Artificial Intelligence

Artificial Intelligence (AI)

AI is an attempt to reproduce intelligent reasoning using machines*

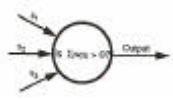
* H. M. Cartwright, Applications of Artificial Intelligence in Chemistry, 1993, pg. 2, Oxford University Press, Oxford

Common AI Methods

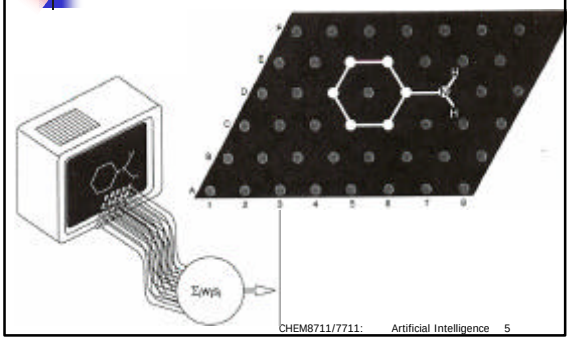
- Artificial Neural Networks: utilize a computational model of the brain (multiple interconnected neurons) in order to learn
- Expert Systems: utilize a knowledge base and set of rules (heuristics) in order to provide 'expert' assistance
- Genetic Algorithms: utilize the concepts of evolution to produce good solutions to a problem from poor random initial guesses

Artificial Neural Networks (ANN)

- ANN uses perceptrons to mimic the functions of simple neurons:
  - Has multiple input connections (s_i) -> adds up signals arriving on these connections ($\Sigma_i w_i s_i$)
  - Remains off unless the sum reaches a threshold (Θ)
  - Returns to off state after a short time



Signals to Perceptrons



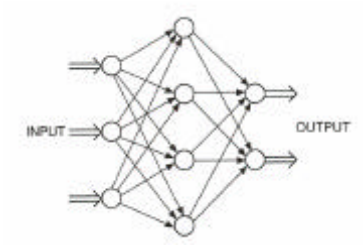
Training

- Training involves both a training stimulus (input to the ANN) and a training target (the desired output)
- Perceptron learning rules:
  - If output is correct, do nothing
  - If incorrect 'on' signal is given, decrease weights on active inputs
  - If incorrect 'off' signal is given, increase weights on active inputs

Pattern Recognition

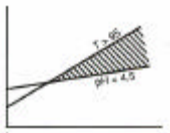
- Simple perceptrons can be trained to recognize simple patterns (molecules containing rings)
- The ability to train a perceptron is dependent on having a common ring orientation and size
- Recognition of rings having different orientations and sizes requires a network of perceptrons (ANN)
- More generally, problems must be linearly separable for a single perceptron to handle

A Simple NN



Example Problem

- Monitor temperature (T) and pH in a reaction vessel and sound an alarm if T>95 OR pH<4.5
- This is not a single linearly separable problem, but is a conjunction of two linearly separable problems



Solving the Problem

- A minimum of two perceptrons are required
- One monitors temperature and ignores the pH signal
- The other monitors pH and ignores the temperature signal

Training Networks

- Networks involve multiple layers of perceptrons, but only the target signals of the output perceptrons are known
- Backpropagation
  - Collects errors from the output perceptrons
  - Errors are divided among the various connections in the network
  - The weights for those connections are adjusted in order to reduce the error

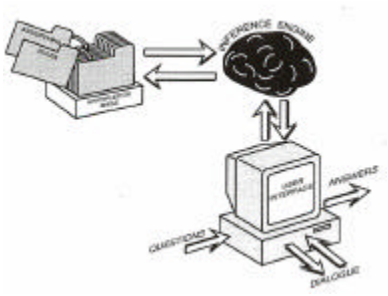
Advantages/Disadvantages

- Advantages
  - A single network can be trained for multiple applications
  - Fault tolerance – ANNs handle noisy data reasonably well
  - Trained networks can deal with previously unseen data
  - ANN operate in parallel
  - ANN discover new relationships among input data
  - ANN can cope with fuzzy data
- Disadvantages
  - Selection of training set determines quality of training
  - Relationships discovered by ANN are not readily translated into human understanding

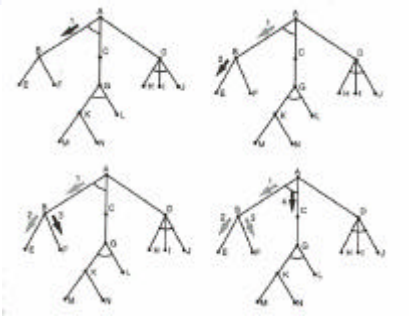
Another Neural Net Example

- Prediction of optimal conditions for protein crystallography – in current use at the Center for Biophysical Sciences and Engineering at UAB
  - Robotics used to set up hundreds of crystal growth experiments – condition combinations determined by N-factorial analysis
  - growth conditions (pH, concentration, etc) used as input for a back-propagation neural network
  - crystal quality (manually graded on 1-10 scale) used as output
  - using first round crystallization trials, can reliably predict optimal untested combination of conditions to produce highest quality crystals

Expert Systems



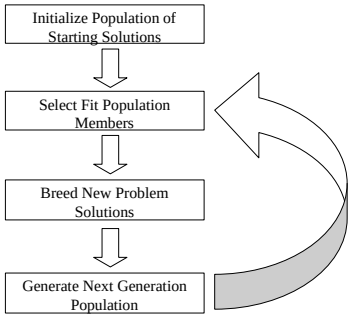
Searching the Knowledge Base



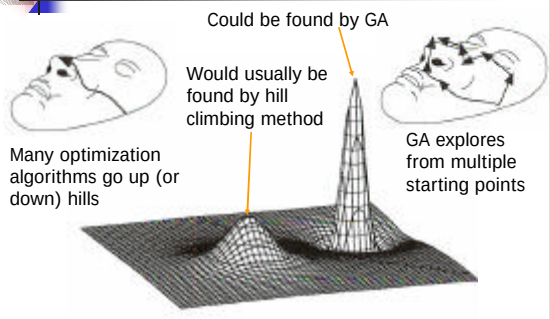
Advantages/Disadvantages

- Advantages
  - Can be used in situations where an expert is not available
  - Can collect input from the user and combine with knowledge base to infer solutions
- Disadvantages
  - Not applicable to new situations
  - Requires considerable expert input to develop
  - Expert knowledge may not easily be easily fed into the knowledge base
  - Requires constant updates in highly active areas (example: synthetic planning)

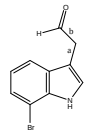
Genetic Algorithm (GA)



GA Applicability



Representing a Solution



Solution Representation Requires 8 Genes:

1. Dihedral Angle Labeled a
2. Dihedral Angle Labeled b
3. Rotation of entire molecule around x axis relative to standard orientation
4. Rotation of entire molecule around y axis relative to standard orientation
5. Rotation of entire molecule around z axis relative to standard orientation
   (Binary example uses 3 bits to encode 360 degrees at 45 degree increments)
6. Distance in x direction from standard orientation
7. Distance in y direction from standard orientation
8. Distance in z direction from standard orientation
   (Binary example uses 3 bits to encode from -2.0 to +1.5 in 0.5 Å increments)

Binary Representation:

Gene:	1	2	3	4	5	6	7	8
	011	011	010	011	100	000	101	110

Real-Valued Representation

Gene:	1	2	3	4	5	6	7	8
	120.0	118.2	45.3	121.2	10.1	1.0	1.3	0.8

Binary Mutation Concern

Few single mutations result in small changes to the actual angle value

Angle Value	Binary Code Value	Gray Code Value
0	000	000
45	001	001
90	010	011
135	011	010
180	100	110
225	101	111
270	110	101
315	111	100

Reproduction: Crossover

Parent 1: 0 1 1 0 1 1 0 1 1 0 0 1 1 1 0 0 0 1 0 1 0

Parent 2: 0 1 0 0 1 0 1 1 1 1 0 1 0 0 0 0 0 1 1 1 0

crossover

Child (Uniform): 0 1 1 0 1 0 0 1 1 0 0 1 1 1 0 0 0 1 1 1 0

Children (One-Point): 0 1 1 0 1 1 0 1 1 1 0 1 0 0 0 0 0 1 1 1 0

0 1 0 0 1 0 1 1 1 1 0 0 1 1 1 0 0 0 1 0 1 0

Children (Two-Point): 0 1 1 0 1 1 0 1 1 1 0 1 0 0 0 0 0 1 0 1 0

0 1 0 0 1 0 1 1 1 1 0 0 1 1 1 0 0 0 1 1 1 0

Reproduction: Mutation

Binary Representation:

Gene:	1	2	3	4	5	6	7	8
	011	011	010	011	100	000	101	110

Mutate bit

	011	011	000	011	100	000	101	110

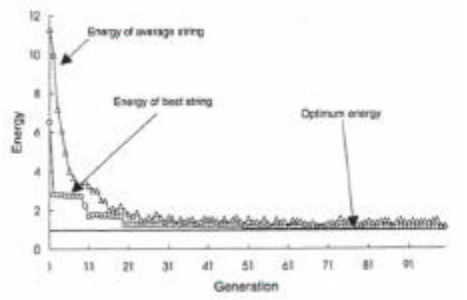
Real-Valued Representation

Gene:	1	2	3	4	5	6	7	8
	120.0	118.2	45.3	121.2	10.1	1.0	1.3	0.8

Mutate real value

	120.0	124.3	45.3	121.2	10.1	1.0	1.3	0.8

GA Behavior



Advantages/Disadvantages

- Advantages
  - Operates in parallel
  - Able to solve problems with complex landscapes
- Disadvantages
  - Requires ability to represent problem as a string
  - The solution must be assembled from segments (schema) that confer high fitness

Related Reading

- 9.9.1
- 12.12.5