Unsupervised Learning in Neural Networks

March 7, 2010

1 Introduction

Unsupervised Learning involves the formation of useful neural wiring patterns despite the lack of external feedback from an instructor or the environment in general. Neural networks (both biological and artificial) that learn by unsupervised means can generally extract useful relationships from sensory/input data. These may be invariant patterns in the data or key variants that allow the system to differentiate important classes of inputs. Either way, the system learns these *concepts* by itself.

In many cases, the result of unsupervised learning is a set of classes or clusters, where each previous input scenario falls into one of them. These facilitate generalization, since new input cases can be ushered into the proper cluster and then handled with the action associated with that group. This ability to generalize behavior is critical for the survival of living organisms and essential for the success of artificial intelligence systems in complex environments (where all possible input scenarios cannot possibly be enumerated and planned for ahead of time).

Unsupervised Learning appears prevalent in the brain, particularly the neocortex and hippocampus. However, basic Hebbian processes occur in many parts of the brain, and in most cases, one sees a rich set of neuronal interactions, some of which have a **cooperative** flavor, with some neurons promoting others, while others have a distinctly *competitive* nature, with neurons actively inhibiting other neurons when they themselves fire. Both processes are clearly important for the neural basis of intelligence. This section summarizes a few of the standard neural network architectures for unsupervised learning, while paying particular attention to the cooperative or competitive nature of the behavior.

1.1 Hopfield Networks

The basic Hebbian notion of firing together and wiring together has a very cooperative connotation: neurons working in concert will tend to promote on another's activity. Thus, networks whose main learning algorithm is the purely Hebbian formula of equation 11 have a strong cooperative feel.

Hopfield networks are perhaps the simplest ANN type that incorporates all three of the basic components (integration, activation and learning). Despite their simplicity, Hopfield networks capture two of the brain's key functions: storage and retrieval of distributed patterns. They do this in a completely **unsupervised** manner by recognizing correlations among neuron firing histories and modifying weights to record those relationships.

In the brain, many forms of information appear to be distributed across large populations of neurons. This *population coding* has several advantages:

1. Storage efficiency - in theory, k neurons with m differentiable states can store m^k patterns.
2. Robustness - if a few neurons die, each pattern may be slightly corrupted, but none is lost completely.
3. Pattern completion - given part of a pattern, the network can often *fill in* the rest.
4. *Content addressable memory* - patterns are retrieved using portions of the pattern (not memory addresses) as keys.

Hopfield nets take advantage of population coding to store many patterns across a shared collection of nodes, with each node representing the same aspect of all stored patterns and each connection weight denoting the average correlation between two aspects across all stored patterns.

Figure 1 displays an auto-associative Hopfield network, where *auto* implies that the correlation is between aspects/components of the **same** pattern. In this case, the components are simply small regions of the image, with components a and b representing small regions centered at distinct locations of the image plane. An auto-associative network encodes the average correlations (across all stored patterns) between all pairs of components.

In Figure 1, the correlation between components a and b is computed for each of the two images. It is positive in the left image, since a and b both contain some black color, but it is negative in the right image, since a contains black but b does not. Thus, the left image contributes a +1 to the average correlation between a and b, while the right image contributes a -1. If there are P patterns to store, then P such correlations will be averaged for every pair of components. This correlation analysis of all P patterns constitutes the *training phase* of the Hopfield algorithm. It is where the learning occurs.

Note that training reflects Hebbian learning at a coarse level: when two components are highly correlated in a pattern, then the link between their nodes in the ANN will be strengthened. Alternatively, a negative correlation (i.e. one component is on/black while the other is off/white) leads to a weight reduction.

The Hopfield network (a small portion of which appears at the bottom of Figure 1) has a *clique* topology, meaning that every node is connected to every other node. Each node represents a component, and each arc weight denotes the average correlation between the components of the arc. In Hopfield networks, the arcs are bidirectional, since a correlation is a symmetric property.

Once trained, the auto-associative Hopfield net can be employed to retrieve one of the P original patterns when given only a portion (or corrupted version) of it, as shown at the bottom of Figure 1.

The retrieval process begins by *loading* the partial pattern into the network: components that are on/black in the partial pattern will have their corresponding ANN nodes set to a high activation level, while those that are off will engender low activation levels. The network is then run, with nodes summing their inputs and using their activation functions to compute new output levels. This continues until either the network reaches a quiescent state (i.e., no nodes are changing activation levels) or a fixed number of update steps have been performed. The final activation levels of the nodes are then mapped back to the image plane to create the output pattern. For example, if node f has a high activation level, then the f component of the image will be painted black.

Similar to a Hopfield net, a hetero-associative net records average correlations between **pairs** of patterns. These are useful for associating one pattern with its typical successor pattern in a sequence. Hence, when given the predecessor pattern, the network can **predict** the successor.

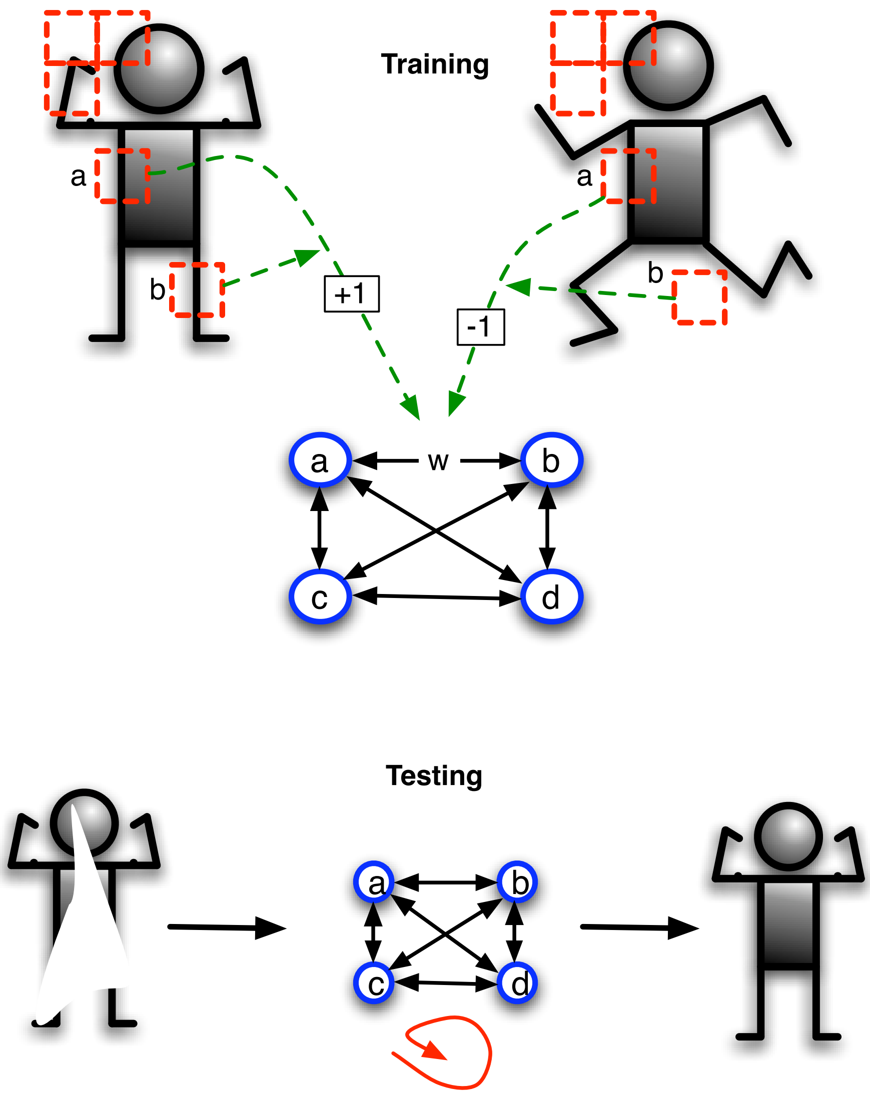


Figure 1: Overview of the training (learning) and testing (pattern retrieval) procedures for auto-associative Hopfield networks.

Figure 2 shows the essence of a hetero-associative network, where correlations between component a in the two figures are computed, as are those between the b regions. In the complete algorithm, all component pairs between the two patterns are examined: (a,a), (a, b), (a, c), etc. Note that the graph has a bipartite topology, meaning that it is split into two halves, with each node connected to all nodes on the other half but none on its own side.

Once trained, the hetero-associative Hopfield network can return a successor pattern when given a partial or corrupted version of its predecessor pattern, as shown at the bottom of Figure 2.

Here, the testing phase begins by loading the partial predecessor pattern onto the input (left) half of the network. Next, the activation levels on the output (right) side are computed based on the integrated inputs from the left side. Then, the left-side activation levels are recomputed, based on both a) the reloaded components of the original input pattern, and b) inputs from the right side of the net.

The process of recomputing activations for the left and right sides continues until quiescence (or a fixed number of steps). The values of the output nodes are then translated into the output image.

1.2 Basic Computations for Hopfield Networks

In Hopfield and many other associative networks, the learning phase is a one-shot, batch process in which all patterns are analyzed and all correlations averaged. The weights of the network are then set to those averages and never modified.

A typical learning (i.e. weight-assignment) scheme for Hopfield networks is:

$$w_{jk} \leftarrow \frac{1}{P}\sum_{p=1}^{P} c_{pk}c_{pj} \tag{1}$$

where P is the number of patterns, c_{pk} is the value of component k in pattern p, and $c_{pk}c_{pj}$ is the local correlation in pattern p between components k and j.

For a hetero-associative network, the corresponding scheme is:

$$w_{jk} \leftarrow \frac{1}{P}\sum_{p=1}^{P} i_{pk}o_{pj} \tag{2}$$

where P is now the number of pattern **pairs**, i_{pk} is the kth component of the predecessor (input) pattern of pair p, and o_{pj} is the jth component of the successor (output) pattern of pair p. The product of the two components is the local (k,j) correlation for pair p.

Once all weights have been computed, the net can be run by loading input patterns and updating activation levels. For discrete Hopfield networks, where firing levels are either +1 or -1, the following activation function is common:

$$c_k(t+1) \leftarrow sign(\sum_{j=1}^{C} w_{kj}c_j(t) + I_k) \tag{3}$$

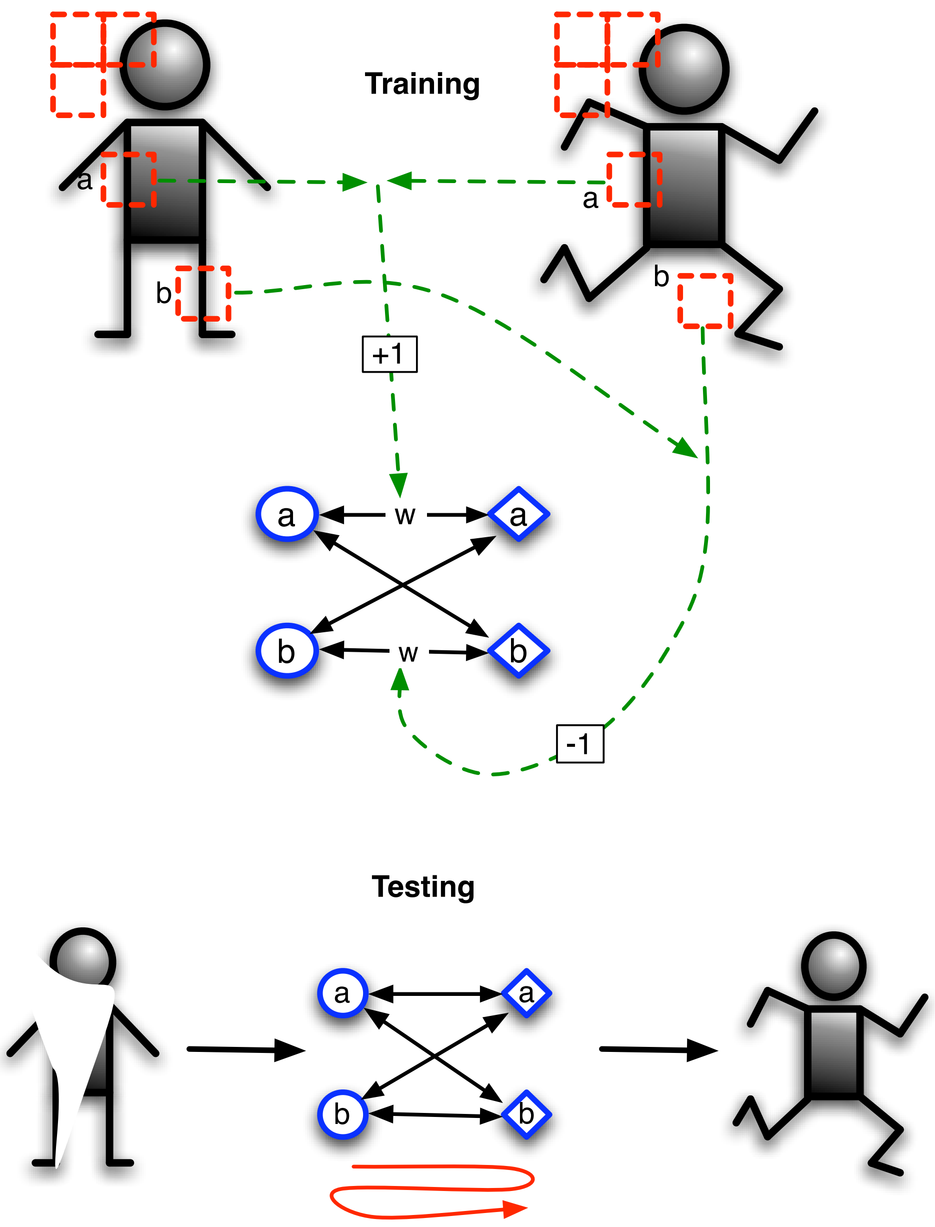


Figure 2: Overview of the training (learning) and testing (pattern retrieval) procedures for hetero-associative networks.

where C is the number of components (for example, 64 in an 8-by-8 image plane), $c_k(t+1)$ is the activation level of the kth component's neuron at time t+1, w_{kj} is the weight on the arc from node j to node k, and I_k is the original input value for component k. The I_k term insures that the original bias imposed by the input pattern has an effect throughout the entire run of the network.

Note that the summation in equation 3 is the standard integration function for computing net_k, as described in the introduction to ANNs.

Figure 3 illustrates the basic training and test procedure for Hopfield networks.

1.3 Search in Hopfield Networks

The process by which a running associative network transitions to quiescence has a search-like quality: the network seeks a stable state. In this case, a state is a vector consisting of the activation levels of each neuron in the ANN.

Unfortunately, stable states do not necessarily correspond to any of the original P patterns. They may be *spurious*, i.e., they map to patterns that were not part of the training set.

Figure 4 illustrates this problem. The original input pattern (top) is loaded into the auto-associative network, but nothing guarantees that the quiescent state will map to the correct pattern (bottom middle) or one of several spurious ones (bottom left and bottom right).

Hopfield [6] quantified the search for quiescence as a search for minima on an energy landscape by defining a function for mapping ANN states to energy levels. The general Hopfield learning procedure (equation **??**) and activation function (equation 3) then insure that low-energy states are those corresponding to patterns on which the net was trained. However, nothing prohibits some spurious patterns from achieving locally-minimal energy as well. Here, a local minimum is defined as a state, M, such that any state M* that is created by updating all activation levels of M **once**, has higher energy than M.

Hopfield's energy function is:

$$E = -a\sum_{k=1}^{C}\sum_{j=1}^{C} w_{jk}c_jc_k - b\sum_{k=1}^{C} I_kc_k \tag{4}$$

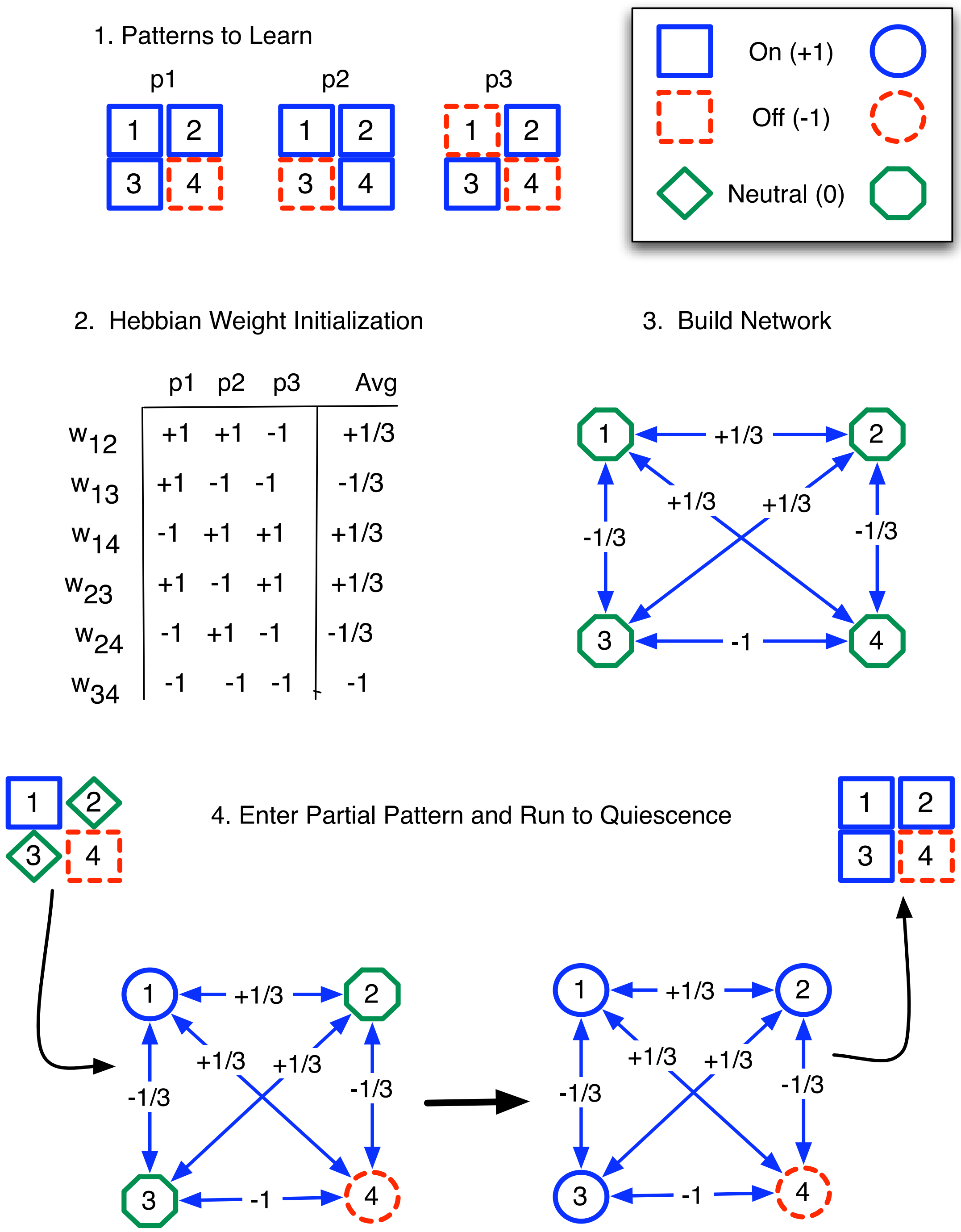
where c_k is the activation level of component k's neuron, I_k is the original input value loaded into the kth component's neuron, and a and b are positive constants.

Albeit complex in appearance, equation 4 is actually quite intuitive. Consider the term:

$$w_{jk}c_jc_k \tag{5}$$

Now, assume that $w_{jk} > 0$, meaning that the jth and kth components had, on average, a positive correlation in the training patterns. Consider two cases:

1. sign(c_j) = sign(c_k), which means that the jth and kth components are both on, or both off. Hence, they are positively correlated in the current state of the ANN. This **agrees** with w_{jk}, which also


1. Patterns to Learn
p1
p2
p3
On (+1)
Off (-1)
Neutral (0)
2. Hebbian Weight Initialization
3. Build Network
+1/3
-1/3
-1
4. Enter Partial Pattern and Run to Quiescence

	p1	p2	p3	Avg
w_{12}	+1	+1	-1	+1/3
w_{13}	+1	-1	-1	-1/3
w_{14}	-1	+1	+1	+1/3
w_{23}	+1	-1	+1	+1/3
w_{24}	-1	+1	-1	-1/3
w_{34}	-1	-1	-1	-1

Figure 3: The basic procedure for encoding patterns in a Hopfield network and then retrieving them via partial patterns. Steps 1-3 involve computing the average correlations between all pairs of components (i.e. pixels) in the input patterns and then using them as weights in the network. Step 4 shows the encoding of a simple partial pattern. All nodes then update their activation levels **simultaneously**, i.e. synchronously, to attain the next state, which turns out to be stable: further updates will not change any activation levels. The final state corresponds to pattern p1.

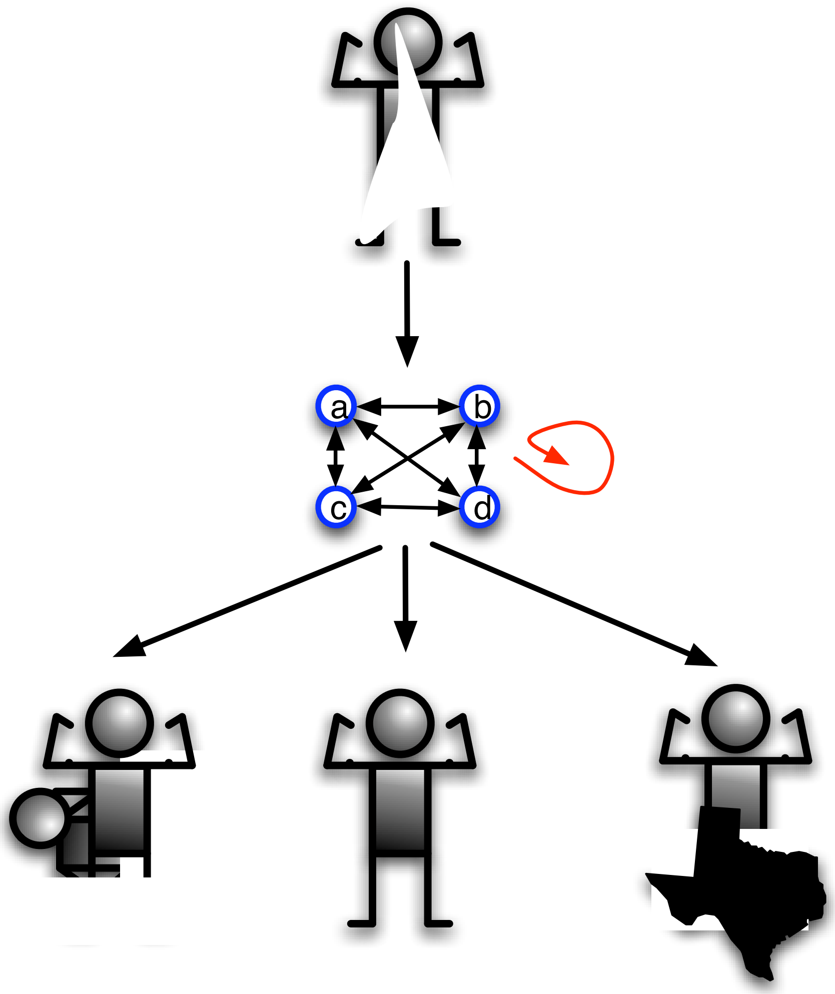


Figure 4: Example of correct (middle) and spurious (left and right) outputs of a Hopfield network when given a corrupted input pattern (top).

indicates a positive correlation between components j and k, since $w_{jk} > 0$. Hence, there is no conflict, only agreement, between c_j, c_k, and w_{jk}. This is reflected in the fact that $w_{jk}c_jc_k > 0$. Since the summations in equation 4 are preceded by negative factors, each pair of activation values that agrees with the corresponding weight will contribute negatively to the total energy, where **lower** total energy means **more** local agreement.

2. $\text{sign}(c_j) \neq \text{sign}(c_k)$, which means that components j and k are negatively correlated in the current state. This **disagrees** with the positive weight between them and is reflected in the fact that $w_{jk}c_jc_k < 0$. Hence, this pair of components will contribute positively to the total energy.

There are a similar set of cases when $w_{jk} < 0$; in those, agreement is signaled when $\text{sign}(c_j) \neq \text{sign}(c_k)$.

Given Hopfield's energy function, we can now sketch an *energy landscape* for an associative network, where network activation states map to energy levels. Figure 5 illustrates a possible landscape for the hypothetical situation of Figure 4. Note that the two spurious patterns occupy local minima and are thus *deceptive* quiescent states for Hopfield search.

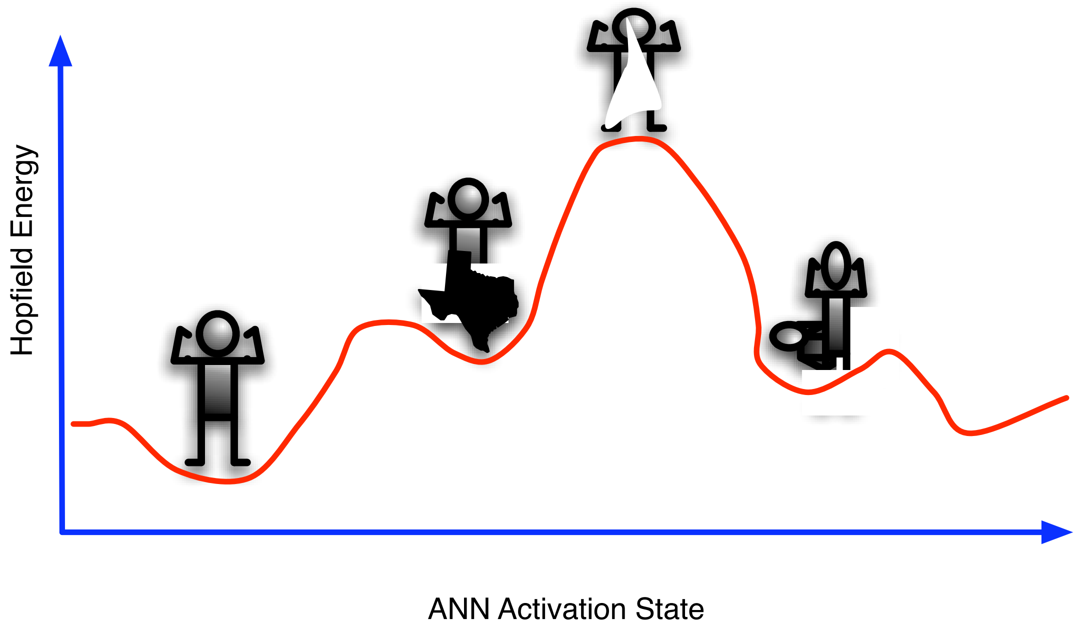


Figure 5: A Hopfield energy landscape in which the initial corrupted pattern from Figure 4 occupies a high-energy point, and the correct pattern resides at the global minimum. Spurious activation states correspond to local minima in the landscape, minima to which the Hopfield network could easily quiesce.

1.4 Hopfield Search in the Brain

The behavior of real brains is believed to exhibit many of the same properties as Hopfield networks in that:

1. The strength of synaptic connections between two neurons (or populations of neurons) often reflects the degree to which the receptive fields of those neurons are correlated, where the *receptive field* of a

neuron is that part of the sensory space (for example, a small region in the upper left quadrant of the visual field) for which the neuron appears to be a detector.

2. Certain activity patterns appear to be *stable attractors*, i.e. quiescent states, to which real neural networks eventually transition. Many believe that these attractors represent salient concepts in the brain.

Consider the duck-rabbit flip-flop picture of Figure 6. Most people cannot view this as both a rabbit and duck simultaneously, but both interpretations seem to alternate, particularly if you stare at the picture for a long period. This is evidence that both interpretations represent stable attractors in memory but that there exists some overlap between the neural states corresponding to each.

The components of each attractor stimulate one another, as shown by the thick links in Figure 6, in much the same way that highly correlated nodes in a Hopfield network excite one another due to their high connection weights. However, due to overlap, when one attractor is active, some of its components (such as the *eyes* and *neck* nodes) also stimulate portions of competing attractors.

In addition, neurons are known to *habituate* to stimuli, meaning that they tend to reduce their AP production in the presence of a continuous stimuli. To see this, try staring at something for a few minutes and feel how hard it is to keep your mind only on that particular item; the mind tends to wander.

Hence, a stable attractor such as the duck pattern will habituate while simultaneously lending some stimulation to the *mouth* and *ears* nodes. Eventually, the balance of firing power shifts and *rabbit* becomes the main interpretation, until it habituates and the duck returns.

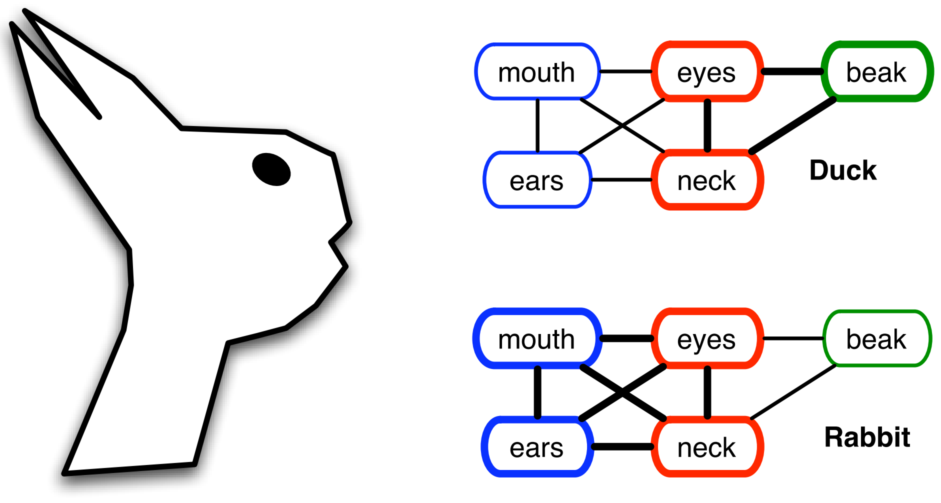


Figure 6: (Left) A flip-flop figure that resembles both a duck and a rabbit, depending upon perspective. (Right) Two copies of the same neural network, with nodes coding for properties of the upper body.

2 Competitive Networks

In certain types of ANNs, the nodes compete for activity such that the most active nodes can both a) inhibit other nodes from firing, and b) localize learning to only their connections, typically the incoming links. In the brain, topologies in which neurons inhibit many of their neighbors (whether immediate or slightly more distant) are commonplace. This often serves the important function of filtering noise, such that the final stable pattern consists of only the neurons that detect meaningful signals. Other competitions lead to useful structural isomorphisms between aspects of the physical world and regions of the brain specialized to handle those properties. These *topological maps* are beautiful examples how the brain encodes much of the inherent structure of the physical world.

Figure 2 illustrates the essence of competitive learning in the brain. In many brain regions, particularly the cortex, the main (often excitatory) neurons are known as *principal cells*. In close proximity are one or several types of interneurons, which are typically inhibitory. Active principal cells tend to stimulate nearby interneurons, which then inhibit all of their post-synaptic targets. This manifests feedback inhibition, wherein the activation of one (or a few) neurons in a layer quickly leads to the inhibition of the rest of the layer. Thus, the principal cells can be viewed as competing; and that neuron which is most active simultaneous to a subset of input neurons can become a detector for that pattern of inputs.

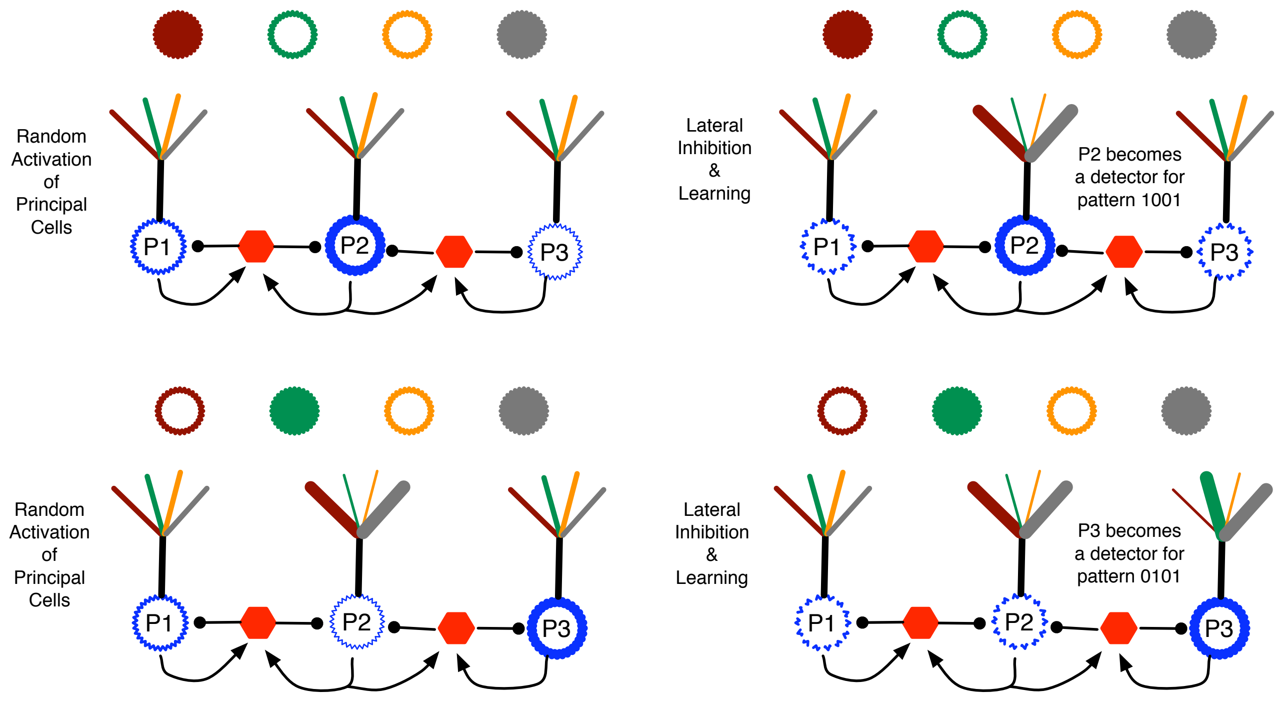

Random Activation of Principal Cells
P1
P2
P3
Lateral Inhibition & Learning
P2 becomes a detector for pattern 1001
Random Activation of Principal Cells
Lateral Inhibition & Learning
P3 becomes a detector for pattern 0101

Figure 7: Competitive learning in a layer of neurons. (Top left) Principal cells fire randomly, and neuron P2 fires approximately coincident to the first and fourth input neurons (top row). (Top right) P2 inhibits its neighbor neurons, thus insuring that very few neurons in its layer fire together. The synapses between the active inputs (shown as filled circles) and P2 strengthen by Hebbian learning. P2 thus becomes a detector for input pattern 1001. (Bottom left and right) A similar process occurs with P3, such that it becomes a detector for 0101.

In practical applications of competitive ANNs, the focus is on the weights of the input arcs to each output node, n_i. The vector of input weights to n_i, $\langle w_i \rangle = \langle w_{i1}, w_{i1}, \ldots w_{im} \rangle$, typically represents a *prototype* of the patterns that n_i is (or has learned to become) specialized to detect. In this sense, each output node represents a class or category, and input patterns can be **clustered** according to the output node that they maximally stimulate.

Figure 8 illustrates a standard topology for artificial competitive networks, with one input and one output layer. The output nodes represent categories/classes that essentially compete to capture the different input vectors, with each such vector falling into the category whose prototype it most closely matches.

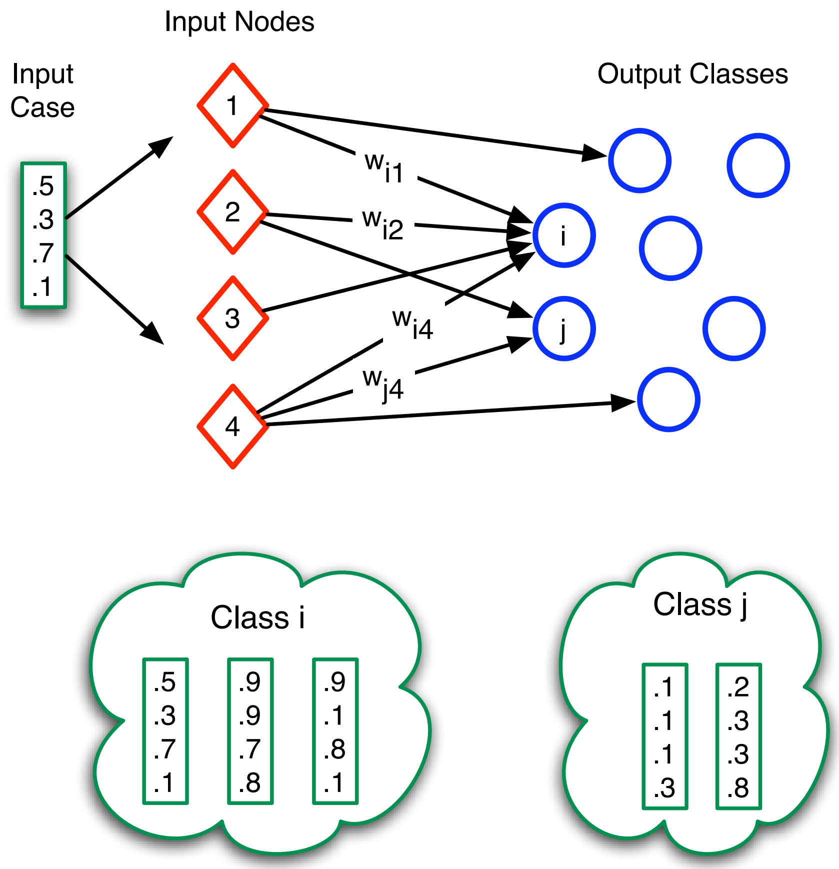


Figure 8: The basic topology of a competitive network, with an input layer and an output layer, with each node in the output layer representing a class whose prototype is given by the input weights to that node. Through learning, input cases become associated with different output nodes and thereby become clustered into instance sets (clouds) of the classes represented by those nodes.

The generic competitive ANN algorithm is quite simple. Patterns are repeatedly presented to the input layer and activations recorded on the output layer. The output node with the highest activation on pattern P *wins* and has its input weights adjusted so that its prototype more closely resembles P. The update formula for the weights into winning node n_i on input pattern P is then:

$$w_{ij} \leftarrow w_{ij} + \eta(P_j - w_{ij}) \tag{6}$$

where P_j is the jth value of pattern P, i.e., the value loaded onto input neuron j. After many epochs (i.e. presentations of the entire training set), the cases often become clearly segregated into classes, with the prototype vector of each class located close to the middle of subspace delineated by its cases. In this way, competitive networks function as clustering mechanisms for complex data sets.

The curious reader surely wonders how adjusting a prototype weight vector, V, to more closely match an input case, C, could possibly insure that the node attached to V, N_v fires harder on the next presentation of C.

In practice, many competitive networks are not really neural networks at all. They are simply lists of prototype vectors that are matched to case vectors. The vector with the closest match, using a standard Euclidian distance metric for n-dimensional space, is updated in the direction of the case.

However, one can capture these same dynamics in an actual neural network that involves a few key components:

1. A multitude of inhibitory links between all output units.
2. Excitatory links between output units and themselves.
3. Normalized case and prototype vectors

The first two features constitute a **Maxnet**, which insures that when all output nodes are activated, they will compete to shut each other off, while stimulating themselves. After a transitory period, the network settles into a state where the only neuron with a non-zero activity level is the one that originally had the highest activation level.

Maxnets are easy to implement, but care must be taken to properly set the (fixed) weights on the inhibitory and self-stimulating arcs, ϵ and θ, respectively. For example, if the network consists of m output neurons, then the following settings work well:

$$\theta = 1 \quad \epsilon \leq \tfrac{1}{m} \tag{7}$$

Normalization is a slightly more complex issue. First consider the basic Euclidean distance between an input pattern vector, P, and the weight vector for output neuron i, $\langle w_i \rangle$:

$$\sqrt{\sum_{j=1}^{n}(P_j - w_{ij})^2} = \sqrt{\sum_{j=1}^{n} P_j^2 - 2P_j w_{ij} + w_{ij}^2} \tag{8}$$

Now, if input vectors and prototype weight vectors are in normalized form, then we know that their unit length is 1. Hence:

$$\sum_{j=1}^{n} P_j^2 = 1 = \sum_{j=1}^{n} w_{ij}^2 \tag{9}$$

Combining equations 8 and 9, we find that:

$$\sqrt{\sum_{j=1}^{n}(P_j - w_{ij})^2} = \sqrt{\sum_{j=1}^{n} P_j^2 - 2P_j w_{ij} + w_{ij}^2} = \sqrt{2 - 2\sum_{j=1}^{n} P_j w_{ij}} \tag{10}$$

Thus, to minimize the distance between P and $\langle w_i \rangle$, we should maximize $\sum_{j=1}^{n} P_j w_{ij}$, which is just the sum of weighted inputs to neuron i. Hence, the prototype vector with the best match to the input case (i.e., that which is closest to it in Euclidean space) will have the highest sum of weighted inputs and thus will have the highest activation level.[1]

Another way of looking at this is that each normalized vector represents a unit vector in n-dimensional space. The term $\sum_{j=1}^{n} P_j w_{ij}$ is the dot product of these vectors, and with unit vectors, the dot product is equal to the cosine of the angle, ϕ, between the vectors. Then, $cos\phi$ is large, i.e., approaches 1, if and only if ϕ approaches 0, i.e. the vectors are similar. Hence, a good match between the normalized input case and prototype is indicated by a large dot product, $\sum_{j=1}^{n} P_j w_{ij}$.

In summary, if a) the application allows a normalization of input patterns and weight vectors, and b) computational resources permit output neurons to participate in Maxnet competitions to determine the largest activation level, then competitive networks can be implemented as true ANNs.

2.1 Self-Organizing Maps

In many competitive maps, the spatial relationships between the output neurons have no significance, and thus it makes no sense to discuss the *neighbors* of a neuron. However, these relationships have meaning inside the brain, since the firing of a neuron in a region of the brain will often have consequences for nearby neurons.

When neurons are viewed as detectors of various phenomena, whether visual, olfactory, auditory or tactile, it is very often the case that nearby neurons in the brain serve as detectors for similar stimuli. Classic examples include the visual and auditory cortices, the latter of which is shown in Figure 9. These are referred to as *topological maps*, and they are abundant in the brain.

The essence of a topological map is the isomorphism between two spaces, at least one of which is a population of neurons. The two spaces are isomorphic when components that are close (distant) in one space map to components that are close (distant) in the other space. This basic idea is shown in Figure 10, where the top mapping is not isomorphic, but the bottom one is.

Invented by Kohonen in the early 1980's, Self-Organizing Maps (SOMs), also known as Kohonen Maps, employ a dynamic mixture of competition and cooperation to enable the emergent formation of an isomorphism between a feature space and an array of neurons [8].

SOMs operate similarly to standard competitive networks in that a case vector is presented, and the best-matching prototype is modified in the direction of the case. However, Kohonen added an interesting twist: neurons have a meaningful spatial relationship to other neurons, and when an output neuron *wins* a case, it *shares the prize* with its neighbors in that both winner and neighbors adjust their prototypes toward the case.

As shown in Figure 11, the neighborhood for sharing changes during the training phase. It typically begins with a large radius that decreases as training progresses and prototypes specialize toward particular subsets of the case patterns. Over time, this sharing results in an isomorphic mapping in which the prototypes of nearby (in neuron space) neurons are more similar to one another than to those of distant neurons, as shown at the bottom of Figure 11.

In addition, SOMs typically have a dynamic learning rate (η in equation 6) that begins large and decreases during the run.

[1]Competitive learning networks often use a linear activation function, so a higher weighted sum of inputs yields a higher activation.

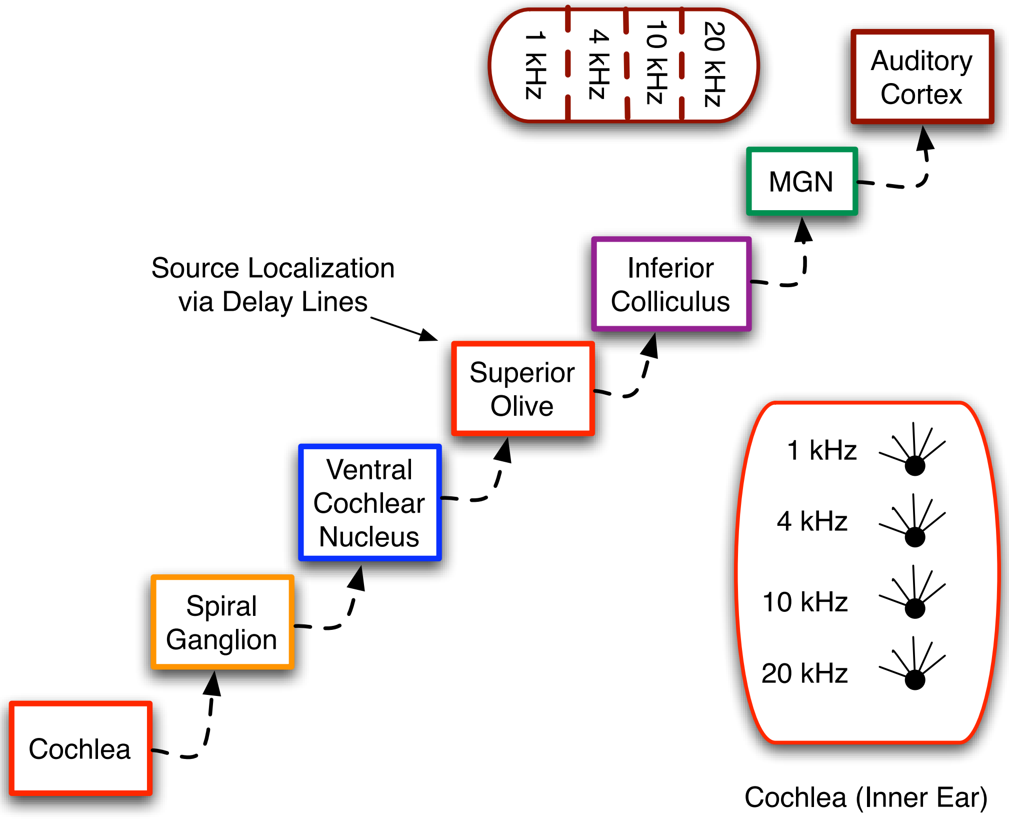


Figure 9: Tonotopic Maps: Topographic mapping between the space of sound frequencies and 7 successive layers of the auditory processing system in the mammalian brain. The correlation between frequencies and neuron locations is preserved through all 7 layers.

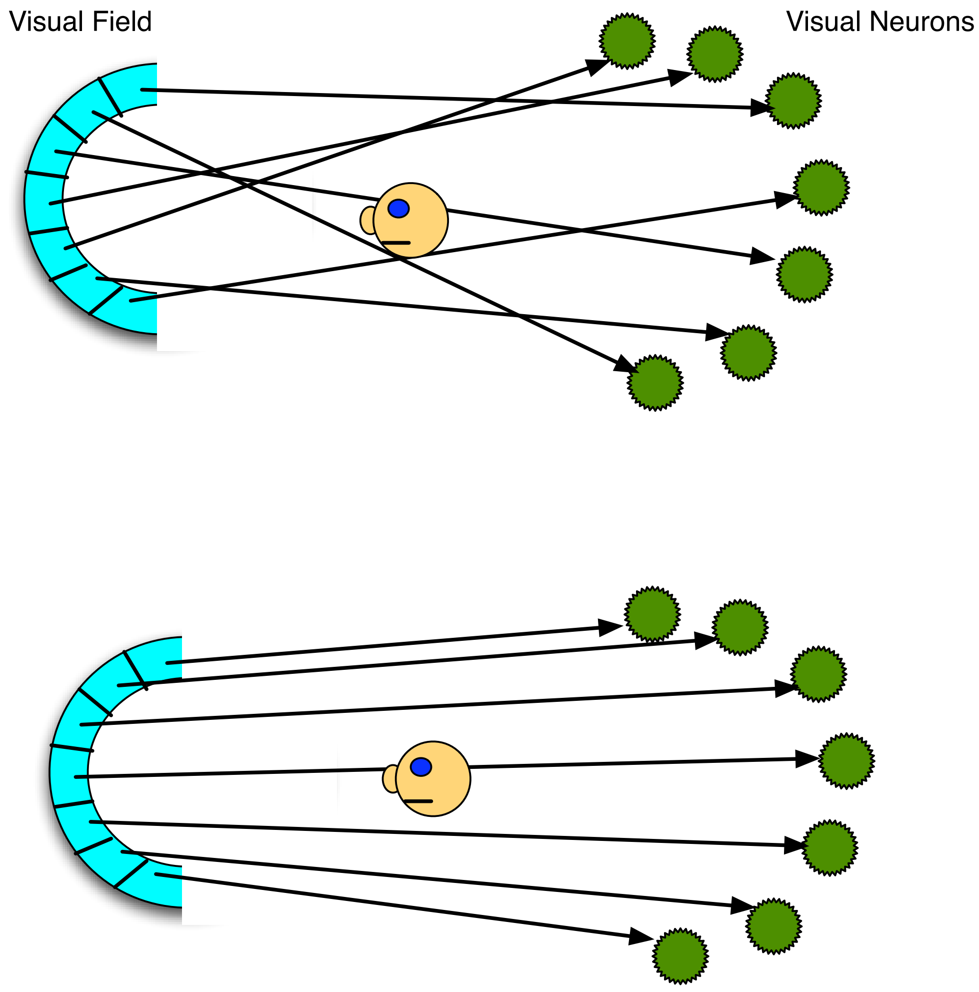


Figure 10: (Above) The typical initial situation for the application of a self-organizing map (SOM), with poor correlation between the two spaces: the visual field and the collection of neurons. (Below) A well-correlated (i.e., isomorphic) mapping between the two spaces.

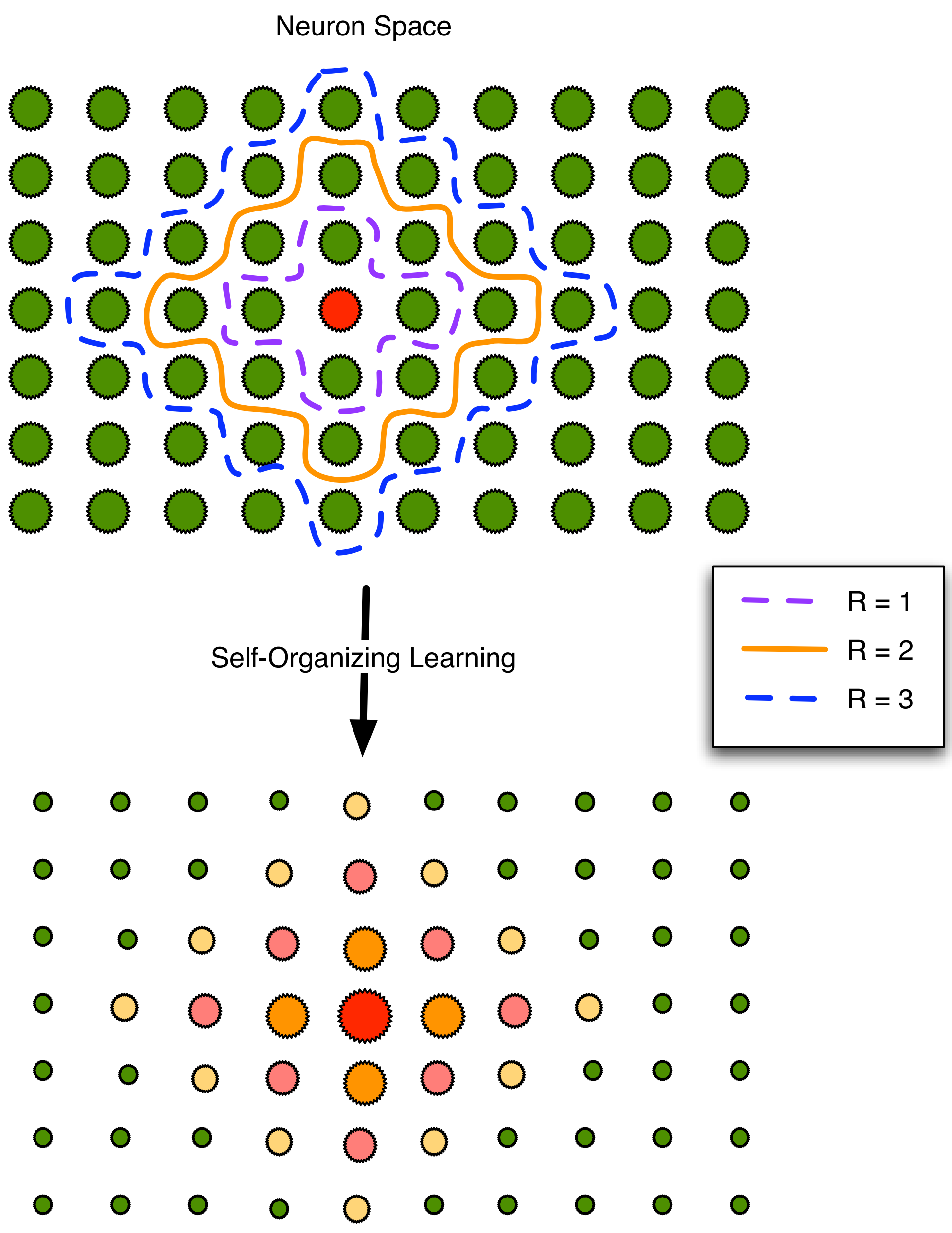


Figure 11: (Top) Illustration of shrinking neighborhoods (about the central red neuron) used to create self-organizing maps (SOMs). R is the radius of the neighborhood, with the Manhattan distance as the metric. (Bottom) After training, the neurons closest to the central neuron, C, have weight vectors that closely ressemble that of C. At greatest distances from C, the resemblance decreases, as denoted by differences in color and size between C and other neurons.

The net result is a convergence of the Euclidean and topological neighborhoods of the neurons in the SOM, as depicted in Figure 12. The significance of this convergence is multi-faceted, including physical factors such as reduced total *wiring* between brain layers, measured in terms of the lengths of axons and dendrites.

In terms of brain function, a key advantage of topological maps is that if situation A_1 maps to neuron (or more likely neuron population) N_1, presumably via a learning process, then situations similar to A_1, such as A_2 and A_3 would map to neighbors of N_1, which would elicit similar behavior. Thus, the topological map allows the brain to reuse and generalize its behaviors to situations similar to those that it has explicitly learned. The neighbors of N_1 may not share all of its functionality, which would seem appropriate, since A_2 and A_3 may require similar, but not exactly the same, actions as N_1 supports.

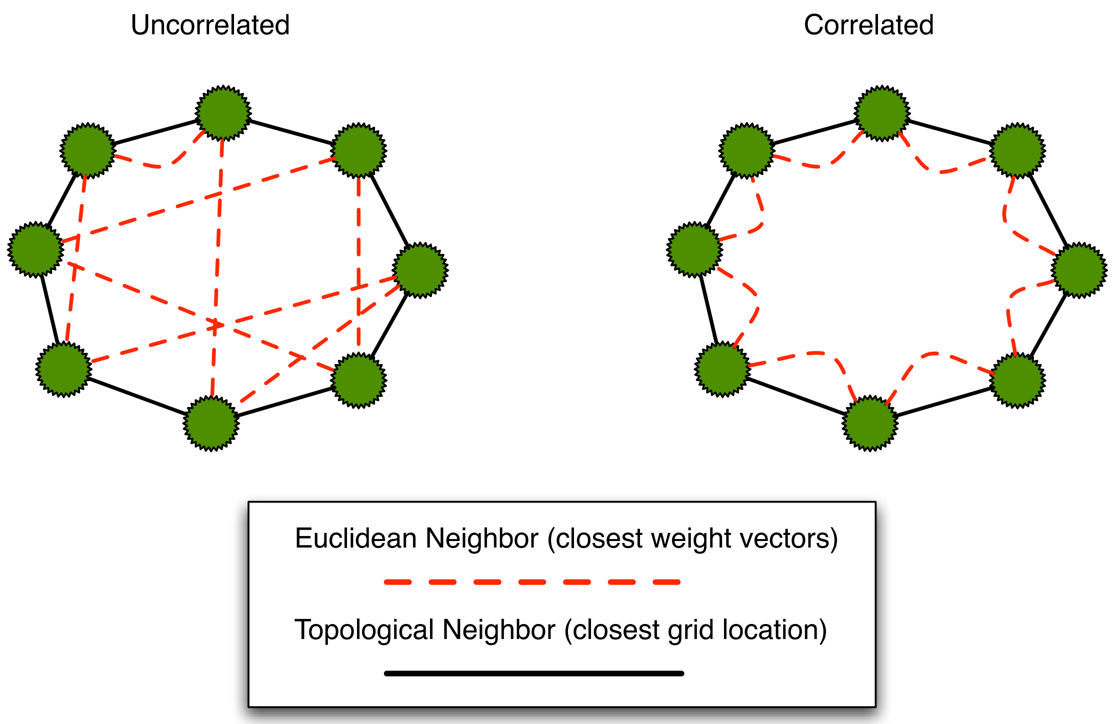

Uncorrelated
Correlated
Euclidean Neighbor (closest weight vectors)
Topological Neighbor (closest grid location)

Figure 12: Neurons in a self-organizing map (SOM) are trained to achieve a high correlation between the Euclidean space (which is the space of prototype vectors, which each vector element representing a feature of, for example, the visual field of Figure 10) and the topological space (which is the space in which the neurons reside). Thus, neighboring elements in neuron space have weight vectors (i.e., prototypes) that are neighbors in Euclidian space.

2.1.1 Self-Organizing Maps and the Traveling Salesman Problem

SOM's have a wide range of applications, both in biology and in engineering. They provide insights for neuroscientists as to the emergence of the brain's many topological maps, while serving as a powerful clustering algorithm for many practical situations where adjacency and neighborhoods in neuron space have significance.

One of the more intriguing applications that exploits the emergent isomorphism between two spaces is the use of an *elastic* ring of neurons to solve the Traveling Salesman Problem (TSP) [4]. As shown in Figure

13, the neuron space consists of a ring, with neighborhoods defined simply by adjacency on the ring. Each neuron has a two-element weight vector which represents a location on the cartesian plane.

As seen at the bottom of Figure 13, the neurons begin with randomly-assigned weight vectors and thus have random locations in cartesian space. The locations of each TSP city are then used as the training patterns for the neuron population, whose members compete to classify the locations, with the winner and its neighbors updating their weights to move closer to the pattern.

After many rounds of training, the neurons tend to move closer to the city locations. A simulation of the learning process, with visualization of the changing neuron locations, gives the population the appearance of an elastic ring that stretches to fit the cities. If the SOM begins with a large enough neighborhood, with a radius of approximately one tenth the neuron-population size, the ring often forms a good scaffold for a TSP solution.

To use the scaffold, simply go through the city list and associate each with its nearest neuron, i.e., the neuron that wins on that city. Once all cities are *attached* to the ring, simply *walk* around the ring and read off the city indices in the order that they appear. The resulting sequence constitutes a TSP solution. If 2 or more cities attach to the same neuron, then the ordering between the cities probably has little consequence and can safely be ignored.[2]

To simplify the implementation, it suffices to use scaled coordinates for the city locations, where all x and y values are real numbers between 0 and 1. The neuron weight vector should also be constrained to lie within the unit (i.e., 1 x 1) plane. Given a TSP city permutation based on the neuron ring in the unit plane (as described above), the actual inter-city distances are easily found by computation (using the original geographic locations), and any efficient solution in the unit plane will translate into a good solution on the original (geographic) map.

3 Hebbian Learning Models

Hebb's key insight, that stronger synaptic bonds form between neurons that fire together, underlies numerous learning rules for artificial neural networks, a few of which are discussed below. These rules are typically *local* in that synaptic change relies solely on the behaviors of the presynaptic and postsynaptic neurons, and not on any global error signals (as in classic supervised ANNs). This locality is appealling from both a biological angle, since the brain appears to employ Hebbian learning, and from an artificial life perspective, wherein complex system functionality *emerges* from the myriad local interactions of simple components, in the total absence of a global controller.

Unfortunately, the naive application of local rules across repeated ANN learning rounds can quickly lead to explosive weight increases and decreases, thus driving networks to states of extreme instability or deeply intrenched stagnation. Only by invoking additional mechanisms, which typically lack biological plausibility and/or strict locality, can the modeller reign in these networks, forcing them into behavioral regimes exhibiting an ample mix of stability and adaptivity.

In the discussion that follows, u_i and v will typically represent either the last activation level or the difference between a) the firing count of the neuron during the past m time steps, and b) the average firing count (per m time steps) computed over M such m-step periods. The term *neural output* will be used as a general reference to u_i or v, without any assumption about the exact nature of the physical variable.

[2]If one seeks the optimal TSP solution, then all orderings must be considered. Alternatively, by adding more and more neurons to the population, the probability of two cities mapping to the same neuron decreases rapidly.

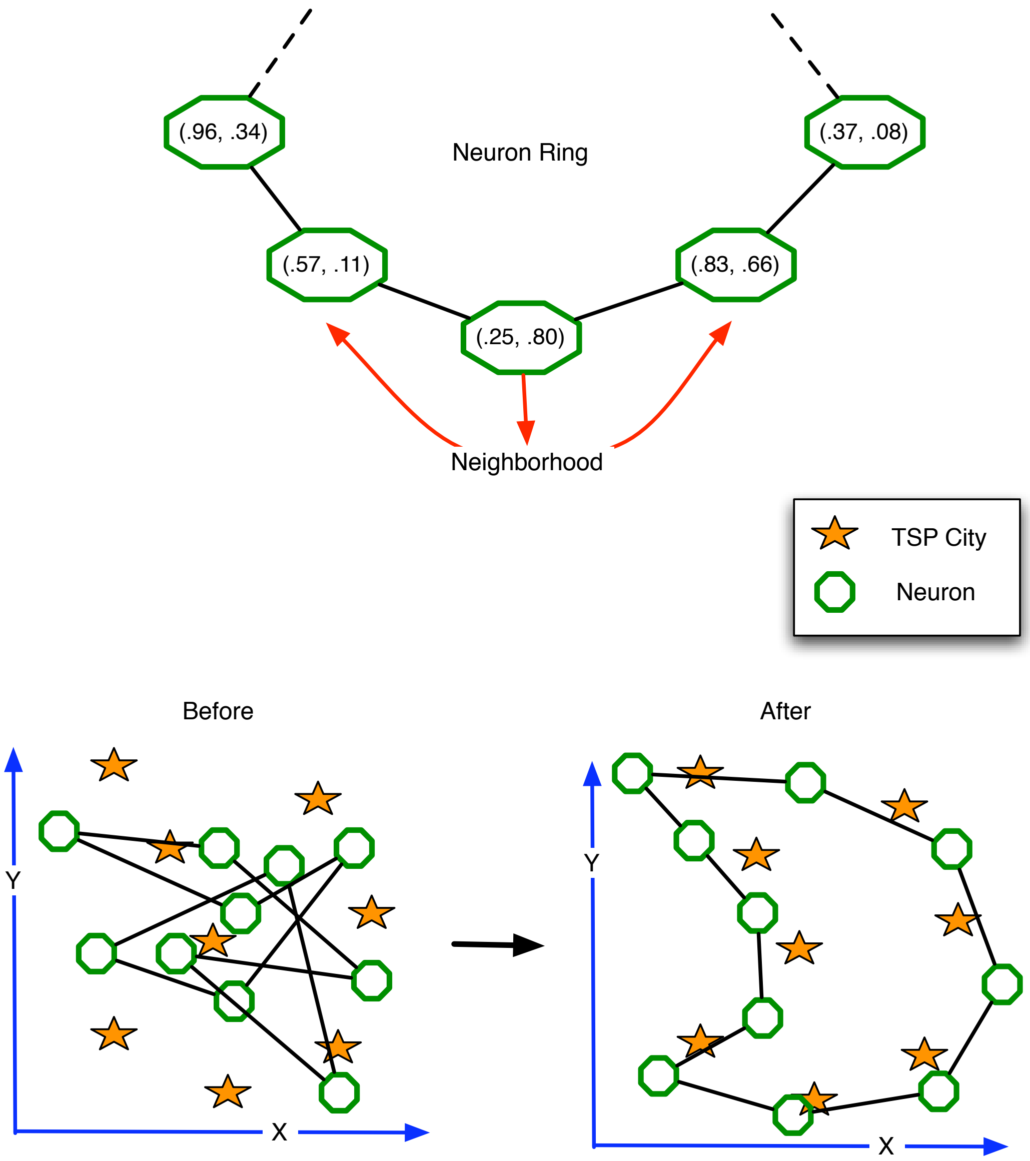


Figure 13: Illustration of the use of a self-organizing map to solve the Traveling Salesman Problem (TSP). (Above) The neuron topology is a ring, with each neuron's weight vector denoting a location in 2-d space. (Bottom) City locations (stars) and neurons (octagons) shown on the cartesian plane, with coordinates corresponding to a) the locations of the cities on a scaled map, and b) the weight vectors of each neuron.

Also, the term long-term potentiation (LTP) refers to a strengthening of a weight, while long-term depression (LTD) denotes a weakening. The *long-term* aspect of each change stems from the biological uses of LTP and LTD, where this type of synaptic change persists for hours, days or longer. In ANNs, there is no such guarantee of the duration of the change.

The classic Hebbian learning rule is simply:

$$\triangle w_i = \lambda u_i v \tag{11}$$

where λ is a positive real number (often less than 1) representing the learning rate. Equation 11 captures the basic proportionality between weight change and the correlation between the two neural outputs.

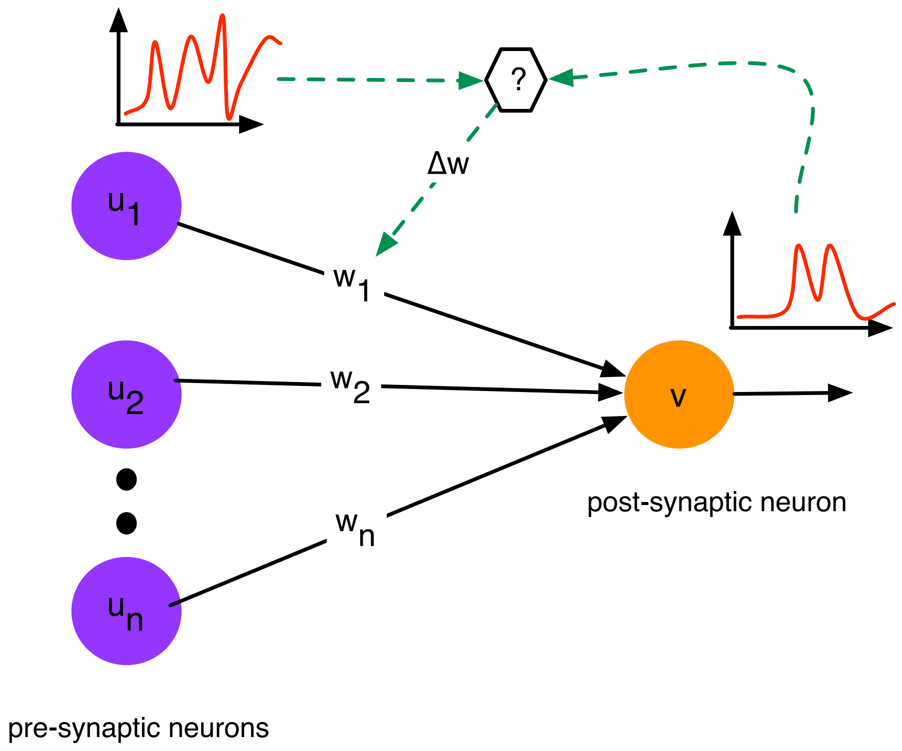


Figure 14: The essence of learning in neural networks: the comparison of pre-synaptic and post-synaptic firing histories determines changes to the connection weight between the two neurons. Here, weights have a single subscript, denoting the pre-synaptic neuron. Graphs are of the neuron's membrane potential as a function of time.

When u_i and v represent recent or time-averaged firing-rates, as they often do, they are never negative. Thus, the right-hand side of equation 11 is always positive, and weights increase without bound. In fact, a positive feedback occurs, since positive firing rates produce weight increases, which insure that the influence of u_i upon v gets stronger, which tends to raise v's firing rate, which then elevates the weight, etc.

One can simply put an upper bound on weight values, but then all weights eventually reach this limit and the ANN has no diversity and hence no interesting information content.

Another attempt to relieve the problem is to view u_i and v as either a) membrane potentials, or b) the differences between current and average firing rates. Both of these interpretations allow u_i and v to be positive or negative. Thus, $u_i v$ will often be negative, and weights should decrease as well as increase.

The latter interpretation has spawned several useful learning rules in which presynaptic, postsynaptic or both firing rates are relativized to a *normal* level. For example, the weight-updating expression, known as a *homosynaptic* rule normalizes only the postsynaptic output to a threshold, θ_v:

$$\triangle w_i = \lambda(v - \theta_v)u_i \tag{12}$$

Notice that this rule can exhibit long-term potentiation LTP or LTD depending upon whether v is above or below θ_v, which typically represents an average firing rate (computed and updated over the course of a simulation. The term *homosynaptic* refers to the fact that if v is above (below) threshold, then **all** presynaptic neurons that have a non-zero firing rate will experience LTP (LTD) along their connection to v. That is, all presynaptic neurons that fire will see the same type of change.

Conversely, the following rule is *heterosynaptic*, since, when $v > 0$, only those presynaptic neurons that fire above threshold will experience LTP, while the others - even those that do not fire at all - will experience LTD:

$$\triangle w_i = \lambda v(u_i - \theta_i) \tag{13}$$

A popular learning scheme that only normalizes the postsynaptic neuron but which requires both pre- and postsynaptic firing is the BCM (Bienenstock, Cooper and Munro) rule:

$$\triangle w_i = \lambda u_i v(v - \theta_v) \tag{14}$$

Rules that normalize both pre- and postsynaptic neurons include:

$$\triangle w_i = \lambda(v - \theta_v)(u_i - \theta_i) \tag{15}$$

and

$$\triangle w_i = \lambda v(v - \theta_v)u_i(u_i - \theta_i) \tag{16}$$

3.0.2 Instability of Hebbian Learning

Returning to the pure Hebbian learning rule of equation 11, as described above, when u_i and v are non-negative numbers, the weights will increase without bound. One seemingly obvious fix is to use activation functions whose outputs can be negative, for example, the hyperbolic tangent function described earlier. Unfortunately, this is not enough to avoid positive feedback and the ensuing unstable increase in weights. The proof, as described in [3] (pp. 286-287) is straightforward and summarized below.

To assess the change of an entire weight vector, in this case, the vector of all input weights to node v, W_v, we can look at the geometric length of that vector, which is simply:

$$\mid W_v \mid = \sqrt{\sum_{i=1}^{n} w_i^2} \tag{17}$$

We are interested in whether that length continually increases, decreases or fluctuates. In other words, we are interested in $\frac{d|W_v|}{dt}$. To simply our analysis, we can look at $\frac{d|W_v|^2}{dt}$, which will have the same sign as $\frac{d|W_v|}{dt}$. Then:

$$\frac{d \mid W_v \mid^2}{dt} = \frac{d(\sum_{i=1}^{n} w_i^2)}{dt} = \frac{dw_1^2}{dt} + \cdots + \frac{dw_n^2}{dt} = 2w_1\frac{dw_1}{dt} + \cdots + 2w_n\frac{dw_n}{dt} = 2W_v \bullet \frac{dW_v}{dt} \tag{18}$$

So the key relationship is:

$$\frac{d \mid W_v \mid^2}{dt} = 2W_v \bullet \frac{dW_v}{dt} \tag{19}$$

Now, if we rewrite equation 11 to account for all input arcs to v, we get:

$$\frac{dW_v}{dt} = \lambda U v \tag{20}$$

where U is the vector composed of $\{u_i : i = 1..n\}$.

Combining equations 19 and 20, we get:

$$\frac{d \mid W_v \mid^2}{dt} = 2W_v \bullet \lambda U v \tag{21}$$

If we assume:

$$v = W_v \bullet U \tag{22}$$

then:

$$\frac{d \mid W_v \mid^2}{dt} = 2\lambda v W_v \bullet U = 2\lambda v^2 \tag{23}$$

Thus, except for the trivial case when v = 0:

$$\frac{d \mid W_v \mid^2}{dt} > 0 \tag{24}$$

Thus, the length of the weight vector is always increasing, which generally means that the positive weights keep getting larger and the negative weights keep getting smaller (i.e. becoming larger negative numbers).

This instability of the weight vector typically leads to a saturation of the network, with many nodes always firing hard and others never firing at all.

It is important to remember that the final step of equation 23 hinges on the assumption in equation 22, which entails that v is the sum of its weighted inputs, net_v. This is equivalent to assuming the linear transfer function of Figure **??**, which, of course, is not always the case.

However, $\frac{d|W_v|^2}{dt}$ remains non-negative as long as v and $W_v \bullet U = net_v$ never have the opposite sign. This is the case for transfer functions with thresholds at $net_v = 0$ and which produce positive outputs above that threshold and non-positive outputs below it. Sigmoidal transfer functions used in ANNs often have this property, although it may be violated in a small neighborhood below the threshold, where small (i.e. near zero) negative net_v values yield small positive outputs.

At any rate, the general argument should be clear: the use of both negative and positive values for u_i and v does not, on its own, prevent the positive feedbacks that lead to instability (i.e., infinite growth in the positive or negative direction) of the ANNs weights.

Furthermore, if $W_v \bullet U$ and v have the same sign for long periods of time, $\triangle W_v$ can easily become dominated by the positive-feedback dynamics. As net_v moves further toward the extremes of the activation function (i.e., *saturates*), this relationship is more likely. Hence, it is wise to design networks that can avoid saturation, but, instead, can allow neurons to work near the thresholds of their activation functions, where the signs of net_v and v often vary.

Similar problems arise with learning rules such as BCM, which is unstable when θ_v is held constant [3] (pg. 288) but becomes stable when θ_v is permitted to grow faster than does the average value of v, as described in [3] (pp. 288-9).

3.1 Weight normalization

To avoid problems of weight-vector instability that occur with so many of the popular learning rules, more direct methods of weight restriction are available.

One of the most direct mechanisms is to simply normalize the weights associated with a particular neuron. Here, the options include:

1. **which** weights to normalize, for instance weights on all incoming (or outgoing) links to (from) each neuron.
2. **how** to normalize, whether by:
   (a) dividing each weight by the sum of the weights or the sum of the absolute values of the weights (in cases where weights can be positive or negative), or
   (b) subtracting the same quantity from each weight.

Another common approach is to randomly initialize the weights and then, for each node, store one of two sums: those of its incoming or outgoing weights to(from) that node. Assume that you choose the input weights, whose initial sum for node i is σ_i. Then, after each round of learning-based weight change, use equation 25 to renormalize each weight such that the input sums for each node equal the originals.

$$w_{ij} \leftarrow \frac{\sigma_i w_{ij}}{\sum_{j=1}^{n} \mid w_{ij} \mid} \tag{25}$$

Although computationally expensive, these methods do have the desired effect of preventing runaway weights.

A simpler and computationally cheaper method is the Oja rule, which includes a *forgetting* term that involves the weight itself:

$$\triangle w_i = \lambda v(u_i - v \mid w_i \mid) = u_i v - v^2 \mid w_i \mid \tag{26}$$

Notice that the forgetting (rightmost) term increases as the postsynaptic firing rate increases. This combats a standard positive-feedback problem with the earlier rules: when neurons fire at high rates, synapses tend to strengthen, which helps neurons to fire even harder in the future.

The Oja rule has nice theoretical properties, including the ability to perform principle component analysis (PCA), though it lacks complete biological plausibility. However, it's stability is easily proven [3] (pg. 289), and thus it is a popular learning mechanism for ANNs designed to solve complex engineering problems by predominantly local learning mechanisms.

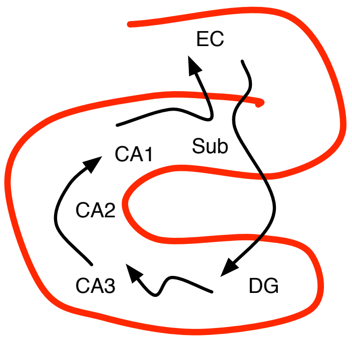
3.2 Unsupervised Episodic Learning in the Hippocampus

There is strong evidence that Hebb's rule applies in many parts of the brain, although certainly not all. In that sense, unsupervised learning occurs throughout the brain. Certainly, many areas, covering a wide spectrum of functionalities, exhibit Hopfield-type memory. These range from early sensory-processing regions to high-level associational sectors; essentially, they span the entire cortex. However, one particular region, CA3 of the Hippocampus, has anatomical and physiological characteristics that make it a prime candidate for the brain's highest-level, unsupervised, associative layer.

Often viewed as the center of long-term memory formation, the hippocampus (HC) resides in the temporal lobe and receives inputs from various cerebral regions, particularly the higher-level associational areas. As shown in Figure 15, the HC and surrounding regions perform a drastic compression (via high convergence) of information between the neocortex (via the entorhinal cortex, EC) and area CA3, and a complementary expansion (via divergence) on the return path through CA1 and Subiculum. The topology of the HC proper is a main loop with several shortcuts from the EC to CA3 and CA1.

Only CA3 contains extensive recurrence, with each neuron connected to approximately 4% of the others [12]. This indicates that CA3 performs associative learning by standard Hebbian means: neurons that fire together wire together. The high convergence from a diverse array of neocortical areas onto CA3 hints of the holistic nature of these patterns. In rats, individual neurons in CA3 and CA1 are known as place cells [2], since they fire only when the animal is at a particular location, while in monkeys, they are called view cells, since they fire when the primate merely looks at such a location [12]. In either case, the cells represent a massive compression of sensory data.

The hippocampus' importance to long-term memory formation is well-established [13, 5], as is the fact that memories reside in the HC only until they can be off-loaded to the cortex for more permanent storage [9]. However, details of the actual learning process remain somewhat vague; the following scenario incorporates some of the more popular theories.



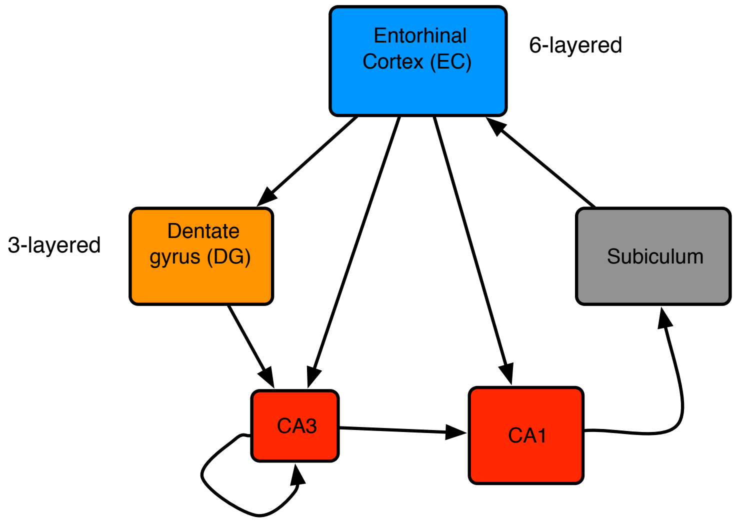


Figure 15: (Above) Basic anatomy of the mammalian hippocampus. (Below) Primary hippocampal areas and their connectivity. Box dimensions roughly illustrate relative sizes of neural populations in each area; all connections are excitatory. Based on pictures and diagrams in [1, 10, 12].

Since particular memorable situations may only occur once, episodic memory formation must involve a snapshot mechanism. However, McClelland et al. [9] point out that forcefully caching a new pattern in an associative network, via extensive synaptic modification (corresponding to a high learning rate in an artificial neural network), can corrupt pre-existing memories. Instead, new patterns should be repeatedly presented to the network in interleaved fashion, with only small synaptic changes occurring each time. The HC acts as the trainer for the cortex by a) temporarily caching snapshots of episodes via very fast Hebbian associative learning and then b) repeatedly re-presenting these patterns to the cortex until it too learns the associations. The basic topology and behavior of the HC indicates how this might work.

Consider a situation, S, summarized by the firing of 10,000 neurons, N1, in different high-level association cortices (many of which are in the temporal lobe along with the HC). The firings of N1 will coincide with the random background firing of certain nodes in pre-HC areas such as the perirhinal cortex, which, in turn, will coincide with random firings in the entorhinal cortex (EC), dentate gyrus (DG), CA3, CA1 and subiculum. Via Hebbian learning, the inter-layer synapses between these simultaneously-active neurons will be strengthened, as will the recurrent connections in CA3. Most HC synapses are capable of Hebbian Learning via long-term potentiation (LTP), but the recurrent collaterals within CA3 and the EC-DG, DG-CA3 and CA3-CA1 links exhibit very fast learning via rapid long-term potentiation (LTP). This learning rate far exceeds that of the cortex. So, although cortical neurons N1 will not initially form strong direct synaptic bonds with one another, their signals will gradually converge through several pre-HC and HC layers until, in CA3, a set of neurons, N2, that summarizes N1, will be co-active and immediately form strong synapses between one another.

Since a) the connections between the pre-HC layers are bi-directional, with both directions being strengthened during S's occurrence, and b) synaptic connections within the HC form a ring that begins and ends at the entorhinal cortex, a return pathway of enhanced synapses from N2 to N1 will form as well. Then, in the future, whenever N2 cells fire, the return pathway will stimulate the N1 cells. Through frequent re-stimulation, the N1 cells will gradually establish intra-cortical connections that will eventually consolidate the memory of S in the cortex. Detailed neural anatomy supports this slow-learning hypothesis, since HC afferents project onto distal (i.e. far from the cell body) portions of cortical dendrites, thus indicating a small effect for each return signal. Restimulation of the cortex may involve repeated waves of CA3 and CA1 activation during sleep.

Prior to long-term memory consolidation, recall could be achieved when portions of N1 send signals through the HC to CA3, stimulating part of N2, which the CA3 association network would then complete; the full N2 would then stimulate the rest of N1 via the return pathway. Rolls and Treves [12] point out that learning and recall are problematic to implement in the same naturally-occurring association layer, since a (complete) pattern to be learned could easily activate recurrent collaterals and be further expanded, based on the memories of other stored patterns. They believe that the two processes are segregated into two pathways, with the direct EC-CA3 connections used for recall, while the EC-DG-CA3 route achieves learning, since the DG neurons are believed to have stronger influences on CA3 cells, thus overshadowing the effects of recurrent stimulation. However, in the same manner that dopamine signals may gate in activation patterns from the posterior cortical areas to the frontal cortex [11], neuromodulators that stimulate the EC-CA3 connections (during learning but not recall) without enhancing the CA3 recurrent collaterals could also explain the bi-modal behavior of CA3.

Evidence of place and view cells in rat and primate HCs, respectively, have motivated a wide variety of ANN models of HC-based navigation, as summarized in [2]. Many of these involve implicit predictive knowledge in CA3 and CA1, wherein place cells fire before the animal arrives at the corresponding location. Place cells are mutually inhibitory and adapt to encode spatial contexts via competitive learning.

In one of the more popular models, Burgess et al. [10] propose a layer of goal cells (possibly in the subiculum) that receive inputs from many CA1 place cells. Goals represent very salient locations, often those involving reinforcements. As a simulated rat moves about, the goal cells fire at frequencies correlated with the rat's proximity to them, so navigation is achieved by choosing movements that increase the firing of focal goal cells.

Another interesting variant [7] posits CA3 as the site of predicted situations and CA1 as the site of real situations (via direct inputs from EC). Mismatches between the two drive learning in CA3 and thus improved predictions in the future.

From this plethora of diverse models and hypotheses, a few general, common themes emerge:

1. The pre-HC and HC compress and integrate huge amounts of sensory data into relatively sparse activation patterns in CA3 and CA1.
2. These patterns represent holistic high-level contexts which can aid the animal during repeated performance trials in the same environment, e.g. by allowing shortcut-taking during navigation.
3. There is an enduring memory for these contexts, whether in the HC or back in the cortex after off-loading.
4. Learning involves LTP in an unsupervised manner, although neuromodulators stemming from emotional experiences may be involved to help solidify memories of more salient contexts.
5. With its abundance of recurrent collaterals, most evidence points to CA3 as the center of this associative learning.

To generalize further, the HC seems instrumental in building memories, possibly quite detailed, of contexts that may later be recalled and analyzed by conscious, cognitive processes. This contrasts sharply with the basal ganglia and cerebellum, which also learn contexts, but these are often so tightly tied to sensorimotor machinery as to be unaccesible for explicit cognitive processing.

4 Conclusion

Unsupervised learning is the most basic form of adaptivity in neural networks, and clearly a mechanism that operates in many areas of the brain., including the hippocampus and neocortex. Whether cooperative or competitive in nature, the process relies heavily on a fundamental feature of neural systems: Hebbian synaptic modification. This Hebbian grounding makes unsupervised learning very easy to implement in artificial neural networks, at least initially. Unfortunately, pure Hebbian learning can quickly lead an ANN away from interesting behavioral regions into hyper- or hypo-active regimes, where all desired functionality evaporates. A clear understanding of the mathematical basis of this problem, along with an overview of potential solution methods such as weight normalization, is essential for successfully implementing Hebbian-based ANNs, particularly those that will perform continuous tasks over long time periods. Biologically-inspired AI involve ANNs requires a thorough command of these issues.

Hopfield networks serve a very useful educational purpose in cutting directly to basic issues of pattern storage and retrieval in neural systems, but they have limited practical utility. However, general competititve learning networks and cooperative Kohonen models have a wide variety of applications in problem domains that require data clustering.

In short, you really can go a long way with the simple Hebbian rule of firing and wiring together. It appears to be the fundamental principle behind associational pattern formation, which, in turn, is touted as one of the premier properties of animal intelligence.

References

[1] P. Andersen, R. Morris, D. Amaral, T. Bliss, and J. O'Keefe, *The Hippocampus Book*, Oxford University Press, New York, NY, 2007.

[2] N. Burgess and J. O'Keefe, *Hippocampus: Spatial models*, in The Handbook of Brain Theory and Neural Networks, M. Arbib, ed., The MIT Press, Cambridge, MA, 2003, pp. 539–543.

[3] P. Dayan and L. Abbott, *Theoretical Neuroscience: Computational and Mathematical Modeling of Neural Systems*, The MIT Press, Cambridge, MA, 2001.

[4] R. Durbin and D. Willshaw, *An analogue approach to the traveling salesman problem using an elastic net method*, Nature (London), 326 (1987), pp. 689–691.

[5] M. Gluck and C. Myers, *Gateway to Learning: An Introduction to Neural Network Modeling of the Hippocampus and Learning*, Kluwer Academic Publishers, Norwell, Massachusetts, 1989.

[6] J. Hopfield, *Neural networks and physical systems with emergent collective computational abilities*, Proceedings of the National Academy of Sciences, 79 (1982), pp. 2554–2558.

[7] S. Kali and P. Dayan, *The involvement of recurrent connections in area ca3 in establishing the properties of place fields: a model*, Journal of Neuroscience, 20 (2000), pp. 7463–7477.

[8] T. Kohonen, *Self-Organizing Maps*, Springer, Berlin, 2001.

[9] J. Mcclelland, B. McNaughton, and R. O'Reilly, *Why there are complementary learning systems in the hippocampus and neocortex: Insights from the successes and failures of connectionist models of learning and memory*, Tech. Rep. PDP.CNS.94.1, Carnegia Mellon University, Mar. 1994.

[10] M. R. N. Burgess and J. O'Keefe, *A model of hippocampal function*, Neural Networks, 7 (1994), pp. 1065–1083.

[11] R. C. O'Reilly and Y. Munakata, *Computational Explorations in Cognitive Neuroscience*, The MIT Press, Cambridge, Massachusetts, 2000.

[12] E. Rolls and A. Treves, *Neural Networks and Brain Function*, Oxford University Press, New York, 1998.

[13] L. Squire and E. Kandel, *Memory: From Mind to Molecules*, Henry Holt and Company, New York, 1999.