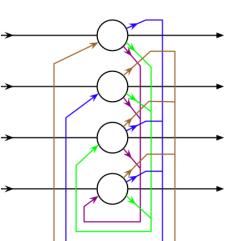
Neural Networks

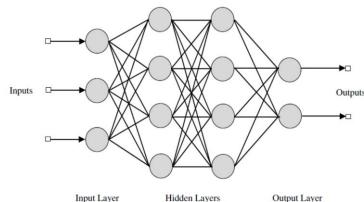
Hopfield Nets and Auto Associators Fall 2017

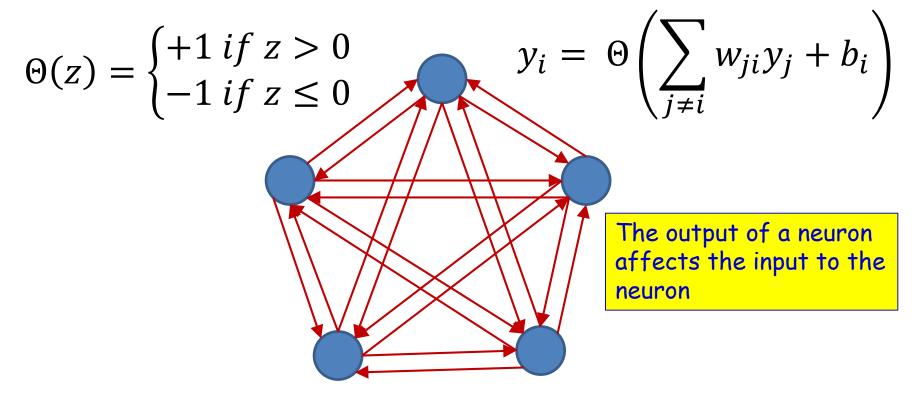
Story so far

- Neural networks for computation
- All feedforward structures

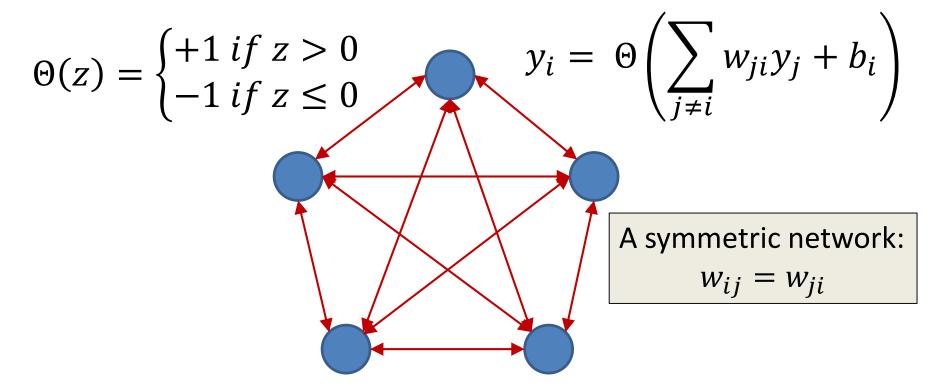
But what about...





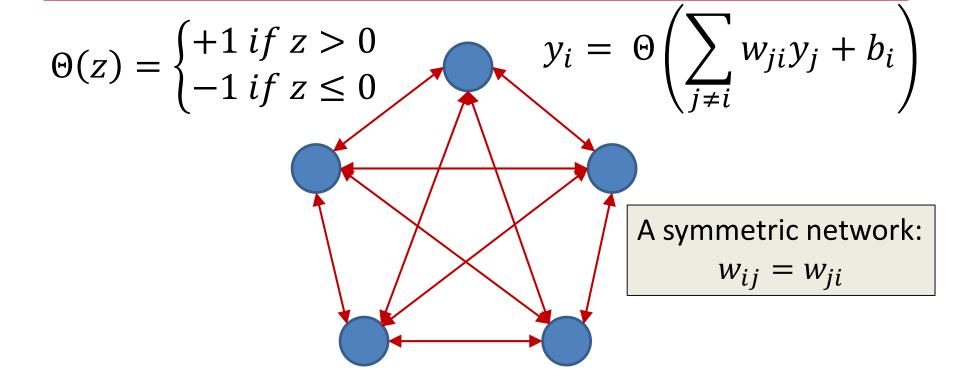


- Each neuron is a perceptron with +1/-1 output
- Every neuron receives input from every other neuron
- Every neuron outputs signals to every other neuron

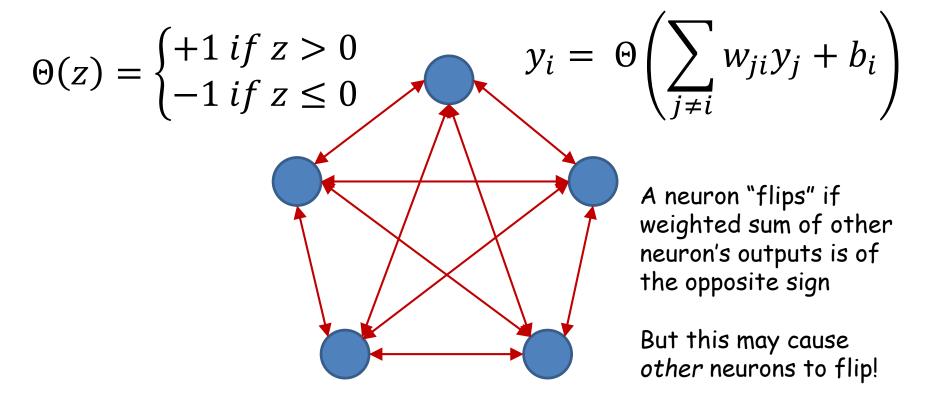


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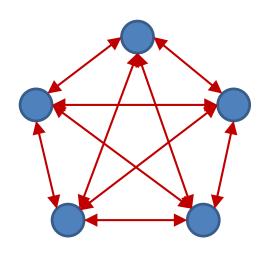
Hopfield Net



- Each neuron is a perceptron with +1/-1 output
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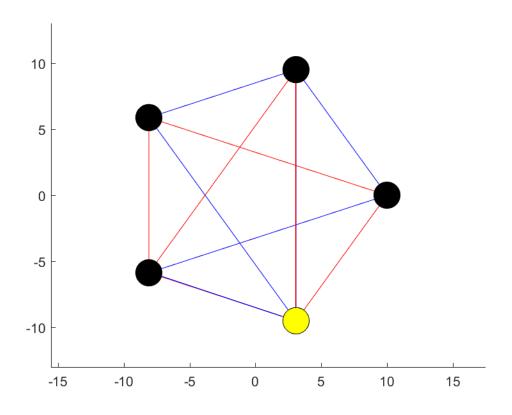
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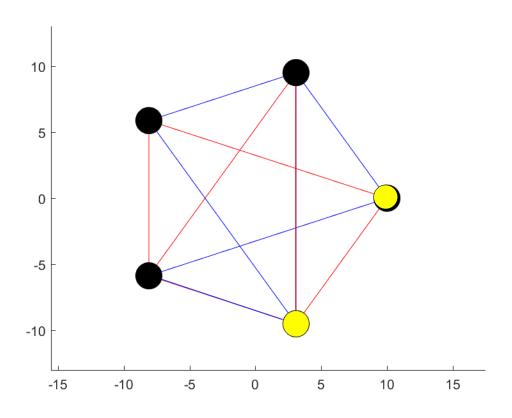
$$y_i = \Theta\left(\sum_{j \neq i} w_{ji} y_j + b_i\right)$$

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

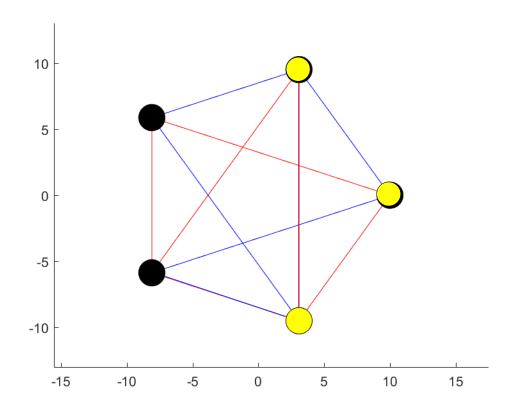
- At each time each neuron receives a "field" $\sum_{j\neq i} w_{ji} y_j + b_i$
- If the sign of the field matches its own sign, it does not respond
- If the sign of the field opposes its own sign, it "flips" to match the sign of the field



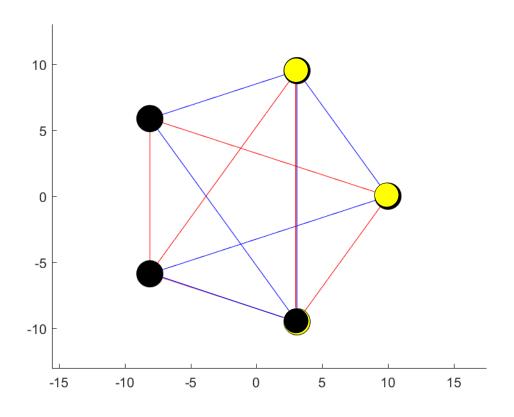
- Red edges are -1, blue edges are +1
- Yellow nodes are +1, black nodes are -1



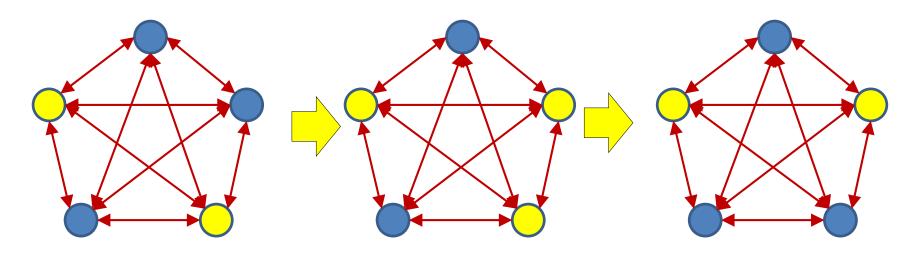
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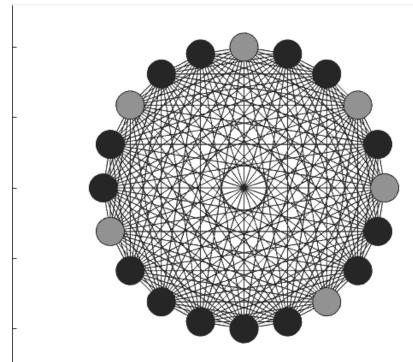


- If the sign of the field at any neuron opposes its own sign, it "flips" to match the field
 - Which will change the field at other nodes
 - Which may then flip
 - Which may cause other neurons including the first one to flip...
 - » And so on...

20 evolutions of a loopy net

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

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

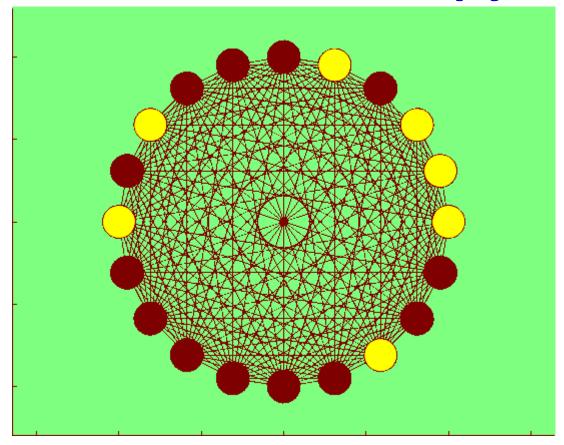


A neuron "flips" if weighted sum of other neuron's outputs is of the opposite sign

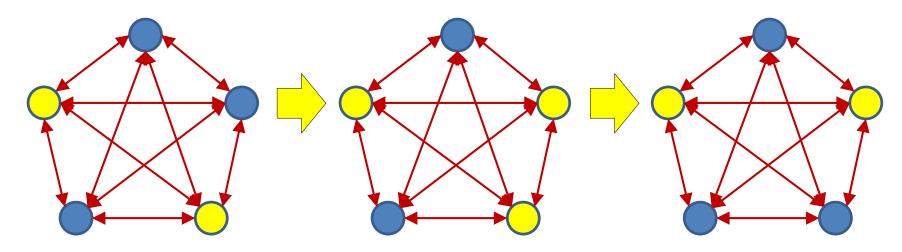
But this may cause other neurons to flip!

 All neurons which do not "align" with the local field "flip"

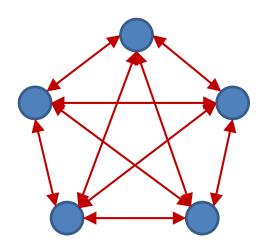
120 evolutions of a loopy net



 All neurons which do not "align" with the local field "flip"



- If the sign of the field at any neuron opposes its own sign, it "flips" to match the field
 - Which will change the field at other nodes
 - Which may then flip
 - Which may cause other neurons including the first one to flip...
- Will this behavior continue for ever??

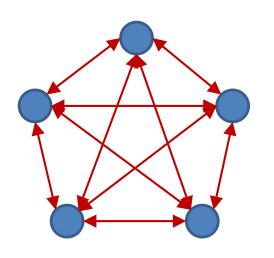


$$y_i = \Theta\left(\sum_{j \neq i} w_{ji} y_j + b_i\right)$$

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

- Let y_i^- be the output of the *i*-th neuron just *before* it responds to the current field
- Let y_i^+ be the output of the *i*-th neuron just *after* it responds to the current field
- If $y_i^- = sign(\sum_{j \neq i} w_{ji} y_j + b_i)$, then $y_i^+ = y_i^-$
 - If the sign of the field matches its own sign, it does not flip

$$y_i^+ \left(\sum_{j \neq i} w_{ji} y_j + b_i \right) - y_i^- \left(\sum_{j \neq i} w_{ji} y_j + b_i \right) = 0$$



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

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

• If $y_i^- \neq sign(\sum_{j\neq i} w_{ji}y_j + b_i)$, then $y_i^+ = -y_i^-$

$$y_i^+ \left(\sum_{j \neq i} w_{ji} y_j + b_i \right) - y_i^- \left(\sum_{j \neq i} w_{ji} y_j + b_i \right) = 2y_i^+ \left(\sum_{j \neq i} w_{ji} y_j + b_i \right)$$

- This term is always positive!
- Every flip of a neuron is guaranteed to locally increase

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

Globally

Consider the following sum across all nodes

$$D(y_1, y_2, ..., y_N) = \sum_{i} y_i \left(\sum_{j < i} w_{ji} y_j + b_i \right)$$

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

- Definition same as earlier, but avoids double counting and assumes $w_{ii}=0$
- For any unit k that "flips" because of the local field

$$\Delta D(y_k) = D(y_1, ..., y_k^+, ..., y_N) - D(y_1, ..., y_k^-, ..., y_N)$$

Upon flipping a single unit

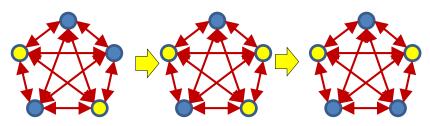
$$\Delta D(y_k) = D(y_1, ..., y_k^+, ..., y_N) - D(y_1, ..., y_k^-, ..., y_N)$$

Expanding

$$\Delta D(y_k) = (y_k^+ - y_k^-) \sum_{j \neq i} w_{jk} y_j + (y_k^+ - y_k^-) b_k$$

- All other terms that do not include y_k cancel out
- This is always positive!
- Every flip of a unit results in an increase in D

Hopfield Net



• Flipping a unit will result in an increase (non-decrease) of

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

• D is bounded

$$D_{max} = \sum_{i,j < i} \left| w_{ij} \right| + \sum_{i} \left| b_i \right|$$

The minimum increment of *D* in a flip is

$$\Delta D_{min} = \min_{i, \{y_i, i=1..N\}} 2 \left| \sum_{j \neq i} w_{ji} y_j + b_i \right|$$

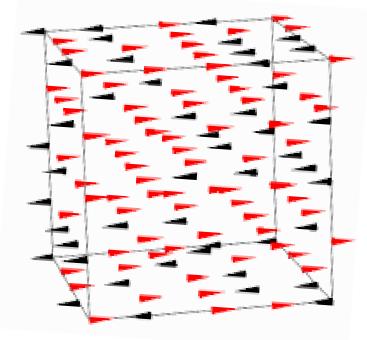
Any sequence of flips must converge in a finite number of steps

The Energy of a Hopfield Net

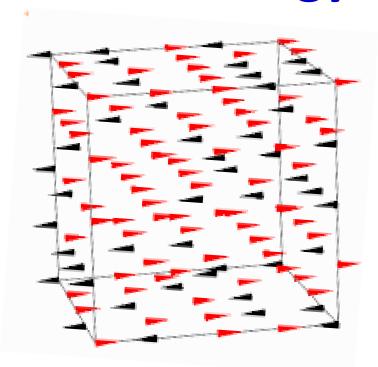
Define the Energy of the network as

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

- Just the negative of D
- The evolution of a Hopfield network constantly decreases its energy
- Where did this "energy" concept suddenly sprout from?



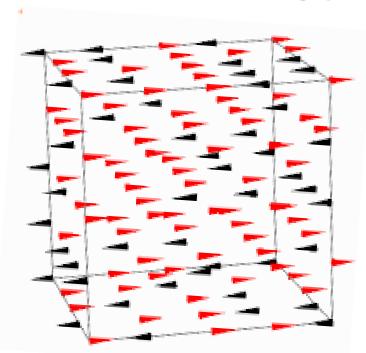
- Magnetic diploes
- Each dipole tries to align itself to the local field
 - In doing so it may flip
- This will change fields at other dipoles
 - Which may flip
- Which changes the field at the current dipole...



Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} \frac{rx_j}{\|p_i - p_j\|^2} + b_i$$
intrinsic
external

- p_i is vector position of i-th dipole
- The field at any dipole is the sum of the field contributions of all other dipoles
- The contribution of a dipole to the field at any point falls off inversely with square of distance



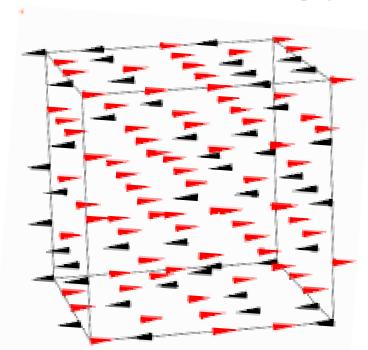
Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} \frac{rx_j}{\|p_i - p_j\|^2} + b_i$$

Response of current diplose

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

A Dipole flips if it is misaligned with the field in its location



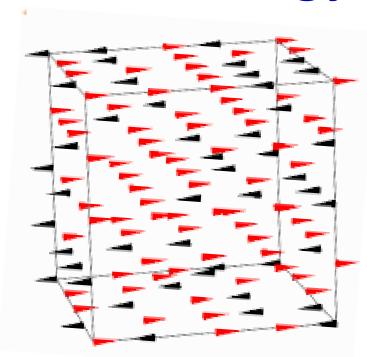
Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} \frac{rx_j}{\|p_i - p_j\|^2} + b_i$$

Response of current diplose

$$x_{i} = \begin{cases} x_{i} & if \ sign(x_{i} f(p_{i})) = 1 \\ -x_{i} & otherwise \end{cases}$$

- Dipoles will keep flipping
 - A flipped dipole changes the field at other dipoles
 - Some of which will flip
 - Which will change the field at the current dipole
 - Which may flip
 - Etc...



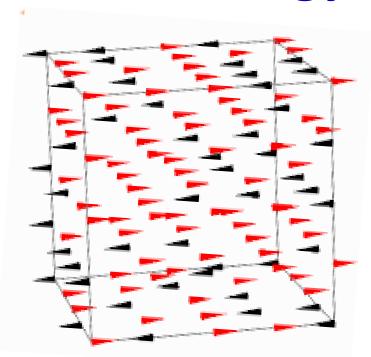
When will it stop???

Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} \frac{rx_j}{\|p_i - p_j\|^2} + b_i$$

Response of current diplose

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



Total field at current dipole:

$$f(p_i) = \sum_{j \neq i} \frac{rx_j}{\|p_i - p_j\|^2} + b_i$$

Response of current diplose

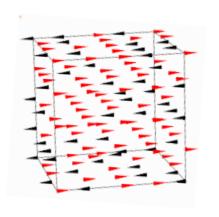
$$x_i = \begin{cases} x_i & if \ sign(x_i f(p_i)) = 1 \\ -x_i & otherwise \end{cases}$$

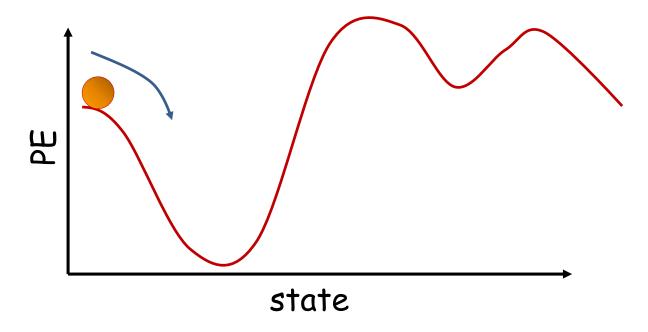
The total potential energy of the system

$$E = C - \frac{1}{2} \sum_{i} x_{i} f(p_{i}) = C - \sum_{i} \sum_{j>i} \frac{r x_{i} x_{j}}{\|p_{i} - p_{j}\|^{2}} - \sum_{i} b_{i} x_{j}$$

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

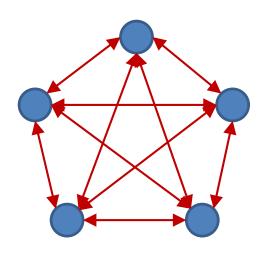
Spin Glasses





- The system stops at one of its stable configurations
 - Where PE 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

Hopfield Network



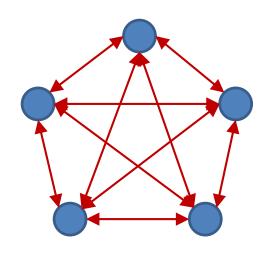
$$y_i = \Theta\left(\sum_{j \neq i} w_{ji} y_j + b_i\right)$$

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

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

- This is analogous to the potential energy of a spin glass
 - The system will evolve until the energy hits a local minimum

Hopfield Network



$$y_{i} = \Theta\left(\sum_{j \neq i} w_{ji} y_{j} + b_{i}\right)$$

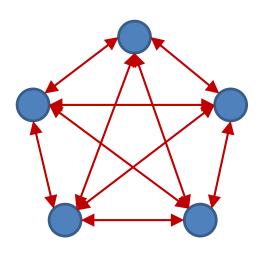
$$\Theta(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z \leq 0 \end{cases}$$

Typically will not utilize bias: The bias is similar to having a single extra neuron that is pegged to 1.0

Removing the bias term does not affect the rest of the discussion in any manner

But not RIP, we will bring it back later in the discussion

Hopfield Network

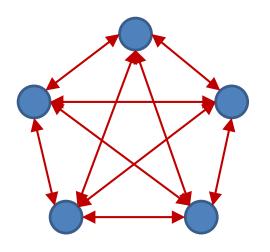


$$y_i = \Theta\left(\sum_{j \neq i} w_{ji} y_j\right)$$

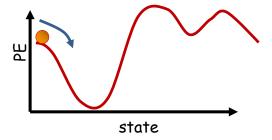
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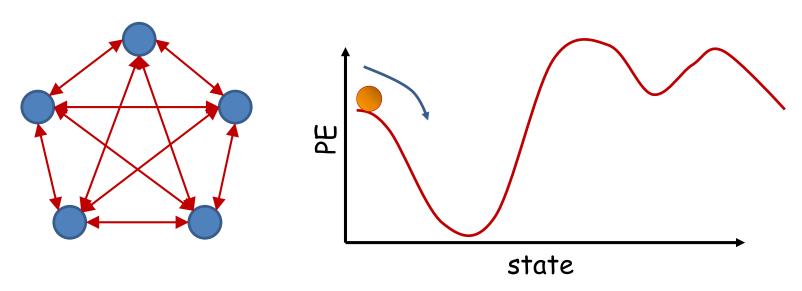


$$E = -\sum_{i,j < i} w_{ij} y_i y_j$$

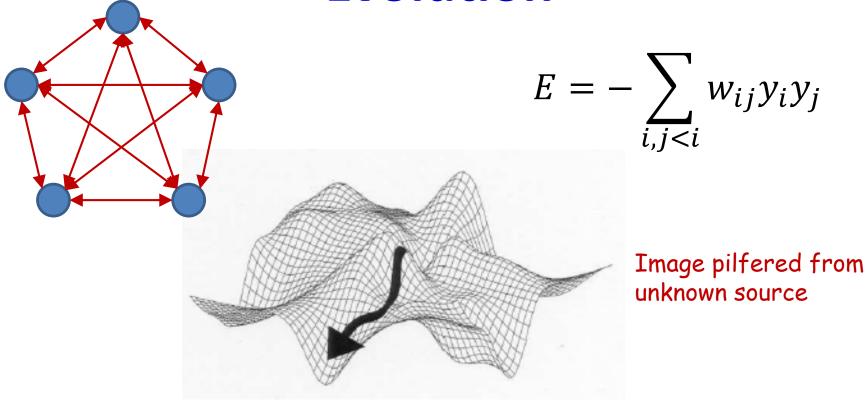


 The network will evolve until it arrives at a local minimum in the energy contour

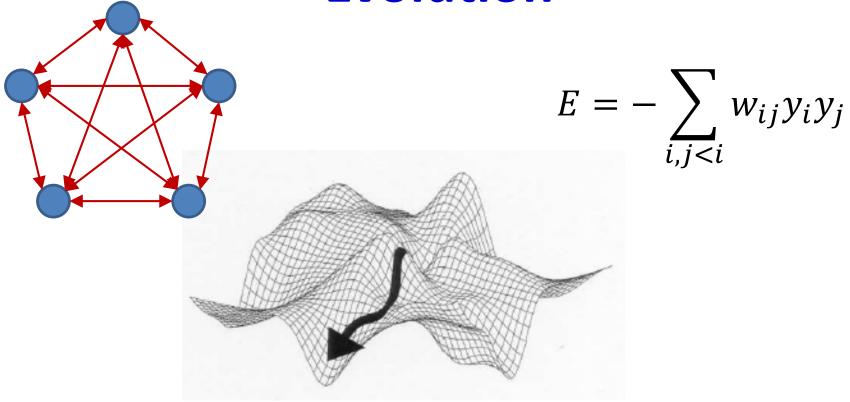
Content-addressable memory



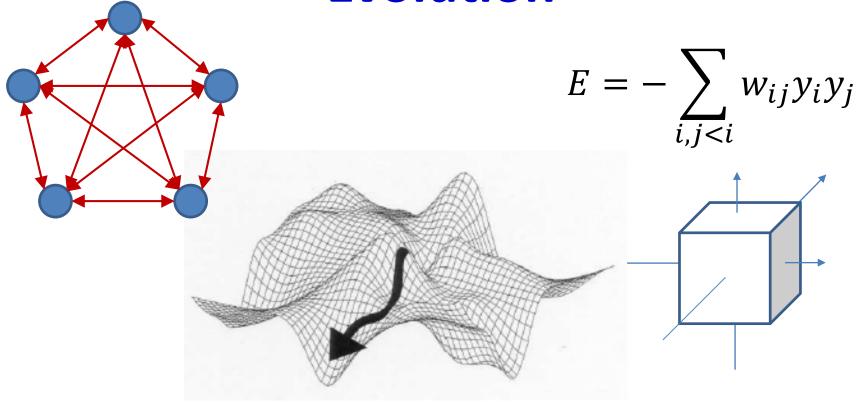
- Each of the minima is a "stored" pattern
 - If the network is initialized close to a stored pattern, it will inevitably evolve to the pattern
- This is a content addressable memory
 - Recall memory content from partial or corrupt values
- Also called associative memory



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

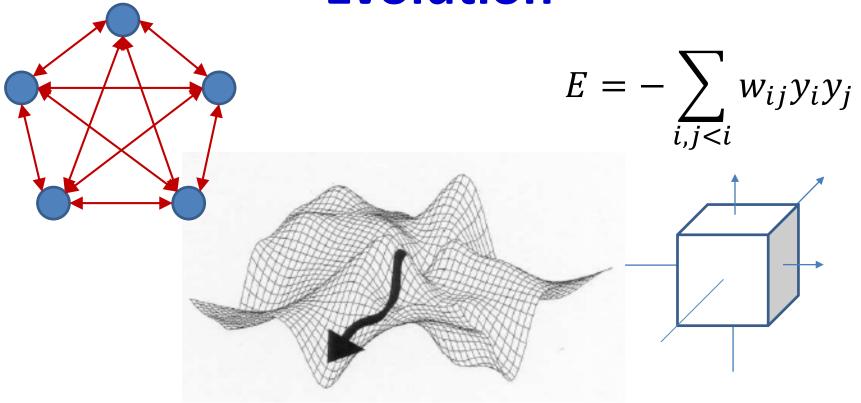


- The network will evolve until it arrives at a local minimum in the energy contour
- We proved that every change in the network will result in decrease in energy
 - So path to energy minimum is monotonic



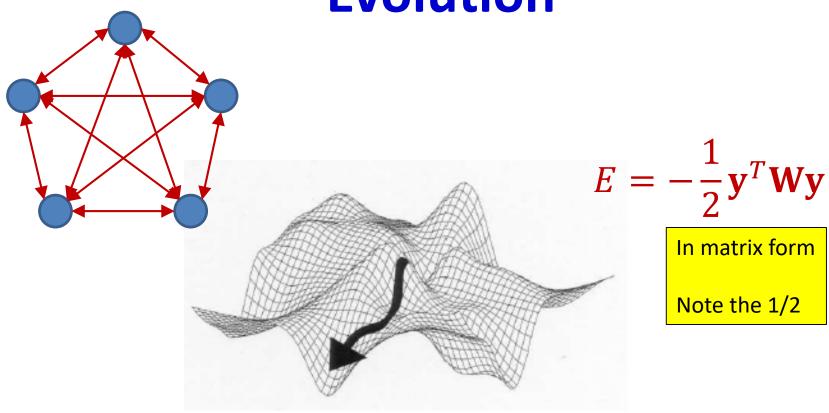
- For threshold activations the energy contour is only defined on a lattice
 - Corners of a unit cube on [-1,1]^N

Evolution



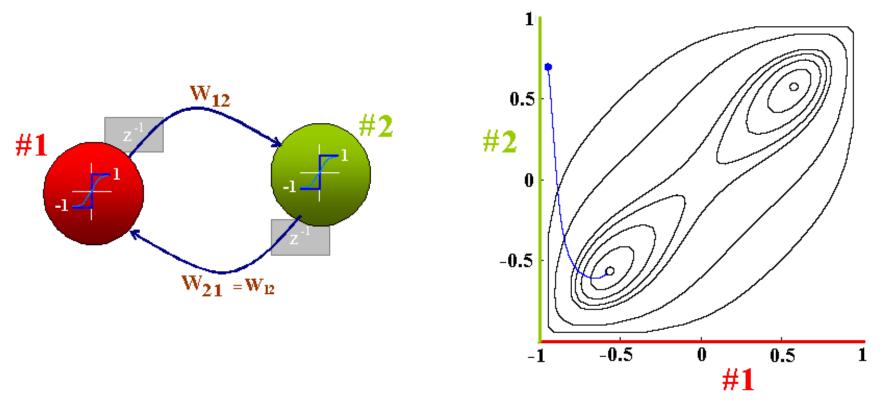
- For threshold activations the energy contour is only defined on a lattice
 - Corners of a unit cube on [-1,1]^N
- For tanh activations it will be a continuous function





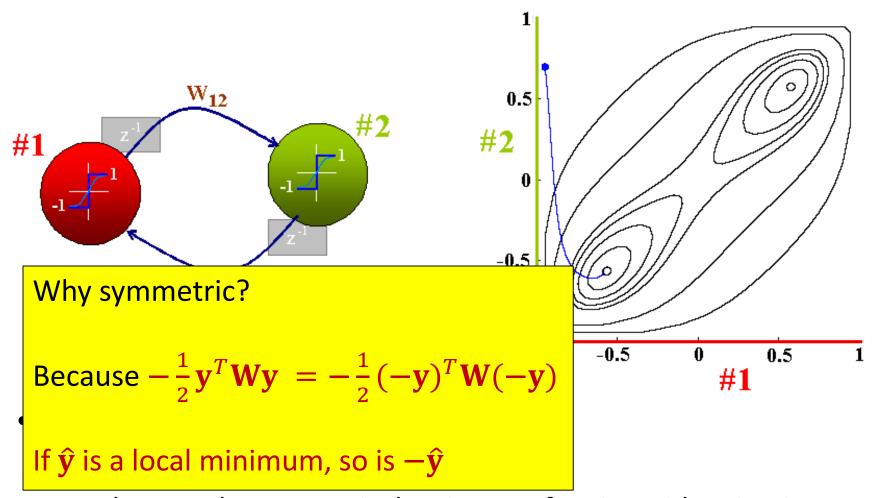
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"Energy" contour for a 2-neuron net



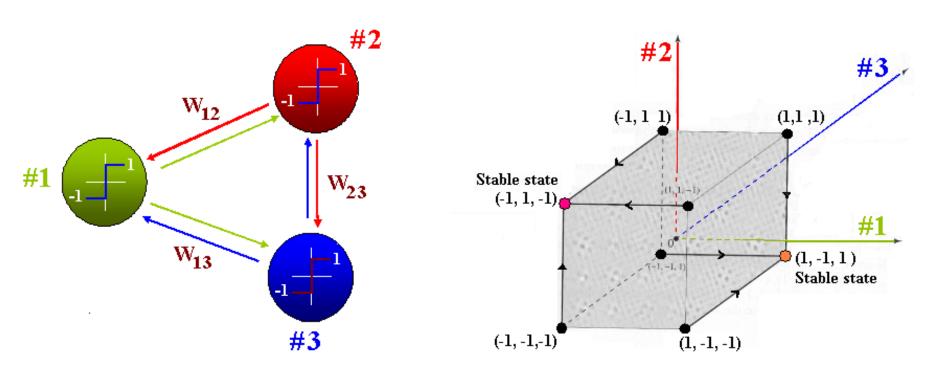
- Two stable states (tanh activation)
 - Symmetric, not at corners
 - Blue arc shows a typical trajectory for sigmoid activation

"Energy" contour for a 2-neuron net



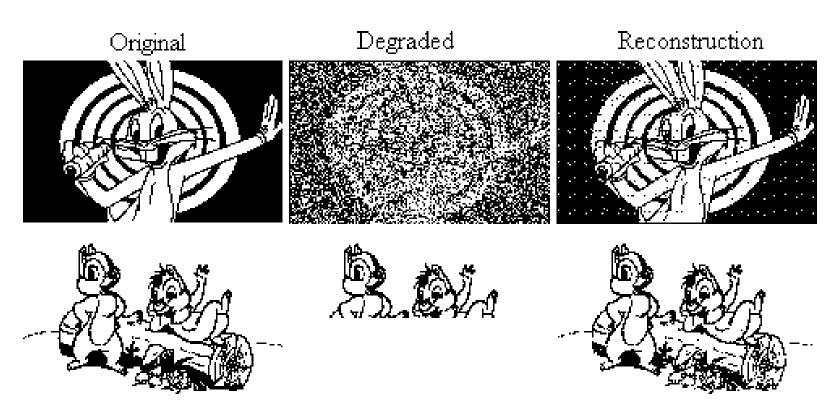
Blue arc shows a typical trajectory for sigmoid activation

3-neuron net



- 8 possible states
- 2 stable states (hard thresholded network)

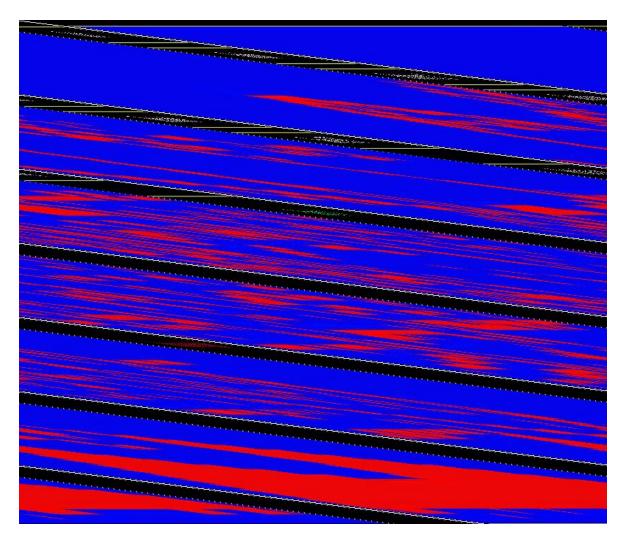
Examples: Content addressable memory



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

http://staff.itee.uq.edu.au/janetw/cmc/chapters/Hopfield/₄₂

Hopfield net examples



Computational algorithm

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

Issues

 How do we make the network store a specific pattern or set of patterns?

How many patterns can we store?

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How many patterns can we store?

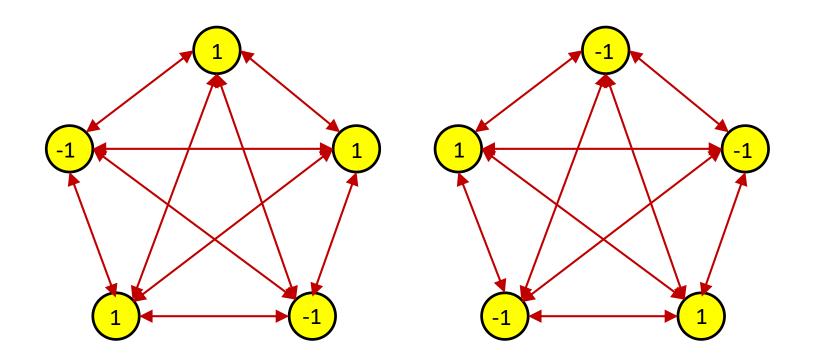
How do we remember a *specific* pattern?

 How do we teach a network to "remember" this image



- For an image with N pixels we need a network with N neurons
- Every neuron connects to every other neuron
- Weights are symmetric (not mandatory)
- $\frac{N(N-1)}{2}$ weights in all

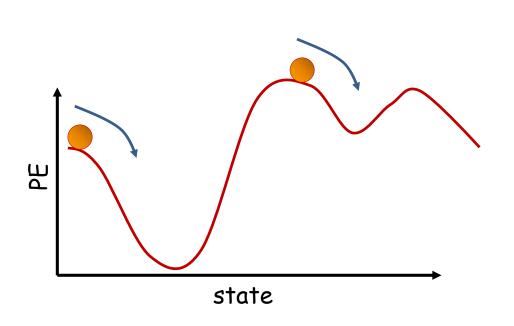
Storing patterns: Training a network

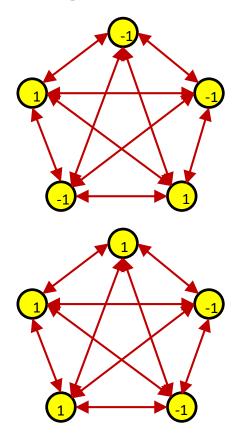


- A network that stores pattern P also naturally stores P
 - Symmetry E(P) = E(-P) since E is a function of $y_i y_j$

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

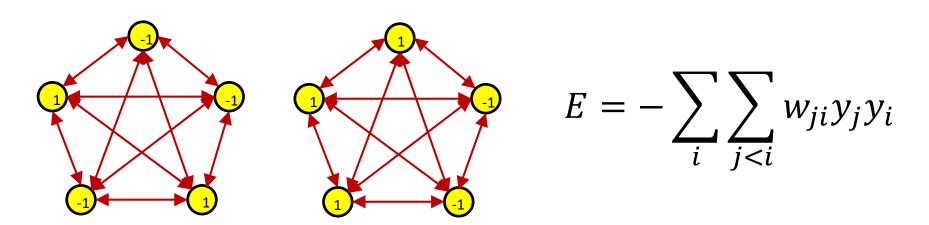
A network can store multiple patterns



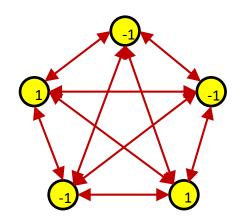


- Every stable point is a stored pattern
- So we could design the net to store multiple patterns
 - Remember that every stored pattern P is actually two stored patterns, P and -P

Storing a pattern



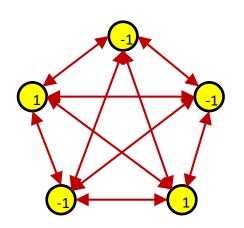
• Design $\{w_{ij}\}$ such that the energy is a local minimum at the desired $P=\{y_i\}$



Storing 1 pattern: We want

$$sign\left(\sum_{j\neq i}w_{ji}y_{j}\right)=y_{i}\quad\forall\ i$$

This is a stationary pattern



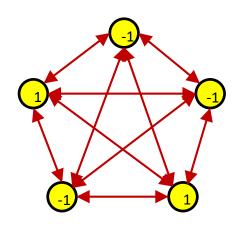
HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

Storing 1 pattern: We want

$$sign\left(\sum_{j\neq i}w_{ji}y_{j}\right)=y_{i}\quad\forall\ i$$

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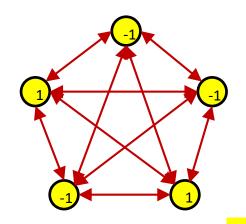


HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

•
$$sign(\sum_{j\neq i} w_{ji}y_j) = sign(\sum_{j\neq i} y_jy_iy_j)$$

= $sign(\sum_{j\neq i} y_j^2y_i) = sign(y_i) = y_i$



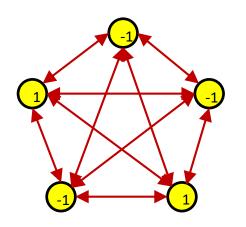
HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

The pattern is stationary

•
$$sign(\sum_{j\neq i} w_{ji}y_j) = sign(\sum_{j\neq i} y_jy_iy_j)$$

= $sign(\sum_{j\neq i} y_j^2y_i) = sign(y_i) = y_i$

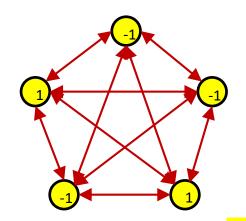


HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

$$E = -\sum_{i} \sum_{j < i} w_{ji} y_{j} y_{i} = -\sum_{i} \sum_{j < i} y_{i}^{2} y_{j}^{2}$$
$$= -\sum_{i} \sum_{j < i} 1 = -0.5N(N - 1)$$

This is the lowest possible energy value for the network



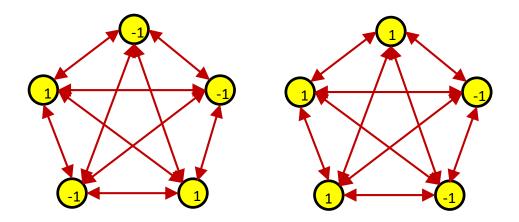
HEBBIAN LEARNING:

$$w_{ji} = y_j y_i$$

The pattern is STABLE

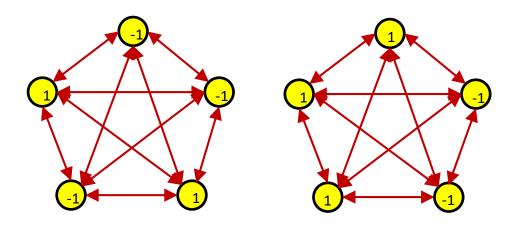
$$E = -\sum_{i} \sum_{j < i} w_{ji} y_{j} y_{i} = -\sum_{i} \sum_{j < i} y_{i}^{2} y_{j}^{2}$$
$$= -\sum_{i} \sum_{j < i} 1 = -0.5N(N - 1)$$

This is the lowest possible energy value for the network



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

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



- Let \mathbf{y}_p be the vector representing p-th pattern
- Let $\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 \ \dots]$ 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

• 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

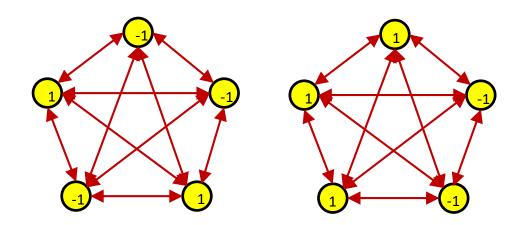
$$\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$$

Energy landscape only differs by an additive constant

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



- 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..

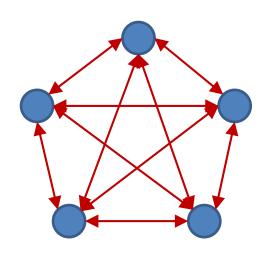
 $\mathbf{W} = \mathbf{Y}\mathbf{Y}^T$

Issues

 How do we make the network store a specific pattern or set of patterns?

How many patterns can we store?

Consider the energy function

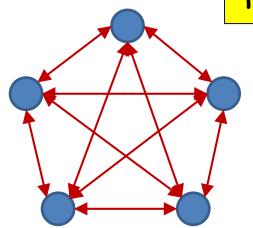


$$E = -\frac{1}{2}\mathbf{y}^T\mathbf{W}\mathbf{y} - \mathbf{b}^T\mathbf{y}$$

- Reinstating the bias term for completeness sake
 - Remember that we don't actually use it in a Hopfield net

Consider the energy function

This is a quadratic!



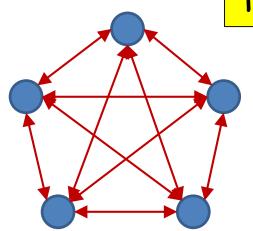
W is positive semidefinite

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

- Reinstating the bias term for completeness sake
 - Remember that we don't actually use it in a Hopfield net

Consider the energy function





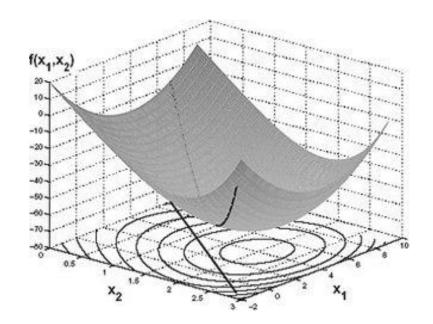
For Hebbian learning W is positive semidefinite

E is convex

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

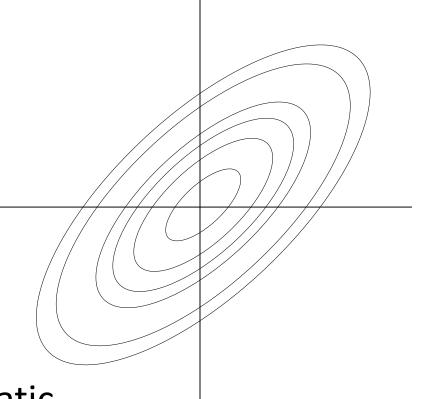
- Reinstating the bias term for completeness sake
 - Remember that we don't actually use it in a Hopfield net

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



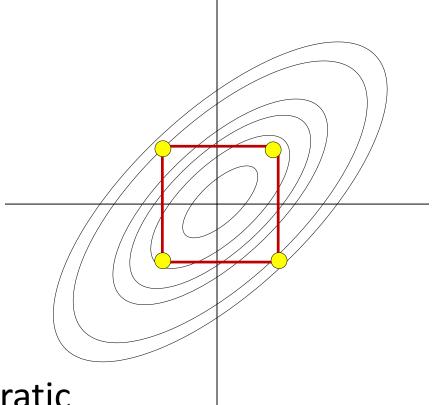
• *E* is a convex quadratic

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

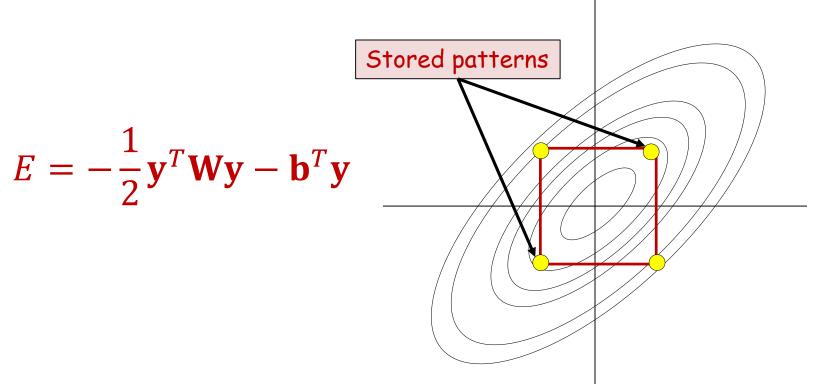


- *E* is a convex quadratic
 - Shown from above (assuming 0 bias)

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

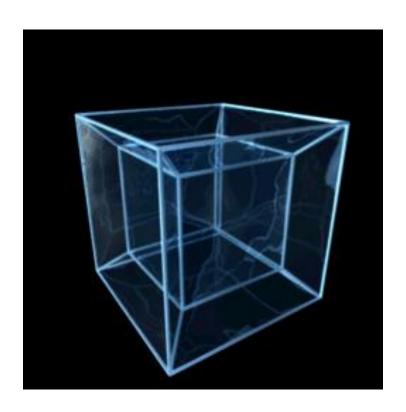


- *E* is a convex quadratic
 - Shown from above (assuming 0 bias)
- But components of y can only take values ± 1
 - I.e y lies on the corners of the unit hypercube



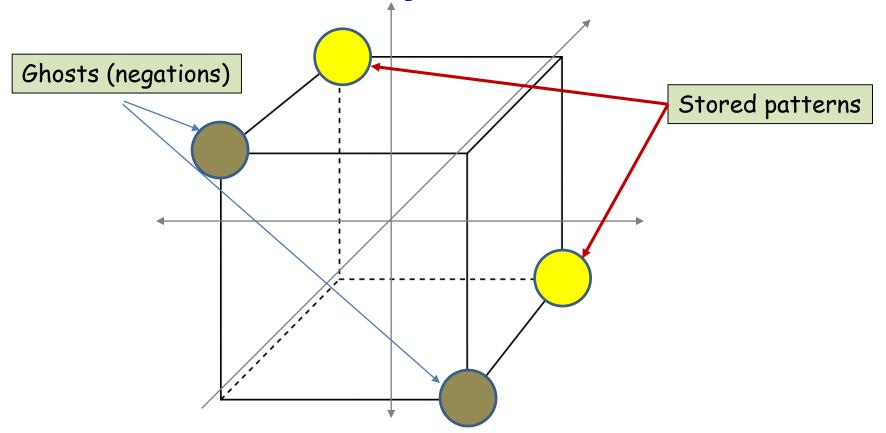
- The stored values of y are the ones where all adjacent corners are higher on the quadratic
 - Hebbian learning attempts to make the quadratic steep in the vicinity of stored patterns

Patterns you can store



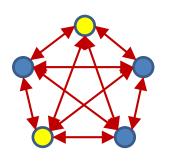
- 4-bit patterns
- Stored patterns would be the corners where the value of the quadratic energy is lowest

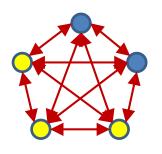
Patterns you can store

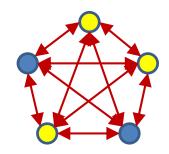


- Ideally must be maximally separated on the hypercube
 - The number of patterns we can store depends on the actual distance between the patterns

How many patterns can we store?

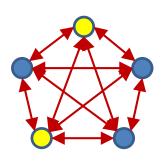


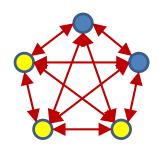


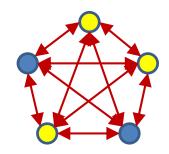


- Hopfield: For a network of N neurons can store up to 0.15N patterns
 - Provided the patterns are random and "far apart"

How many patterns can we store?







- Problem with Hebbian learning: Focuses on patterns that must be stored
 - What about patterns that must not be stored?
- More recent work: can actually store up to N patterns
 - Non Hebbian learning
 - *W* loses positive semi-definiteness

Storing N patterns

- Non Hebbian
- 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

• I.e. $y_1, y_2, ..., y_P$ are the only binary Eigenvectors of W, and the corresponding eigen values are positive

Storing N patterns

- Simple solution: Design W such that $y_1, y_2, ..., y_P$ are the Eigen vectors of W
- Easily achieved if $y_1, y_2, ..., y_P$ are orthogonal to one another
 - Let $Y = [\mathbf{y}_1 \ \mathbf{y}_2 \dots \mathbf{y}_P \ \mathbf{r}_{P+1} \dots \mathbf{r}_N]$
 - N is the number of bits
 - $-\mathbf{r}_{P+1} \dots \mathbf{r}_N$ are "synthetic" non-binary vectors
 - $-\mathbf{y}_1\mathbf{y}_2...\mathbf{y}_P\mathbf{r}_{P+1}...\mathbf{r}_N$ are all orthogonal to one another

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

- Eigen values λ in diagonal matrix Λ determine the steepness of the energy function around the stored values
 - What must the Eigen values corresponding to the \mathbf{y}_P s be?
 - What must the Eigen values corresponding to the " \mathbf{r} "s be?
- Under no condition can more than N values be stored

Storing N patterns

- For non-orthogonal W, solution is less simple
- $y_1, y_2, ..., y_P$ can no longer be Eigen values, but now represent *quantized* Eigen directions

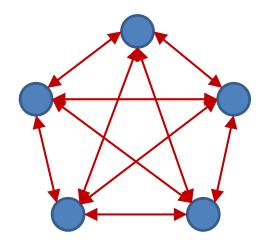
$$sign(\mathbf{W}\mathbf{y}_p) = \mathbf{y}_p$$

Note that this is not an exact Eigen value equation

- Optimization algorithms can provide Ws for many patterns
- Under no condition can we store more than N patterns

Alternate Approach to Estimating the Network

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



- Estimate W (and b) such that
 - E is minimized for $y_1, y_2, ..., y_P$
 - -E is maximized for all other y
- We will encounter this solution again soon
- Once again, cannot store more than N patterns

Storing more than N patterns

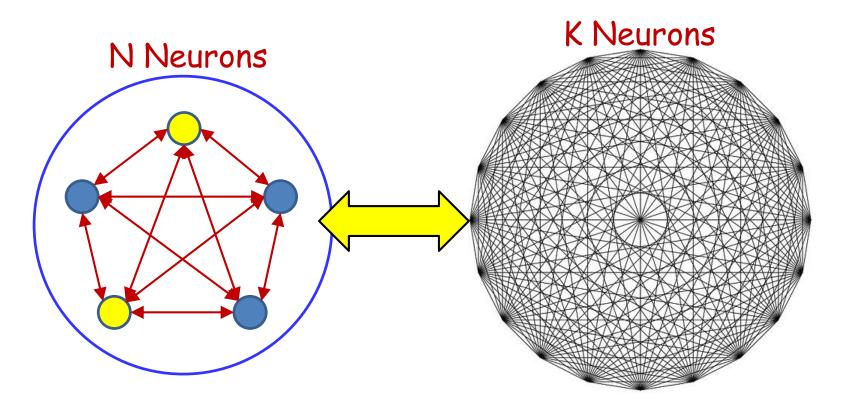
How do we even solve the problem of storing
 N patterns in the first place

- How do we increase the capacity of the network
 - Store more patterns
- Common answer to both problems..

Lookahead...

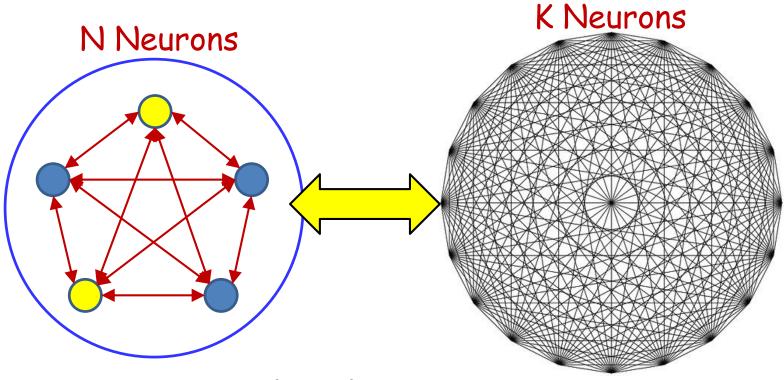
Adding capacity to a Hopfield network

Expanding the network



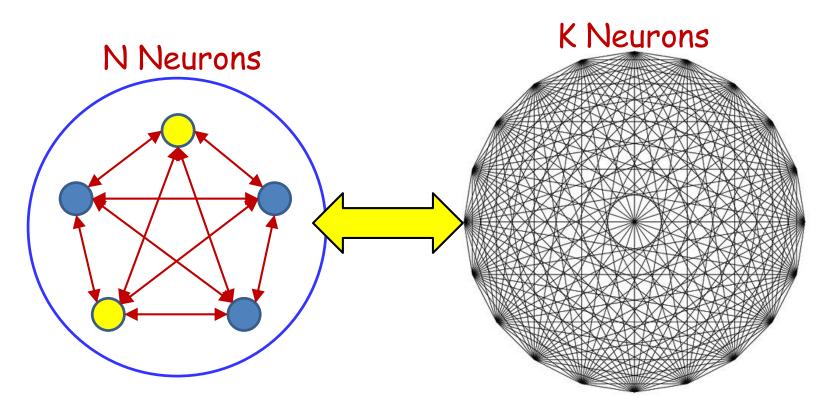
 Add a large number of neurons whose actual values you don't care about!

Expanded Network



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

Introducing...



- · The Boltzmann machine...
- Next regular class...