Catalytic Networks

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Introduction

Summary

- Artificial Chemistry review
- Self organization
- Catalytic Networks
  - Autocatalytic Sets
  - Self Reproduction
  - Self Maintenance
- Evolving autocatalytic sets (in a catalytic network)
- Training autocatalytic sets (in a catalytic network)

Artificial Chemistry Review

Artificial Life (AL)

- Artificial Life (AL)
  - Hypothesis – “Biotic phenomena can be modeled by using complex systems of many interacting components”
  - Emergence
    - Deduce global properties of a system from local interactions

Artificial Chemistry(AC)

- AC tries to investigate the dynamics of complex systems
  - Organization
  - Self Maintenance
  - Self Construction

What is an AC?

- Man made system which is similar to real chemical systems
- A triple (S, R, A)
  - S - The set of possible molecules
  - R - The set of collision rules
  - A - Algorithm describing reaction vessel

The Molecules - S

$$S = \{S_1, S_2, \ldots, S_n\}$$

- Abstract symbols
- Character sequences
- Lambda Expressions
- Binary strings
- Numbers
- Etc…

Rule Set - R

- Example:

$$S_1 + S_2 + \ldots + S_n = S_1' + S_2' + \ldots + S_m'$$

  - Based on
    - Neighborhood
    - Rate constants
    - Probability
    - Energy Consumption

Reaction Vessel - A

- Determines how rules are applied
- 2 separate models
  - Molecules are either separate [Stochastic]
  - Similar molecules are grouped [Differential]

Self Organization

- “Sufficiently complex mixes of chemicals can spontaneously crystallize into systems with the ability to collectively catalyze the network of chemical reactions by which the molecules themselves are formed. Such collectively autocatalytic sets sustain themselves and reproduce”[1]

Self Organization(2)

- “Something is self organizing, if left to itself, it tends to become more organized.” [2]

- Mechanisms which lead to self-organization
  - Self Replication
  - Replication of several types by cooperation

Catalytic Networks Introduction

- Catalyst – A substrate that enhances a reaction without being consumed itself
  - Is a mechanism for cooperation
- Catalytic Network – A network where catalysts speed up certain reactions without being consumed

Catalytic Networks

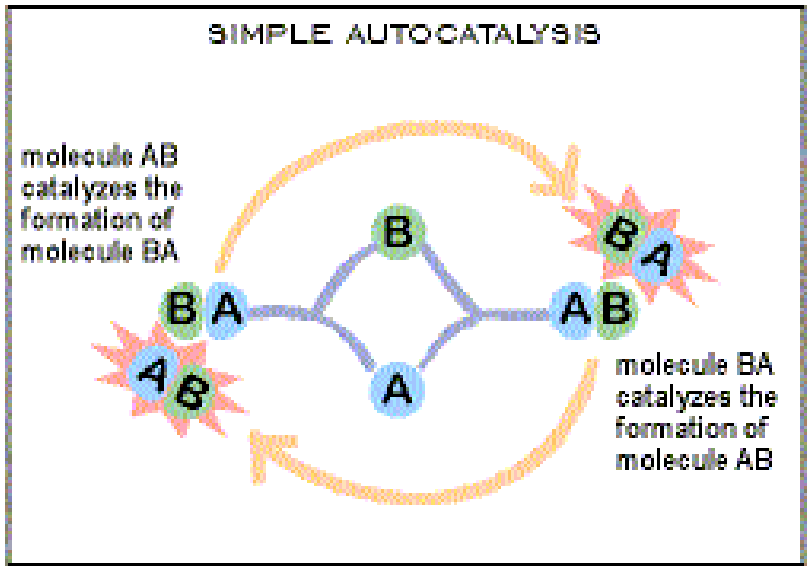
- Used to explain the cooperation of several types of molecules, which may be been precursors to the first cells
- Allows cooperation to feed back to the same set of molecules that act as catalysts
  - This can create a cycle
  - Provides positive feedback that lets selected molecules grow

Autocatalytic Sets Introduction

- Reaction – A process by which substrates (molecules) combine or split to form products
  - Reactions are slow
  - Catalyst plays role of facilitator
    - Dynamically increases speed of reaction
- Catalyst is unaffected by reaction
  - A single catalyst can aid in many reactions

Autocatalytic Sets

- A collection of molecules which catalyze each others reactions
  - "Help bring each other into existence"



Source:www.mgtaylor.com/mgtaylor/jotm/summer97/Complexity.html

Self Reproduction Introduction

- Replicator:
  - "Any entity in the universe which interacts with it's world in such a way that copies of itself are made"[8]
  - Basics done by John von Neumann
    - System that could support self-replicating machines
    - Could withstand some mutation and pass these on
    - These machines could therefore participate in evolution

Self reproduction(2)

$$A + \square(X)\square > X$$

$$B + \square(X)\square > \square(X)$$

$$A + B + C + \square(X)\square > X + \square(X)$$

$$A + B + C + \square(A + B + C)\square > A + B + C + \square(A + B + C)$$

- + = A single machine composed of components to left and right
- --> = Process of construction

Self maintenance

- Not self replication

$$j + k \not\to i + j + k$$

$$\neg i \to K(\neg j, k \to K)$$

- The set K maintains itself
  - It doesn't copy itself it makes more of itself

Catalytic Networks

- S, R, A
- Population P
- Two different types
  - Stochastic
  - Differential

Stochastic

- Stochastic molecular collisions
- Typical algorithm [Simple]
  - Draw a sample of molecules from population P
  - Check if a rule applies
  - If so, molecules are replaced by right hand side of rule

Stochastic

- Advantages
  - Very realistic
- Disadvantages
  - Complexity drastically rises with
    - Concentrations of molecular species
    - Constants of reactions
  - Inefficient
    - The number of species is low or population P is large

Differential

- Continuous differential collisions
  - Example:

$$r : a_1 s_1 + a_2 s_2 + \ldots + a_n s_n \rightarrow b_1 s_1 + b_2 s_s + \ldots + b_n s_n$$

- a_i, b_i
  - Stoichiometric factors
    - a_i is zero if s_i is not a reactant
    - b_i is zero if s_i is not a product

Differential

- Application of all all rules

$$\frac{ds_i}{dt} = \sum_{r \in R} \left((b_i^r - a_i^r) \prod_{j=1}^{N} s_j^{a_j^r} \right)$$

$$i = 1..N$$

Spatial Topology

- Spatial structure of the reactor is a parameter of the algorithm A of {S,R,A}
- Usually
  - Reactor is modeled as a well-stirred tank reactor
  - Probability of Si to participate in a reaction R is independent of position in reactor
  - Size of reactor (number of molecules) is held constant

Competition

- Competition is achieved by limiting the population numbers
  - Originally keeping the rum of all population variables constant
  - Population Numbers are scaled relative to total population

Autocatalytic Sets

- A particular type of dynamics that occur naturally in biochemical or ecosystems
- Characterized by cooperation in a competitive environment
  - Several population dynamic variables maintaining a high level through cooperation in a competitive environment

Evolving Catalytic Networks

- "Evolving Catalytic Reaction sets using Genetic Algorithms"[7]
- Goal: Study emergence of a chemical reaction network
  - Starting from a state of relative disorder
  - Thought to be a crucial step in the evolution of metabolisms

Protocell Model

- Simple mass-conserving, well-stirred reactor
- Molecules(S) – Linear Polymers (chains)
- Rules (R)
  - Bonding (condensation)
  - Breaking (cleavage)
- Ex: Bonding monomer with 4-mer

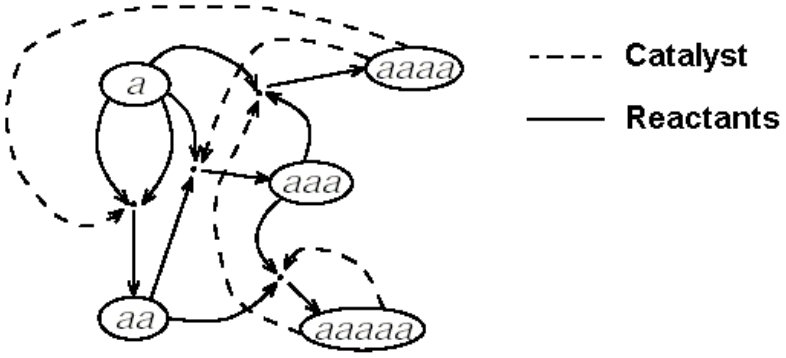
$$a + aaaa \rightleftharpoons aaaaa$$

Protocell Model (2)

- Algorithm (A)
  - Stochastic Model
  - Well-stirred reactor
  - Fixed initial distribution
  - Interactions must be catalytic
- Reactions $A + B \xrightarrow{C} P$
- A,B,C,P are polymers

Protocell Model (3)

- An autocatalytic set will occur when one of the reactants also catalyzes the reaction



$$a + a \overset{aaaa}{\rightleftharpoons} aa \qquad a + aaa \overset{aaaaa}{\rightleftharpoons} aaaa$$

$$a + aa \overset{aaaa}{\rightleftharpoons} aaa \qquad aa + aaa \overset{aaaaa}{\rightleftharpoons} aaaaa$$

Example of a catalytic reaction set: graphical depiction (top) and reaction set (bottom). Reverse reactions are not shown explicitly in graph.

Goal

- Automatically produce reactions sets
  - Input: An initial disordered distribution
  - Output: A distribution biased towards building up long polymers
- Two Target distributions
  - Peak
  - Target

Peak vs Target

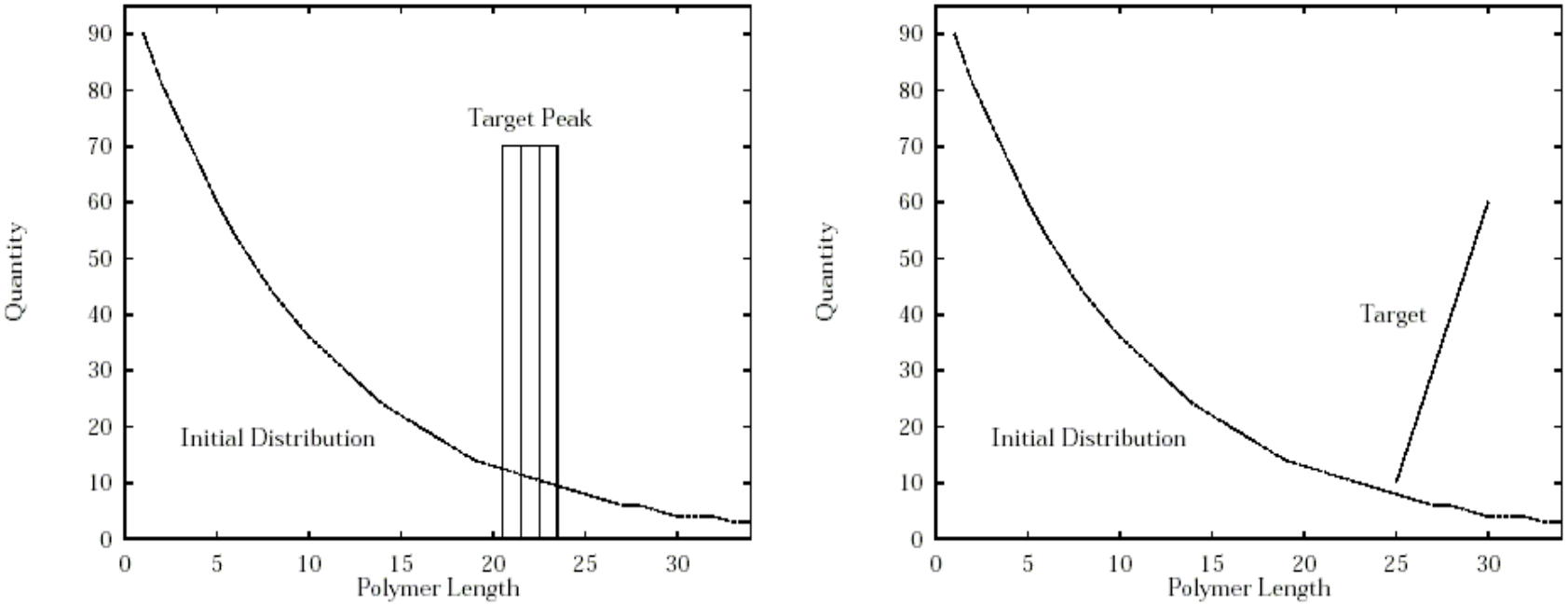


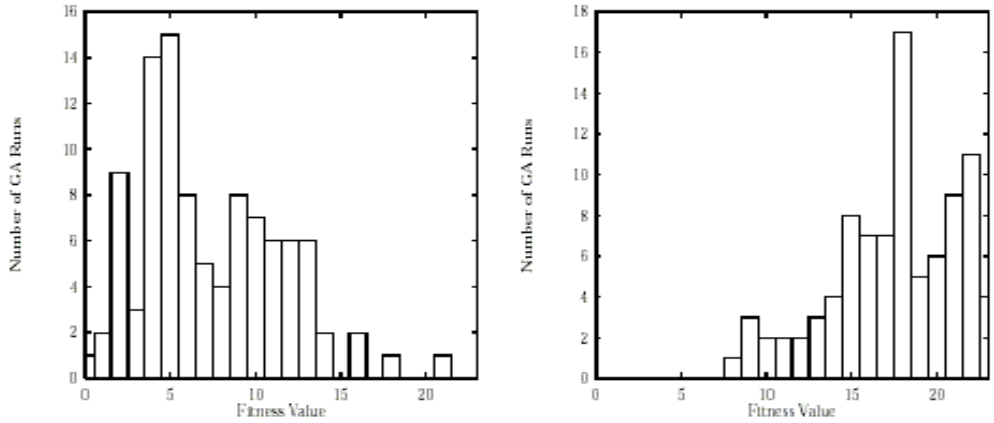
Fig. 3. The peak target distribution.

Genetic Algorithm

- Genetic algorithm is used to change reaction rules towards biased distribution
- Reaction Set represented by Boolean arrays
- Max polymer size is 34
  - 289 combinations of A and B
  - 289*34 possible different reactions
  - 9826^{100} possible reactions sets

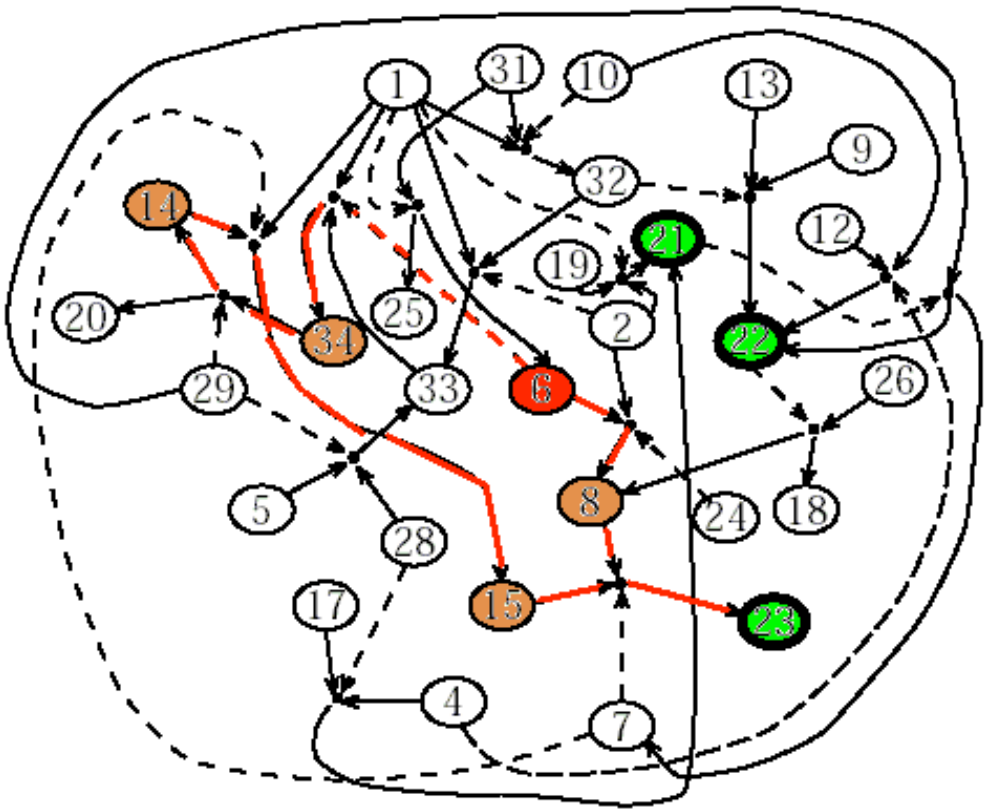
Fitness function

- Absolute different between target distribution and simulation distribution



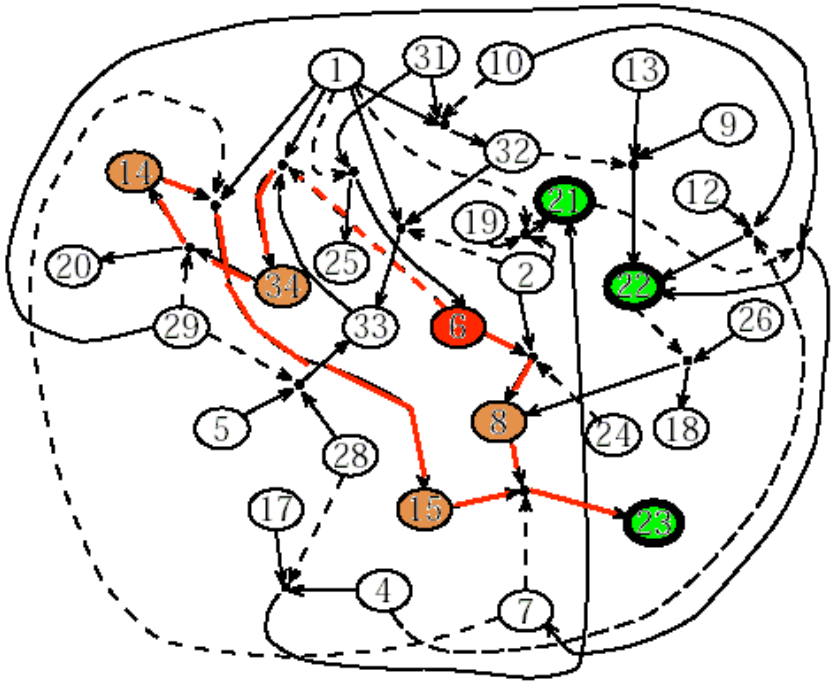
Histogram showing frequency of best fitness values found in 100 genetic algorithm runs. The left graph is for the `peak` experiment and the `slope` experiment is shown on the right. Lower fitness values correspond to lower error and improved fitness.

The result



Reaction Graph - Peak Experiment

Reaction Graph



Reaction Graph - Peak Experiment

- Characteristics
  - Shows Complexity
    - Produces large polymers
    - Then breaks these down
  - Short Cycle formation
  - Key polymers act as both reactants/catalysts
  - Target polymers act only as catalysts

Conclusion

- Highly simplified models of interaction
- Can move to a system of increasing complexity
- Reactions sets robust in producing desirable behavior

Association

- Autocatalytic sets are a result of self organization
  - Specifically in a catalytic network
- Can we do anything with them?

Learning

- Goal
  - Develop a mathematical model of learning in autocatalytic sets
  - Achieve some degree of the adaptability of evolving systems
- Example Task
  - Association of word symbols with letters

The network

- Differential model

$$\hat{x}_i = g_i(x)\left(\frac{x_i}{0.5}\right)\max(g_1(x), g_2(x), \ldots, g_n(x))$$

$$g_i(x) = \max(b_{i1}x_1^{w_{i11}}x_2^{w_{i21}}\ldots x_s^{w_{is1}}, b_{i2}x_1^{w_{i12}}x_2^{w_{i22}}\ldots x_s^{w_{is2}}, \ldots, b_{im}x_1^{w_{i1m_i}}x_1^{w_{i2m_i}}\ldots x_1^{w_{ism_i}})$$

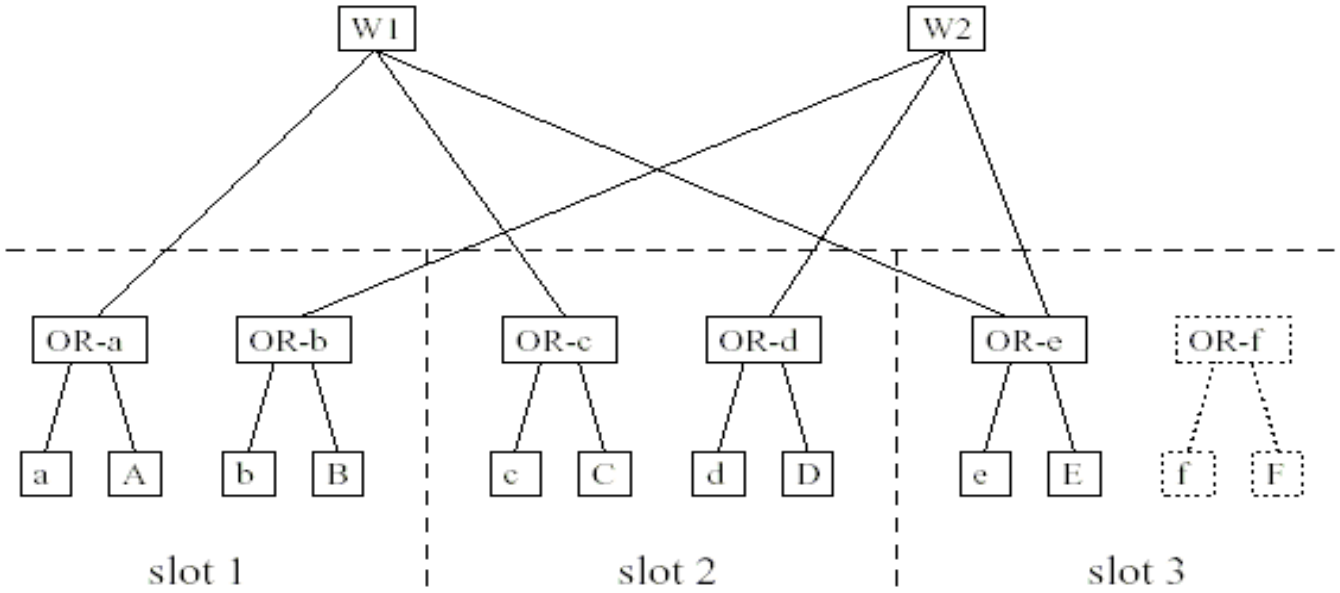
  - Models growth of population variables
  - Each input/connected node is weighted
- Competition through limiting population size

Output

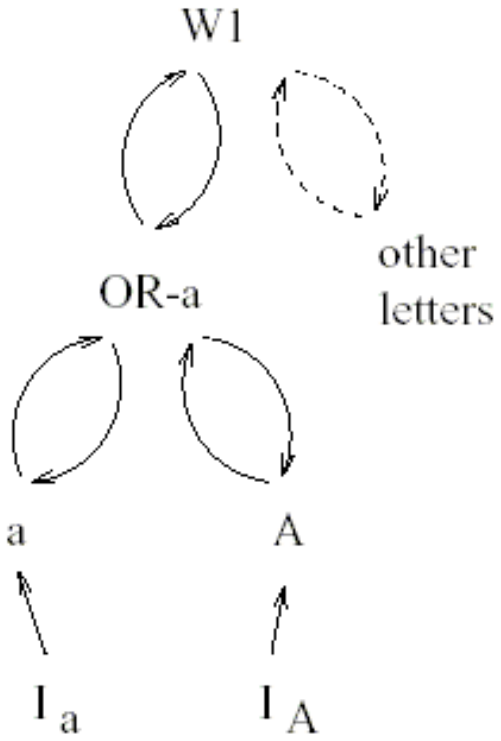
- Output should be some learned response
  - Based off of inputs (bi-directional)
- Training Phase
  - Apply some input
  - Allow chemical reactions to occur (with competition)
  - Learning: Apply a learning algorithm (Based off of population numbers)

A picture(Initial architecture)

Input - W1: ace & ACE W2: bde & BDE



Doctored Stochastic version



- OR-a,Ia => a
- OR-a,IA => A
- a,W1 => OR-a
- A,W1 => OR-a
- OR-a, other => W1

Learning in catalytic networks

- The learning rules
  - Adjusts the weights (connections)
  - Adjusts the biases of equations

$$\Delta w_{ijk} = \frac{1}{n}(x_j - w_{ijk})$$

$$\Delta b_{ik} = \beta(\frac{1}{g_i} - 1)$$

Goal

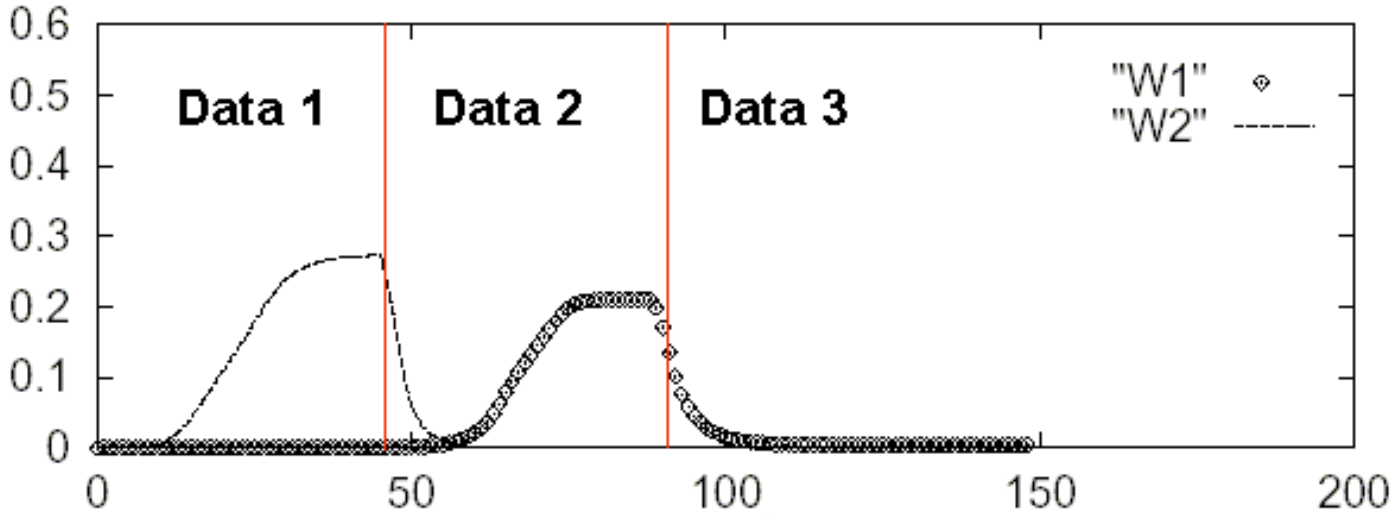
- Task of learning
  - Find a suitable bias for the word nodes
- The biased nodes
  - Are in terms of large population size
  - Caused by some sort of organization

Example

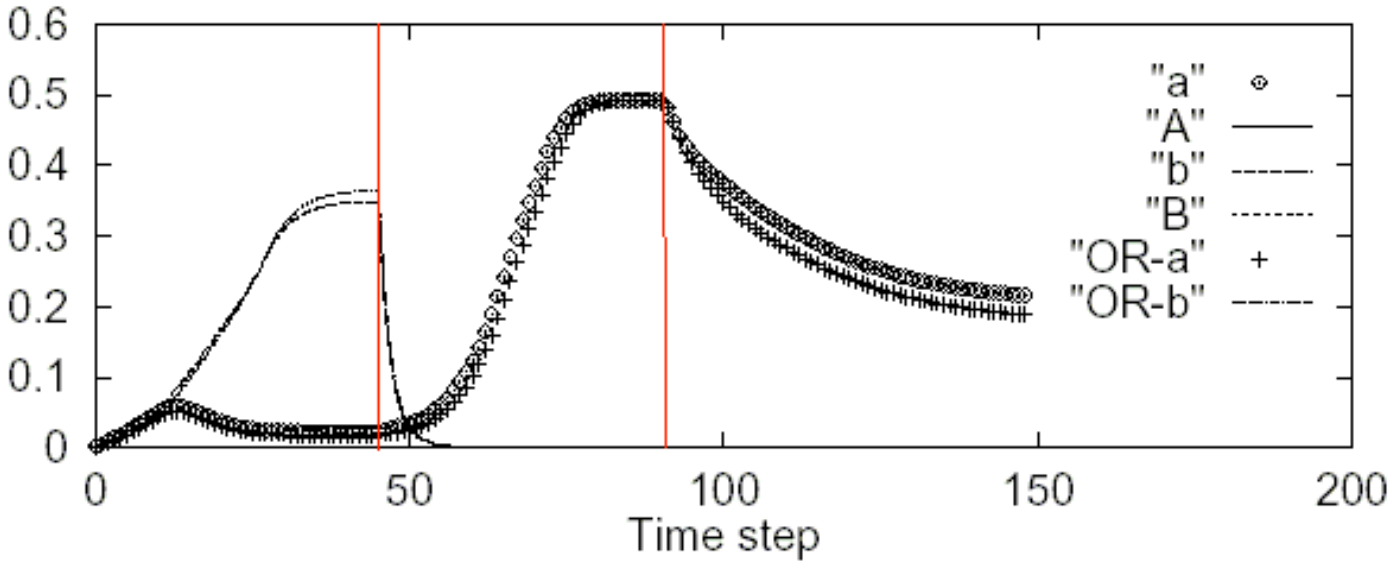
Data item	Input 1	Input 2
1	W2 = 01	xde = 0.5 0.5 0.5 0 0 0 010000 100000
2	WX = 0.5 0.5	ace = 100000 100000 100000
3	WX = 0.5 0.5	ade = 100000 010000 100000

- Data 1: An incomplete word
- Data 2: A word that has been trained
- Data 3: A word that has not been trained

Word response



Slot 1 response



Conclusion

- Creating a system which can be ‘taught’
  - Much like neural network
- Has bi-directional associations
  - Top-down and bottom-up activations can be combined
  - Can perform logical AND and OR
    - In a branching tree structure

Conclusion(2)

- Output shows
  - Word recognition
  - Word rejection
  - Disambiguation of letters
- Potential view of how some mechanisms underlying evolution may take place in the living brain

Summary

- Artificial Chemistry review
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- Autocatalytic Set / Self Reproduction
- Evolving autocatalytic sets (in a catalytic network)
- Training autocatalytic sets (in a catalytic network)

References

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Thanks

Questions?