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# A Rosetta Stone for Connectionism

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## Abstract

The term connectionism is usually applied to neural networks. There are, however, many other models that are mathematically similar, including classifier systems, immune networks, autocatalytic chemical reaction networks, and others. In view of this similarity, it is appropriate to broaden the term connectionism. I define a connectionist model as a dynamical system with two properties: (1) The interactions between the variables at any given time are explicitly constrained to a finite list of connections. (2) The connections are fluid, in that their strength and/or pattern of connectivity can change with time.

This paper reviews the four examples listed above and maps them into a common mathematical framework, discussing their similarities and differences. It also suggests new applications of connectionist models, and poses some problems to be addressed in an eventual theory of connectionist systems.

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ΠΤΟΛΕΜΑΙΟΣ

Figure 1: “Ptolemy”, in hieroglyphics, Demotic, and Greek. This cartouche played a seminal role in deciphering hieroglyphics, by providing a hint that the alphabet was partially phonetic [12]. (The small box is a “p”, and the half circle is a “t” – literally it reads “ptolmis”.)

## 1 Introduction

This paper has several purposes. The first is to identify a common language across several fields in order to make their similarities and differences clearer. A central goal is that practitioners in neural nets, classifier systems, immune nets, and autocatalytic nets will be able to make correspondences between work in their own field as compared to the others, more easily importing mathematical results across disciplinary boundaries. This paper attempts to provide a coherent statement of what connectionist models are and how they differ in mathematical structure and philosophy from conventional “fixed” dynamical systems models. I hope that it provides a first step toward clarifying some of the mathematical issues needed for a generally applicable theory of connectionist models. Hopefully this will also provide a natural framework for connectionist models in other areas, such as ecology, economics, and game theory.

### 1.1 Breaking the jargon barrier

Language is the medium of cultural evolution. To a large extent differences in language define culture groupings. Someone who speaks Romany, for example, is very likely a Gypsy; the existence of a common and unique language is one of the most important bonds preserving Gypsy culture. At times, however, communication between sub-cultures becomes essential, so that we must map one language to another.

The language of science is particularly specialized. It is also particularly fluid; words are tools onto which we map ideas, and which we invent or redefine as necessary. Our jargon evolves as science changes. Although jargon is a necessary feature of communication in science, it can also pose a barrier impeding scientific progress.

When models are based on a given class of phenomena, such as neurobiology or ecology, the terminology used in the models tends to reflect the phenomenon being modeled rather than the underlying mathematical structure. This easily obscures similarities in the mathematical structure. "Neural activation" may appear quite different from "species population", even though relative to given mathematical models the two may be identical. Differences in jargon place barriers to communication that prevent results in one field from being transparent to workers in another field. Proper nomenclature should identify similar things but distinguish those that are genuinely different.

At present this problem is particularly acute for adaptive systems. The class of mathematical models that are employed to understand adaptive systems contain subtle but nonetheless significant new features that are not easily categorized by conventional mathematical terminology. This adds to the problem of communication between disciplines, since there are no standard mathematical terms to identify the features of the models.

## 1.2 What is connectionism?

Connectionism is a term that is currently applied to neural network models such as those described in references [58,15]. The models consist of elementary units, which can be "connected" together to form a network. The form of the resulting connection diagram is often called the *architecture* of the network. The computations performed by the network are highly dependent on the architecture. Each connection carries information in its weight, which specifies how strongly the two variables it connects interact with each other. Since the modeler has control over how the connections are made, the architecture is plastic.

This contrasts with the usual approach in dynamics and bifurcation theory, where the dynamical system is a fixed object whose variability is concentrated into a few parameters. The plasticity of the connections and connection strengths means that we must think about the entire family of dynamical systems described by all possible architectures and all possible combinations of weights. Dynamics occurs on as many as three levels, that of the states of the network, the values of connection strengths, and the architecture of the connections themselves.

Mathematical models with this basic structure are by no means unique to neural networks. They occur in several other areas, including classifier systems, immune networks, and autocatalytic networks. They also have potential applications in other areas, such as economics, game-theoretic models and ecological models. I propose that the term connectionism be extended to this wider class of models.

By comparing connectionist models for different phenomena using a common nomenclature, we get a clear view of the extent to which these models are similar or different. We also get a *glimpse* of the extent to which the underlying phenomena are similar or different. I emphasize the word *glimpse* to make it clear that we are simplifying a complicated phenomenon when we model it in connectionist terms. Comparing two connectionist models of, for example, the nervous system and the

immune system, provides a means of extracting certain aspects of their similarities, but we must be very careful in doing this; much richness and complexity is lost at this level of description.

Connectionism represents a particular level of abstraction. By reducing the state of a neuron to a single number, we are collapsing its properties relative to a real neuron, or relative to those of another potentially more comprehensive mathematical formalism. For example, consider fluid dynamics. At one level of description the state of fluid is a function whose evolution is governed by a partial differential equation. At another level we can model the fluid as a finite collection of spatial modes whose interactions are described by a set of ordinary differential equations. The partial differential equation is not a connectionist model; there are no identifiable elements to connect together; a function simply evolves in time. The ordinary differential equations are *more* connectionist; the nature of the solution depends critically on the particular set of modes, their connections, and their coupling parameters. In fluid dynamics we can sometimes calculate the correct couplings from first principles, in which case the model is just a fixed set of ordinary differential equations. In contrast, for a connectionist model there are dynamics for the couplings and/or connections. In a fully connectionist model, the connections and couplings would be allowed to change, to find the best possible model with a given degree of complexity.

Another alternative is to model the fluid on a grid with a finite difference scheme or a cellular automaton. In this case each element is "connected" to its neighbors, so there might be some justification for calling these connectionist models. However, the connections are fixed, completely regular, and have no dynamics. I will not consider them as "connectionist".

Just as there are limits to what can be described by a finite number of distinct modes, there are also limits to what can be achieved by connectionist models. For more detailed descriptions of many adaptive phenomena we may need models with explicit spatial structure, such as partial differential equations or cellular automata. Nonetheless, connectionism is a useful level of abstraction, which solves some problems efficiently.

The Rosetta Stone is a fragment of rock in which the same text is inscribed in several different languages and alphabets. It provides a key that greatly facilitated the decoding of these languages, but it is by no means a complete description of them. My goal is similar; by presenting several connectionist models side by side, I hope to make it clear how some aspects of the underlying phenomena compare with one another, but I offer the warning that quite a bit has been omitted in the process.

### 1.3 Organization of this paper

In section 2, I describe the basic mathematical framework that is common to connectionist models. I then discuss four different connectionist models: neural networks, classifier systems, immune networks, and autocatalytic networks. In each case I begin with a background discussion, make a correspondence to the generic framework described in section 2, and then discuss general issues. Finally, the conclusion con-

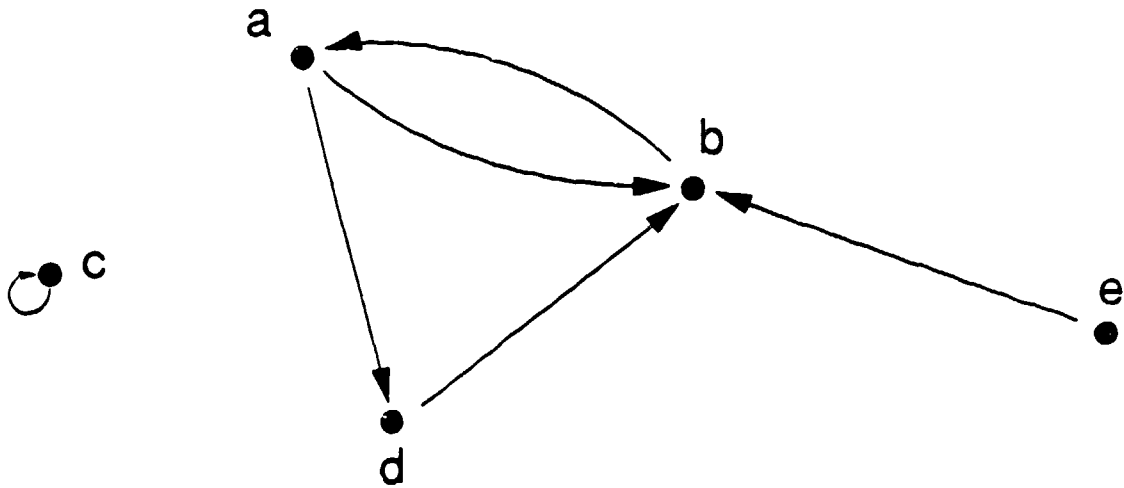


Figure 2: A directed graph.

tains the “rosetta stone”, a table mapping the jargon of each area into a common nomenclature. I also make a few suggestions for applications of connectionist models and comment on what I learned in writing this paper.

Connectionist models are ultimately dynamical systems. Readers who are not familiar with terms such as automaton, map, or lattice model may wish to refer to the Appendix.

## 2 The general mathematical framework of connectionist models

In this section I present the mathematical framework of a “generic” connectionist model. I make some arbitrary choices about nomenclature, in order to provide a standard language, noting common synonyms whenever appropriate.

To first approximation a connectionist model is a pair of coupled dynamical systems living on a graph. In some cases the graph itself may also have dynamics. The remainder of this section explains this in more detail.

### 2.1 The graph

The foundation of any connectionist model is a graph, consisting of *nodes* (or *vertices*) and *connections*, *links*, or *edges* between them as shown in Figure (2). The graph describes the architecture of the system and provides the channels in which the dynamics takes place. There are different types of graphs; for example, the links can be either directed (with arrows), or undirected (without arrows). For some purposes,

such as modeling catalysis, it is necessary to allow more complicated graphs with more than one type of node or more than one type of link.

For many purposes it is important to specify the pattern of connections, with a *graph representation*. The simplest way to represent a graph is to draw a picture of it, but for many purposes a more formal description is necessary. One common graph representation is a *connection matrix*. The nodes are assigned an arbitrary order, corresponding to the rows and columns of a matrix. The row corresponding to each node contains a nonzero entry, such as "1", in the columns corresponding to the nodes to which it makes connections. For example, if we order the nodes of Figure (2) lexicographically, the connection matrix is

$$C = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \quad (1)$$

If the graph is undirected then the connection matrix is symmetric. It is sometimes economical to combine the representation of the graph and the connection parameters associated with it into a matrix of connection parameters.

A *connection list* is an alternative of a graph representation. For example, the graph of Figure (2) can also be represented as

$$\begin{array}{l} a \rightarrow b \\ a \rightarrow d \\ b \rightarrow a \\ c \rightarrow c \\ d \rightarrow b \\ e \rightarrow b \end{array} \quad (2)$$

Note that the nodes are implicitly contained in the connection list. In some cases, if there are isolated nodes, it may be necessary to provide an additional list of nodes that do not appear on the connection list. For the connectionist models discussed here isolated nodes, if any, can be ignored.

For a *dense* graph almost every node is connected to almost every other node. For a *sparse* graph most nodes are connected to only a small fraction of the other nodes. A connection matrix is a more efficient representation for a dense graph, but a connection list is a more efficient representation for a sparse graph.

## 2.2 Dynamics

In conventional dynamical models the form of the dynamical system is fixed. The only part of the dynamical system that changes is the state, which contains all the information we need to know about the system to determine its future behavior. The possible ways the "fixed" dynamical form "might change" are encapsulated as



parameters. These are usually thought of as fixed in any given experiment, but varying from experiment to experiment. Alternatively we can think of the parameters as knobs that can be slowly changed in the background. In reality the quantities that we incorporate as parameters are usually aspects of the system that change on a time scale slower than those we are modeling with the dynamical system.

Connectionist models extend this view by giving the parameters an explicit dynamics of their own, and in some cases, by giving the list of variables and their connections a dynamic of its own. Typically this also involves a separation of time scales. Although a separation of time scales is not necessary, it provides a good starting point for the discussion. The fast scale dynamics, which changes the *states* of the system, is usually associated with short term information processing. This is the *transition rule*. The intermediate scale dynamics changes the *parameters*, and is usually associated with learning. I will call this the *parameter dynamics* or the *learning rule*. On the longest time scale, the graph itself may change. I will call this the *graph dynamics*. The graph dynamics may also be used for learning; hopefully this will not lead to confusion.

Of course, strictly speaking the states, parameters, and graph representation described above are just the states of a larger dynamical system with multiple time scales. Reserving the word *state* for the shortest time scale is just a convenience. The association of time scales given above is the natural generalization of "conventional" dynamical systems, in which the states change quickly, the parameters change slowly, and the graph is fixed. For some purposes, however, it might prove to be useful to relax this separation, for example, letting the graph change at a rate comparable to that of the states. Although all the models discussed here have at most three time scales, in principle this framework could be iterated to higher levels to incorporate an arbitrary number of time scales.

The information that resides on the graph typically consists of integers, real numbers, or vectors, but could in principle be any mathematical objects<sup>1</sup>. The state transition and learning rules can potentially be any type of dynamical system. For systems with continuous states and continuous parameters the natural dynamics are ordinary differential equations or discrete time maps. In principle, the states or parameters could also be functions whose dynamics are partial differential equations or functional maps. This might be natural, for example, in a more realistic model of neurons where the spatio-temporal form of pulse propagation in the axon is important [59]. When the activities or parameters are integers, their dynamics are naturally automata, although it is also common to use continuous dynamics even when the underlying states are discrete.

Since the representation of the graph is intrinsically discrete, the graph dynamics usually has a different character. Often, as in classifier systems, immune networks, or autocatalytic networks, the graph dynamics contains random elements. In other cases, it may be a deterministic response to statistical properties of the node states or the connection strengths, for example, as in pruning algorithms. Dynamical systems

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<sup>1</sup>The *states* could conceivably be more complicated mathematical objects, such as functions.

with graph dynamics are sometimes called *metadynamical systems* [20,8].

In all of the models discussed here the states of the system reside on the nodes of the graph<sup>2</sup>. The states are denoted  $x_i$ , where  $i$  is an integer labeling the node. The parameters reside at either nodes or connections;  $\theta_i$  refers to a *node parameter* residing at node  $i$ , and  $w_{ij}$  refers to a *connection parameter* residing at the connection between node  $i$  and node  $j$ .

The degree to which the activity at one node influences the activity at another node, or the *connection strength*, is an important property of connectionist models. Although this is often controlled largely by the connection parameters,  $w_{ij}$ , the node parameters  $\theta_i$  may also have an influence, and in some cases, such as B-cell immune networks, provide the *only* means of changing the average connection strength. Thus, it is misleading to assume that the connection parameters are equivalent to the connection strengths. Since the connection strength at any given instant may vary depending on the states of the system, and since the form of the dynamics may differ considerably in different models, we need to discuss connection strength in terms of a quantity that is representation-independent, which is well defined for any dynamical model.

For a continuous transition rule the natural way to discuss the connection strength is in terms of the Jacobian. When the transition rule is an ordinary differential equation, of the form  $\frac{d}{dt}x_i = f_i(x_1, x_2, \dots, x_N)$ , the *instantaneous connection strength* of the connection from node  $i$  to node  $j$  (where  $i$  is an input to  $j$ ) is the corresponding term in the Jacobian matrix  $J_{ji} = \frac{\partial x_j}{\partial x_i} = \frac{\partial f_j}{\partial x_i}$ . A connection is excitatory if  $J_{ji} > 0$  and inhibitory if  $J_{ji} < 0$ . Similarly, for discrete time dynamical systems (continuous maps), of the form  $x_j(t+1) = f_j(x_1, x_2, \dots, x_N)$ , a connection is excitatory if  $|J_{ji}| > 1$  and inhibitory if  $|J_{ji}| < 1$ . In a continuous system, the average connection strength is  $\langle J_{ji} \rangle$ , where  $\langle \rangle$  denotes an appropriate average; in a discrete system it is  $\langle |J_{ji}| \rangle$ . To make this more precise it is necessary to specify the ensemble over which the average is taken.

For automaton transition rules, since the states  $x_i$  are discrete the notion of instantaneous connection strength no longer makes sense. The average connection strength may be defined in one of many ways; for example, as the fraction of times node  $j$  changes state when node  $i$  changes state. In situations where  $x_i$  is an integer but nonetheless approximately preserves continuity, if  $|\Delta x_i(t)|$  is the magnitude of the change in  $x_i$  at time  $t$ , the average connection strength can be defined as  $\langle \frac{|\Delta x_j(t+1)|}{|\Delta x_i(t)|} \rangle_{|\Delta x_i(t)| > 0}$ .

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<sup>2</sup>It is also possible that states could be attached to connections, but this is not the case in any of the models discussed here.

## 3 Neural nets

### 3.1 Background

Neural networks originated with early work of McCulloch and Pitts [42], Rosenblatt [57], and others. Although the form of neural networks was originally motivated by neurophysiology, their properties and behavior are not constrained by those of real neural systems, and indeed are often quite different. There are two basic applications for neural networks: one is to understand the properties of real neural systems, and the other is for machine learning. In either case, a central question for developing a theory of learning is: Which behaviors of real neurons are essential to their information processing capabilities, and which are simply irrelevant side effects?

For machine learning problems neural networks have many uses that go considerably beyond the problem of modeling real neural systems. There are several reasons for dropping the constraints of modeling real neurons:

- We do not understand the behavior of real neurons.
- Even if we understood them, it would be computationally inefficient to implement the full behavior of real neurons.
- It is unlikely that we need the full complexity of real neurons in order to solve problems in machine learning.
- By experimenting with different approaches to simplified models of neurons, we can hope to extract the basic principles under which they operate, and discover which of their properties are truly essential for learning.

Because of the factors listed above, for machine learning problems there has been a movement towards simpler artificial neural networks that are less motivated by real neural networks. Such networks are often called “artificial neural networks”, to distinguish them from the real thing, or from more realistic models. Similar arguments apply to all the models discussed here; it might also be appropriate to say “artificial immune networks” and “artificial autocatalytic networks”. However, this is cumbersome and I will assume that the distinction between the natural and artificial worlds is taken for granted.

Neural networks are constructed with simple units, often called “neurons”. Until about five years ago, there were almost as many different types of neural networks as there were active researchers in the field. In the simplest and probably currently most popular form, each neuron is a simple element that sums its inputs with respect to weights, subtracts a threshold, and applies an *activation function* to the result. If we assume that time is discrete so that we can write the dynamics as a map, then we have

- $t = 1, 2, \dots = \text{time}$
- $x_i(t) = \text{state of neuron } i$

- $w_{ij}$  = weight of connection from  $i$  to  $j$
- $\theta_j$  = threshold
- $S$  = the activation function, often a sigmoidal function such as  $\tanh$ .

The response of a single neuron can be characterized as

$$x_j(t+1) = S\left(\sum_i w_{ij}x_i(t) - \theta_j\right). \quad (3)$$

We could also write the dynamics in terms of automata, differential equations, or, if we assume that the neurons have a refractory period during which they do not change their state, as delay differential equations.

The instantaneous connection strength is

$$\frac{\partial x_j(t+1)}{\partial x_i(t)} = w_{ij}S'\left(\sum_i w_{ij}x_i(t) - \theta_j\right). \quad (4)$$

where  $S'$  is the derivative of  $S$ . If  $S$  is a sigmoid, then  $S'$  is always positive and a connection with  $w_{ij} > 0$  is always excitatory and a connection with  $w_{ij} < 0$  is always inhibitory.

A currently popular procedure for constructing neural networks is to line the neurons up in rows, or "layers". A standard architecture has one layer of input units, one or two layers of "hidden" units, and a layer of output units, with full connections between adjacent layers. For a *feed-forward* architecture the graph has no loops so that with fixed parameters information flows only in one direction, from the inputs to the outputs. If the graph has loops so that the activity of a neuron feeds back on itself then the network is *recurrent*.

For layered networks it is sometimes convenient to assign the neurons an extra label that indicates which layer they are in. For feed-forward networks the dynamics across layers is particularly simple, since first the input layer is active, then the first hidden layer, then the next, etc., until the output layer is reached. If, for definiteness, we choose  $\tanh$  as the activation function, and let 1 refer to the input layer, 2 to the first hidden layer, etc., the dynamics can be described by Equation (5). Note that because the activity of each layer is synchronized and depends only on that of the previous layer at the previous time step, the role of time is trivial. Since each variable only changes its value once during a given feed-forward step, we can drop time labels without ambiguity.

$$\begin{aligned} x_{2j} &= \tanh\left(\sum_i w_{1j,i}x_{1i} - \theta_{1j}\right) \\ x_{3k} &= \tanh\left(\sum_j w_{2k,j}x_{2j} - \theta_{2k}\right) \\ x_{4l} &= \tanh\left(\sum_k w_{3l,k}x_{3k} - \theta_{3l}\right). \end{aligned} \quad (5)$$

From this point of view the neural network simply implements a particular family of nonlinear functions, parameterized by the weights  $w$  and the thresholds  $\theta$  [22]. For feed-forward networks the transition rule dynamics is equivalent to a single (instantaneous) mapping. For a recurrent network, in contrast, the dynamics is no longer trivial; any given neuron can change state more than once during a computation. This more interesting dynamics effectively gives the network a memory, so that the set of functions that can be implemented with a given number of neurons is much larger. However, it becomes necessary to make a decision as to when the computation is completed, which complicates the learning problem.

To solve a given problem we must select values of the parameters  $w$  and  $\theta$ , *i.e.*, we must select a particular member of the family of functions specified by the network. This is done by a learning rule.

The Hebbian learning rules are perhaps the simplest and most time honored. They do not require detailed knowledge of the desired outputs, and are easy to implement locally. The idea is simply to strengthen neurons with coincident activity. A simple implementation changes the weights according to the product of the activities on each connection,

$$\Delta w_{ij} = cx_i x_j \quad (6)$$

Hebbian rules are appealing because of their simplicity and particularly because they are local. They can be implemented under very general circumstances. However, learning with Hebbian rules can be ineffective, particularly when there is more detailed knowledge available for training. For example, in some situations we have a training set of patterns for which we know both the correct input and the correct output. Hebbian rules fail to exploit this information, and are correspondingly inefficient when compared with algorithms that do.

Given a learning set of desired input/output vectors, the parameters of the network can be determined to match these input/output vectors by minimizing an error function based on them. The back-propagation algorithm, for example, minimizes the least mean square error and is effectively a nonlinear least-squares fitting algorithm. For more on this, see reference [58].

Since there is an extensive and accessible literature on neural networks, I will not review it further [58,15].

### 3.2 Comparison to a generic network

Neural networks are the canonical example of connectionism and their mapping into generic connectionist terms is straight forward.

- **Nodes** correspond to neurons.
- **Connections** correspond to the axons, synapses, and dendrites of real neurons. The average connection strength is proportional to the weight of each connection.

- **Node dynamics.** There are many possibilities. For feed-forward networks the dynamics is reduced to function evaluation. For recurrent networks the node dynamics may be an automaton, a system of coupled mappings, or a system of ordinary differential equations. The attractors of such systems can be fixed points, limit cycles, or chaotic attractors. More realistic models of the refractory periods of the neurons yield systems of delay-differential equations.
- **Learning rules .** Again, there are many possibilities. For feed-forward networks with carefully chosen neural activation functions such as radial basis functions [11,13,54] where the weights can be solved through a linear algorithm, the dynamics reduces to a function evaluation. Nonlinear search algorithms such as back-propagation are nonlinear mappings which usually have fixed point attractors. Nondeterministic algorithms such as simulated annealing have stochastic dynamics.
- **Graph dynamics.** For real neural systems this corresponds to plasticity of the synapses. There is increasing evidence that plasticity plays an important role, even in adults [2]. As currently practiced, most neural networks do not have explicit graph dynamics; the user simply tinkers with the architecture attempting to get good results. This approach is clearly limited, particularly for large problems where the graph must be sparse and the most efficient way to restrict the architecture is not obvious from the symmetries of the problem. There is currently a great deal of interest in implementing graph dynamics for neural networks, and there are already some results in this direction [26,43,46, 64,66]. This is likely to become a major field of interest in the future.

## 4 Classifier Systems

### 4.1 Background

The classifier system is an approach to machine learning introduced by John Holland [30]. It was inspired by many influences, including production systems in artificial intelligence [48], population genetics, and economics. The central motivation was to avoid the problem of brittleness encountered in expert systems and conventional approaches to artificial intelligence. The classifier system learns and adapts using a low-level abstract representation that it constructs itself, rather than a high-level explicit representation constructed by a human being.

On the surface the classifier system appears quite different from a neural network, and at first glance it is not obvious that it is a connectionist system at all. On closer examination, however, classifier systems and neural networks are quite similar. In fact, by taking a sufficiently broad definition of "classifier systems" and "neural networks", any particular implementation of either one may be viewed as a special case of the other. Classifier systems and neural networks are part of the same class

of models, and represent two different design philosophies for the connectionist approach to learning. The analogy between neural networks and classifier systems has been explored by Compiani *et al.* [14], Belew and Garrity [9], and Davis [16]. There are many different versions of classifier systems; I will generally follow the version originally introduced by Holland [30], but with a few more recent modifications such as intensity and support [31].

At its core, the classifier system has a rule-based language with content addressable memories. The addressing of instructions occurs by matching of patterns or rules rather than by the position of the instructions, as it does in traditional von Neumann languages. Each rule or *classifier* consists of a condition and an action, both of which are fixed length strings. One rule invokes another when the action part of one matches the condition part of the other. This makes it possible to set up a chain of associations; when a given rule is active it may invoke a series of other rules, effecting a computation. The activity of the rules is mediated by a *message list*, which serves as a blackboard or short term memory on which the rules post messages for each other. While many of the messages on the list are posted by other classifiers, some of them are also external messages, inputs to the program posted by activity from the outside world. In the most common implementations the message list is of fixed length, although there are applications where its length may vary. See the schematic diagram shown in Figure (3). You may also want to refer to the example in Section 5.

The conditions, actions, and messages are all strings of the same fixed length. The messages are strings over the binary alphabet  $\{0, 1\}$ , while the conditions and actions are over the alphabet  $\{0, 1, \#\}$ , where  $\#$  is a "wildcard" or "don't care" symbol. The length of the message list controls how many messages can be active at a given time, and is typically much smaller than the total number of rules.

The way in which a classifier system "executes programs" is apparent by examining what happens during a cycle of its operation. At a given time, suppose there is a set of messages on the message list, some of which were posted by other classifiers, and some of which are inputs from the external world. The condition parts of all the rules are matched against all the messages on the message list. A match occurs if each symbol matches with the symbol in the corresponding position. The symbol  $\#$  matches everything. The rules that make matches on a given time step post their actions as messages on the next time step. By going through a series of steps like this, the classifier system can perform a computation. Note that in most implementations of the classifier system each rule can have more than one condition part; a match occurs only when both conditions are satisfied.

In general, because of the  $\#$  symbol, more than one rule may match a given message. The parameters of the classifier system (frequency of  $\#$ , length of messages, length of message list, *etc.*) are usually chosen so that the number of matches typically exceeds the size of the message list. The rules then *bid* against each other to decide which of them will be allowed to post messages. The bids are used to compute a threshold, which is adjusted to keep the number of messages on the message list (that

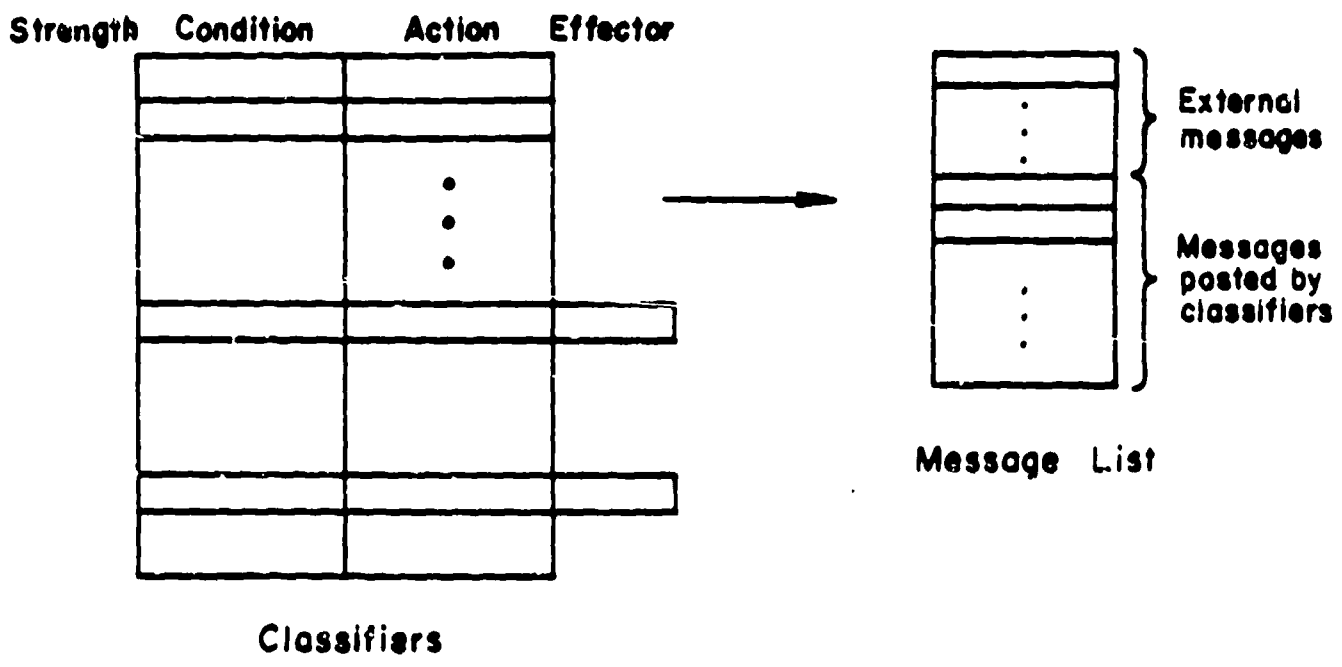


Figure 3: A schematic diagram of the classifier system.



will be posted on the next step) less than or equal to the size of the message list. Only those rules whose bids exceed the threshold are allowed to post their messages on the next time step<sup>3</sup>.

An important factor determining the size of the bid is the *strength* of a classifier, which is a real number attached to each classifier rule. The strength is a central part of the learning mechanism. If a classifier wins the bidding competition and successfully posts a message, an amount equal to the size of its bid is subtracted from its strength and divided among the classifiers that (on the previous time step) posted the messages that match the bidding classifier's condition parts on the current time step<sup>4</sup>.

Another factor in determining the size of bids is the *specificity* of a classifier, which is defined as the percentage of characters in its condition part that are either zero or one, i.e., that are not #. The motivation is that when there are "specialists" to solve a problem, their input is more valuable than that of "generalists".

The final factor that determines the bid size is the *intensity*  $x_i(t)$  associated with a given message. In older implementations of the classifier system, the intensity is a boolean variable, whose value is one if the message is on the message list, and zero otherwise. In newer implementations the intensity is allowed to take on real values  $0 \leq x_i \leq 1$ . Thus, some messages on the list are "more intense" than others, which means they have more influence on subsequent activity. Under the *support rule*, the intensity of a message is computed by taking the sum over all the matching messages on the previous time step, weighted by the strength of the classifier making the match.

The size of a bid is

$$bid = Const \times w \times specificity \times F(intensity), \quad (7)$$

where *Const* is a constant.  $F(intensity)$  is a function of the intensities of the matching messages. There are many options; for example, it can be the intensity of the message generating the highest bid, or the sum of all the matching messages [50].

To produce outputs the classifier system must have a means of deciding when a computation halts. The most common method is to designate certain classifiers as outputs. When these classifiers become active the classifier system makes the output associated with that classifier's message. If more than one output classifier becomes active it is necessary to resolve the conflict. There are various means of doing this; a simple method is to simply pick the output with the largest bid.

Neglecting the learning process, the state of a classifier system is determined by the intensities of its messages (most of which may be zero). In many cases it is important to be able to pass along a particular set of information from one time step to another. This is done by a construction called *pass-through*. The # symbol in the action part of the rule has a different meaning than it does in the condition part of the rule. In the action part of the rule it is used to "pass through" information

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<sup>3</sup>Some implementations allow stochastic bidding.

<sup>4</sup>Other variants are also used. Many authors think that this step is unnecessary, or even harmful; this is a topic of active controversy.

from the message list on one time step to the message list on the next time step; anywhere there is a # symbol in the action part, the message that is subsequently posted contains either a zero or one according to whether the *message matched by the condition part* on the previous time step contained a zero or a one.

The procedure described above allows the classifier system to implement any finite function, as long as the necessary rules are present in the system with the proper strengths (so that the correct rules will be evoked). The transfer of strengths according to bid size defines a learning algorithm, called the *bucket brigade*. The problem of making sure the necessary rules are present is addressed by the use of *genetic algorithms* that operate on the bit strings of the rules as though they were haploid chromosomes. For example, *point mutation* randomly changes a bit in one of the rules. *Crossover* or *recombination* mimics sexual reproduction. It is performed by selecting two rules, picking an arbitrary position, and interchanging substrings so that the left part of the first rule is concatenated to the right part of the second rule and *visa versa*. When the task to be performed has the appropriate structure, crossover can speed up the time required to generate a good set of rules, as compared to pure point mutation<sup>5</sup>.

## 4.2 Comparison to generic network

The classifier system is rich with structure, nomenclature, and lore, and has a literature of its own that has evolved more or less independently of the neural network literature. Nonetheless, the two are quite similar, as can be seen by mapping the classifier system to standard connectionist terms.

For the purpose of this discussion we will assume that the classifiers only have one condition part. The extension to classifiers with multiple condition parts has been made by Compiani *et al.* [14].

- **Nodes.** The messages are labels for the nodes of the connectionist network. For a classifier system with word length  $N$  the  $2^N$  possible messages range from  $i = 0, 1, \dots, 2^N - 1$ . (In practice, for a given set of classifiers, only a small subset of these may actually occur.) The state of the  $i^{\text{th}}$  node is the intensity  $x_i$ . The node activity also depends on a globally defined threshold  $\theta(t)$ , which varies in time.
- **Connections.** The condition and action parts of the classifier rules are a connection list representation of a graph, in the form of Equation (2). Each classifier rule connects a set of nodes  $\{i\}$  to a node  $j$  and can be written  $\{i\} \rightarrow j$ . A rule consisting entirely of ones and zeros corresponds to a single connection; a rule with  $n$  don't care symbols represents  $2^n$  different connections. Note that if two rules share their output node  $j$  and some of their input nodes  $i$  then there are multiple connections between two nodes. The connection parameters  $w_{ij}$

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<sup>5</sup>Several specialized graph manipulation operators, for example triggered cover operators, have also been developed for classifier systems [56].

are computed as the product of the classifier rule strength and the classifier rule specificity i.e.,  $w_{ij} = \text{specificity} \cdot \text{strength}$ . When the graph is sparse there are many nodes that have no rule connecting them so that implicitly  $w_{ij} = 0$ .

Note that only the connections are represented explicitly; the nodes are implicitly represented by the right hand parts of the connection representations, which give all the nodes that could ever conceivably become active. Thus nodes with no inputs are not represented. This can be very efficient when the graph is sparse.

Although on the surface pass-through appears to be a means of keeping recurrent information, as first pointed out by Miller and Forrest [44], in connectionist terms it is a mechanism for efficient graph representation. Pass-through occurs when a classifier has # symbols at the same location in both its condition and action parts. (If the # is only in the action part, then the pass-through value is always the same, and so it is irrelevant.) The net effect is that the node that is activated on the output depends on the node that was active on the input. This amounts to representing more than one connection with a single classifier. For example, consider the classifier  $0\# \rightarrow 1\#$ . If node 00 becomes active, then the second 0 is "passed through", so the output is 10. Similarly, if 01 becomes active, the output is 11. The net result is that two connections are represented by the same classifier. From the point of view of the network, the classifier  $0\# \rightarrow 1\#$  is equivalent to the two classifiers  $00 \rightarrow 10$  and  $01 \rightarrow 11$ . The net effect is thus a more efficient graph representation, and pass-through is just a representational convenience.

- **Transition rule.** In traditional classifier systems a node  $j$  becomes active on time step  $t + 1$  if it has an input connection  $i$  on time step  $t$  such that  $x_i(t)w_{ij} > \theta$ . Using the support rule,

$$x_j(t + 1) = \sum_i x_i(t)w_{ij}, \quad (8)$$

where the sum is taken over all  $i$  that satisfy  $x_i(t)w_{ij} > \theta$ . With the support rule the dynamics is thus piecewise linear, with nonlinearity due to the effect of the threshold  $\theta$ . Without the support rule the intensity is  $x_j(t + 1) = \max_i \{x_i(t)\}$ .

There are two approaches to computing the threshold  $\theta$ . The simplest approach is to simply set it to a constant value  $\theta$ . A more commonly used approach in traditional classifier systems is to adjust  $\theta(t)$  on each time step so that the number of messages that are active on the message list is less than or equal to a constant, which is equivalent to requiring that the number of nodes active on a given time step is less than or equal to a constant. In connectionist terms this may be visualized as adding a special thresholding unit that has input and output connections to every node.

- **Learning rule.** The traditional learning algorithm for classifier systems is the bucket brigade, which is a particular modified Hebbian learning rule. (See

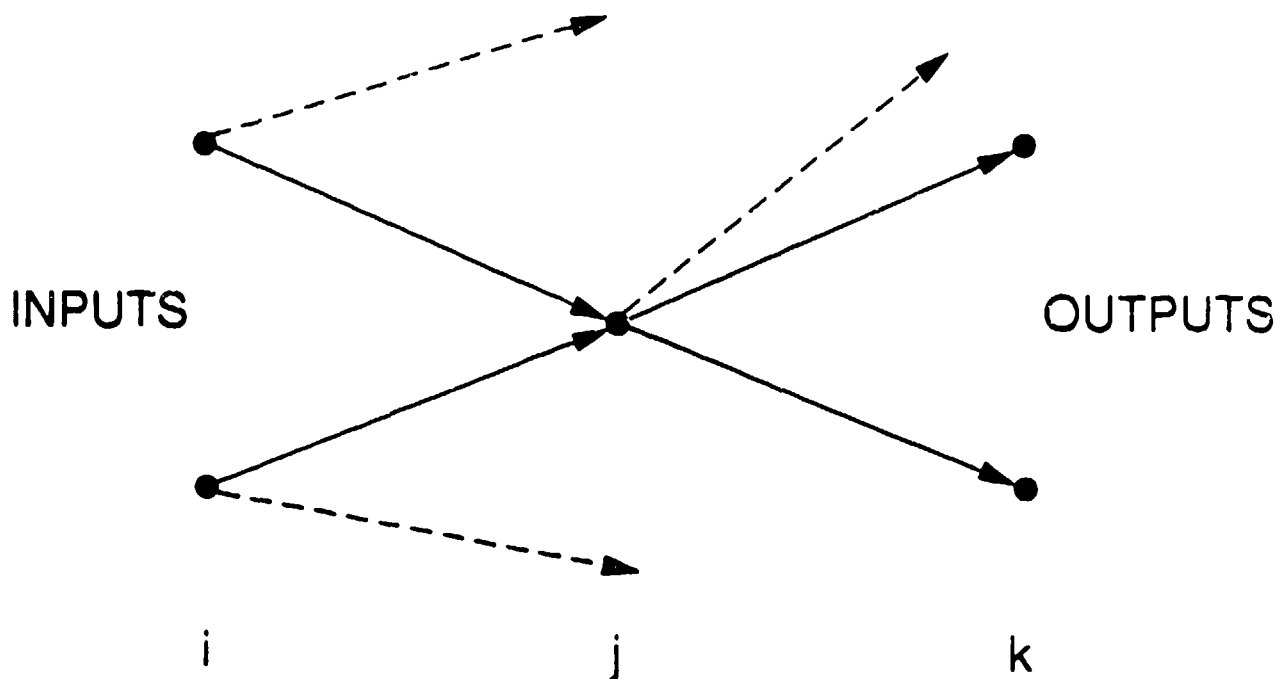


Figure 4: *The bucket brigade learning algorithm.* A wave of activity propagates from nodes  $\{i\}$  at time  $t - 1$  through node  $j$  at time  $t$  to nodes  $\{k\}$  at time  $t + 1$ . The solid lines represent active connections, and the dashed lines represent inactive connections. Strength is transferred from the input connections of  $j$  to output connections of  $j$  according to Equation (11). The motivation is that connections “pay” the connections that activate them.

Equation (6)). When a node becomes active, strength is transferred from its active output connections to its active input connections. This transfer occurs on the time step after it was active. To be more precise, consider a wave of activity  $x_j(t) > 0$  propagating through node  $j$ , as shown in Figure (4).

Suppose this activity is stimulated by  $m$  activities  $x_i(t - 1) > 0$  through input connection parameters  $w_{ij}$ , and in turn stimulates activities  $x_k(t + 1) > 0$  through output connection parameters  $w_{jk}$ . Letting  $H$  be the Heaviside function  $H(x) = 1$  for  $x > 0$ ,  $H(x) = 0$  for  $x \leq 0$ , the input connections gain strength according to

$$\Delta w_{ij} = \frac{x_j}{m} \sum_k w_{jk} H(x_j w_{jk} - \theta) \quad (9)$$

$$\Delta w_{jk} = -x_j w_{jk} H(x_j w_{jk} - \theta) \quad (10)$$

(11)

where  $\Delta w_{ij} = w_{ij}(t+1) - w_{ij}(t)$ . All the quantities on the right hand side are evaluated at time  $t$ .

This is only one of several variants of the bucket brigade learning algorithm; for discussion of other possibilities see Reference [10].

In order to learn, the system must receive feedback about the quality of its performance<sup>6</sup>. To provide feedback about the overall performance of the system, the output connections of the system, or the *effectors*, are given strength according to the quality of their outputs. Judgements as to the quality must be made according to a predefined evaluation function. To prevent the system from accumulating useless classifiers, causing isolated connections, there is an activity tax which amounts to a dissipation term. Putting all of these effects together and following reference [21] we can write the bucket brigade dynamics (the learning rule) as

$$\Delta w_{ij} = \frac{1}{m} \sum_k x_j w_{jk} H(x_j w_{jk} - \theta) - x_i w_{ij} H(x_i w_{ij} - \theta) + x_i P(t) - k w_{ij}, \quad (12)$$

where  $k$  is the dissipation rate for the activity tax, and  $P(t)$  is the evaluation function for outputs at time  $t$ .

- **Graph dynamics.** The graph dynamics occurs through manipulations of the graph representation (the classifier rules) through genetic algorithms such as point mutation and crossover. These operations are stochastic and are highly nonlocal; they preserve either the input or the output of each connection, but the other part can move to a very different part of the graph. The application of these operators generates new connections, which is usually accompanied by the removal of other connections.

### 4.3 An example

An example makes the graph-theoretic view of classifier systems clearer. For example, consider the classic problem of exclusive-or. (See also Belew and Gherrity [9].) The exclusive-or function is 0 if both inputs are the same and 1 if both inputs are different. The standard neural net solution of this problem is easily implemented with three classifiers:

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<sup>6</sup>It is clearly important to maintain an appropriate distribution of strength within a classifier system, which does not overly favor input or output classifiers, and which can set up chains of appropriate associations. Strength is added to classifiers that participate in good outputs, and then the bucket brigade causes a local transfer of feedback, in the form of connection strength, from outputs to inputs. This is further complicated by the recursive structure of classifier systems, which corresponds to loops in the graph. Maintaining an appropriate gradient of strength from outputs to inputs has proved to be a difficult issue in classifier systems.

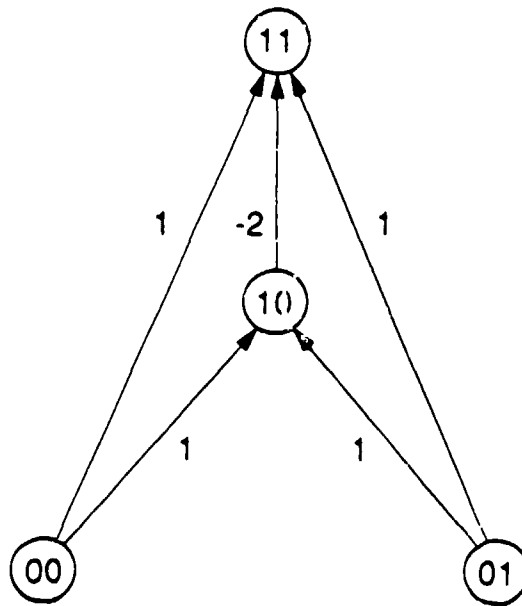


Figure 5: A classifier network implementing the exclusive-or in standard neural net fashion. The binary numbers, which in classifier terms would be messages on the message list, label the nodes of the network.

- $0\# \rightarrow 10 : +1$
- $0\# \rightarrow 11 : +1$
- $10 \rightarrow 11 : -2.$

(The number after the colon is  $w = \text{strength} \times \text{the specificity.}$ ) Although there are only three classifiers, because of the  $\#$  symbols they make five connections, as shown in Figure (5).

With this representation the node 00 represents one of the inputs, and 01 represents the other input; the state of each input is its intensity. If both inputs are 1, for

node	intensity			
00	1	1	1	1
01	1	1	1	1
10	0	1	1	1
11	0	1	0	0

Table 1: A wave of activity caused by the inputs (1,1) is shown in the following table. The numbers from left to right are the intensities on successive iterations. Initially the two input messages have intensity 1, and the others are 0. The input messages activate messages 10 and 11, and then 10 switches 11 off. For the input (0,0), in contrast, the network immediately settles to a fixed point with the intensities of all the nodes at zero.

example, then nodes 00 and 01 become active, in other words, they have intensity  $> 0$ , which is equivalent to saying that the messages 00 and 01 are placed on the message list. Assume that we use the support rule, Equation (8), that outputs occur when the activity on the message list settles to a fixed point, and that the message list is large enough to accommodate at least four messages. An example illustrating how the computation is accomplished is shown in the table of Figure (5).

This example is unusual from the point of view of common classifier system practice in several respects. (1) The protocol of requiring that the system settle to a fixed point in order to make an output. A more typical practice would be to make an output whenever one of the output classifiers becomes active. (2) The message list is rather large for the number of classifiers, so the threshold is never used. (3) There are no recursive connections (loops in the graph).

There are simpler ways to implement exclusive-or with a classifier system. For example, if we change the input protocol and let the input message be simply the two inputs, then the classifier system can solve this with four classifiers whose action parts are the four possible outputs. This always solves the problem in one step with a message list of length one. Note that in network terms this corresponds to unary inputs, with the four possible input nodes representing each possible input configuration. While this is a cumbersome way to solve the problem with a network, it is actually quite natural with a classifier system.

#### 4.4 Comparison of classifiers and neural networks

There are many varieties of classifier systems and neural networks. Once the classifier system is described in connectionist terms, it becomes difficult to distinguish between them. In practice, however, there are significant distinctions between neural nets *as they are commonly used* and classifier systems *as they are commonly used*. The appropriate distinction is not between classifiers and neural networks, but rather between the two design philosophies represented by the typical implementations of connectionist networks within the classifier system and neural net communities. A comparison of classifier systems and neural networks in a common language illustrates their differences more clearly and suggests a natural synthesis of the two approaches.

- **Graph topology and representation.** The connection list graph representation of the classifier system is efficient for sparse graphs, in contrast to the connection matrix representation usually favored by neural net researchers. This issue is not critical on small problems that can be solved by small networks which allow the luxury of a densely connected graph. On larger problems, use of a sparsely connected graph is essential. If a large problem cannot be solved with a sparsely connected network, then it cannot feasibly be implemented in hardware or on parallel machines where there are inevitable constraints on the number of connections to a given node.

To use a sparse network it is necessary to discover a network topology suited to a given problem. Since the number of possible network topologies is exponen-

tially large, this can be difficult. For a classifier system the sparseness of the network is controlled by the length of each message, and by the number of classifiers and their specificity. Genetic algorithms provide a means of discovering a good network, while maintaining the sparseness of the network throughout the learning process. (Of course, there may be problems with convergence time.) For neural nets, in contrast, the most commonly used approach is to begin with a network that is fully wired across adjacent layers, train the network, and then prune connections if their weights decay to zero. This is useless for a large problem because of the dense network that must be present at the beginning.

The connection list representation of the classifier system, which can be identified with that of production systems, potentially makes it easier to incorporate prior knowledge. For example, Forrest has shown that the semantic networks of KL-ONE can be mapped into the classifier system [23]. On the other hand, another common form of prior knowledge occurs in problems such as vision, when there are group invariances such as translation and rotation symmetry. In the context of neural nets, Giles *et al.* [25] have shown that such invariances can be hard-wired into the network by restricting the network weights and connectivity in the proper manner. This could also be done with a classifier system by imposing appropriate restrictions on the rules produced by the genetic algorithm.

- **Transition rule.** Typical implementations of the classifier system apply a threshold to each input separately, before it is processed by the node, whereas in neural networks it is more common to combine the inputs and then apply thresholds and activation functions. It is not clear which of these approaches is ultimately more powerful, and more work is needed.

Most implementations of the classifier system are restricted to either linear threshold activation functions or maximum input activation functions. Neural nets, in contrast, utilize a much broader class of activation functions. The most common example is probably the sigmoid, but in recent work there has been a move to more flexible functions, such as radial basis functions [11,13,47,54] and local linear functions [22,35,67]. Some of these functions also have the significant speed advantage of linear learning rules<sup>7</sup>. In smooth environments, smooth activation functions allow more compact representations. Even in environments where *a priori* it is not obvious that smoothness plays a role, such as learning boolean functions, smooth functions often yield better generalization results and accelerate the learning process [67]. Implementation of smoother activation functions may improve performance of classifier systems in some problems.

Traditionally, classifier systems use a threshold computed on each time step in order to keep the number of active nodes below a maximum value. Computation of the threshold in this way requires a global computation that is expensive from

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<sup>7</sup>Linear learning rules are sometime criticized as "not local". Linear algorithms are, however, easily implemented in parallel by systolic arrays, and converge in logarithmic time.



a connectionist point of view. Future work should concentrate on constant or locally defined thresholds.

From a connectionist point of view, classifiers with the # symbol correspond to multiple connections constrained to have the same strength. There is no obvious reason why their lack of specificity should give them less connection strength. This intuition seems to be borne out in numerical experiments using simplified classifier systems [65].

- **Learning rule.** The classifier system traditionally employs the bucket brigade learning algorithm, whose feedback is condensed into an overall performance score. In problems where there is more detailed feedback, for example a set of known input-output pairs, the bucket-brigade algorithm fails to use this information. This, combined with the lack of smoothness in the activation function, causes it to perform poorly in problems such as learning and forecasting smooth dynamical systems<sup>8</sup>. Since there are now recurrent implementations of back-propagation [53], it makes sense to incorporate this into a classifier system with smooth activation functions, to see whether this gives better performance on such problems [9].

For problems where there is only a performance score, the bucket brigade is more appropriate. Unfortunately, there have been no detailed comparisons of the bucket brigade algorithm against other algorithms that use "learning with a critic". The form of the bucket brigade algorithm is intimately related to the activation dynamics, in that the size of the connection strength transfers are proportional to the size of the input activation signal (the bid). Although coupling of the connection strength dynamics to the activation dynamics is certainly necessary for learning, it is not clear that the threshold activation level is the correct or only quantity to which the learning algorithm should be coupled. Further work is needed in this area.

## 5 Immune networks

### 5.1 Background

The basic task of the immune system is to distinguish between self and non-self, and to eliminate non-self. This is a problem of pattern learning and pattern recognition in the space of chemical patterns. This is a difficult task, and the immune system performs it with high fidelity, with an extraordinary capacity to make subtle distinctions between molecules that are quite similar.

The basic building blocks of the immune system are *antibodies*, "y" shaped molecules that serve as identification tags for foreign material; *lymphocytes*, cells that produce antibodies and perform discrimination tasks; and *macrophages*, large cells that remove material tagged by antibodies. Lymphocytes have antibodies attached to their

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<sup>8</sup>Stephen Pope, unpublished research.

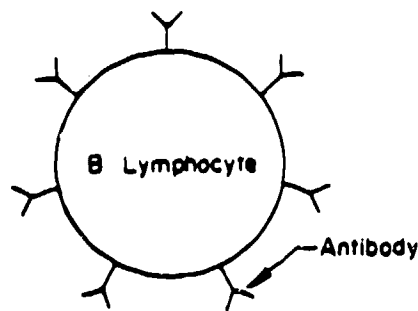
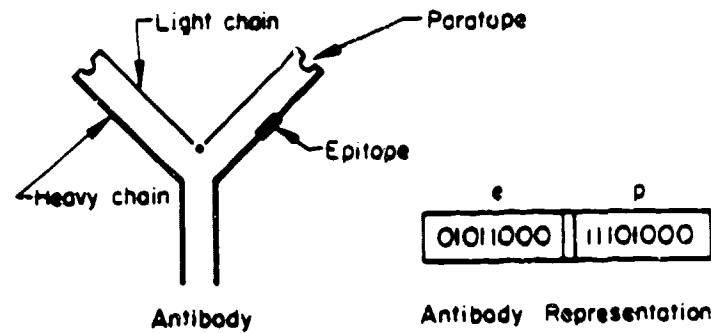


Figure 6: A schematic representation of the structure of an antibody, an antibody as we represent it in our model, and a B-lymphocyte with antibodies on its surface that function as antigen detectors.

surface which serve as antigen detectors. (See Figure 6.) Foreign material is called *antigen*. A human contains roughly  $10^{20}$  antibodies and  $10^{12}$  lymphocytes, organized into roughly  $10^8$  distinct *types*, based on the chemical structure of the antibody. Each lymphocyte has only one type of antibody attached to it. Its type is equivalent to the type of its attached antibodies. The majority of antibodies are *free antibodies*, i.e. not attached to lymphocytes. The members of a given type form a *clone*, i.e., they are chemically identical.

The difficulty of the problem solved by the immune system can be estimated from the fact that mammals have roughly  $10^5$  genes, coding for the order of  $10^9$  proteins. An *antigenic determinant* is a region on the antigen that is recognizable by an antibody. The number of antigenic determinants on a protein such as myoglobin is the order of 50, with 6 – 8 amino acids per region. We can compare the difficulty of telling proteins apart to a more familiar task by assuming that each antigenic determinant is roughly as difficult to recognize as a face. In this case the pattern recognition task performed by the immune system is comparable to recognizing a million different faces. A central question is the means by which this is accomplished.

Does the immune system function as a gigantic look up table, like a neural network with billions of "grandmother cells"? Or, does it have an associative memory with computational capabilities?

The argument given above neglects the important fact that there are  $10^5$  distinct proteins only *if we neglect the immune system*. Each antibody is itself a protein, and there are  $10^8$  distinct antibodies, which appear to be a contradiction: How do we generate  $10^8$  antibodies with only  $10^5$  genes? The answer lies in combinatorics. Each antibody is chosen from seven gene segments, and each gene segment is chosen from a "family" or set of possible variants. The total number of possible antibody types is then the product of the sizes of each gene family. This is not known exactly, but is believed to be on the order of  $10^7 - 10^8$ . Additional diversity is created by *somatic mutation*. When the lymphocytes replicate, they do so with an unusually large error rate in their antibody genes. Although it is difficult to estimate the number of *possible* types precisely, it is probably much larger than the number of types that are actually present in a given organism.

The ability to recognize and distinguish self is *learned*. How the immune system accomplishes this task is unknown. However, it is clear that one of the main tools the immune system uses is *clonal selection*. The idea is quite simple: A particular lymphocyte can be stimulated by a particular antigen if it has a chemical reaction with it. Once stimulated it replicates, producing more lymphocytes of the same type, and also secreting free antibodies. These antibodies bind to the antigen, acting as a "tag" instructing macrophages to remove the antigen. Lymphocytes that do not recognize antigen do not replicate and are eventually removed from the system.

While clonal selection explains how the immune system recognizes and removes antigen, it does not explain how it distinguishes it from self. From both experiments and theoretical arguments, it is quite clear that this distinction is learned rather than hard-wired. Clonal selection must be suppressed for the molecules of self. How this actually happens is unknown.

A central question for self-nonself discrimination is: Where is the seat of computation? It is clear that a significant amount of computation takes place in the lymphocytes, which have a sophisticated repertoire of different behaviors. It is also clear that there are complex interactions between lymphocytes of the same type, for example, between the different varieties of T-lymphocytes and B-lymphocytes. These interactions are particularly strong during the early stages of development.

Niels Jerne proposed that a significant component of the computational power of the immune system may come from the interactions of different types of antibodies and lymphocytes *with each other* [33,34]. The argument for this is quite simple: Since antibodies are after all just molecules, then from the point of view of a given molecule other molecules are effectively indistinguishable from antigens. He proposed that much of the power of the immune system to regulate its own behavior may come from interacting antibodies and lymphocytes of many different types<sup>9</sup>.

There is good experimental evidence that network interactions take place, particu-

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<sup>9</sup>Such networks are often called *idiotypic networks*.

larly in young animals. Using the nomenclature that an antibody that reacts directly with antigen is AB1, an antibody that reacts directly with AB1 is AB2, *etc.*, antibodies in categories as deep as AB4 have been observed experimentally<sup>10</sup>. Furthermore, rats raised in sterile environments have active immune systems, with activity between types. Nonetheless, the relevance of networks in immunology is highly controversial.

## 5.2 Connectionist models of the immune system

While Jerne proposed that the immune system could form a network similar to that of the nervous system, his proposal was not specific. Early work on immune networks put this proposal into more quantitative terms, assuming that a given AB1 type interacted only with one antigen and one other AB2 type. These interactions were modeled in terms of simple differential equations whose three variables represented antigen, AB1, and AB2 [55,28]. A model that treats immune interactions in a connectionist network<sup>11</sup>, allowing interactions between arbitrary types, was proposed in reference [21]. The complicated network of chemical interactions between different antibody types, which are impossible to model in detail from first principles, was taken into account by constructing an artificial antibody chemistry. Each antigen and antibody type is assigned a random binary string, describing its "chemical properties". Chemical interactions are assigned based on complementary matching between strings. The strength of a chemical reaction is proportional to the length of the matching substrings, with a threshold below which no reaction occurs. Even though this artificial chemistry is unrealistic in detail, hopefully it correctly captures some essential qualitative features of real chemistry.

A model of gene shuffling provides metadynamics for the network. This is most realistically accomplished with a gene library of patterns, mimicking the gene families of real organisms. These families are randomly shuffled to produce an initial population of antibody types. This gives an initial assignment of chemical reactions, through the matching procedure described above, including rate constants and other parameters<sup>12</sup>. Kinetic equations implement clonal selection; some types are stimulated by their chemical reactions, while others are suppressed. Types with no reactions are slowly flushed from the system so that they perish. Through reshuffling of the gene library new types are introduced to the system. It is also possible to simulate somatic mutation through point mutations of existing types, proportional to their rate of replication.

It is difficult to model the kinetics of the immune system realistically. There are five different classes of antibodies, with distinct interactions and properties. There are

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<sup>10</sup>This classification of antibodies should not be confused with their type: a given type can simultaneously be AB1 and AB2 relative to different antigens, and many different types may be AB1.

<sup>11</sup>Another connectionist model with a somewhat different philosophy was also proposed by Hoffmann [29].

<sup>12</sup>The genetic operations described here are more sophisticated than those actually used in reference [21]; more realistic mechanisms have been employed in subsequent work [50,17,18].

different types of lymphocytes, including helper, killer and suppressor T-cells, which perform regulatory functions, as well as B-cells, which can produce free antibodies. All of these have developmental stages, with different responses in each stage. Chemical reactions include cell-cell, antibody-antibody, and cell-antibody interactions. Furthermore, the responses of cells are complicated and often state dependent. Thus, any kinetic equations are necessarily highly approximate, and applicable to only a subset of the phenomena.

In our original model we omitted T-cells, treating only B-cells. (This can also be thought of as modeling the response to certain polymeric antigens, for which T-cells seem to be irrelevant.) We assumed that the concentration of free antibodies is in equilibrium with the concentration of lymphocytes, so that their populations can be lumped together into a single concentration variable. Since the characteristic time scale for the production of free antibodies is minutes or hours, while that of the population of lymphocytes is days, this is a good approximation for some purposes. It turns out, however, that separating the concentration of lymphocytes and free antibodies and considering the cell-cell, antibody-antibody, and cell-antibody reactions separately gives rise to new phenomena that are important for the connectionist view. In particular, this generates a more interesting repertoire of steady states, including "mildly excited" self-stimulated states suggestive of those observed in real immune systems [50,17,18].

### 5.3 Comparison to a generic network

As with classifier systems and neural networks, there are several varieties of immune networks [21,17,29,63], and it is necessary to choose one in order to make a comparison. The model described here is based on that of Farmer, Packard and Perelson [21], with some modifications due to later work by Perelson [50] and DeBoer and Hogeweg [17]. Also, since this model only describes B-cells, whenever necessary I will refer to it as a B-cell network, to distinguish it from models that also incorporate the activity of T-cells.

To discuss immune networks in connectionist terms it is first necessary to make the appropriate map to nodes and connections. The most obvious mapping is to assign antibodies and antigens to nodes. However, since antibodies and antigens typically have more than antigenic determinant, and each region has a distinct chemical shape<sup>13</sup>, we could also make the regions (or chemical shapes) the fundamental variable. Since all the models discussed above treat the concentration of antibodies and lymphocytes as the fundamental variables, I shall make the identification at this level. This leads to the following connectionist description:

- **Nodes** correspond to antibodies, or more accurately, to distinct antibody types. Antigens are another type of node with different dynamics; from a certain point of view the antigen concentrations may be regarded as the input and output

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<sup>13</sup>"Chemical shape" here means all the factors that influence chemical properties, including geometry, charge, polarization, etc.

nodes of the network<sup>14</sup>. The free antibody concentrations, which can change on a rapid time scale, are the states of the nodes. They are the immediate indicators of information processing in the network. The lymphocyte concentrations, which change on an intermediate time scale, are node parameters. (Recall that there is a one-to-one correspondence between free antibody types and lymphocyte types). Changes in lymphocyte concentration are the mechanism for learning in the network.

- **Connections.** The physical mechanisms which cause connections between nodes are chemical reactions between antibodies, lymphocytes, and antigens. The strength of the connections depends on the strength of the chemical reactions. This is in part determined by chemical properties, which are fixed in time, and in part by the concentrations of the antibodies, lymphocytes, and antigens, which change with time. Thus the instantaneous connection strength changes in time as conditions change in the network. The precise way of representing and modeling the connections is explained in more detail in the following.
- **Graph representation.** To model the notion of “chemical properties” we assign each antibody type a binary string. To determine the rate of the chemical reaction between type  $i$  and type  $j$ , the binary string of type  $i$  is compared to binary string of type  $j$ . A match strength matrix  $m_{ij}$  is assigned to this connection, which depends on the degree of complementary matching between the two strings. Types whose strings have a high degree of complementary matching are assigned large reaction rates. Since the matching algorithm is symmetric<sup>15</sup>  $m_{ij} = m_{ji}$ .

There is a threshold for the length of the complementary matching region below which we assume that no reaction occurs and set  $m_{ij} = 0$ . Since  $m_{ij}$  is the connection matrix of the graph, setting  $m_{ij} = 0$  amounts to deleting the corresponding connection from the graph. We thus neglect reactions that are so weak that they have an insignificant effect on the behavior of the network. The match threshold together with the length of the binary strings determines the sparseness of the graph. When the system is sparse the matrix  $m_{ij}$  can also be represented in the form of a connection list. The match strength for a given pair of immune types does not change with time. However, as new types are added or deleted from the system, the  $m_{ij}$  that are relevant to the types in the network change.

The graph dynamics provides a mechanism of learning in the immune system; as new types are tested by clonal selection, the graph changes, and the system “evolves”. Another mechanism for dynamical learning depends on the lymphocyte concentrations, as discussed below.

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<sup>14</sup>Future models should include chemical types identified with self as yet another type of node.

<sup>15</sup>In our original paper [21] we also considered the case of asymmetric interactions. However, this is difficult to justify chemically, and it is probably safe to assume that the connections are symmetric [28].

- **Dynamics.** The  $m_{ij}$  are naturally identified as connection parameters for the network. For any given  $i$  and  $j$ , however, the  $m_{ij}$  are fixed. Thus, learning in B-cell immune networks occurs not by changing connection parameters, but rather by changing the lymphocyte concentration, which is a parameter of the nodes. The net reaction flux (or strength of the reaction) is a nonlinear function of the lymphocyte concentration. Thus changing the lymphocyte concentration changes the effective connection strength. This is a fundamental difference between neural networks and B-cell immune networks; while the connection strength is changeable in both cases, in B-cell immune networks all the connection strengths to a given node change in tandem as the lymphocyte concentration varies. However, since the reaction rates are nonlinear functions, a change in lymphocyte concentration may effect each connection differently, depending on the concentration of the other nodes.

The dynamics of the real immune system are not well understood. The situation is similar to that of neural networks; we construct simplified heuristic immune dynamics based on a combination of chemical kinetics and experimental observations, attempting to recover some of the phenomena of real immune systems. The real complication arises because lymphocytes are cells, and understanding their kinetics requires understanding how they respond to stimulation and suppression by antigens, antibodies, and other cells. At this point our understanding of this is highly approximate and comes only from experimental data. The kinetic equations used in our original paper were highly idealized [21]. The more realistic equations quoted here are due to DeBoer and Hogeweg<sup>16</sup> [17].

Let  $i$  label the nodes of the system,  $x_i$  the concentration of antibodies, and  $\theta_i$  the concentration of lymphocytes<sup>17</sup>. The amount of stimulation received by lymphocytes of type  $i$  is approximated as

$$s_i = \sum_j m_{ij} x_j \quad (13)$$

The rate of change of antibody concentration is due to production by lymphocytes, removal from the system, and binding with other antibodies. The equations are

$$\frac{dx_i}{dt} = \theta_i f(s_i) - kx_i - cx_i s_i. \quad (14)$$

$k$  is a dissipation constant and  $c$  the binding constant.  $f$  is a function describing the degree of stimulation of a lymphocyte. Experimental observations show that  $f$  is bell-shaped. A function with this rough qualitative behavior can be

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<sup>16</sup>More realistic equations have also proposed by Segel and Perelson [80], Perelson [51,50], and Varela et al. [63].

<sup>17</sup>Note that we use  $\theta$  to represent lymphocytes because they play the role of node parameters. However, they are not thresholds, but rather quantities whose primary function is to modify connection strength.

constructed by taking the product of a sigmoid with an inverted sigmoid, for example

$$f(z) = \frac{zk_2}{(k_1 + z)(k_2 + z)}. \quad (15)$$

The production of lymphocytes is due to replenishment by the bone marrow, cell replication, and removal from the system. The equations are

$$\frac{d\theta_i}{dt} = r + p\theta_i f(s_i) - k\theta_i. \quad (16)$$

$r$  is the rate of replenishment and  $p$  is a rate constant for replication.

## 5.4 Comparison to neural networks and classifier systems

There are significant differences between the dynamics of immune networks and neural networks. The most obvious is in the form of the transition and learning rules. The nodes of the immune network are activated by a bell-shaped function rather than a sigmoid function. Since the bell-shaped function undergoes an inflection and its derivative changes sign, the dynamics are potentially more complicated.

B-cell immune networks differ from neural networks in that there is no variable which acts as a connection parameter. Instead, the connection strength is indirectly determined by the node parameters (concentrations and kinetic equations). The instantaneous connection strength is

$$\frac{\partial \dot{x}_i}{\partial x_j} = (\theta_i f'(s_i) - cx_i)m_{ij} - cs_i - k\delta_{ij} \quad (17)$$

where  $\delta_{ij} = 0$  for  $i \neq j$ ,  $\delta_{ii} = 1$ . All of the terms in this equation except for  $f'$  are greater than or equal to zero. For low values of  $s_i$ ,  $f'(s_i) > 0$ , but for large values of  $s_i$ ,  $f'(s_i) < 0$ . Given the structure of these equations, as  $s_i$  increases, at some point before  $f$  reaches a maximum, all the connections to a given node change from excitatory to inhibitory. The point at which this happens depends on the lymphocyte concentration of  $i$ , the antibody concentration, the concentration of the other antibodies, and on the exact form of the stimulation function. Thus, in contrast to neural networks or the classifier system, a given connection can be either excitatory or inhibitory depending on the state of the system.

The connections in the immune system are chemical reactions. Insofar as the immune system is well-stirred, this allows a potentially very large connectivity, as high as the number of different chemical types a given type can react with. In practice, the number of types that a given type reacts with can be as high as about 1000. Thus, the connectivity of real immune networks is apparently of the same order of magnitude as that of real neural networks.

One of the central differences between the B-cell immune networks and neural or classifier networks is that for the immune system there are no independent parameters on the connections. If the average strength of a connection to a given node cannot be



adjusted independently of that of other nodes, the learning capabilities of the network may be much weaker or more inefficient than those of networks where the connection parameters are independent. As discussed in the next section, this may be altered by the inclusion of T-cells in the models.

## 5.5 Directions for future research

Whether immune networks are a major component of the computational machinery of the immune system is a subject of great debate. The analogy between neural networks and immune networks suggests that immune networks potentially possess powerful capabilities, such as associative memory, that could be central to the functioning of the immune system. However, before this idea can reach fruition we need more demonstrations of what immune networks can do. At this point the theory of immune networks is still in its infancy and their utility remains an open question.

The immune network may be able to perform tasks that would be impossible for individual cells. Consider, for example, a large antigen such as a bacterium with many distinct antigenic determinants. If each region is chemically distinct, a single type can interact with at most a few of them (and thus a single cell can interact with at most a few of them). Network interactions, in contrast, potentially allow different cells and cell types to communicate with each other and make a collective computation to reinforce or suppress each other's immune responses. For example, suppose A, B, C and D are active sites. It might be useful for a network to implement an associative memory rule such as: If any three of A, B, C, and D are present, then generate an immune response; otherwise do not. Such an associative memory requires the capability to implement a repertoire of Boolean functions. A useful rule might be: Generate an immune response if active site A is present, or active site B is present, but not if both are present simultaneously". Such a rule, which is equivalent to taking the exclusive-or function of A and B, might be useful for implementing self tolerance. Such logical rules are easily implemented by networks. It is difficult to see how they could be implemented by individual cells all of the same type.

Immune memory is another task in which networks may play an essential role. Currently the prevailing belief is that immune memory comes about because of special memory cells. It is certainly true that some cells go into developmental states that are indicative of memory. Although the typical lifetime of a lymphocyte is about five days, there are some lymphocytes that have been demonstrated to persist for as long as a month. This is a far cry, however, from the eighty or more years that a human may display an immune memory. Since cells are normally flushed from the system at a steady rate, it is difficult to believe that any individual cell could last this long. It is only the type, then, that persists, but in order to achieve this individual cells must periodically replicate themselves. However, in order to hold the population stable the replication rate must be perfectly balanced against the removal rate. This is an unstable process unless there is feedback holding the population stable. It is difficult to see how feedback on the population size can be given unless there are network interactions.

In an immune network a memory can potentially be modeled by a fixed point of the network. The concentrations at the fixed point are held constant through the feedback of one type to another type. Models of the form of Equations (14) and (16) contain fixed points that might be appropriate for immune memory. However, it is clear from experiments that T-cells are necessary for memory, and so must be added to immune networks to recover this effect.

T-cells are a key element missing from most current immune network models. T-cells play an important role in stimulating or suppressing reactions between antibodies and antigens, and are essential to immune memory. From the point of view of learning in the network, they may also indirectly act as specific connection parameters.

One of the most interesting activities of the immune system is "antigen presentation". When a B-cell or macrophage reacts with an antigen it may process it, discarding all but the antigenic determinants. It then presents the antigenic determinant on its surface (as a peptide bound to an MHC molecule). The T-cell reacts with the antigenic determinant and the B-cell, and based on this information may either stimulate or suppress the B-cell. Note that antigen presentation provides information about *both* the B-cell *and* an antigen, and thus potentially about a specific connection in the network.

In a connectionist model, this may amount to a connection strength parameter; a B-cell presenting a given active site contains information that is specific to two nodes, one for the B-cell of the same type as the T-cell, and one for the antigen whose active site is being presented (which may also be another antibody). Due to their interactions with T-cells, the B-cell populations of type  $i$  presenting antigenic determinants from type  $j$  may play the roles of the connection parameters  $w_{ij}$ .

At this point, it is not clear how strongly the absence of explicit connection parameters limits the computational and learning power of immune networks. However, it seems likely that before they can realize their full potential, connection parameters must be included, taking into account the operation of T-cells. T-cells act like catalysts, either suppressing or enhancing reactions. Since catalytic activity is one of the primary tools used to implement the internal functions of living organisms, it is not surprising that it should play a central role in the immune system as well. Autocatalytic activity is discussed in more detail in the next section.

## 6 Autocatalytic networks

### 6.1 Background

All the models discussed so far are designed to perform learning tasks. The autocatalytic network model of this section differs in that it is designed to solve a problem in evolutionary chemistry. Of course, evolution may also be regarded as a form of learning. For autocatalytic networks there are significant differences in the way this happens.

The central goal of the autocatalytic network is to solve a classic problem in

the origin of life, namely, to demonstrate an evolutionary pathway from a soup of monomers to a polymer metabolism with selected autocatalytic properties, which in turn could provide a substrate for the emergence of contemporary (or other) life forms. When Miller and Urey discovered that amino acids could be synthesized *de novo* from the hypothetical primordial constituents "earth, fire and water" [45], it seemed but a small step to the synthesis of polymers built out of amino acids (polypeptides and proteins). It was hoped that RNA and DNA could be created similarly. However, under normal circumstances longer polymers are not favored at equilibrium. Living systems, in contrast, contain DNA, RNA, and proteins, specific long polymers which exist in high concentration. They are maintained in abundance by their symbiotic relationship with each other: Proteins help replicate RNA and DNA, and DNA and RNA help synthesize proteins. Without the other, neither would exist. How did such a complex system ever get started, unless there were proteins and RNA to begin with? The question addressed in references [36,20,8] is: Under what circumstances can the synthesis of specific long polymers be achieved beginning with simple constituents such as monomers and dimers?

The model here applies to any situation in which unbranched polymers are built out of monomers through a network of catalytic activity. The monomers come from a fixed alphabet,  $a, b, c, \dots$ . They form one-dimensional chains which are represented as a string of monomers,  $acabbacbc \dots$ . The monomer alphabet could be the twenty amino acids, or it could equally well be the four nucleotides. This changes the parameters but not the basic properties of the model. The model assumes that the polymers have catalytic properties, *i.e.*, that they can undergo reactions in which one polymer catalyzes the formation of another. If  $A, B, C$ , and  $E$  are polymers, and  $H$  is water, then the basic reaction is:



where  $E$  is written over the arrows to indicate that it catalyzes the reaction.

Our purpose is to model a chemostat, a reaction vessel into which monomers are added at a steady rate. The chemical species that are added to the chemostat are called the *food set*. We assume that the mass in the vessel is conserved, for example, by simply letting the excess soup overflow. For convenience we assume that the soup is well-stirred, so that we can model it by a system of ordinary differential equations.

In any real system it is extremely difficult to determine from first principles which reactions will be catalyzed, and with what affinity. Very few if any of the relevant properties have been measured experimentally in any detail, and the number of measurements or computations that would have to be made in order to predict all the chemical properties is hopelessly complex. Our approach is to invent an artificial chemistry and attempt to make its properties at least qualitatively similar to those of a real chemical system. Actually we use one of two different artificial chemistries, based on two different principles:

- Random assignment of catalytic properties.

- Assignment of catalytic properties based on string matching.

These two simple artificial chemistries lie on the borders of extreme behavior in real chemistry. In some cases, we know that changing one monomer can have a dramatic effect on the chemical properties of a polymer, either because it causes a drastic change in the configuration of the polymer or because it alters a critical site. If this were always the case, then random chemistry would be a reasonable model.

In other cases, changing a monomer has only a small effect on the chemical properties. Our string matching model is closer to this case; altering a single monomer will only change the quality of matching between two strings by an incremental amount, and should never cause a dramatic alteration in the chemical properties of the polymer.

Another difficulty of modeling real chemistry is that there is an extraordinarily large number of possible reactions. In a vessel with all polymers of length  $l$  or less, for example, the total number of polymer species is  $\sum_{i=1}^l m^i$ , where  $m$  is the number of distinct monomers. For example, with  $m = 20$  and  $l = 100$ , the number of polymer species is in excess of  $20^{100}$ , an extremely large number, and the number of possible reactions is far larger than this. To get around this problem, to first approximation, we neglect spontaneous reactions, and assume that the catalytic properties are sufficiently strong that all catalyzed reactions are much faster than spontaneous reactions<sup>18</sup>.

Once we have assigned chemical properties, we can represent the network of catalyzed chemical reactions as a graph, or more precisely, as a poly-graph with two types of nodes and two types of connections [20]. Because of catalysis the graph must be more complicated than for any of the other networks discussed so far. An example is shown in Figure (7). One type of node is labeled by ovals containing the string representation of the polymer species. The other type of node corresponds to catalyzed reactions, and is labeled by black dots. The dark black connections are undirected (because the reactions are reversible), and connect each reaction to the three polymer species that participate in it; the dotted connections are directed, and connect the reaction to its catalysts. All the edges connect polymers to reactions, and each reaction has at least four connections, three connections for the reaction products and one or more for the catalyst(s). In this illustration we have labeled the members of the food set by double ovals.

If we use the random method of assigning chemical properties, then the graph is a random graph and can be studied using standard techniques. The probability  $p$  that a reaction selected at random will be catalyzed controls the ratio of connections to nodes. As  $p$  increases so does this ratio. As  $p$  grows the graph becomes more and more connected, i.e., more dense. At a critical threshold almost every node becomes connected to at least one other node. As studied in references [36,20], the critical

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<sup>18</sup>In more recent work [7] we make a tractable model for approximate treatment of spontaneous reactions by lumping together all the polymer species of a given length that are not in the autocatalytic network, assuming that they all have the same concentration. These can be viewed as a new type of node in the network. This allows us to include the effect of spontaneous reactions when necessary.

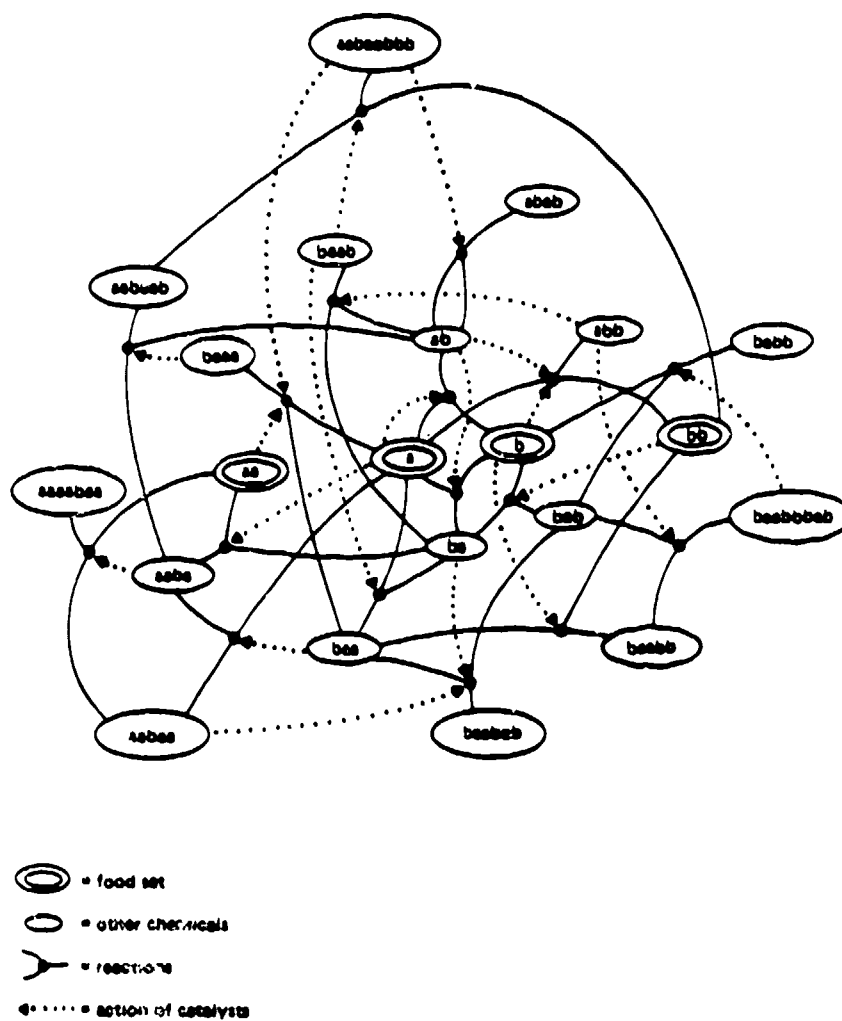


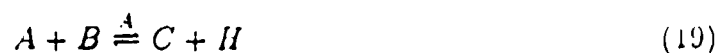
Figure 7: The graph for an autocatalytic network. The ovals represent polymer species, labeled by strings. The black dots represent reactions. The solid lines are connections from polymer nodes to the reactions in which they participate. The dotted lines go from polymer species to the reactions they catalyze. The double ovals are special polymer nodes corresponding to the elements of the food set, whose concentrations are supplied externally.

threshold also depends on the size of the food set, *i.e.*, how many chemical species are in the food set. Using a very approximate estimate of a physically reasonable value of  $p$ , we can make a connected graph from a food set of monomers and dimers [20]. Note that spontaneous reactions create a significant number of dimers, so that supplying monomers automatically produces a supply of dimers as well.

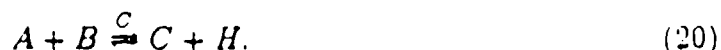
The graph-theoretic analysis only addresses the question of who reacts with whom, and begs the central (and much more difficult) question of concentrations. Numerical modeling of the kinetics *for any given catalyzed reaction* is straightforward but cumbersome. We introduced a simplified technique for treating catalyzed reactions of this type in reference [20] that approximates the true catalyzed kinetics fairly well.

Modeling of the complete kinetics for an entire reaction graph is impossible, since the graph is infinite and under the laws of continuous mass action, even if we initialize all but a finite number of the species to zero concentration, an instant later they will all have non-zero concentrations. From a practical point of view, however, it is possible to circumvent this problem by realizing that any chemical reaction vessel is finite, and species whose continuous concentrations are significantly below the concentration corresponding to the presence of a single molecule are unlikely to participate in any reactions. Thus, to cope with this problem we introduce a concentration threshold, and only consider reactions where all the members on either side of the reaction equation (either  $A$ ,  $B$ , and  $E$ , or  $C$  and  $E$ ) are above the concentration threshold. This then becomes a metadynamical system: At any given time, only a finite number of species are above the threshold, and we only consider a finite graph. As the kinetics act, species may rise above the concentration threshold, so that the graph grows, or they may drop below the threshold, so that the graph shrinks.

One of the main goals of this model is to obtain closure in the form of an *autocatalytic set*. This is a set of polymer species such that each member of the set is produced by at least one catalyzed reaction involving only other members of the set (including the catalysts). Since the reactions are reversible, a species can be "produced" either by cleavage or condensation, depending on which side of equilibrium it finds itself. Thus an autocatalytic set can be quite simple; for example,



is an autocatalytic set, and so is



$A$ ,  $B$ , and  $C$  will be regenerated by supplying either  $A$  and  $B$ , or by supplying  $C$ . Note, however, that such simple autocatalytic sets are only likely to occur when the probability of catalysis is very high. As  $p$  decreases the average size of the smallest autocatalytic set (in a finite population) increases. Depending on the connectivity of the autocatalytic set it may be possible to sustain a large reaction network by supplying only a few polymer species.

There are three notions of the formation of autocatalytic sets, depending on what we mean by "produced by" in the definition given above:

	a	b	ab	bb
v	5	5	5	5
w	5	0	5	7.5
x	0	0	10	5
y	10	20	0	0
z	0	10	10	0

Table 2: An experiment in varying the food set of an autocatalytic set. The table shows the four species of the food set, and the concentration of each that is supplied externally per unit time. Case *v* is used to “grow” the autocatalytic set, and cases *w* - *z* are four changes made once the autocatalytic set is established. *x* and *z* kill the autocatalytic set, while *w* and *y* sustain it with only minimal alteration, as shown in Figure (8).

- *Graph theoretic.* The subgraph defined by the autocatalytic set is closed, so that each member is connected (by a solid connection) to at least one reaction catalyzed by another member.
- *Kinetics.* Each member is produced at a level exceeding a given concentration threshold.
- *Robust.* The autocatalytic set is robust under at least some changes in its food set, *i.e.*, its members are at concentrations sufficiently large and there are enough pathways so that for some alterations of the food set it remains a kinetic autocatalytic set, capable of regenerating removed elements at concentrations above the threshold.

These notions are arranged in order of their strength, *i.e.*, an autocatalytic set in the sense of kinetics is automatically an autocatalytic set in the graph-theoretic sense, and a robust autocatalytic set is automatically a kinetic autocatalytic set.

Describing the details of the conditions under which autocatalytic sets can be created is outside of the scope of this paper. Suffice it to say that, within our artificial chemistry we can create robust autocatalytic sets. Consider, for example, an autocatalytic set based on the monomers *a* and *b*, originally formed by a food set consisting of the species *a*, *b*, *ab*, and *bb*, as shown in Figure (8).

We plot the concentrations of the 21 polymer species in the reactor against an index that orders the species according to their length. We compare four different alterations of the original food set, all of which have the same rate of mass input. For two of the altered food sets the concentration of the members of the autocatalytic set remains almost the same; they are all maintained at high concentration. For the other two, the autocatalytic set “dies” in that some of the members of the set fall below the concentration threshold, and most of the concentrations decrease dramatically. [7]

Our numerical evidence suggests that any fixed reaction network always approaches a fixed point where the concentrations are constant. However, since spontaneous re-

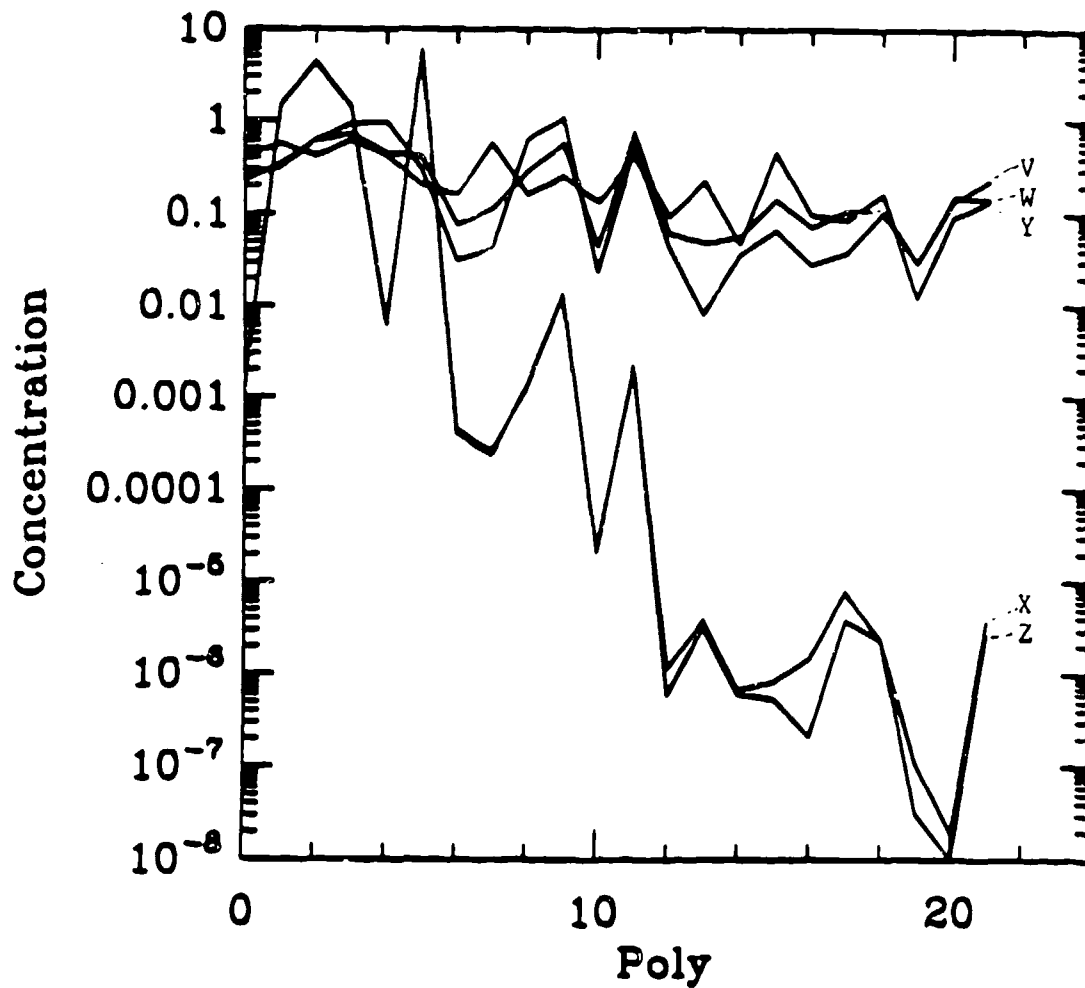


Figure 8: An experiment demonstrating the robust properties of an autocatalytic set. The food set is originally  $a$ ,  $b$ ,  $ab$ , and  $bb$ . The food set is altered in four different ways, as shown in Table 2. For each alteration of the food set the concentrations of all 21 polymers in the autocatalytic set are plotted against the "polymer index". (The polymer index assigns a unique label to each polymer. It is ordered according to length, but is otherwise arbitrary.) Two of the alterations of the food set cause the autocatalytic set to die, while the other two hardly change it. Like a robust metabolism, the autocatalytic set can digest a variety of different foods.



actions always take place, there is the possibility that a new species will be created that is on the graph of the autocatalytic set, but which the kinetics did not yet reach. If the catalyzed pathway is sufficiently strong, then the new species may be regenerated and added to the (kinetic) autocatalytic set. This is the way the autocatalytic sets evolve; spontaneous reactions provide natural variation, and kinetics provides selection.

Autocatalytic networks create a rich, focused set of enzymes at high concentration. They form simple metabolisms, which might have provided a substrate for contemporary life.

The results discussed here, as well as many others, will be described in more detail in a future paper [7]. We intend to study the evolution of autocatalytic sets, and to make a closer correspondence to experimental parameter values.

## 6.2 Comparison to generic network

- **Nodes** correspond to both polymer species and to reactions. The states are determined by the concentrations of the polymers.
- **Connections.** The graph connections are quite different in this system, in that there are no direct reaction connections to the same types of nodes. Each reaction node is connected by undirected links to exactly three polymer nodes, and contains one (directed) catalytic link to one or more polymer nodes. A polymer node can be connected by a solid link to any number of reaction nodes, and can have any number of catalytic links to reaction nodes.
- **Dynamics.** The dynamics is based on the laws of mass action. The equations are physically realistic, and are considerably more complicated than those of the other networks we have discussed. Arbitrarily label all the polymer species by an index  $i$ , and let  $x_i$  represent the concentration of the  $i^{\text{th}}$  species. Assume that all the forward reactions in Equation (18) have the same rate constant  $k_f$ , all the backward reactions have the same rate constant  $k_r$ , and that all catalyzed reactions have the same velocity  $\nu$ . Let the quantity  $m_{ijk_e}$  represent the connections in the two graphs, where  $i$  and  $j$  refer to the two species that join together to form  $k$  under enzyme  $e$ .  $m_{ijk_e} = 1$  when there is a catalyzed reaction, and  $m_{ijk_e} = 0$  otherwise.  $m_{ijk_e} = m_{jik_e}$ . Let the dissipation constant be  $k$ , let the rate at which elements are added to the foodset be  $d$ , and let  $h$  be the concentration of water. Neglecting the effects of enzyme saturation, the equations can be written

$$\begin{aligned} \frac{dx_k}{dt} = & \sum_{e,i,j} m_{ijk_e} (1 + \nu x_e) (k_f x_i x_j - k_r h x_k) \\ & + 2 \sum_{l,m,e} m_{klm_e} (1 + \nu x_e) (k_r h x_m - k_f x_k x_l) - k x_k + d f(x_k) \end{aligned} \quad (21)$$

$f$  is a function whose value is one if  $x_k$  is in the food set, and is zero otherwise. More accurate equations incorporating the effect of enzyme saturation are given in reference [20].

An effective instantaneous connection strength can be computed by evaluating  $\frac{\partial \dot{x}_k}{\partial x_p}$ . The resulting expression is too complicated to write here. Like the immune network, the instantaneous connection strength can be either excitatory or inhibitory depending on where the network is relative to its steady state value. In contrast to the other networks we have studied, there are no special variables in Equation (21) that explicitly play the role of either node or connection parameters. The concentration of the enzymes  $x_e$  that catalyze a given reaction is suggestive of the connection parameters in other connectionist networks. However, since any species can be a reactant in one equation and an enzyme in another, there is no explicit separation of time scales between  $x_e$  and the other variables.

- **Graph dynamics.** The separation of time scales usually associated with learning occurs entirely through modification of the graph. The deterministic behavior for any given graph goes to a fixed point. However, in a real autocatalytic system there are always spontaneous reactions creating new species not contained in the catalytic reaction graph. It occasionally happens that one of the new species catalyzes a pathway that feeds back to create that species. Such a fluctuation can be amplified enormously, altering the part of the catalyzed graph that is above the concentration threshold. This provides a mechanism for the evolution of autocatalytic networks.

Autocatalytic networks are interesting from a connectionist point of view because of their rich graph structure and because of the possibilities opened up by catalytic activity. Catalytic activity is analogous to amplification in electronic circuits; it results in multiplicative terms that either amplify or suppress the activity of a given node. The fixed points of the network may be thought of as self-sustaining memories, caused by the feedback of catalytic activity. The dynamical equations that we use here are based on reversible chemical reactions, and lead to unique fixed points. However, other chemical reaction networks can have multiple fixed points, and it seems likely that when we alter the model to study irreversible reactions such as those observed in contemporary metabolisms, we will see multiple fixed points. In this case the computational possibilities of such networks become much more complex.

## 7 Other potential examples and applications

The four examples discussed here are by no means the only ones where connectionist models have been used, or could be used. Limitations of space and time prevent a detailed examination of all of the possibilities, but a few deserve at least cursory mention.

- **Bayesian inference networks, markov networks, and constraint networks** are procedures used in artificial intelligence and decision theory for organizing and codifying causal relationships in complex systems [49]. Each variable corresponds to a node of the network. Each node is connected to the other variables on which it depends. Bayesian networks are based on conditional probability distributions, and use directed graphs; markov networks are based on joint probability and have undirected graphs; constraint networks assume deterministic constraints between variables. These networks are most commonly used to incorporate prior knowledge, make predictions and test hypotheses. Learning good graph representations is an interesting problem where further work is needed.
- **Boolean networks.** A neural network whose transition rule is a binary automaton is an example of a boolean network. In general there is no need to restrict the dynamics to the sum and threshold rules usually used in neural nets (other than the fact that this may make the learning problem simpler). Instead, the nodes can implement arbitrary logical (Boolean) functions. Kauffman studied the emergent properties of networks in which each node implements a random Boolean function [38,37]. (The functions are fixed in time, but each node implements a different function.) More recently, Miller and Forrest [44] have shown that the dynamics of classifier systems can be mapped into Boolean networks. This allows them to describe the emergent properties of classifier systems. Their work implicitly maps Boolean networks to the generic connectionist framework. The formulation of learning rules for general Boolean networks is an interesting problem that deserves further study. Kauffman has done some work using point mutation to modify the graph [39].
- **Ecological models and population genetics** are a natural area for the application of connectionism. There is a large body of work modeling plant and animal populations and their interactions with their environment in terms of differential equations. In these models it is necessary to explicitly state how the populations interact, and translate this into mathematical form. An alternative is to let these interaction *evolve*. A natural framework for such models is provided by the work of Maynard Smith in the application of game-theoretic models to population genetics and ethology [62]. The interactions of the populations with each other are modeled as game-theoretic strategies. In these models, however, it is necessary to state in advance what these strategies are. A natural alternative is to let the strategies evolve. Some aspects of this have been addressed in the fledgling theory of evolutionary games [24]. A connectionist approach is a natural extension of this work. The immune networks discussed here are very similar to predator-prey models. The strings encoding chemical properties are analogous to genotypes of a given population, and the matrix of interactions are analogous to phenotypes.

- **Economics** is another natural area of application. Again, existing game-theoretic work suggests a natural avenue for a connectionist approach, which could be naturally implemented along the lines of the immune model. The binary strings can be viewed as encoding simple strategies, specifying the interactions of economic agents. Indeed, there are already investigations of models of this type based on classifier systems [4,5,41].
- **Game theory** is a natural area of application. For example, Axelrod [6] has studied the game of iterated prisoner's dilemma. His approach was to encode recent past moves as binary variables, and encode the strategy of the player as a Boolean function. He demonstrated that genetic algorithms can be used to evolve Boolean functions that correspond to good strategies. An alternative approach would be to distribute the strategy over many nodes, and use a connectionist model instead of a look-up table. Such models may have applications in many different problems where evolutionary games are relevant, such as economics and ethology.
- **Molecular evolution models.** The autocatalytic model discussed in detail here is by no means the only connectionist model for molecular evolution. Perhaps one of the earliest example is the hypercycle model of Eigen and Schuster [19], which has recently been compared to the Hopfield neural network models [32,52]. For a review see Hofbauer and Sigmund [27].

## 8 Conclusions

I hope that presenting four different connectionist systems in a common framework and notation will make it easier to transfer results from one field to another. This should be particularly useful in areas such as immune networks, where connectionist models are not as well developed as they are in other areas, such as neural networks. By showing how similar mathematical structure manifests itself in quite different contexts, I hope that I have conveyed the broad applicability of connectionism. Finally, I hope that these mathematical analogies make the underlying phenomena clearer. For example, comparing the role of the lymphocyte in these models to the role of neurons may give more insight into the construction of immune networks, with more computational power.

### 8.1 Open questions

Hopefully the framework for connectionist models presented here will aid the development of a broader mathematical theory of connectionist systems. From an engineering point of view, the central question is: What is the most effective way to construct good connectionist networks? Questions that remain unclear include:

- In  $\dots$  systems, such as neural networks and classifier systems, a connection is always either inhibitory or excitatory. In others, such as immune networks

and autocatalytic networks, a connection can be either inhibitory or excitatory, depending on the state of the system. Does the latter more flexible approach complicate learning? Does it give the network any useful additional computational power?

- Is it essential to have independent parameters for each connection? In neural nets, each connection has its own parameter. In classifier systems, the use of the “don't care” symbol means that many connections are represented by one classifier, and thus share a common connection parameter. This decreases the flexibility of the network, but at the same time gives an efficient graph representation, and aids the genetic algorithms in finding good graphs. In B-cell immune networks the parameters reside entirely in the nodes, and thus as a single parameter changes many different connections are effected. Does this make it impossible to implement certain functions? How does this effect learning and evolution? (It is conceivable that the reduction of parameters may actually cause some improvements.)
- What is the optimal level of complexity for the transition rule? Some neural nets and classifier systems employ simple activation functions, such as linear threshold rules. Somewhat more complicated nonlinear functions, such as sigmoids, have the advantage of being smooth; immune networks have even more complicated activation functions. An alternative is to make each node a flexible function approximation box, for example, with its own *set* of local linear functions, so that the node can approximate functions with more general shapes [22.67]. However, complexity also increases the number of free parameters and potentially increases the amount of data needed for learning.
- A related question concerns the role of catalysis. In autocatalytic networks, a node can be switched on or off by another node through *multiplicative* coupling terms. In contrast to networks in which inputs can only be summed, this allows a single unit to exert over-riding control over another. A similar approach has been suggested in  $\Sigma - \Pi$  neural networks [58]; T-cells and neuro-transmitters may play a similar role in real biological systems. How valuable is specific catalysis to a network? How difficult is the learning problem when it is employed?
- What are the optimal approaches to evolving good graph representations? Most of the work in this area has been done for classifier systems, although even here many important issues remain to be clarified. All known algorithms that can *create* connections and nodes, such as the genetic algorithms, are stochastic; there are deterministic pruning algorithms that can only *destroy* connections, such as orthogonal projection. Are there efficient deterministic algorithms for *creating* new graph connections?
- What are the best learning algorithms? A great deal of effort has been devoted to answering this question, but the answer is still obscure. A perusal of

the literature suggests certain general conclusions. For example, in problems with detailed feedback, *e.g.* a list of known input-output pairs, deterministic function fitting algorithms such as least-squares minimization (of which back-propagation is an example) can be quite effective. However, if the search space is not smooth, for example because the samples are too small to be statistically stable, stochastic algorithms such as crossover are often more effective [1]. In more general situations where there is no detailed feedback, there seems to be no general consensus as to which learning algorithms are superior.

Thus far, very few connectionist networks make use of nontrivial computational capabilities. In typical applications most connectionist networks end up functioning as stimulus-response systems, simply mapping inputs to outputs without making use of conditional looping, subroutines, or any of the power we take for granted in computer programs. Even in systems that clearly have a great deal of computational power *in principle*, such as classifier systems, the solutions actually learned are usually close to look-up tables. It seems to be much easier to implement effective learning rules in simpler architectures that sacrifice computational complexity, such as feed-forward networks.

It may be that there is an inherent trade-off between the complexity of learning and the complexity of computation, so that the difficulty of learning increases with with computational power. At one end of the spectrum is a look-up table. Learning is trivial; examples are simply inserted as they occur. Unfortunately, all too often neural network applications have not been compared to this simple approach. In the infamous NET-talk problem [61], for example, a simple look-up table gives better performance than a sum/sigmoid back-propagation network [3]. Simple function approximation is one level above a look-up table in computational complexity: functions can at least attempt to interpolate between examples, and generalize to examples that are not in the learning data set. Learning is still *fairly* simple, although already the subtleties of probability and statistics begin to complicate the matter. However, simple function approximation has less computational capability than a finite state machine. There are no good learning algorithms for finite state machines. Without counting, conditional looping, *etc.*, many problems will simply remain insoluble.

It is probably more likely that learning is *possible* with more sophisticated computational power, and that we simply do not yet know how to accomplish it. I suspect that the connectionist networks of the future will be full of loops.

Connectionist models are a useful tool for solving problems in learning, adaptation. They make it possible to deal with situations in which there are an infinite number of possible variables, but in which only a finite number are active at any given time. The connections are explicit but changeable. We have only recently begun to acquire the computational capabilities to realize their potential. I suspect that the next decade will witness an enormous explosion in the application of the connectionist methodology.

However, connectionism represents a level of abstraction that is ultimately limited by such factors as the need to specify connections explicitly, and the lack of built in

spatial structure. Many problems in adaptive systems ultimately require models such as partial differential equations or cellular automata with spatial structure [40]. The molecular evolution models of Fontana *et al.*, for example, explicitly model the spatial structure of individual polymers in an artificial chemistry. As a result the phenotypes emerge more naturally than in the artificial chemistry discussed here. On the other hand, this requires more computational resources. For many problems connectionism may provide a good compromise between accurate modeling and tractability, appropriate to the study of adaptive phenomena during the last decade of this millenium.

## 8.2 Rosetta stone

This paper is a modest start toward creating a common vocabulary for connectionist systems, and unifying work on adaptive systems. Like the Rosetta Stone, it contains only a small fragment of knowledge. I hope it will nonetheless lead to a deeper understanding in the future.

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I urge the reader to use these results for peaceful purposes.

## 9 Appendix: A superficial taxonomy of dynamical systems

Dynamical systems can be trivially classified according to the continuity or locality of the underlying variables. A variable either can be discrete, *i.e.* describable by a finite integer, or continuous. There are three essential properties:

- **Time.** All dynamical systems contain time as either a discrete or continuous variable.
- **State.** The state can either be a vector of real numbers, as in an ordinary differential equation, or integers, as for an automaton.
- **Space** plays a special role in dynamical systems. Some dynamical models, such as automata or ordinary differential equations, do not contain the notion of space. Other models, such as lattice maps or cellular automata, contain a notion of locality and therefore space even though they are not fully continuous. Partial differential equations or functional maps have continuous spatial variables.

This is summarized in table 4.

<b>Generic</b>	<b>Neural Net</b>	<b>Classifier System</b>	<b>Immune Net</b>	<b>Autocatalytic Net</b>
<b>node</b>	neuron	message	antibody type	polymer species
<b>state</b>	activation level	intensity	free antibody/antigen concentration	polymer concentration
<b>connection</b>	axon/synapse/dendrite	classifier	chemical reaction of antibodies	catalyzed chemical reaction
<b>parameters</b>	connection weight	strength and specificity	reaction affinity lymphocyte concentration	• catalytic velocity
<b>interaction rule</b>	sum/sigmoid	linear threshold and max	bell-shaped	mass action
<b>learning algorithm</b>	Hcbb, back-prop	bucket brigade (gen. Hcbb)	clonal selection (gen. Hcbb)	approach to attractor
<b>graph dynamics</b>	synaptic plasticity	genetic algorithms	genetic algorithms	• artificial chemistry rules • spontaneous reactions

Table 3: A Rosetta Stone for connectionism.



type of dynamical system	space	time	representation
partial differential equations	continuous	continuous	continucus
computer representation of a p.d.e.	local	local	local
functional maps	continuous	discrete	continuous
ordinary differential equations	none	continuous	continuous
lattice models	local	discrete or continuous	continuous
maps (difference equations)	none	discrete	continuous
cellular automata	local	discrete	discrete
automata	none	discrete	discrete

Table 4: Types of dynamical systems, characterized by the nature of time, space, and state. "Local" means that while this property is discrete, there is typically some degree of continuity and a clear notion of neighborhood.

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