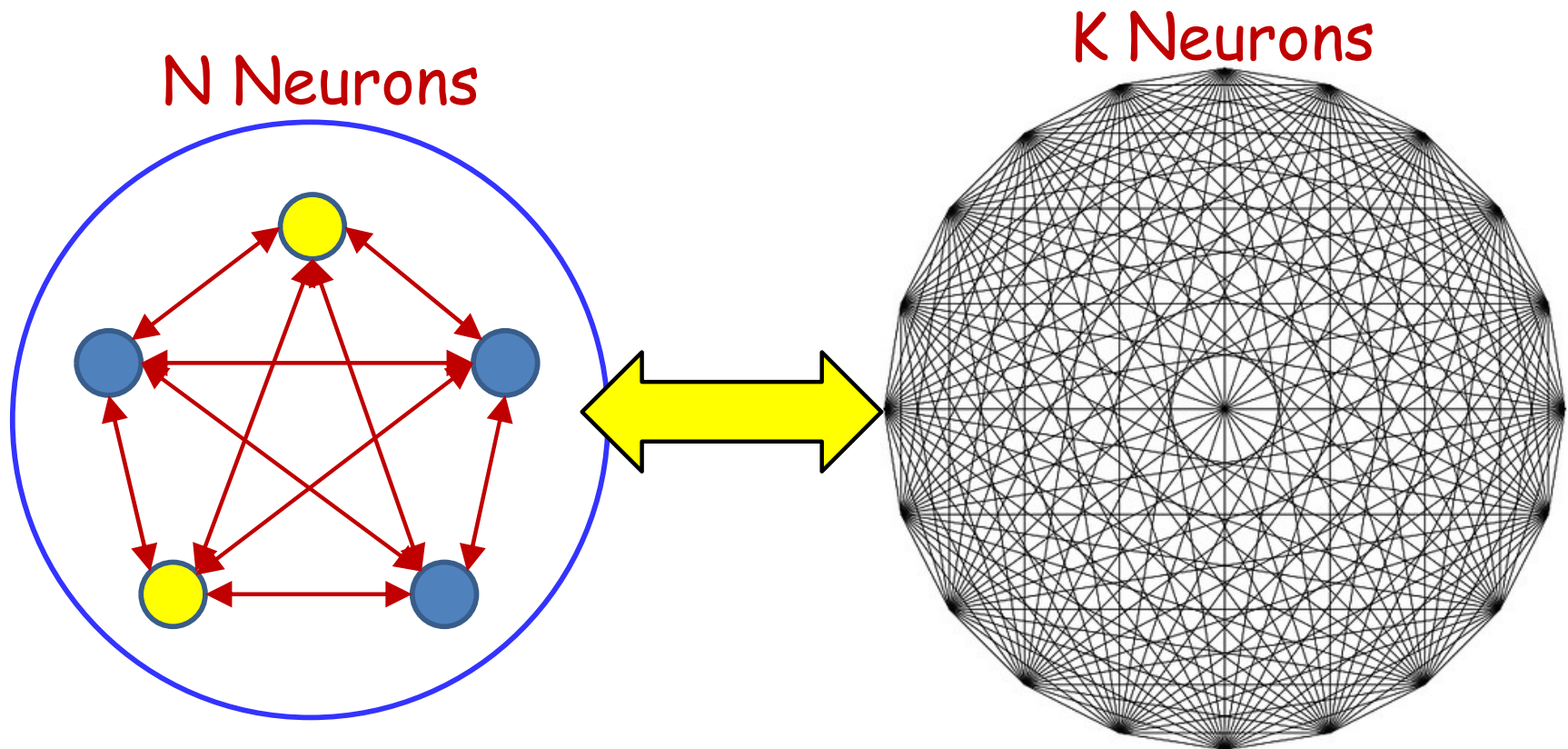
- The network can store up to N N -bit patterns
- How do we increase the capacity

Expanding the network



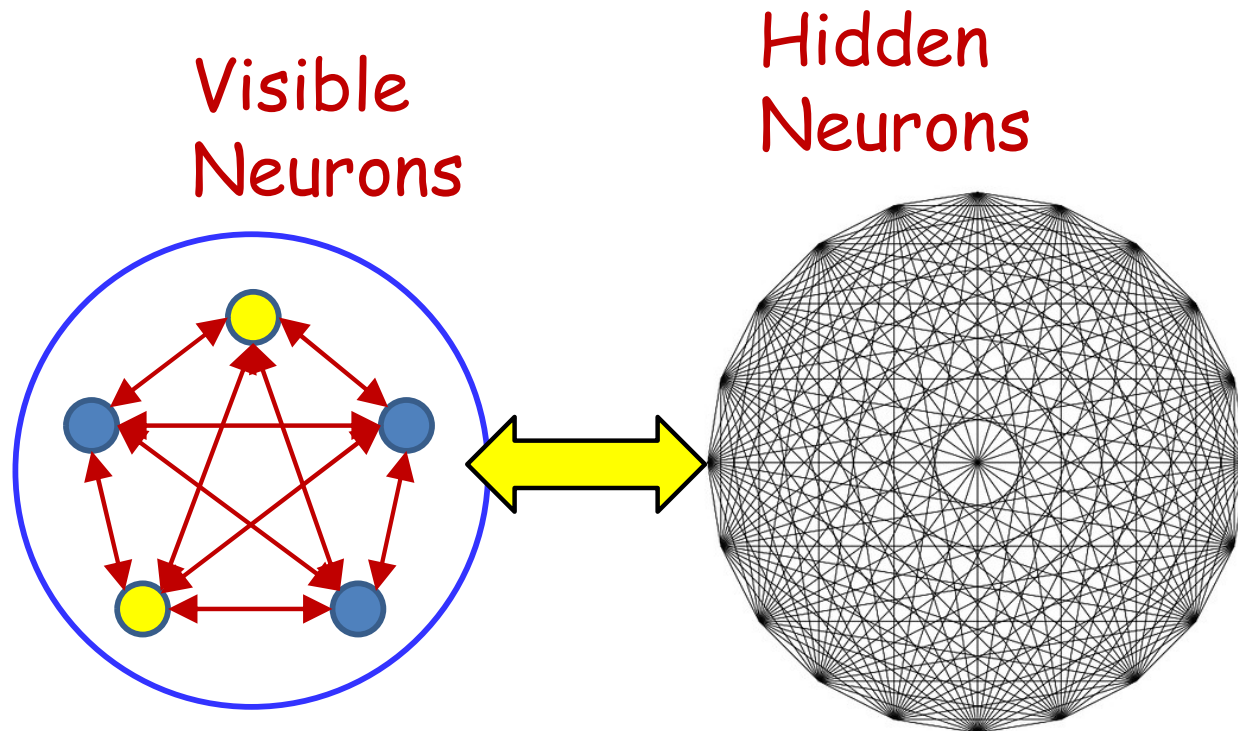
- Add a large number of neurons whose actual values you don't care about!

Expanded Network



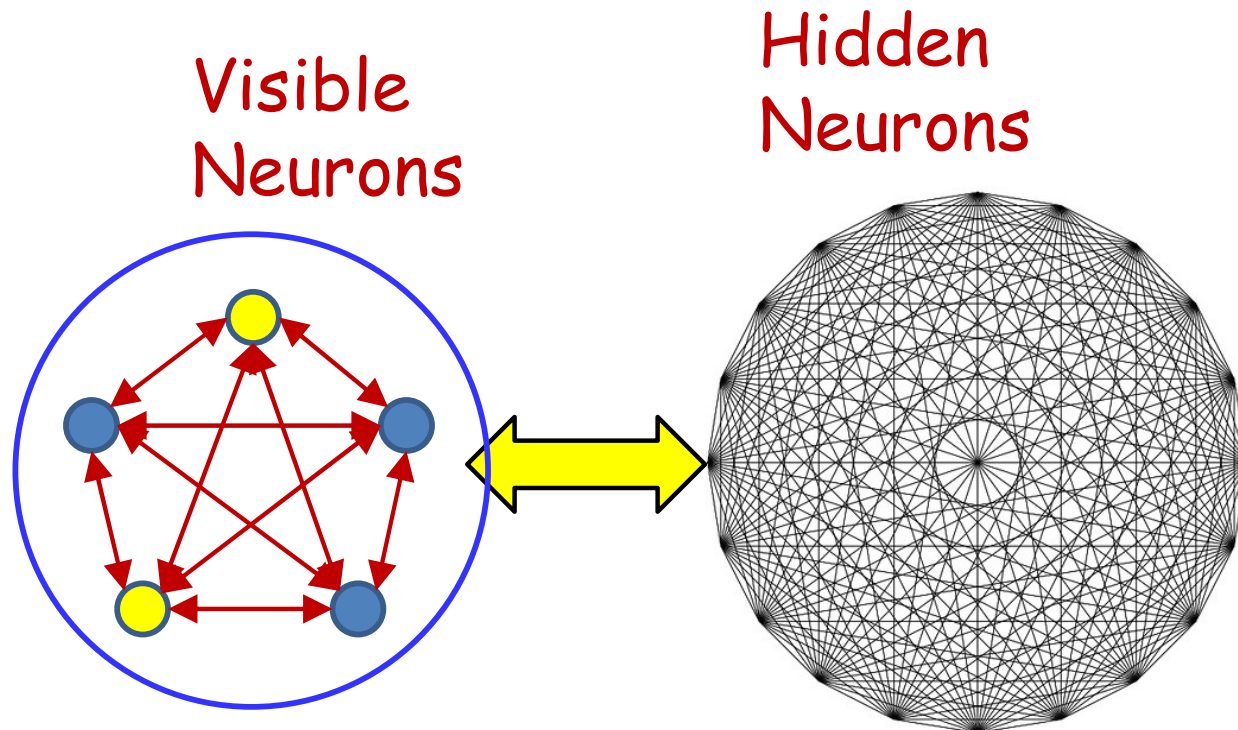
- New capacity: $\sim(N + K)$ patterns
 - Although we only care about the pattern of the first N neurons
 - We're interested in N -bit patterns

Terminology



- Terminology:
 - The neurons that store the actual patterns of interest: *Visible neurons*
 - The neurons that only serve to increase the capacity but whose actual values are not important: *Hidden neurons*
 - These can be set to anything in order to store a visible pattern

Training the network

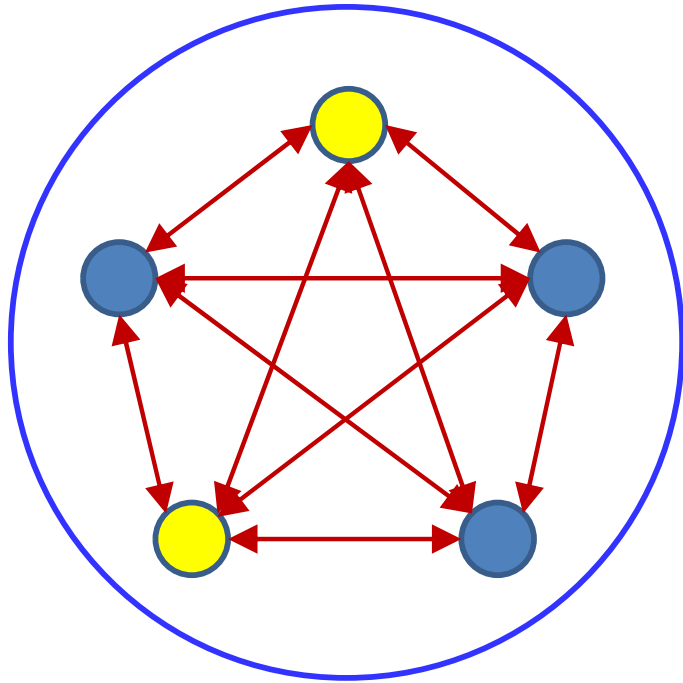


- For a given pattern of *visible* neurons, there are any number of *hidden* patterns (2^K)
- Which of these do we choose?
 - Ideally choose the one that results in the lowest energy
 - But that's an exponential search space!

The patterns

- In fact we could have *multiple* hidden patterns coupled with any visible pattern
 - These would be multiple stored patterns that all give the same visible output
 - How many do we permit
- Do we need to specify one or more particular hidden patterns?
 - How about *all* of them
 - What do I mean by this bizarre statement?

Boltzmann machine without hidden units



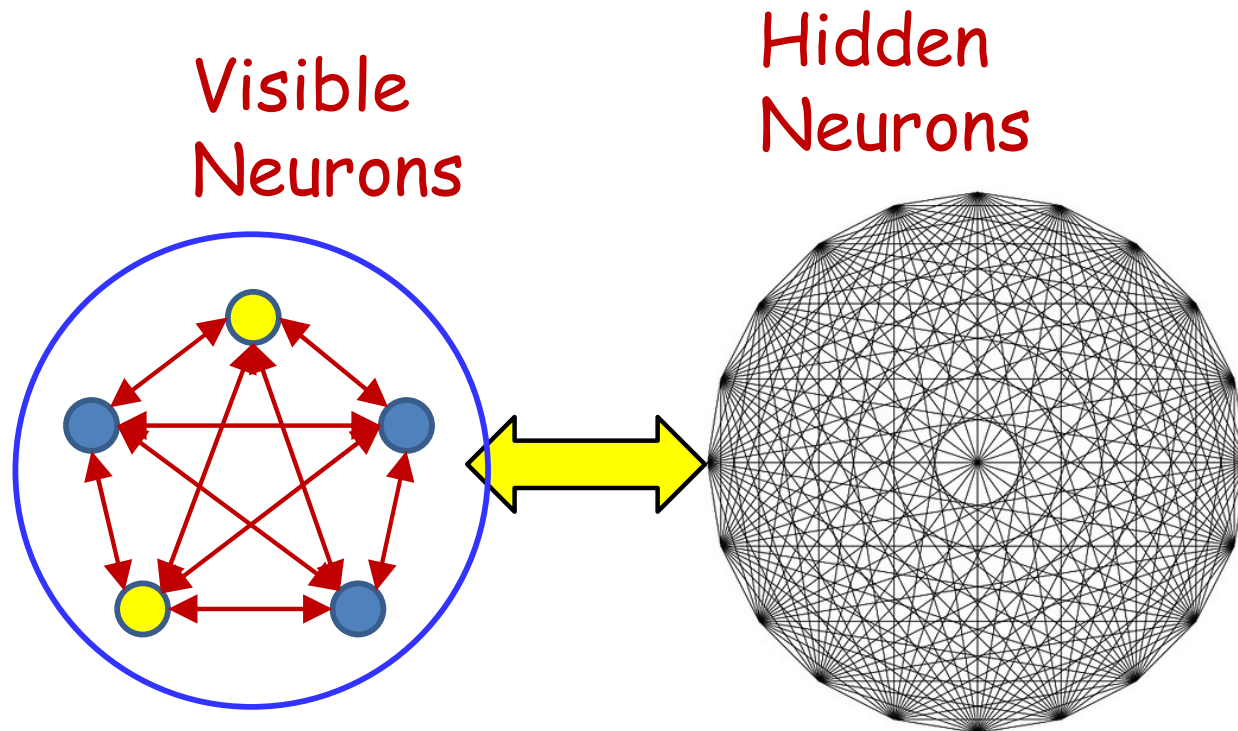
units

$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{N} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{simul}} s'_i s'_j$$

$$w_{ij} = w_{ij} + \eta \frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}}$$

- This basic framework has no hidden units
- Extended to have hidden units

With hidden neurons

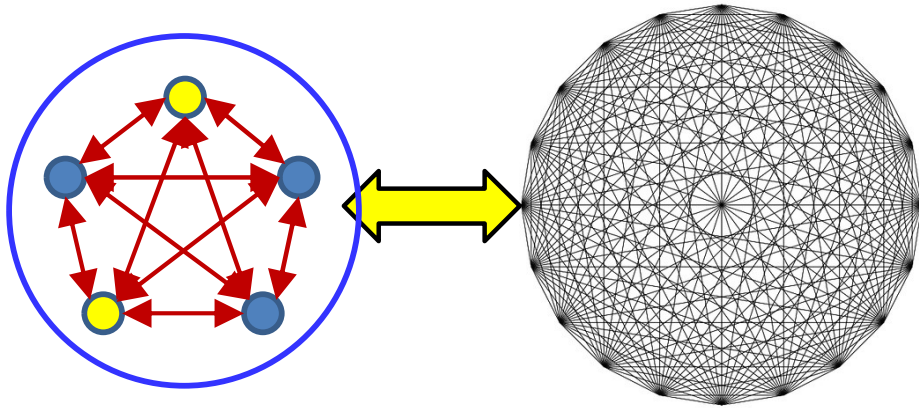


- Now, with hidden neurons the complete state pattern for even the *training* patterns is unknown
 - Since they are only defined over visible neurons

With hidden neurons

Visible
Neurons

Hidden
Neurons



$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

$$P(S) = P(V, H)$$

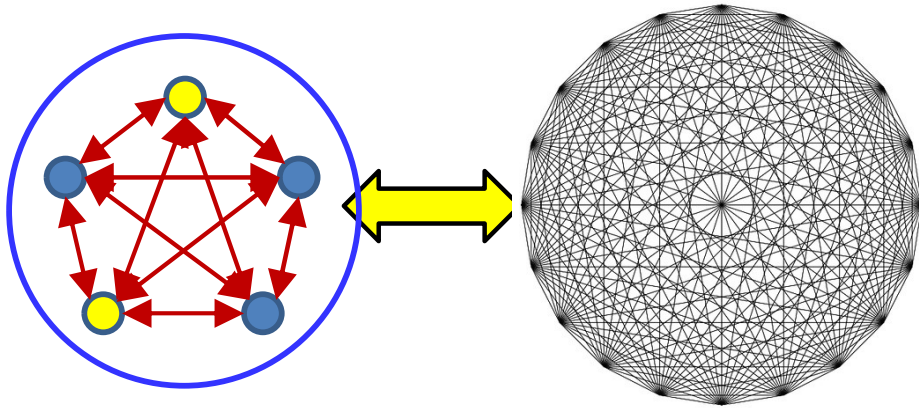
$$P(V) = \sum_H P(S)$$

- We are interested in the *marginal* probabilities over *visible* bits
 - We want to learn to represent the visible bits
 - The hidden bits are the “latent” representation learned by the network
- $S = (V, H)$
 - V = visible bits
 - H = hidden bits

With hidden neurons

Visible
Neurons

Hidden
Neurons



$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

$$P(S) = P(V, H)$$

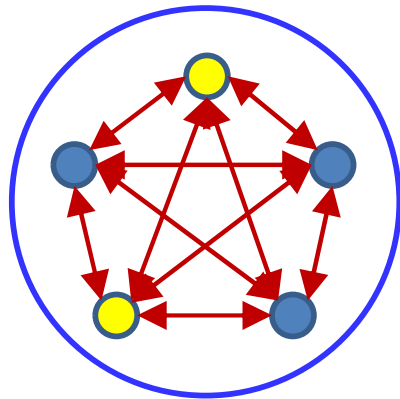
$$P(V) = \sum_H P(S)$$

- We are interested in the *marginal* probabilities over *visible* bits
 - We want to learn to represent the visible bits
 - The hidden bits are the “latent” representation learned by the network
- $S = (V, H)$
 - V = visible bits
 - H = hidden bits

Must train to maximize probability of desired patterns of *visible* bits

Training the network

Visible
Neurons



$$E(S) = - \sum_{i < j} w_{ij} s_i s_j$$

$$P(S) = \frac{\exp(\sum_{i < j} w_{ij} s_i s_j)}{\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}$$

$$P(V) = \sum_H \frac{\exp(\sum_{i < j} w_{ij} s_i s_j)}{\sum_{S'} \exp(\sum_{i < j} w_{ij} s'_i s'_j)}$$

- Must train the network to assign a desired probability distribution to *visible* states
- Probability of visible state sums over all hidden states

Maximum Likelihood Training

$$\log(P(V)) = \log \left(\sum_H \exp \left(\sum_{i < j} w_{ij} s_i s_j \right) \right) - \log \left(\sum_{S'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

$$\mathcal{L} = \frac{1}{N} \sum_{V \in \mathbf{V}} \log(P(V))$$

Average log likelihood of training vectors
(to be maximized)

$$= \frac{1}{N} \sum_{V \in \mathbf{V}} \log \left(\sum_H \exp \left(\sum_{i < j} w_{ij} s_i s_j \right) \right) - \log \left(\sum_{S'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

- Maximize the average log likelihood of all visible bits of “training” vectors $\mathbf{V} = \{V_1, V_2, \dots, V_N\}$
 - The first term also has the same format as the second term
 - Log of a sum
 - Derivatives of the first term will have the same form as for the second term

Maximum Likelihood Training

$$\mathcal{L} = \frac{1}{N} \sum_{V \in \mathbf{V}} \log \left(\sum_H \exp \left(\sum_{i < j} w_{ij} s_i s_j \right) \right) - \log \left(\sum_{S'} \exp \left(\sum_{i < j} w_{ij} s'_i s'_j \right) \right)$$

$$\frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_{V \in \mathbf{V}} \sum_H \frac{\exp(\sum_{k < l} w_{kl} s_k s_l)}{\sum_{H'} \exp(\sum_{k < l} w_{kl} s'_k s'_l)} s_i s_j - \sum_{S'} \frac{\exp(\sum_{k < l} w_{kl} s'_k s'_l)}{\sum_{S''} \exp(\sum_{k < l} w_{kl} s''_k s''_l)} s'_i s'_j$$

$$\frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_{V \in \mathbf{V}} \sum_H P(S|V) s_i s_j - \sum_{S'} P(S') s'_i s'_j$$

- We've derived this math earlier
- But now *both* terms require summing over an exponential number of states
 - The first term fixes visible bits, and sums over all configurations of hidden states for each visible configuration in our training set
 - But the second term is summed over *all* states

The simulation solution

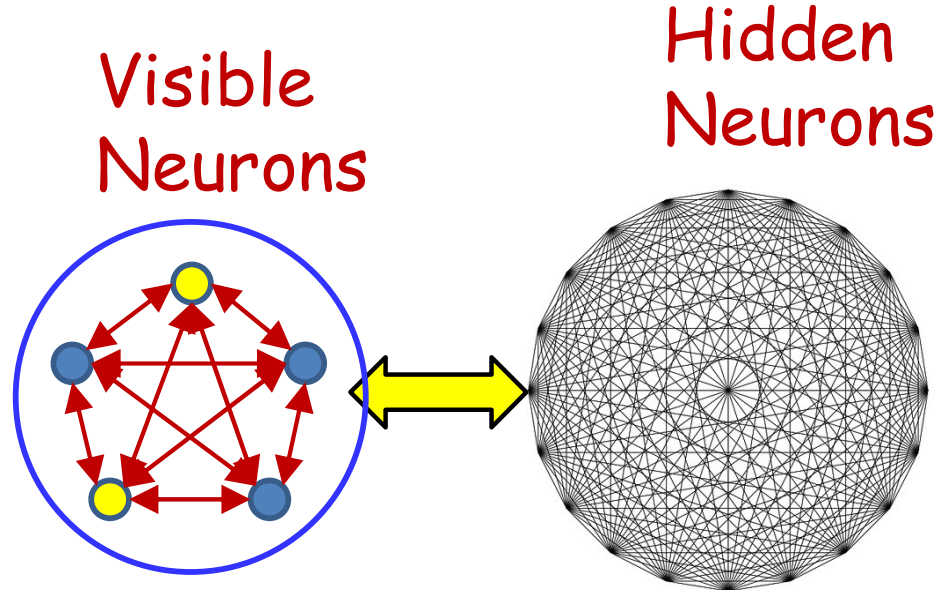
$$\frac{d\mathcal{L}}{dw_{ij}} = \frac{1}{N} \sum_{V \in \mathbf{V}} \sum_H P(S|V) s_i s_j - \sum_{S'} P(S') s'_i s'_j$$

$$\sum_H P(S|V) s_i s_j \approx \frac{1}{K} \sum_{H \in \mathbf{H}_{simul}} s_i s_j$$

$$\sum_{S'} P(S') s'_i s'_j \approx \frac{1}{M} \sum_{S' \in \mathbf{S}_{simul}} s'_i s'_j$$

- The first term is computed as the average sampled *hidden* state with the visible bits fixed
- The second term in the derivative is computed as the average of sampled states when the network is running “freely”

More simulations



$$P(S) = \frac{\exp(-E(S))}{\sum_{S'} \exp(-E(S'))}$$

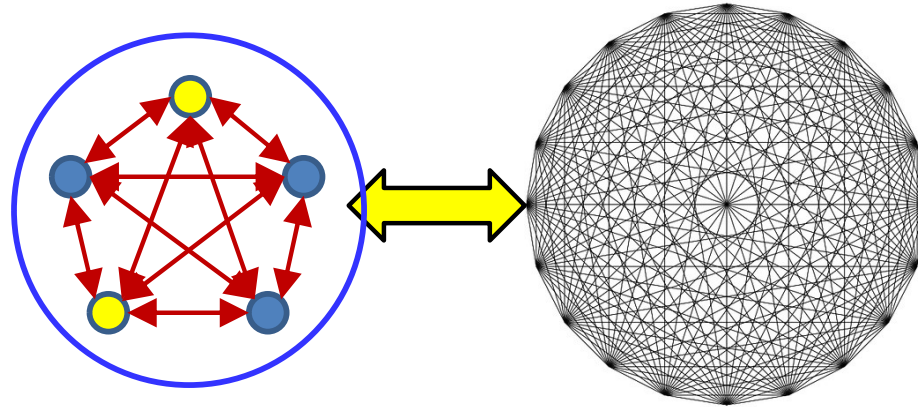
$$P(V) = \sum_H P(S)$$

- Maximizing the marginal probability of V requires summing over all values of H
 - An exponential state space
 - So we will use simulations again

Step 1

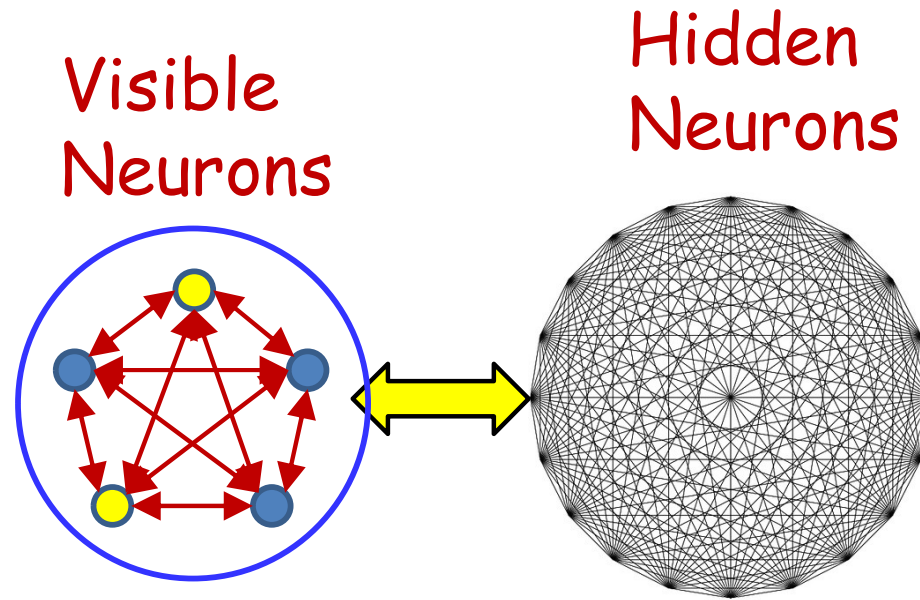
Visible
Neurons

Hidden
Neurons



- For each training pattern V_i
 - Fix the visible units to V_i
 - Let the hidden neurons evolve from a random initial point to generate H_i
 - Generate $S_i = [V_i, H_i]$
- Repeat K times to generate synthetic training
$$\mathbf{S} = \{S_{1,1}, S_{1,2}, \dots, S_{1K}, S_{2,1}, \dots, S_{N,K}\}$$

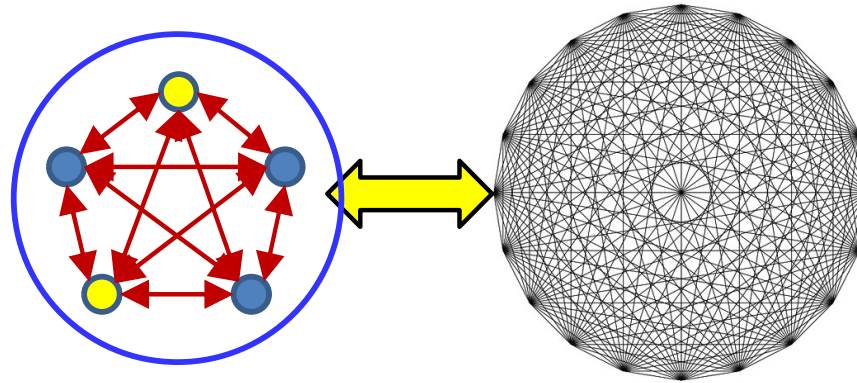
Step 2



- Now *unclamp* the visible units and let the entire network evolve several times to generate

$$\mathbf{S}_{simul} = \{S_{simul,1}, S_{simul,1=2}, \dots, S_{simul,M}\}$$

Gradients

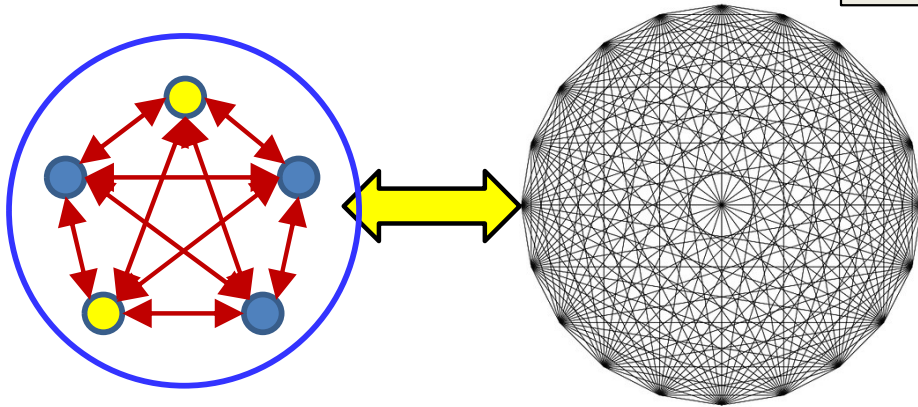


$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{simul}} s'_i s'_j$$

- Gradients are computed as before, except that the first term is now computed over the *expanded* training data

Overall Training

$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{simul}} s'_i s'_j$$



$$w_{ij} = w_{ij} - \eta \frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}}$$

- Initialize weights
- Run simulations to get clamped and unclamped training samples
- Compute gradient and update weights
- Iterate

Boltzmann machines

- Stochastic extension of Hopfield nets
- Enables storage of many more patterns than Hopfield nets
- But also enables computation of probabilities of patterns, and completion of pattern

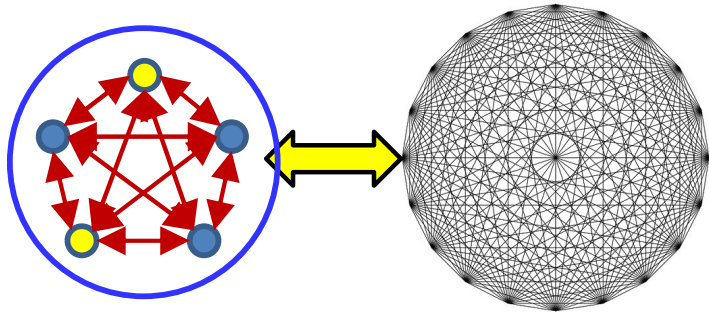
Boltzmann machines: Overall

$$z_i = \sum_j w_{ji} s_i + b_i$$

$$P(s_i = 1) = \frac{1}{1 + e^{-z_i}}$$

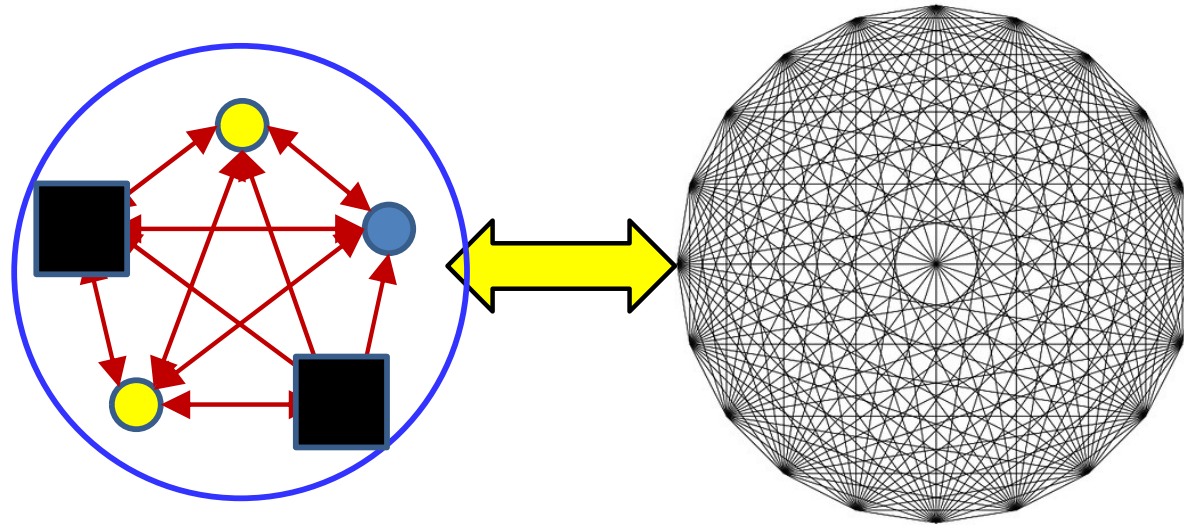
$$\frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}} = \frac{1}{NK} \sum_{\mathbf{S}} s_i s_j - \frac{1}{M} \sum_{\mathbf{S}' \in \mathbf{S}_{simul}} s'_i s'_j$$

$$w_{ij} = w_{ij} - \eta \frac{d\langle \log(P(\mathbf{S})) \rangle}{dw_{ij}}$$



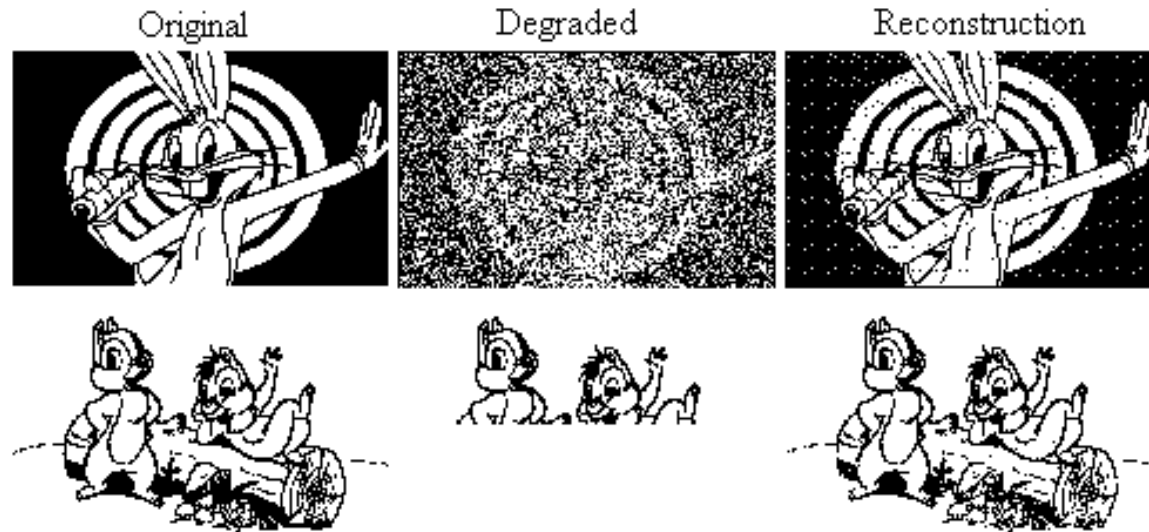
- **Training:** Given a set of training patterns
 - Which could be repeated to represent relative probabilities
- Initialize weights
- Run simulations to get clamped and unclamped training samples
- Compute gradient and update weights
- Iterate

Boltzmann machines: Overall



- Running: Pattern completion
 - “Anchor” the *known* visible units
 - Let the network evolve
 - Sample the unknown visible units
 - Choose the most probable value

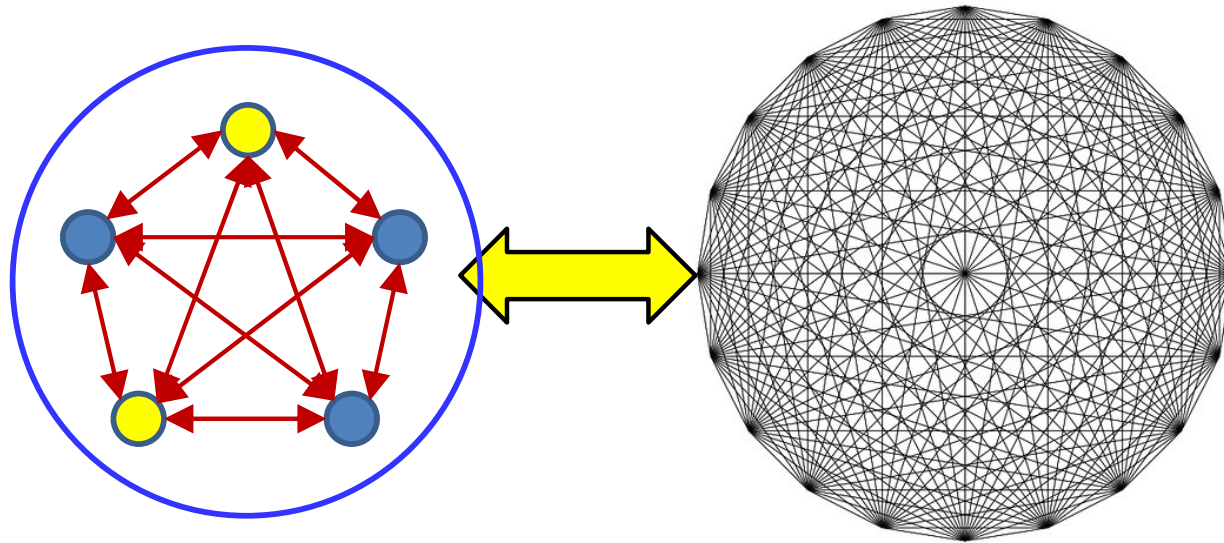
Applications



Hopfield network reconstructing degraded images
from noisy (top) or partial (bottom) cues.

- Filling out patterns
- Denoising patterns
- *Computing conditional probabilities of patterns*
- ***Classification!!***
 - *How?*

Boltzmann machines for classification

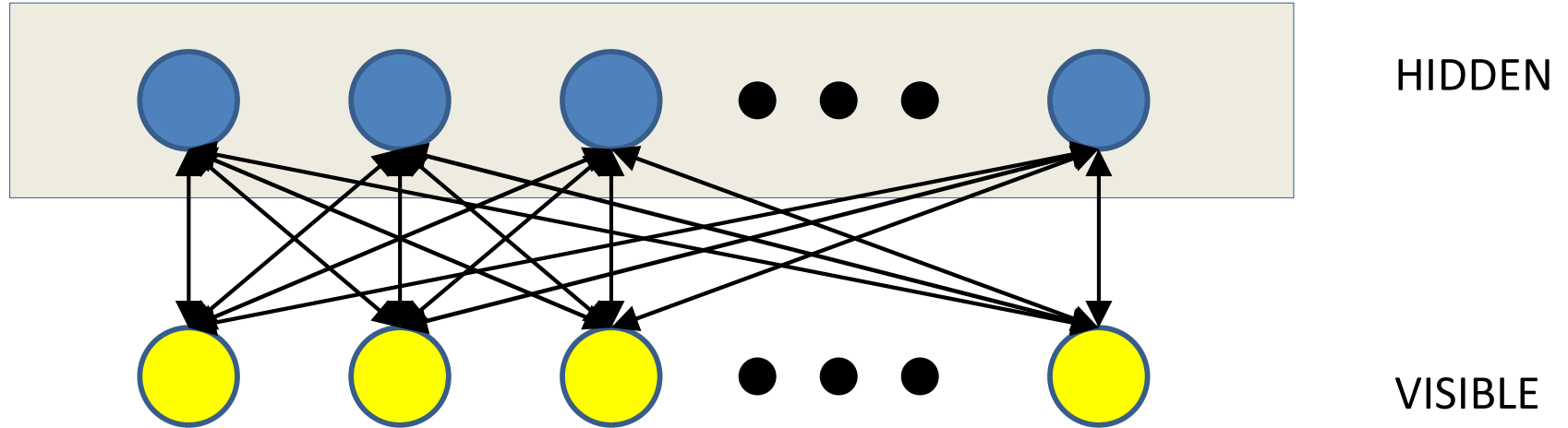


- Training patterns:
 - $[f_1, f_2, f_3, \dots, \text{class}]$
 - Features can have binarized or continuous valued representations
 - Classes have “one hot” representation
- Classification:
 - Given features, anchor features, estimate a posteriori probability distribution over classes
 - Or choose most likely class

Boltzmann machines: Issues

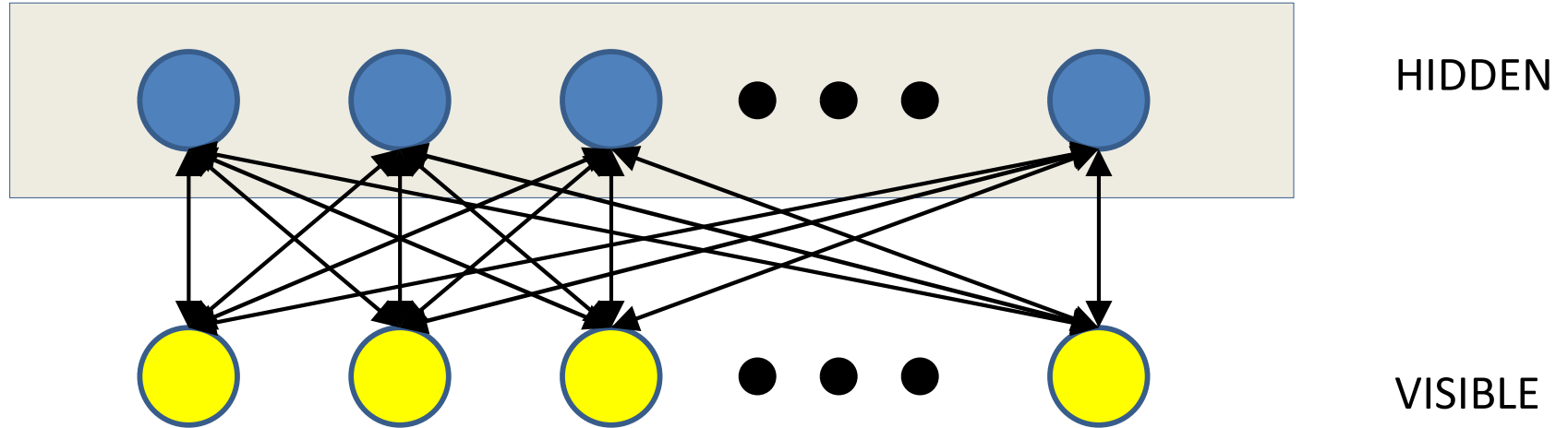
- Training takes for ever
- Doesn't really work for large problems
 - A small number of training instances over a small number of bits

Solution: *Restricted Boltzmann Machines*



- Partition visible and hidden units
 - Visible units **ONLY** talk to hidden units
 - Hidden units **ONLY** talk to visible units
- Restricted Boltzmann machine..
 - **Originally proposed as “Harmonium Models” by Paul Smolensky**

Solution: *Restricted Boltzmann Machines*

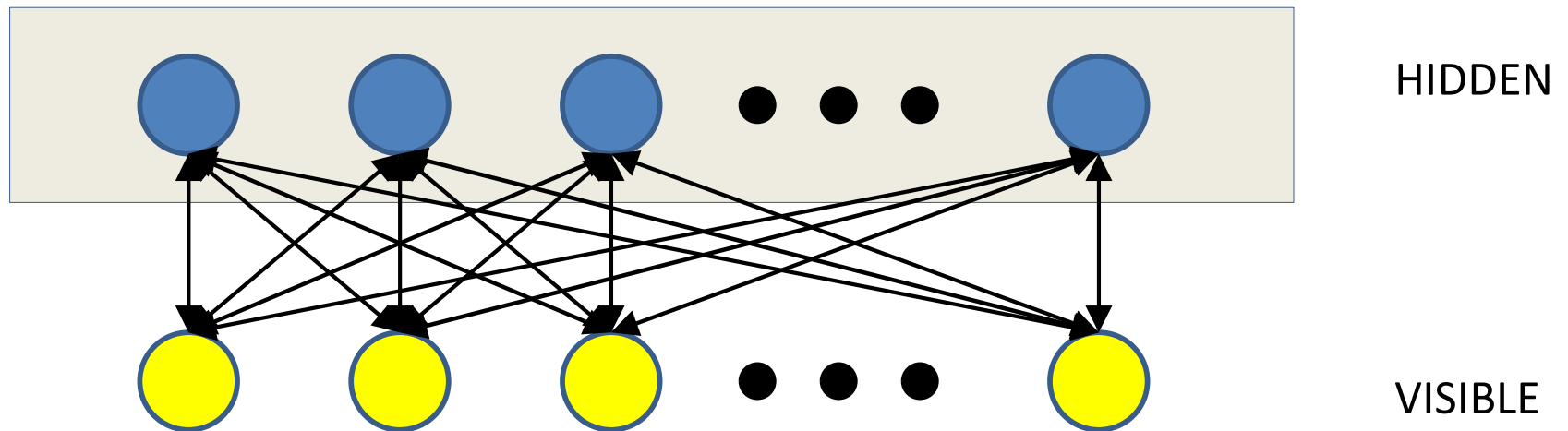


$$z_i = \sum_j w_{ji} s_i + b_i$$

$$P(s_i = 1) = \frac{1}{1 + e^{-z_i}}$$

- Still obeys the same rules as a regular Boltzmann machine
- But the modified structure adds a big benefit..

Solution: *Restricted Boltzmann Machines*



HIDDEN

$$z_i = \sum_j w_{ji} v_i + b_i$$

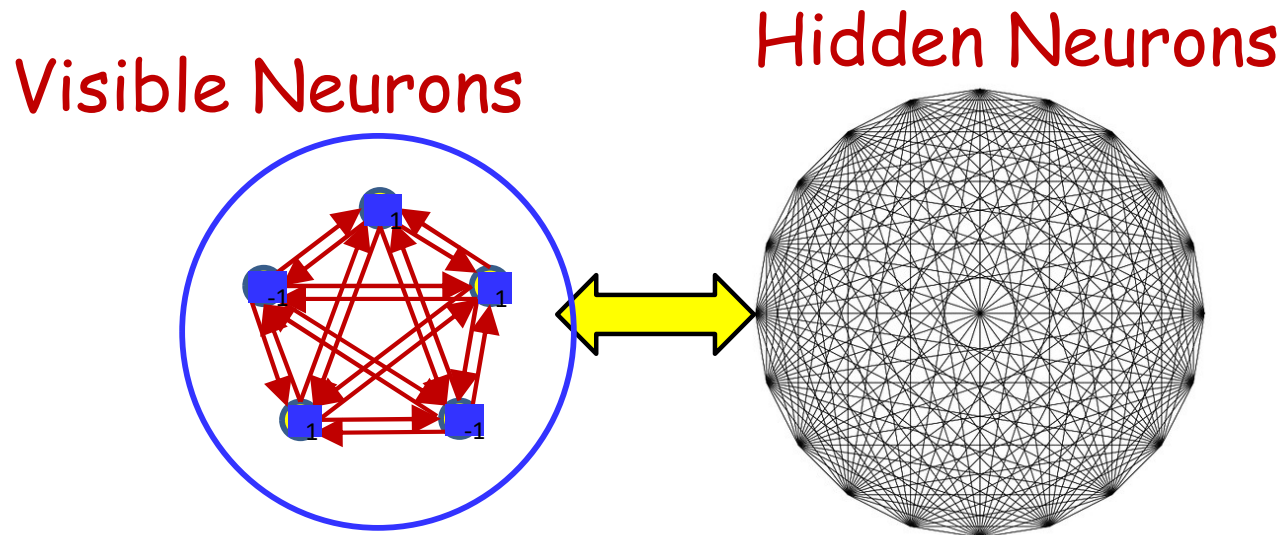
$$P(h_i = 1) = \frac{1}{1 + e^{-z_i}}$$

VISIBLE

$$y_i = \sum_j w_{ji} h_i + b_i$$

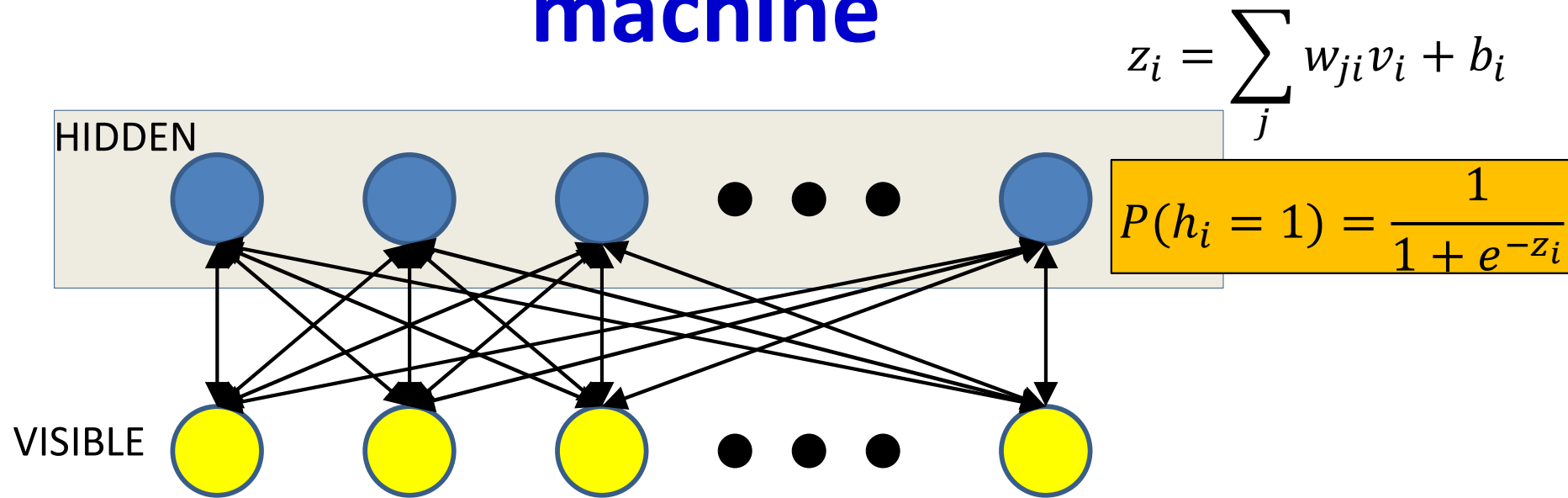
$$P(v_i = 1) = \frac{1}{1 + e^{-y_i}}$$

Recap: Training full Boltzmann machines: Step 1



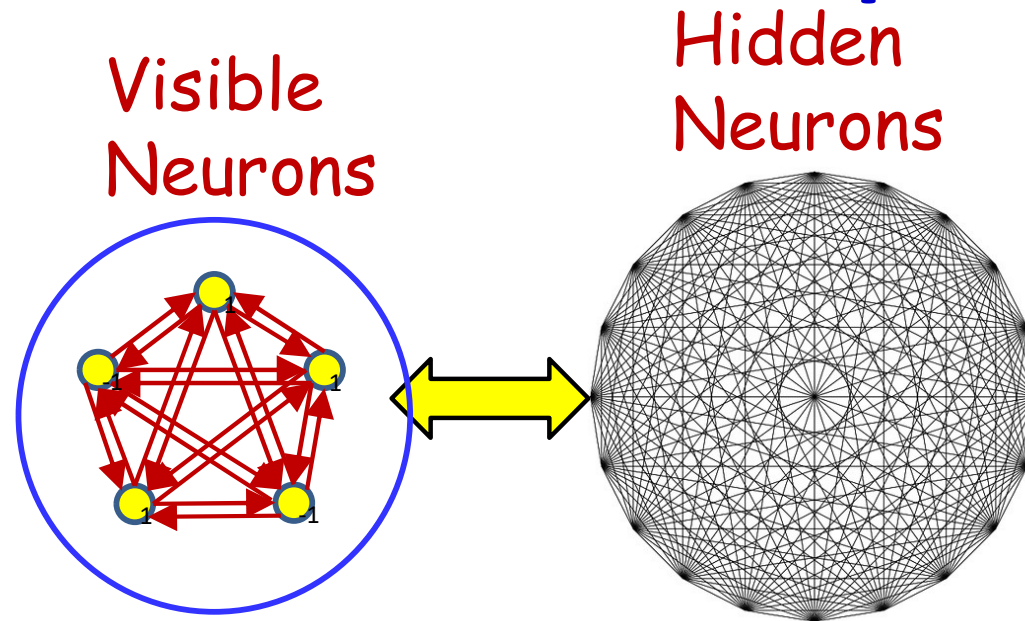
- For each training pattern V_i
 - Fix the visible units to V_i
 - Let the hidden neurons evolve from a random initial point to generate H_i
 - Generate $S_i = [V_i, H_i]$
- Repeat K times to generate synthetic training
$$\mathbf{S} = \{S_{1,1}, S_{1,2}, \dots, S_{1K}, S_{2,1}, \dots, S_{N,K}\}$$

Sampling: Restricted Boltzmann machine



- For each sample:
 - Anchor visible units
 - Sample from hidden units
 - No looping!!

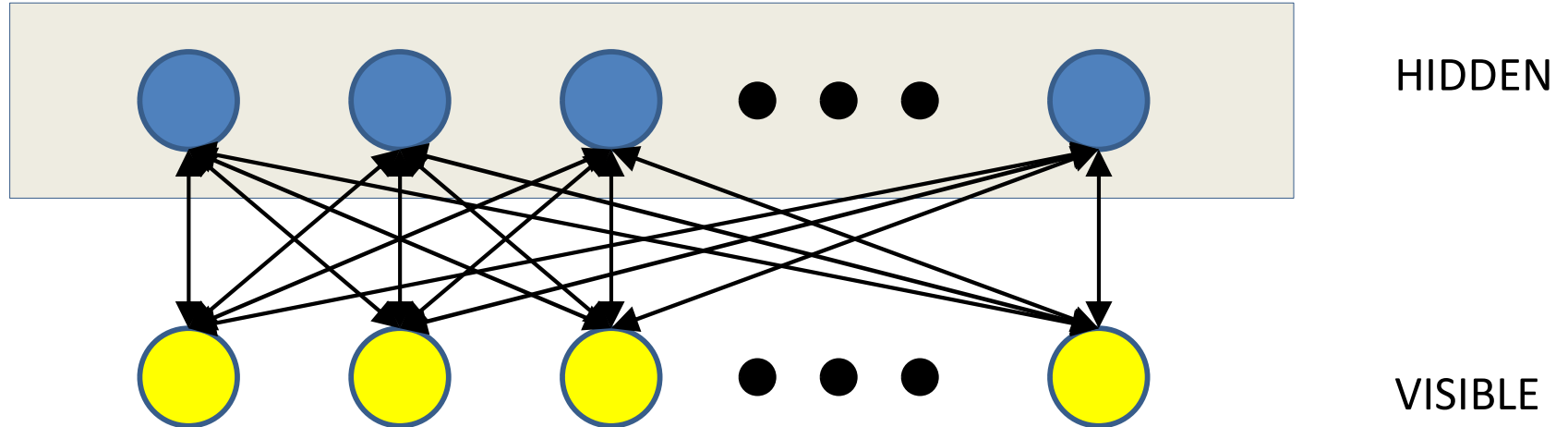
Recap: Training full Boltzmann machines: Step 2



- Now *unclamp* the visible units and let the entire network evolve several times to generate

$$\mathbf{S}_{simul} = \{S_{simul,1}, S_{simul,1=2}, \dots, S_{simul,M}\}$$

Sampling: Restricted Boltzmann machine



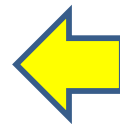
$$z_i = \sum_j w_{ji} v_i + b_i$$

$$P(h_i = 1) = \frac{1}{1 + e^{-z_i}}$$



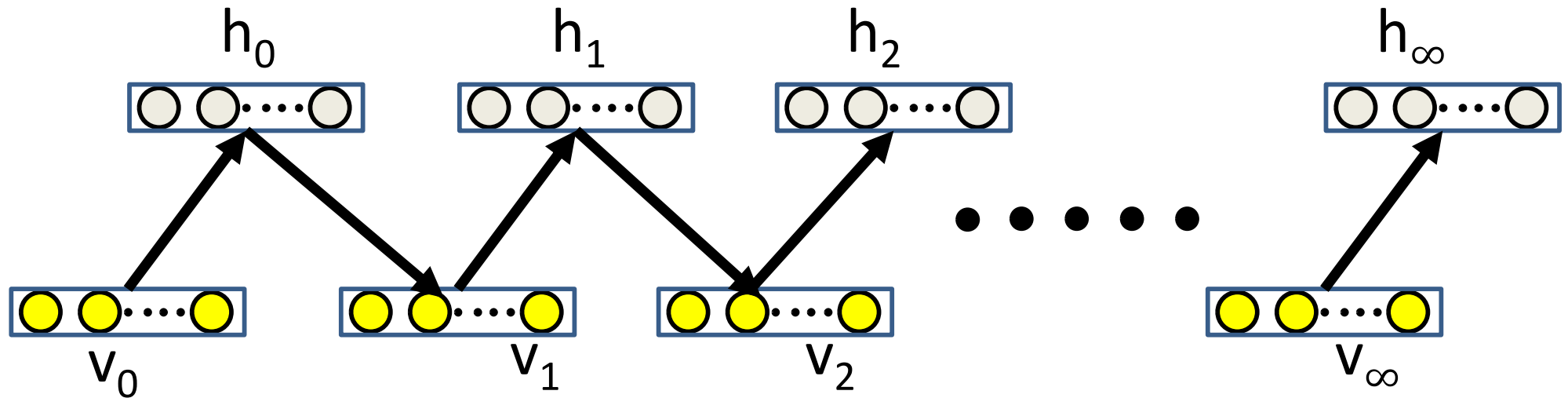
$$y_i = \sum_j w_{ji} h_i + b_i$$

$$P(v_i = 1) = \frac{1}{1 + e^{-y_i}}$$



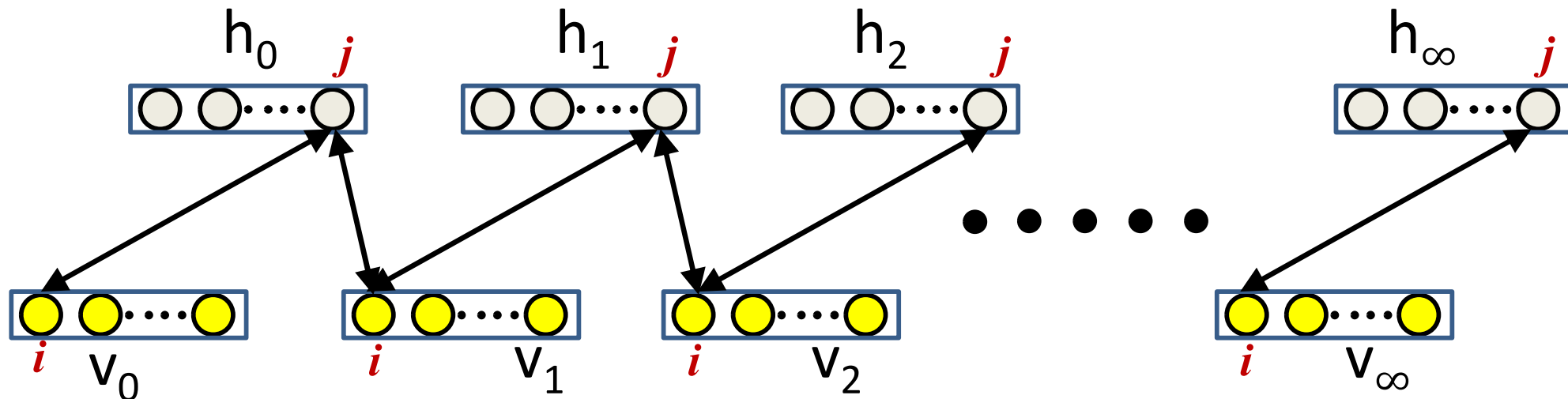
- For each sample:
 - Iteratively sample hidden and visible units for a long time
 - Draw final sample of both hidden and visible units

Pictorial representation of RBM training



- For each sample:
 - Initialize V_0 (visible) to training instance value
 - Iteratively generate hidden and visible units
 - For a very long time

Pictorial representation of RBM training



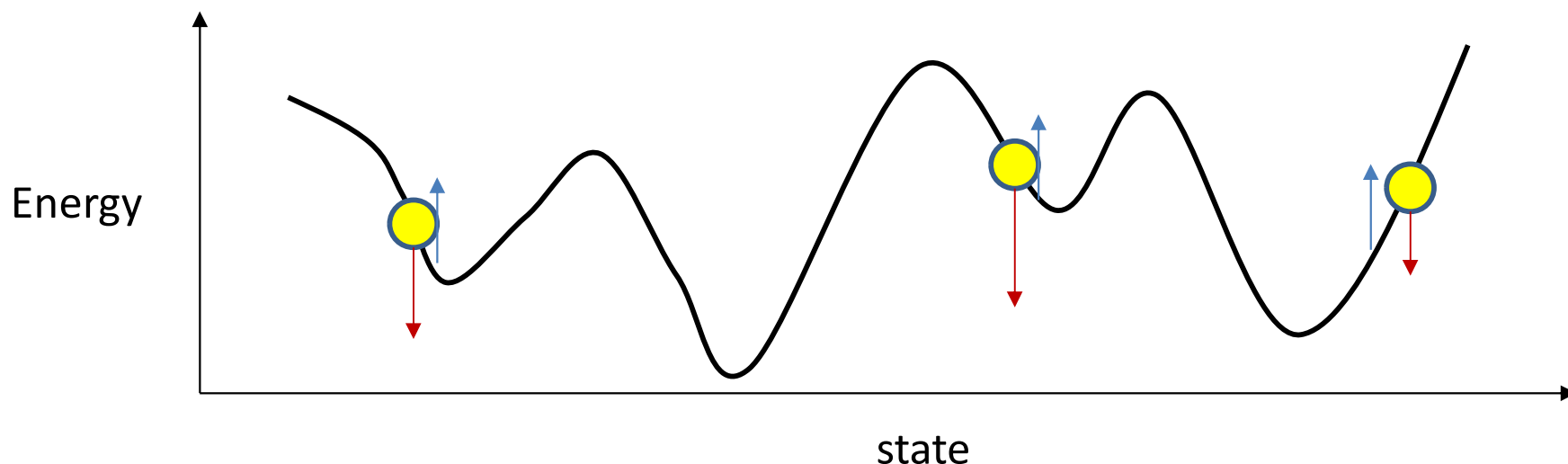
- Gradient (showing only one edge from visible node i to hidden node j)

$$\frac{\partial \log p(v)}{\partial w_{ij}} = \langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^\infty$$

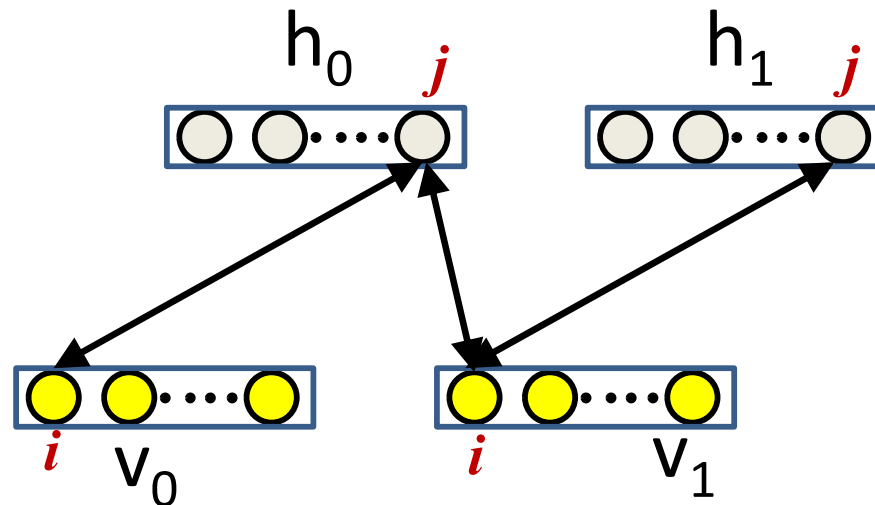
- $\langle v_i, h_j \rangle$ represents average over many generated training samples

Recall: Hopfield Networks

- Really no need to raise the entire surface, or even every valley
- Raise the *neighborhood* of each target memory
 - Sufficient to make the memory a valley
 - The broader the neighborhood considered, the broader the valley



A Shortcut: Contrastive Divergence



- Sufficient to run one iteration!

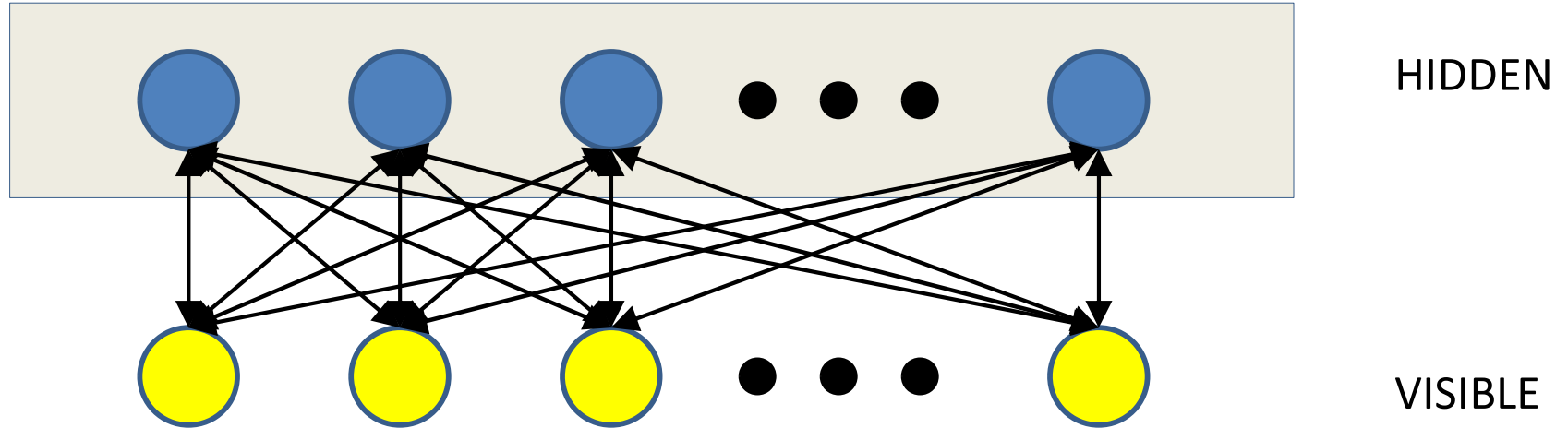
$$\frac{\partial \log p(v)}{\partial w_{ij}} = \langle v_i h_j \rangle^0 - \langle v_i h_j \rangle^1$$

- This is sufficient to give you a good estimate of the gradient

Restricted Boltzmann Machines

- Excellent generative models for binary (or binarized) data
- Can also be extended to continuous-valued data
 - “Exponential Family Harmoniums with an Application to Information Retrieval”, Welling et al., 2004
- Useful for classification and regression
 - How?
 - More commonly used to *pretrain* models

Continuous-values RBMs



HIDDEN

$$z_i = \sum_j w_{ji} v_i + b_i$$

$$P(h_i = 1) = \frac{1}{1 + e^{-z_i}}$$

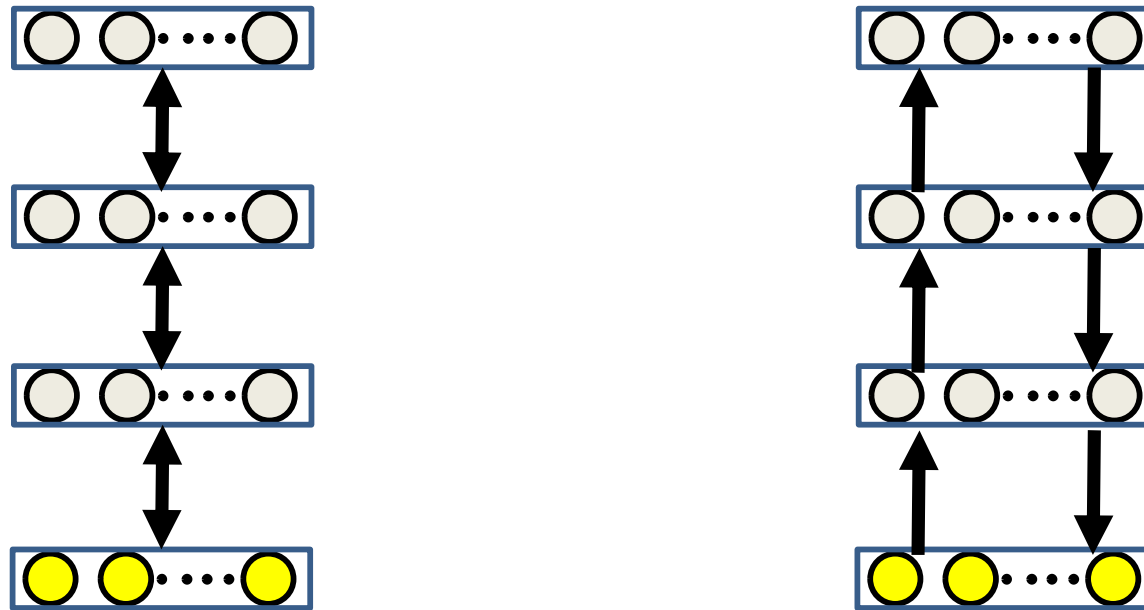
VISIBLE

$$y_i = \sum_j w_{ji} h_i + b_i$$

$$P(v_i) = r(y_i) \exp(y_i)$$

Hidden units may also be continuous values

Other variants



- Left: “Deep” Boltzmann machines
- Right: Helmholtz machine
 - Trained by the “wake-sleep” algorithm

Topics missed..

- Other algorithms for Learning and Inference over RBMs
 - Mean field approximations
- RBMs as feature extractors
 - Pre training
- RBMs as generative models
- More structured DBMs
- ...