Bioinformatics CSM17
Week 8: Simulations (1)
Soft Computing:

- Genetic Algorithms
- Evolutionary Computation
- Neural Networks

Genetic Algorithms (GAs)

- simulate sexual reproduction
- use artificial 'chromosomes'
- simulate evolution

'Real' Chromosomes

- humans have 46 in total
  - 23 homologous pairs
- half from each parent

Mitosis

- normal cell division e.g. for growth, repair
- all cells are diploid (usually)
- i.e. they are said to be '2n'

Meiosis

- cell division to produce gametes
  - gametes
  - Female: eggs or ova (singular ovum)
  - Male: sperm
- daughter cells are haploid (n)

Main features of GAs

- crossover (chiasma)
- 'chromosomes'
- population containing individuals
- successive generations
- survival of the 'fittest'
- only the 'most fitted' reproduce
- (removal of the worst)
- mutation

A Simple Example

- population of 4
- attributes are simple numbers
- fitness function is a minimisation function
- only 2 best fitted survive to reproduce

Mutation

- changes of nucleotide bases
- caused by
  - ionizing radiation, mutagenic chemicals
- usually harmful (damaging)
- may be
  - single base (changing one amino acid)
  - frameshift (more serious)

Karl Sims

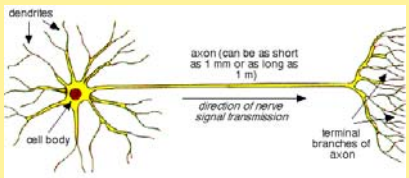
- Evolved creatures
- Swimming
- Jumping
- Walking
- Following....etc.

Neural Networks

- biological neurons
- natural neural networks
- artificial neural networks
- applications

A Biological Neuron has…

- soma (the 'body' of the neuron)
- dendrites (for inputs)
- axon (for output)
- synapses



Natural Neural Networks

- nerve net
  - in Coelenterates
  - *e.g. Hydra,* sea anemones

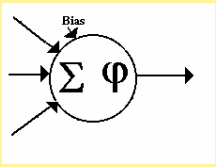
The Human Brain

- ~100 billion neurons
- about as many trees in Amazon Rain Forest
- the number of connections is about the same as the total number of leaves
- up to 100 thousand inputs per cell

The Human Brain (from the visible human project)

Artificial Neurons

- McCulloch & Pitts
  - single neuron model (1943)
- … with weights becomes Hebbian Learning



- Rosenblatt's Perceptron
  - multi-neuron model (1957)

Artificial Neural Networks

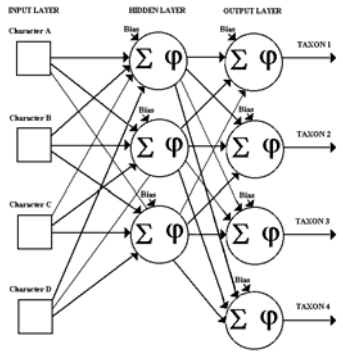
- supervised
  - known classes
- unsupervised
  - unknown classes

Supervised Neural Networks

- multilayer perceptron (MLP)
- used where classes are known
- trained on known data
- tested on unknown data
- useful for identification or recognition

MLP Architecture

- usually 3-layered (I:H:O)
  - one node for each attribute / character
- input layer
  - one node for each attribute / character
- hidden layer
  - variable number of nodes
- output layer
  - one node for each class



MLP Learning Algorithms

- summation is carried out by

$$v_j = \sum_{i=0}^{n} w_i \cdot x_i$$

- where w_i is the weight and x_i is the input value for input i.

MLP Learning Algorithms

- the non-linear *activation function* (φ) is given by

$$\varphi(v_j) = \frac{1}{1+\exp(-v_j)}$$

- where v_j is the weighted sum over n inputs for node j

MLP Learning Algorithms

- backpropagation
  - (Werbos) Rummelhart & McClelland 1986
- contribution of each weight to the output is calculated
- weights are adjusted to be 'better' next time…using the delta rule

MLP Learning Algorithms

- delta rule

$$w_{ij}(t+1) = w_{ij}(t) + \eta \delta_j y_i$$

- … for output nodes

$$\delta_k = y_k[1-y_k] \bullet (t_k - y_k)$$

- … for hidden nodes

$$\delta_j = y_j[1-y_j] \bullet \sum_{k=1}^{K} [\delta_k w_{kj}]$$

Applications

- identification / recognition
- fault diagnosis e.g. teabag machine
- medical diagnosis
- decision making

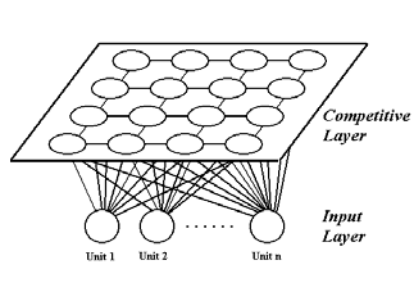
Unsupervised NNs

- self-organising (feature) maps
- 'Kohonen' maps
- topological maps

Kohonen Self-Organising Feature Map (SOM, SOFM)

- Teuvo Kohonen (1960s)
- input layer
  - one node for each attribute / character
- competitive 'Kohonen' layer

Kohonen SOM Architecture



Kohonen Learning Algorithm

- initially random weights between input layer and Kohonen layer
- data records (input vectors) presented one at a time
- each time there is one 'winner' (closest Euclidean distance)
- the weights connected to the winner and its neighbours are adjusted so they are closer
- learning rate and neighborhood size are reduced

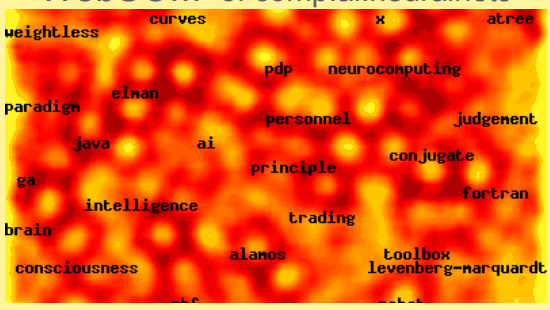
SOM Learning Algorithm

$$i(x) = \arg\min \| x(t) - w(t)_j \|$$

$$\| x(t) - w(t)_j \| = \sqrt{[\sum_1^I (x(t)_i - w(t)_{ji})^2]}$$

$$w_j(t+1) = w_j(t) + \eta[x(t) - w_j(t)]$$

WebSOM of comp.ai.neuralnets



Summary

- biological neurons
- natural neural networks incl. the brain
- artificial neural networks
- applications

Useful Websites GAs

- Evolutionary design by computers: http://www.cs.ucl.ac.uk/staff/P.Bentley/evdes.html
- Evolving creatures (Karl Sims): http://www.genarts.com/karl/evolved-virtual-creatures.html

Useful Websites: Neural Nets

Visible Human Project
http://www.nlm.nih.gov/research/visible/

Stuttgart Neural Network Simulator (Unix)
http://www-ra.informatik.uni-tuebingen.de/SNNS/

Microsoft's List of Neural Network Websites
http://research.microsoft.com/~jplatt/neural.html

Neural Network FAQ
ftp://ftp.sas.com/pub/neural/FAQ.html

WebSOM
http://websom.hut.fi/websom/

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