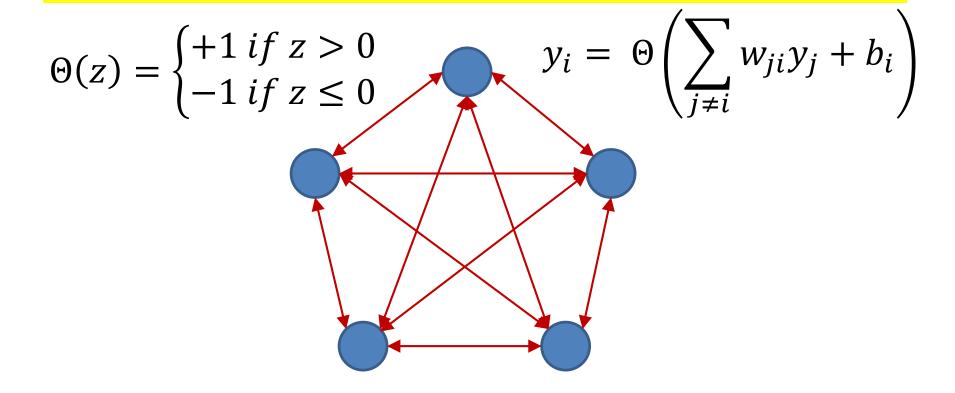
Neural Networks

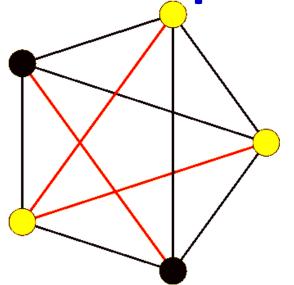
Hopfield Nets and Boltzmann Machines Spring 2018

Recap: Hopfield network



- Symmetric loopy network
- Each neuron is a perceptron with +1/-1 output

Recap: Hopfield network

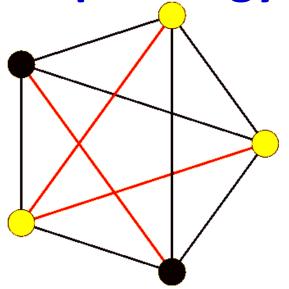


$$y_i = \Theta\left(\sum_{j \neq i} w_{ji} y_j + b_i\right)$$

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

- 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



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

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

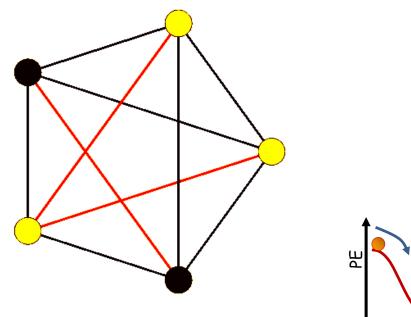
Not assuming node bias

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

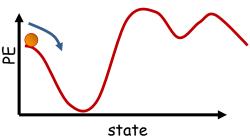
- The system will evolve until the energy hits a local minimum
- In vector form, including a bias term (not typically used in Hopfield nets)

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

Recap: Evolution

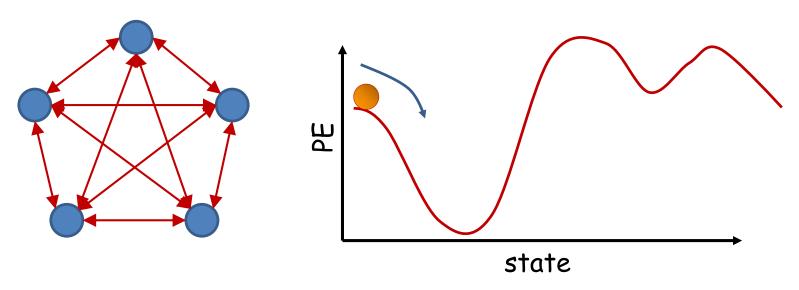


$$E = -\frac{1}{2}\mathbf{y}^T\mathbf{W}\mathbf{y}$$



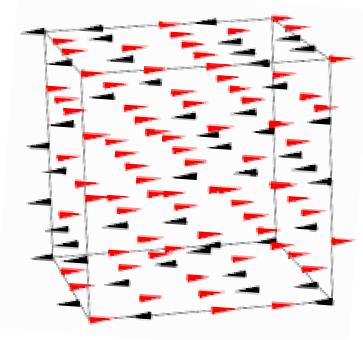
 The network will evolve until it arrives at a local minimum in the energy contour

Recap: Content-addressable memory



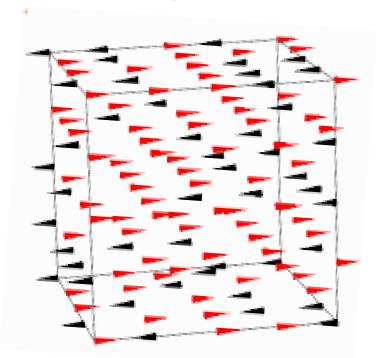
- Each of the minima is a "stored" pattern
 - If the network is initialized close to a stored pattern, it will inevitably evolve to the pattern
- This is a content addressable memory
 - Recall memory content from partial or corrupt values
- Also called associative memory

Recap – Analogy: Spin Glasses



- Magnetic diploes
- Each dipole tries to align itself to the local field
 - In doing so it may flip
- This will change fields at other dipoles
 - Which may flip
- Which changes the field at the current dipole...

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 diplose

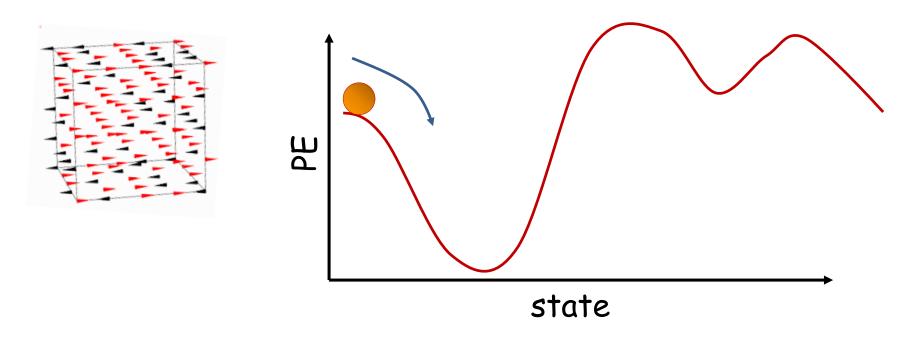
$$x_i = \begin{cases} x_i & if \ sign(x_i f(p_i)) = 1 \\ -x_i & otherwise \end{cases}$$

The total energy of the system

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

- 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
- Any small jitter from this stable configuration returns it to the stable configuration
 - I.e. the system remembers its stable state and returns to it

Recap: Hopfield net computation

1. Initialize network with initial pattern

$$y_i(0) = x_i, \qquad 0 \le i \le N - 1$$

2. Iterate until convergence

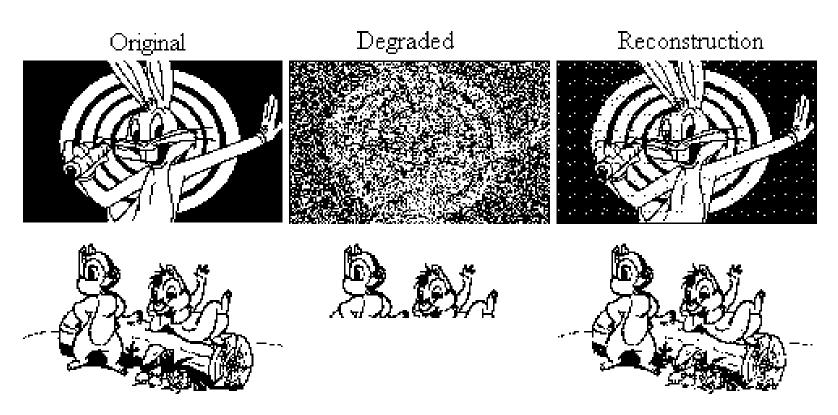
$$y_i(t+1) = \Theta\left(\sum_{j \neq i} w_{ji} y_j\right), \qquad 0 \le i \le N-1$$

- 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

Examples: Content addressable memory



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

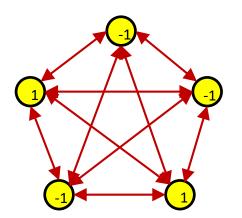
http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/₁₁

"Training" the network

- How do we make the network store a specific pattern or set of patterns?
 - Hebbian learning
 - Geometric approach
 - Optimization

- Secondary question
 - How many patterns can we store?

Recap: Hebbian Learning to Store a Specific Pattern



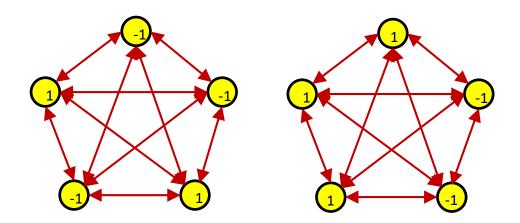
HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

$$\mathbf{W} = \mathbf{y}_p \mathbf{y}_p^T - \mathbf{I}$$

 For a single stored pattern, Hebbian learning results in a network for which the target pattern is a global minimum

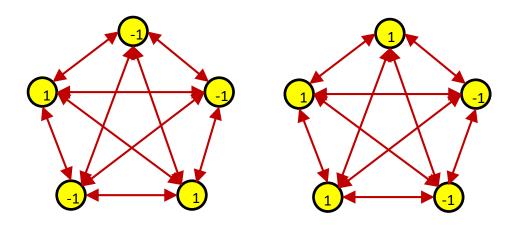
Storing multiple patterns



$$w_{ji} = \sum_{p \in \{y_p\}} y_i^p y_j^p$$

- $\{y_p\}$ is the set of patterns to store
- Superscript p represents the specific pattern

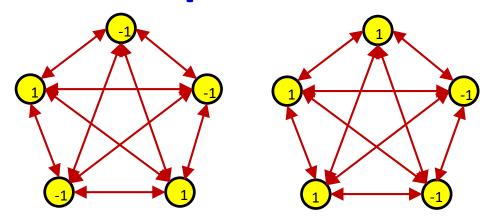
Storing multiple patterns



- Let \mathbf{y}_p be the vector representing p-th pattern
- Let $\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ ...]$ be a matrix with all the stored pattern
- Then..

$$\mathbf{W} = \sum_{p} (\mathbf{y}_{p} \mathbf{y}_{p}^{T} - \mathbf{I}) = \mathbf{Y} \mathbf{Y}^{T} - N_{p} \mathbf{I}$$
Number of patterns

Recap: Hebbian Learning to Store Multiple Patterns

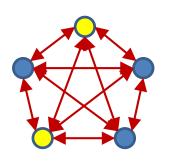


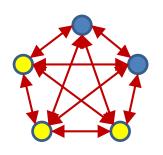
$$w_{ji} = \sum_{p \in \{p\}} y_i^p y_j^p$$

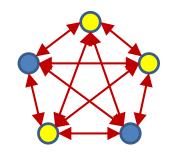
$$\mathbf{W} = \sum_{p} (\mathbf{y}_{p} \mathbf{y}_{p}^{T} - \mathbf{I}) = \mathbf{Y} \mathbf{Y}^{T} - N_{p} \mathbf{I}$$

- {p} is the set of patterns to store
 - Superscript p represents the specific pattern
- N_p is the number of patterns to store

How many patterns can we store?







- Hopfield: For a network of N neurons can store up to 0.14N patterns
- In reality, seems possible to store K > 0.14N patterns
 - i.e. obtain a weight matrix W such that K > 0.14N patterns are stationary

Bold Claim

- I can always store (upto) N orthogonal patterns such that they are stationary!
 - Although not necessarily stable

• Why?

"Training" the network

- How do we make the network store a specific pattern or set of patterns?
 - Hebbian learning
 - Geometric approach
 - Optimization

- Secondary question
 - How many patterns can we store?

A minor adjustment

• Note behavior of $\mathbf{E}(\mathbf{y}) = \mathbf{y}^T \mathbf{W} \mathbf{y}$ with

$$\mathbf{W} = \mathbf{Y}\mathbf{Y}^T - N_p \mathbf{I}$$

Is identical to behavior with

$$\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$$

Energy landscape only differs by an additive constant

Gradients and location of minima remain same

Since

$$\mathbf{y}^{T}(\mathbf{Y}\mathbf{Y}^{T} - N_{p}\mathbf{I})\mathbf{y} = \mathbf{y}^{T}\mathbf{Y}\mathbf{Y}^{T}\mathbf{y} - NN_{p}$$

• But $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$ is easier to analyze. Hence in the following slides we will use $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$

A minor adjustment

• Note behavior of $\mathbf{E}(\mathbf{y}) = \mathbf{y}^T \mathbf{W} \mathbf{y}$ with

Both have the same Eigen vectors $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T - N_p \mathbf{I}$ $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$ $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$

Energy landscape only differs by an additive constant

Gradients and location of minima remain same

Since

$$\mathbf{y}^{T}(\mathbf{Y}\mathbf{Y}^{T} - N_{p}\mathbf{I})\mathbf{y} = \mathbf{y}^{T}\mathbf{Y}\mathbf{Y}^{T}\mathbf{y} - NN_{p}$$

• But $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$ is easier to analyze. Hence in the following slides we will use $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$

A minor adjustment

• Note behavior of $\mathbf{E}(\mathbf{y}) = \mathbf{y}^T \mathbf{W} \mathbf{y}$ with

 $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T - N_p \mathbf{I}$ Both have the same Eigen vectors behavior with

$$\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$$

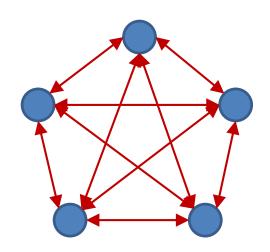
NOTE: This is a positive semidefinite matrix $\mathbf{y} = \mathbf{y}^T \mathbf{Y} \mathbf{y}^T \mathbf{y} - NN_p$

Energy landscape only differs by an additive constant

Gradients and location of minima remain same

• But $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$ is easier to analyze. Hence in the following slides we will use $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$

Consider the energy function

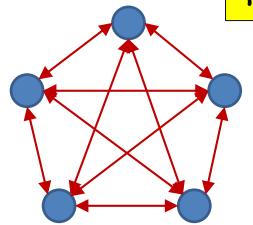


$$E = -\frac{1}{2}\mathbf{y}^T\mathbf{W}\mathbf{y} - \mathbf{b}^T\mathbf{y}$$

Reinstating the bias term for completeness sake

Consider the energy function





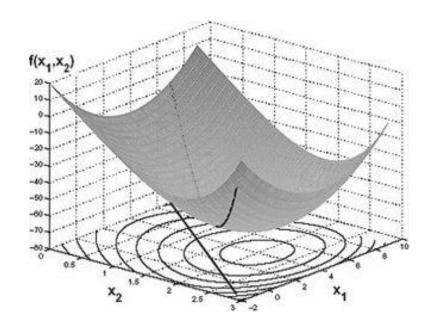
For Hebbian learning W is positive semidefinite

E is convex

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

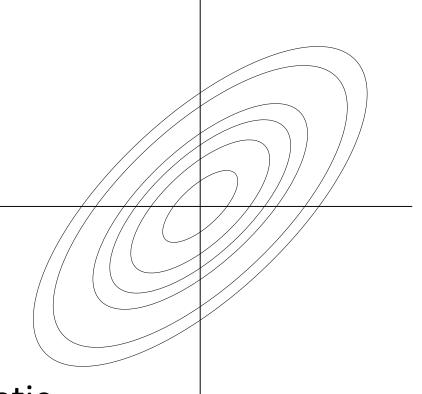
Reinstating the bias term for completeness sake

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



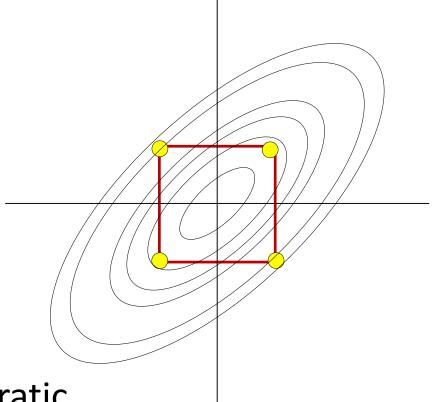
• *E* is a convex quadratic

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

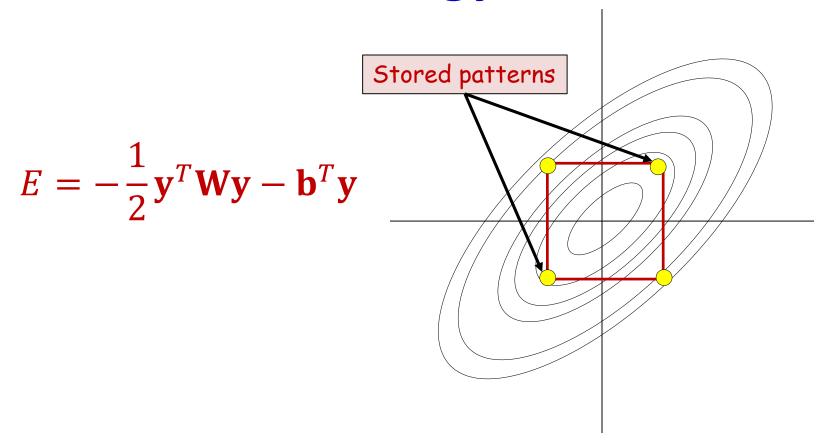


- *E* is a convex quadratic
 - Shown from above (assuming 0 bias)

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

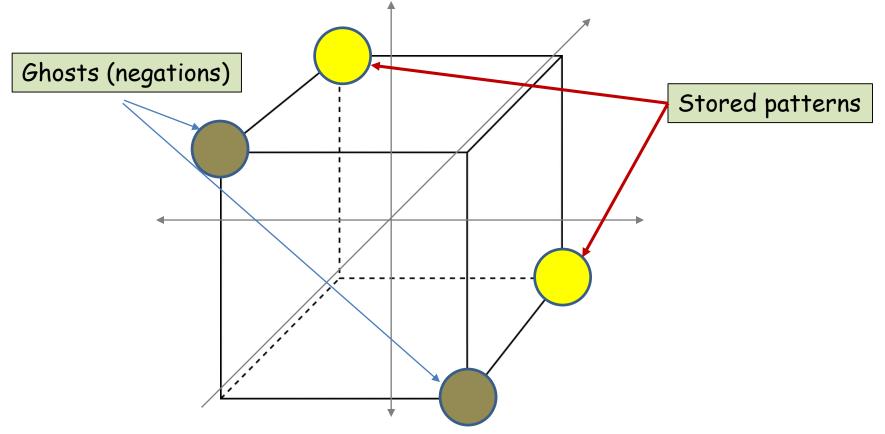


- *E* is a convex quadratic
 - Shown from above (assuming 0 bias)
- But components of y can only take values ± 1
 - I.e y lies on the corners of the unit hypercube



 The stored values of y are the ones where all adjacent corners are lower on the quadratic

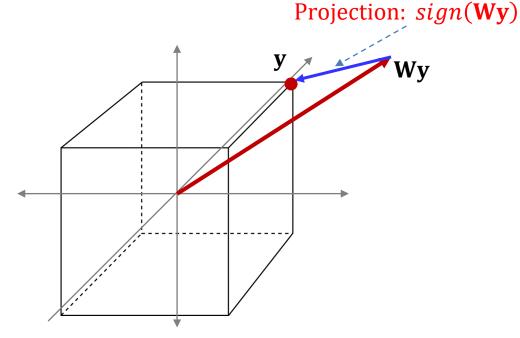
Patterns you can store



- All patterns are on the corners of a hypercube
 - If a pattern is stored, it's "ghost" is stored as well
 - Intuitively, patterns must ideally be maximally far apart
 - Though this doesn't seem to hold for Hebbian learning

Evolution of the network

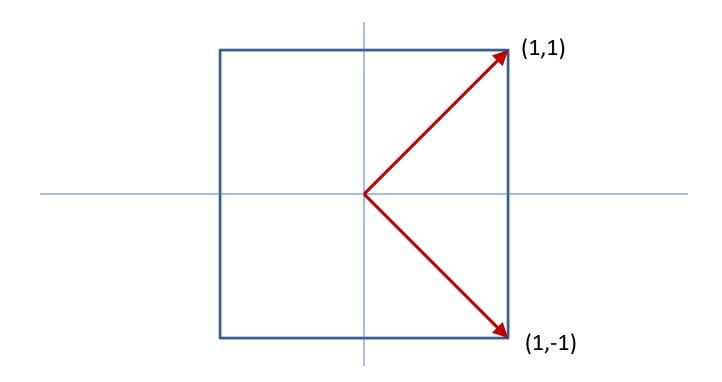
- Note: for binary vectors sign(y) is a projection
 - Projects y onto the nearest corner of the hypercube
 - It "quantizes" the space into orthants
- Response to field: $\mathbf{y} \leftarrow sign(\mathbf{W}\mathbf{y})$
 - Each step rotates the vector \mathbf{y}_P and then projects it onto the nearest corner



Storing patterns

- A pattern \mathbf{y}_P is stored if:
 - $-sign(\mathbf{W}\mathbf{y}_p) = \mathbf{y}_p$ for all target patterns
- Training: Design W such that this holds
- Simple solution: \mathbf{y}_p is an Eigenvector of \mathbf{W}
 - And the corresponding Eigenvalue is positive $\mathbf{W}\mathbf{y}_p = \lambda\mathbf{y}_p$
 - More generally orthant($\mathbf{W}\mathbf{y}_p$) = orthant(\mathbf{y}_p)
- How many such \mathbf{y}_p can we have?

Only N patterns?



- Patterns that differ in N/2 bits are orthogonal
- You can have max N orthogonal vectors in an N-dimensional space

Another random fact that should interest you

The Eigenvectors of any symmetric matrix W are orthogonal

• The Eigenvalues may be positive or negative

Storing more than one pattern

- Requirement: Given $y_1, y_2, ..., y_P$
 - Design W such that
 - $sign(\mathbf{W}\mathbf{y}_p) = \mathbf{y}_p$ for all target patterns
 - There are no other binary vectors for which this holds

 What is the largest number of patterns that can be stored?

Storing K orthogonal patterns

- Simple solution: Design \mathbf{W} such that \mathbf{y}_1 , \mathbf{y}_2 , ..., \mathbf{y}_K are the Eigen vectors of \mathbf{W}
 - $\text{ Let } \mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_K]$

$$\mathbf{W} = \mathbf{Y} \wedge \mathbf{Y}^T$$

- $-\lambda_1, \dots, \lambda_K$ are positive
- For $\lambda_1=\lambda_2=\lambda_K=1$ this is exactly the Hebbian rule
- The patterns are provably stationary

Hebbian rule

In reality

- Let
$$Y = [y_1 \ y_2 \ ... \ y_K \ r_{K+1} \ r_{K+2} \ ... \ r_N]$$

$$\mathbf{W} = \mathbf{Y} \Lambda \mathbf{Y}^T$$

- $\mathbf{r}_{K+1} \mathbf{r}_{K+2} \dots \mathbf{r}_N$ are orthogonal to $\mathbf{y}_1 \mathbf{y}_2 \dots \mathbf{y}_K$
- $-\lambda_1 = \lambda_2 = \lambda_K = 1$
- $-\lambda_{K+1}$,..., $\lambda_N=0$
- All patterns orthogonal to $y_1 y_2 ... y_K$ are also stationary
 - Although not stable

Storing N orthogonal patterns

• When we have N orthogonal (or near orthogonal) patterns $\mathbf{y}_1, \mathbf{y}_2, ..., \mathbf{y}_N$

$$-Y = [\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_N]$$

$$\mathbf{W} = \mathbf{Y} \wedge \mathbf{Y}^T$$

$$-\lambda_1 = \lambda_2 = \lambda_N = 1$$

- The Eigen vectors of W span the space
- Also, for any \mathbf{y}_k

$$\mathbf{W}\mathbf{y}_k = \mathbf{y}_k$$

Storing N orthogonal patterns

- The N orthogonal patterns $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N$ span the space
- Any pattern y can be written as

$$\mathbf{y} = a_1 \mathbf{y}_1 + a_2 \mathbf{y}_2 + \dots + a_N \mathbf{y}_N$$

$$\mathbf{W} \mathbf{y} = a_1 \mathbf{W} \mathbf{y}_1 + a_2 \mathbf{W} \mathbf{y}_2 + \dots + a_N \mathbf{W} \mathbf{y}_N$$

$$= a_1 \mathbf{y}_1 + a_2 \mathbf{y}_2 + \dots + a_N \mathbf{y}_N = \mathbf{y}$$

- All patterns are stable
 - Remembers everything
 - Completely useless network

Storing K orthogonal patterns

- Even if we store fewer than N patterns
 - Let $Y = [\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_K \ \mathbf{r}_{K+1} \ \mathbf{r}_{K+2} \ ... \ \mathbf{r}_N]$

$$W = Y\Lambda Y^T$$

- $\mathbf{r}_{K+1} \mathbf{r}_{K+2} \dots \mathbf{r}_N$ are orthogonal to $\mathbf{y}_1 \mathbf{y}_2 \dots \mathbf{y}_K$
- $-\lambda_1=\lambda_2=\lambda_K=1$
- $-\lambda_{K+1}$, ..., $\lambda_N=0$
- All patterns orthogonal to $y_1 y_2 ... y_K$ are stationary
- Any pattern that is *entirely* in the subspace spanned by $y_1 y_2 ... y_K$ is also stable (same logic as earlier)
- Only patterns that are *partially* in the subspace spanned by $\mathbf{y_1} \ \mathbf{y_2} \ ... \ \mathbf{y_K}$ are unstable
 - Get projected onto subspace spanned by $\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_K$

Problem with Hebbian Rule

Even if we store fewer than N patterns

- Let
$$Y = [\mathbf{y}_1 \ \mathbf{y}_2 \ ... \ \mathbf{y}_K \ \mathbf{r}_{K+1} \ \mathbf{r}_{K+2} \ ... \ \mathbf{r}_N]$$

$$W = Y\Lambda Y^T$$

- $\mathbf{r}_{K+1} \mathbf{r}_{K+2} \dots \mathbf{r}_N$ are orthogonal to $\mathbf{y}_1 \mathbf{y}_2 \dots \mathbf{y}_K$

$$-\lambda_1 = \lambda_2 = \lambda_K = 1$$

- Problems arise because Eigen values are all 1.0
 - Ensures stationarity of vectors in the subspace
 - What if we get rid of this requirement?

Hebbian rule and general (nonorthogonal) vectors

$$w_{ji} = \sum_{p \in \{p\}} y_i^p y_j^p$$

- What happens when the patterns are not orthogonal
- What happens when the patterns are presented more than once
 - Different patterns presented different numbers of times
 - Equivalent to having unequal Eigen values...
- Can we predict the evolution of any vector y
 - Hint: Lanczos iterations
 - Can write $\mathbf{Y}_P = \mathbf{Y}_{ortho} \mathbf{B}$, $\rightarrow \mathbf{W} = \mathbf{Y}_{ortho} \mathbf{B} \wedge \mathbf{B}^T \mathbf{Y}_{ortho}^T$

The bottom line

- With an network of N units (i.e. N-bit patterns)
- The maximum number of stable patterns is actually exponential in N
 - McElice and Posner, 84'
 - E.g. when we had the Hebbian net with N orthogonal base patterns, all patterns are stable
- For a *specific* set of K patterns, we can *always* build a network for which all K patterns are stable provided $K \leq N$
 - Mostafa and St. Jacques 85'
 - For large N, the upper bound on K is actually N/4logN
 - McElice et. Al. 87'
 - But this may come with many "parasitic" memories

The bottom line

- With an network of N units (i.e. N-bit patterns)
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 patterns, all patterns are stable

How do we find this network?

- For a *specific* set of K patterns, we can *always* build a network for which all K patterns are stable provided $K \leq N$
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The bottom line

- With an network of N units (i.e. N-bit patterns)
- The maximum number of stable patterns is actually exponential in N
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 - E.g. when we had the K
 patterns, all patterns are stable

How do we find this network?

Can we do something

- For a *specific* set of K patterns, we can *always* build a network for which all K patterns are stable provided $K \leq N$
 - Mostafa and St. Jacques 85'

• For large N, the upper bound on K is actually 19

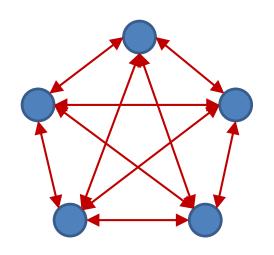
- McElice et. Al. 87'
- But this may come with many "parasitic" memories

A different tack

- How do we make the network store a specific pattern or set of patterns?
 - Hebbian learning
 - Geometric approach
 - Optimization

- Secondary question
 - How many patterns can we store?

Consider the energy function



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

- This must be maximally low for target patterns
- Must be maximally high for all other patterns
 - So that they are unstable and evolve into one of the target patterns

Alternate Approach to Estimating the Network

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

- Estimate W (and b) such that
 - E is minimized for $y_1, y_2, ..., y_P$
 - -E is maximized for all other y
- Caveat: Unrealistic to expect to store more than N patterns, but can we make those N patterns memorable

Optimizing W (and b)

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

$$E(\mathbf{y}) = -\frac{1}{2}\mathbf{y}^T\mathbf{W}\mathbf{y}$$
 $\widehat{\mathbf{W}} = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{\mathbf{y} \in \mathbf{Y}_P} E(\mathbf{y})$

The bias can be captured by another fixed-value component

- Minimize total energy of target patterns
 - Problem with this?

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

$$\widehat{\mathbf{W}} = \underset{\mathbf{W}}{\operatorname{argmin}} \sum_{\mathbf{y} \in \mathbf{Y}_P} E(\mathbf{y}) - \sum_{\mathbf{y} \notin \mathbf{Y}_P} E(\mathbf{y})$$

- Minimize total energy of target patterns
- Maximize the total energy of all non-target patterns

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

Simple gradient descent:

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

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

- Can "emphasize" the importance of a pattern by repeating
 - More repetitions → greater emphasis

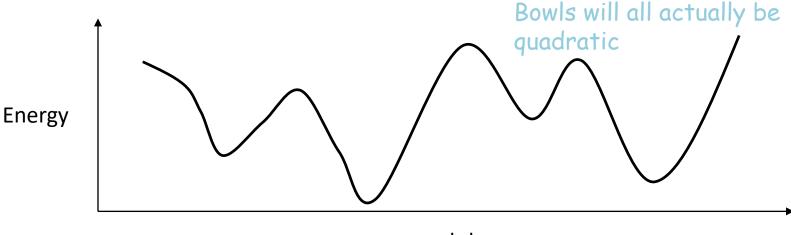
$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P} \mathbf{y} \mathbf{y}^T \right)$$

- Can "emphasize" the importance of a pattern by repeating
 - More repetitions → greater emphasis
- How many of these?
 - Do we need to include all of them?
 - Are all equally important?

The training again...

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

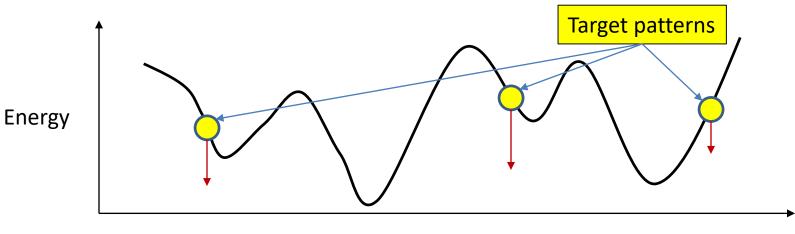
 Note the energy contour of a Hopfield network for any weight W



The training again

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

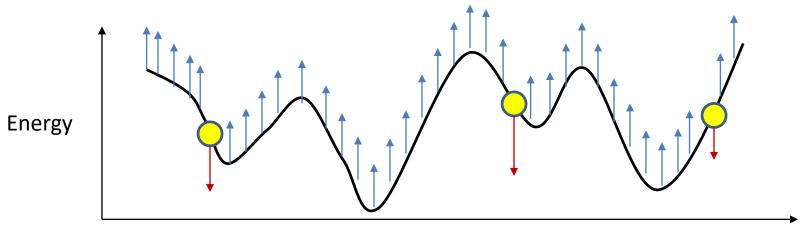
- The first term tries to minimize the energy at target patterns
 - Make them local minima
 - Emphasize more "important" memories by repeating them more frequently



The negative class

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

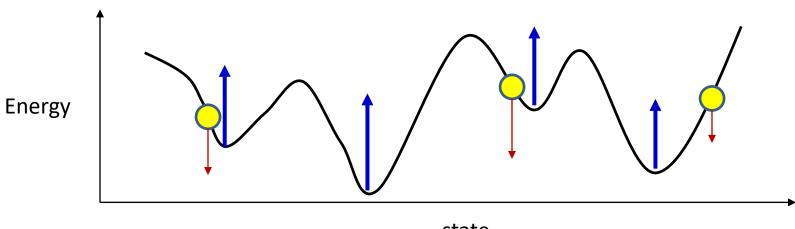
- The second term tries to "raise" all non-target patterns
 - Do we need to raise everything?



Option 1: Focus on the valleys

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

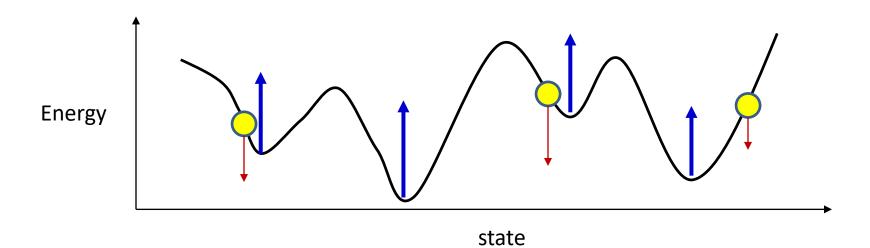
- Focus on raising the valleys
 - If you raise every valley, eventually they'll all move up above the target patterns, and many will even vanish



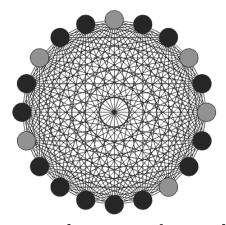
Identifying the valleys...

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

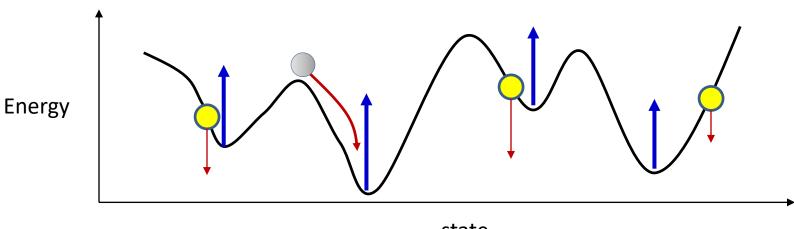
 Problem: How do you identify the valleys for the current W?



Identifying the valleys...



- Initialize the network randomly and let it evolve
 - It will settle in a valley



Training the Hopfield network

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

- Initialize W
- Compute the total outer product of all target patterns
 - More important patterns presented more frequently
- Randomly initialize the network several times 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

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

- Initialize 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
 - Randomly initialize the network and let it evolve
 - And settle at a valley \mathbf{y}_{v}
 - Update weights

•
$$\mathbf{W} = \mathbf{W} + \eta (\mathbf{y}_p \mathbf{y}_p^T - \mathbf{y}_v \mathbf{y}_v^T)$$

Training the Hopfield network

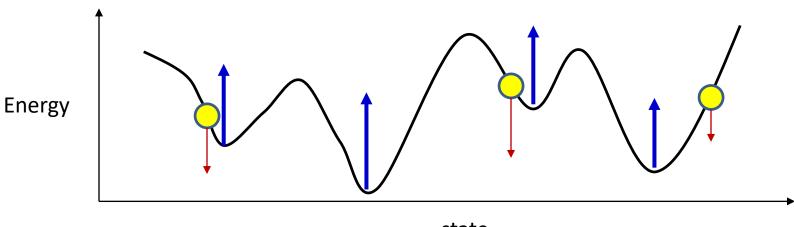
$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = valley} \mathbf{y} \mathbf{y}^T \right)$$

- Initialize 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
 - Randomly initialize the network and let it evolve
 - And settle at a valley \mathbf{y}_v
 - Update weights

•
$$\mathbf{W} = \mathbf{W} + \eta (\mathbf{y}_p \mathbf{y}_p^T - \mathbf{y}_v \mathbf{y}_v^T)$$

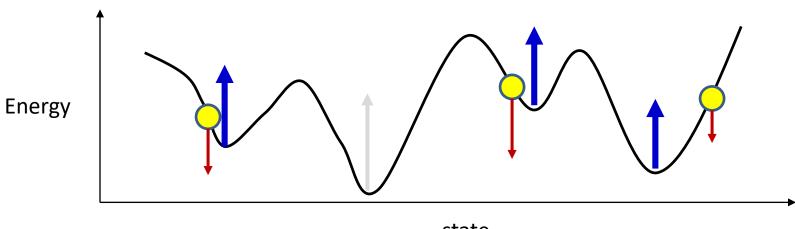
Which valleys?

- Should we randomly sample valleys?
 - Are all valleys equally important?

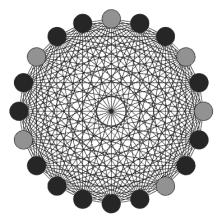


Which valleys?

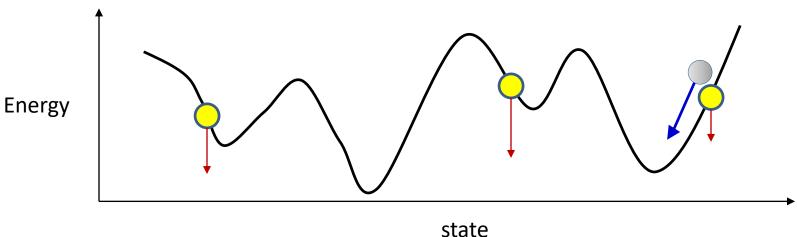
- Should we randomly sample valleys?
 - Are all valleys equally important?
- Major requirement: memories must be stable
 - They must be broad valleys
- Spurious valleys in the neighborhood of memories are more important to eliminate



Identifying the valleys...



- 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

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

- Initialize 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

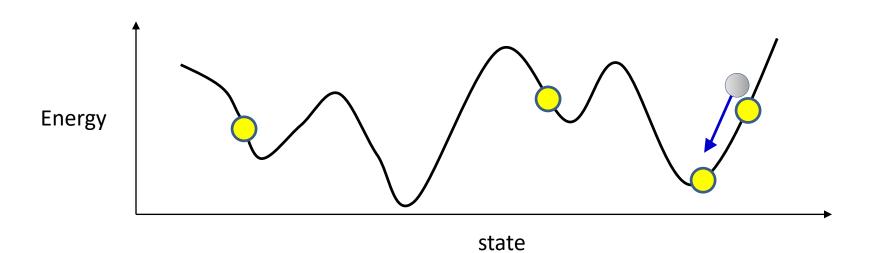
$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P \& \mathbf{y} = valley} \mathbf{y} \mathbf{y}^T \right)$$

- Initialize 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

•
$$\mathbf{W} = \mathbf{W} + \eta (\mathbf{y}_p \mathbf{y}_p^T - \mathbf{y}_v \mathbf{y}_v^T)$$

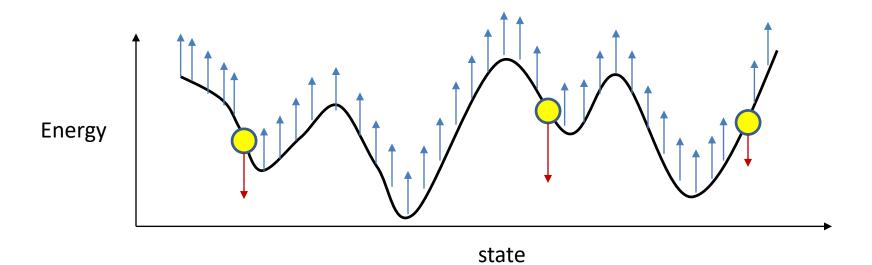
A possible problem

- What if there's another target pattern downvalley
 - Raising it will destroy a better-represented or stored pattern!



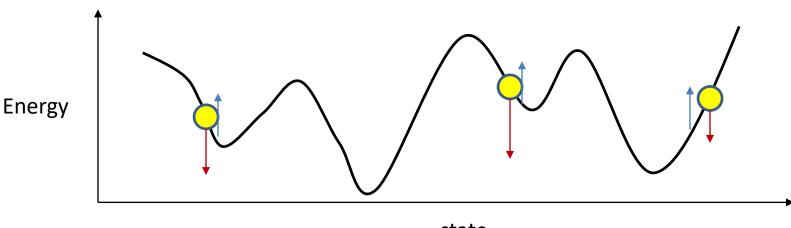
A related issue

 Really no need to raise the entire surface, or even every valley



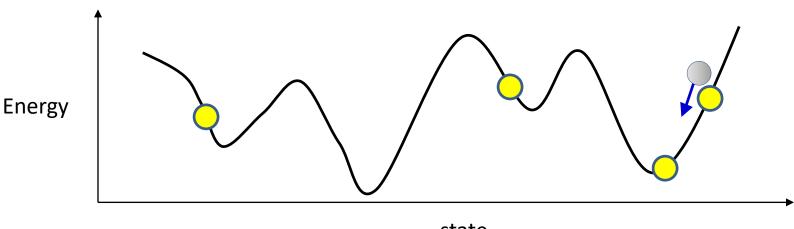
A related issue

- 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



Raising the neighborhood

- Starting from a target pattern, let the network evolve only a few steps
 - Try to raise the resultant location
- Will raise the neighborhood of targets
- Will avoid problem of down-valley targets



Training the Hopfield network: SGD version

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

- Initialize 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

•
$$\mathbf{W} = \mathbf{W} + \eta (\mathbf{y}_p \mathbf{y}_p^T - \mathbf{y}_d \mathbf{y}_d^T)$$

A probabilistic interpretation

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

- For continuous y, the energy of a pattern is a perfect analog to the negative log likelihood of a Gaussian density
- For binary y it is the analog of the negative log likelihood of a Boltzmann distribution
 - Minimizing energy maximizes log likelihood

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

The Boltzmann Distribution

$$E(\mathbf{y}) = -\frac{1}{2}\mathbf{y}^T \mathbf{W} \mathbf{y} - \mathbf{b}^T \mathbf{y} \qquad P(\mathbf{y}) = Cexp\left(\frac{-E(\mathbf{y})}{kT}\right)$$

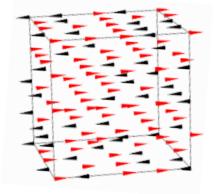
$$P(\mathbf{y}) = Cexp\left(\frac{-E(\mathbf{y})}{kT}\right)$$

$$C = \frac{1}{\sum_{\mathbf{v}} P(\mathbf{y})}$$

- k is the Boltzmann constant
- T is the temperature of the system
- The energy terms are like the loglikelihood of a Boltzmann distribution at T=1
 - Derivation of this probability is in fact quite trivial...

Continuing the Boltzmann analogy

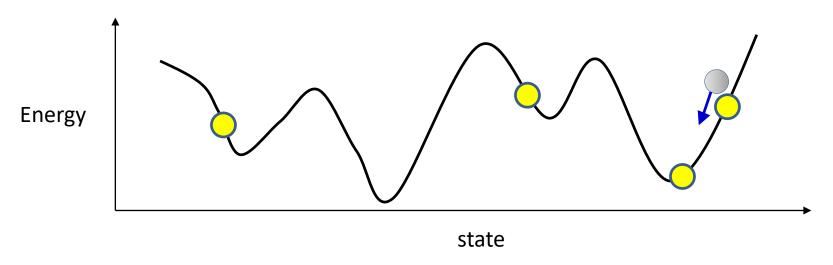
$$E(\mathbf{y}) = -\frac{1}{2}\mathbf{y}^{T}\mathbf{W}\mathbf{y} - \mathbf{b}^{T}\mathbf{y} \qquad P(\mathbf{y}) = Cexp\left(\frac{-E(\mathbf{y})}{kT}\right)$$



$$C = \frac{1}{\sum_{\mathbf{y}} P(\mathbf{y})}$$

- The system probabilistically selects states with lower energy
 - With infinitesimally slow cooling, at T=0, it arrives at the global minimal state

Spin glasses and Hopfield nets



• Selecting a next state is akin to drawing a sample from the Boltzmann distribution at T=1, in a universe where k=1

Optimizing W

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

Simple gradient descent:

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \alpha_{\mathbf{y}} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P} \beta(E(\mathbf{y})) \mathbf{y} \mathbf{y}^T \right)$$

More importance to more frequently presented memories

More importance to more attractive spurious memories

Optimizing W

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

Simple gradient descent:

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \alpha_{\mathbf{y}} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P} \beta(E(\mathbf{y})) \mathbf{y} \mathbf{y}^T \right)$$

More importance to more frequently presented memories

More importance to more attractive spurious memories

Optimizing W

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

Update rule

$$\mathbf{W} = \mathbf{W} + \eta \left(\sum_{\mathbf{y} \in \mathbf{Y}_P} \alpha_{\mathbf{y}} \mathbf{y} \mathbf{y}^T - \sum_{\mathbf{y} \notin \mathbf{Y}_P} \beta(E(\mathbf{y})) \mathbf{y} \mathbf{y}^T \right)$$
$$\mathbf{W} = \mathbf{W} + \eta \left(E_{\mathbf{v} \sim \mathbf{Y}_P} \mathbf{y} \mathbf{y}^T - E_{\mathbf{v} \sim Y} \mathbf{y} \mathbf{y}^T \right)$$

Natural distribution for variables: The Boltzmann Distribution

Continuing on...

- The Hopfield net as a Boltzmann distribution
- Adding capacity to a Hopfield network
 - The Boltzmann machine

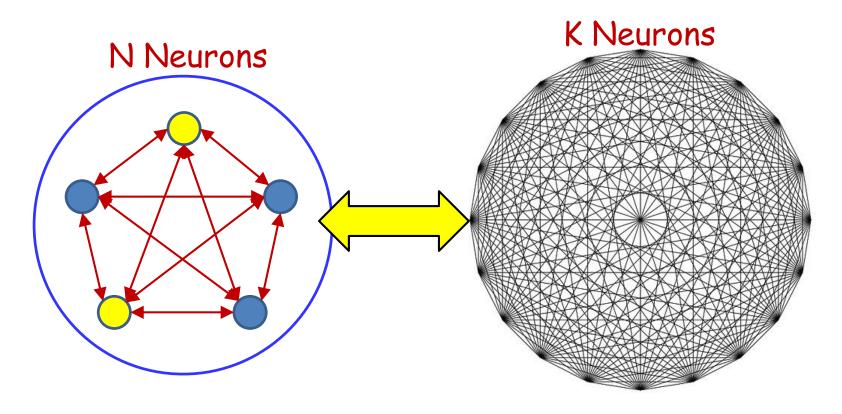
Continuing on...

- The Hopfield net as a Boltzmann distribution
- Adding capacity to a Hopfield network
 - The Boltzmann machine

Storing more than N patterns

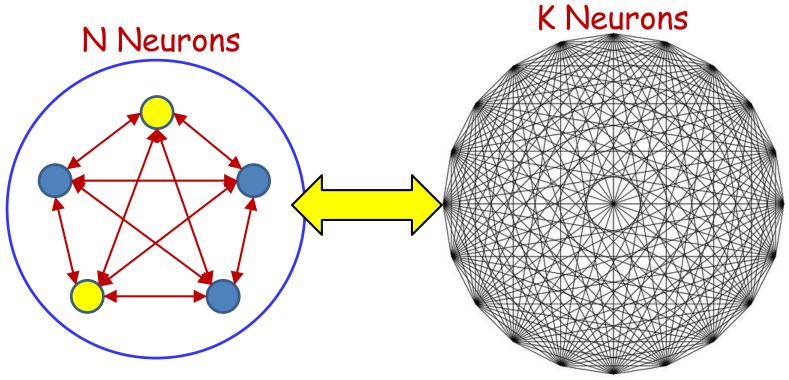
- The memory capacity of an N-bit network is at most N
 - Stable patterns (not necessarily even stationary)
 - Abu Mustafa and St. Jacques, 1985
 - Although "information capacity" is $\mathcal{O}(N^3)$
- How do we increase the capacity of the network
 - Store more patterns

Expanding the network



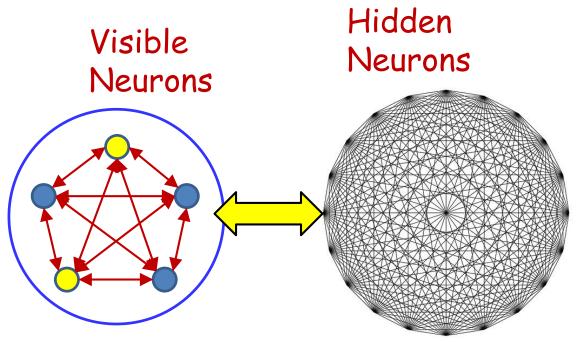
 Add a large number of neurons whose actual values you don't care about!

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

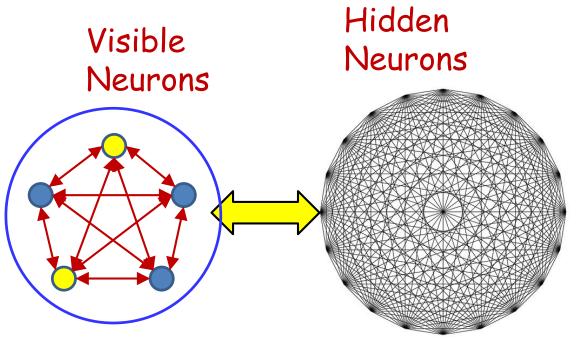
Terminology



• 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!
 - Solution: Combinatorial optimization
 - Simulated annealing

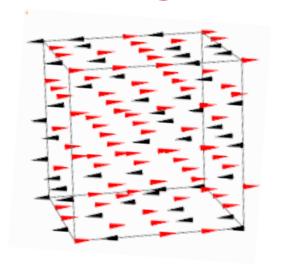
The patterns

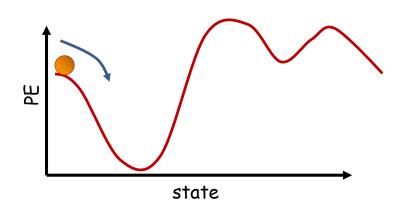
- In fact we could have multiple hidden patterns coupled with any visible pattern
 - These would be multiple stored patterns that all give the same visible output
 - How many do we permit
- Do we need to specify one or more particular hidden patterns?
 - How about all of them
 - What do I mean by this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

But first...

• The Hopfield net as a distribution..

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
 - And the expected value of the state

- 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 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

$$F_T = U_T + kTH_T$$

$$= \sum_{s} P_T(s) E_s - kT \sum_{s} P_T(s) \log P_T(s)$$

$$F_T = \sum_{S} P_T(s) E_S - kT \sum_{S} P_T(s) \log P_T(s)$$

- 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

$$F_T = \sum_{S} P_T(s) E_S - kT \sum_{S} P_T(s) \log P_T(s)$$

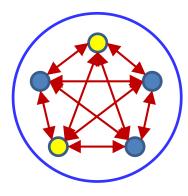
• Minimizing this w.r.t $P_T(s)$, we get

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

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

The Energy of the Network

Visible Neurons



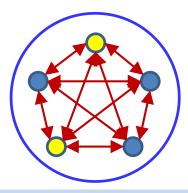
$$E(S) = -\sum_{i < j} w_{ij} s_i s_j - b_i s_i$$

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

- We can define the energy of the system as before
- Since neurons are stochastic, there is disorder or entropy (with T = 1)
- The equilibribum probability distribution over states is the Boltzmann distribution at T=1
 - This is the probability of different states that the network will wander over at equilibrium

The Hopfield net is a distribution

Visible Neurons



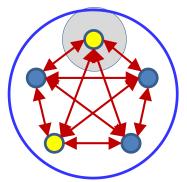
$$E(S) = -\sum_{i < j} w_{ij} s_i s_j - b_i s_i$$

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

- 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)

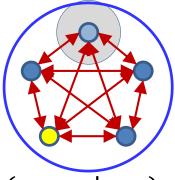
The field at a single node

- 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



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

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



$$logP(S) - logP(S') = logP(s_i = 1|s_{j\neq i}) - logP(s_i = 0|s_{j\neq i})$$

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

The field at a single node

• Let S and S ' be the states with the ith bit in the +1 and -1 states

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

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

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

•
$$log P(S) - log P(S') = E(S') - E(S) = \sum_{j \neq i} w_j s_j + b_i$$

The field at a single node

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

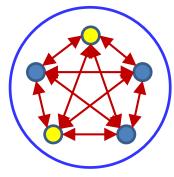
Giving us

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

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

Redefining the network

Visible Neurons



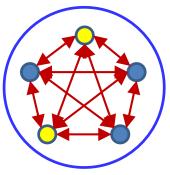
$$z_i = \sum_j w_{ji} s_j + b_i$$

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

- 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





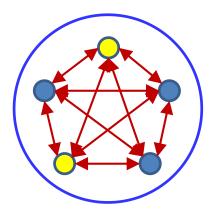
$$z_i = \sum_j w_{ji} s_j + b_i$$

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

- 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



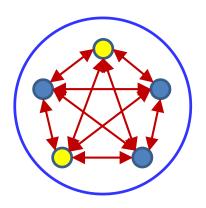
$$z_i = \sum_j w_{ji} s_j + b_i$$

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

- Initialize the neurons
- Cycle through the neurons and randomly set the neuron to 1 or -1 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

Training the network

Visible Neurons



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

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

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

- As in Hopfield nets, in order to train the network, we need to select weights such that those states are more probable than other states
 - Maximize the likelihood of the "stored" states

Maximum Likelihood Training

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

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

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

- Maximize the average log likelihood of all "training" vectors $\mathbf{S} = \{S_1, S_2, ..., SN\}$
 - In the first summation, s_i and s_j are bits of S
 - In the second, s_i and s_i are bits of S'

Maximum Likelihood Training

$$\langle \log(P(\mathbf{S})) \rangle = \frac{1}{N} \sum_{S} \left(\sum_{i < j} w_{ij} s_i s_j + b_i s_i(S) \right) - \log \left(\sum_{S'} exp \left(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i' \right) \right)$$

$$\frac{d\langle \log(P(\mathbf{S}))\rangle}{dw_{ij}} = \frac{1}{N} \sum_{S} s_i s_j -???$$

- We will use gradient descent, 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!

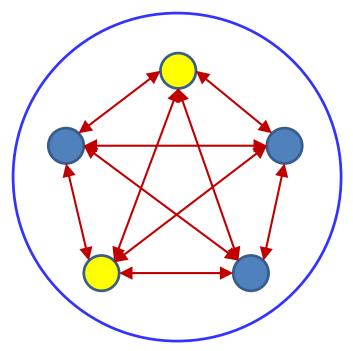
The second term

$$\frac{d\log(\sum_{S'} exp(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i'))}{dw_{ij}} = \sum_{S'} \frac{exp(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i')}{\sum_{S'} exp(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i')} s_i' s_j'$$

$$\frac{d\log(\sum_{S'} exp(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i'))}{dw_{ij}} = \sum_{S'} P(S') s_i' s_j'$$

- 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!

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

$$\frac{d\log(\sum_{S'} exp(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i'))}{dw_{ij}} = \sum_{S'} P(S') s_i' s_j'$$

$$\sum_{S'} P(S') s_i' s_j' \approx \frac{1}{M} \sum_{S' \in \mathbf{S}_{simul}} s_i' s_j'$$

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

Maximum Likelihood Training

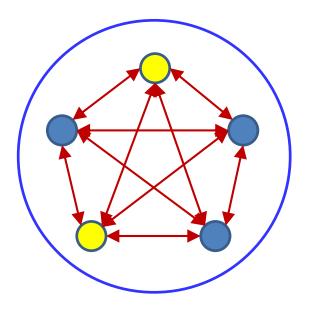
$$\left\langle \log \left(P(\mathbf{S}) \right) \right\rangle = \frac{1}{N} \sum_{S} \left(\sum_{i < j} w_{ij} s_i s_j + b_i s_i(S) \right) - \log \left(\sum_{S'} exp \left(\sum_{i < j} w_{ij} s_i' s_j' + b_i s_i' \right) \right)$$

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

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

The overall gradient ascent rule

Overall Training



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

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

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

Lookahead...

- Boltzmann Machines
- Training strategies
- RBMs
- DBMs..