Evolutionary Neural Networks Design

- Motivation
- Evolutionary training
- Evolutionary design of the architecture
- Evolutionary design of the learning rules

Evolutionary Neural Networks Design

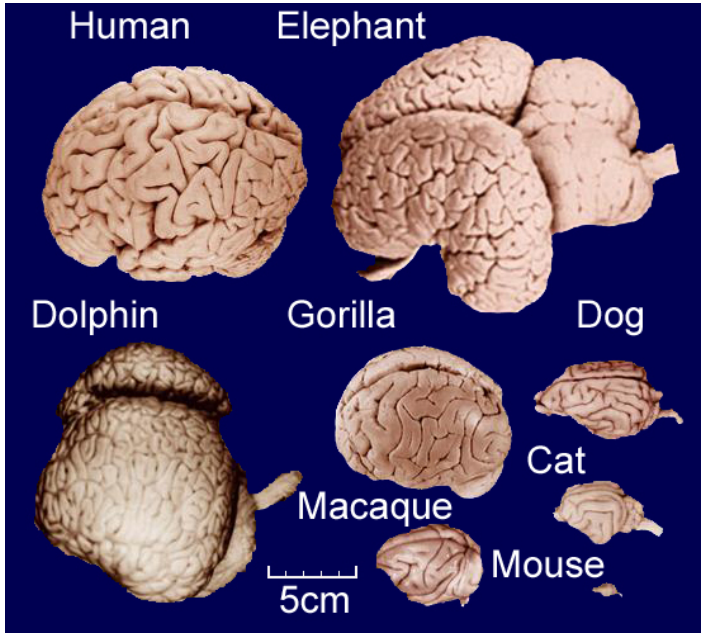
Motivation. Neural networks design consists of:

- Choice of the architecture (network topology+connectivity)
  - Has an influence on the network ability to solve the problem
  - Usually is a trial-and-error process

- Train the network
  - Is an optimization problem = find the parameters (weights) which minimize the error on the training set
  - The classical methos (ex: BackPropagation) have some drawbacks :
    - If the activation functions are not differentiable
    - Risk of getting stuck in local minima

Evolutionary Neural Networks Design

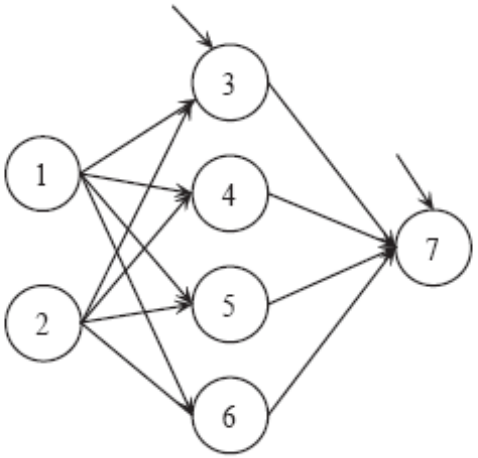
Idea: use an evolutionary process



- Inspired by the biological evolution of the brain
- The system is not explicitely designed but its structure derives by an evolutionary process involving a population of encoded neural networks
  - Genotype = the network codification (structural description)
  - Phenotype = the network itself, which can be simulated (functional description)

Evolutionary Training

- Use an evolutionary algorithm to solve the problem of minimizing the mean squared error on the training set



- Parameters: synaptic weights and biases

$$\text{Training set}: \{(x^1, d^1), ..., (x^L, d^L)\}$$

$$\text{Error function}: E(W) = \frac{1}{L}\sum_{l=1}^{L}(d^l - y^l)^2$$

$$W = \{w_{31}, w_{32}, w_{30}, w_{41}, w_{42}, w_{40}, ..., w_7, w_{71}, ..., w_{76}\}$$

Evolutionary Training

Evolutionary algorithm components:

- Encoding: each element of the population is a real vector containing all adaptive parameters (similar to the case of evolution strategies)
- Evolutionary operators: typical to evolution strategies or evolutionary programming
- Evaluation: the quality of an element depends on the mean squared error (MSE) on the training/validation set; an element is better if the MSE is smaller

Evolutionary Training

Aplications:

- For networks with non-differentiable or non-continuous activation functions
- For recurrent networks (the output value cannot be explicitely computing from the input value, thus the derivative based learning algorithms cannot be applied

Drawbacks:

- More costly than traditional non-evolutionary training
- It is not appropriate for fine tuning the parameters

Hybrid versions:

- Use an EA to explore the parameter space and a local search technique to refine the values of the parameters

Evolutionary Training

Remark. EAs can be used to preprocess the training set

- Selection of attributes
- Selection of examples

Evolutionary Pre-processing

Selection of attributes (for classification problems)

- Motivation: if the number of attributes is large the training is difficult
- It is important when some of the attributes are not relevant for the classification task
- The aim is to select the relevant attributes
- For initial data having N attributes the encoding could be a vector of N binary values (0 – not selected, 1 – selected)
- The evaluation is based on training the network for the selected attributes (this corresponds to a wrapper-like technique of attributes selection)

Evolutionary Pre-processing

Example: identify patients with cardiac risk

Total set of attributes:

(age, weight, height, body mass index, blood pressure, cholesterol, glucose level)

Population element: (1,0,0,1,1,1,0)

Corresponding subset of attributes:

(age, body mass index, blood pressure, cholesterol)

Evaluation: train the network using the subset of selected attributes and compute the accuracy; the fitness value will be proportional to the accuracy

Remark:

- This technique can be applied also for non neural classifiers (ex: Nearest-Neigbhor)
- It is called “wrapper based attribute selection”

Evolutionary Pre-processing

Selection of examples

- Motivation: if the training set is large the training process is costly and there is a higher risk of overfitting
- It is similar to attribute selection
- Binary encoding (0 – not selected, 1 – selected)
- The evaluation is based on training the network (using any training algorithm) for the subset specified by the binary encoding

Evolving architecture

Non-evolutionary approaches:

- Growing networks
  - Start with a small size network
  - If the training stagnates add a new unit
  - The assimilation of the new unit is based on adjusting, in a first stage, only its weights

- Pruning networks
  - Start with a large size network
  - The units and connection which do not influence the training process are eliminated

Evolving architecture

Elements which can be evolved:

- Number of units
- Connectivity
- Activation function type

Encoding variants:

- Direct
- Indirect

Evolving architecture

Direct encoding: each element of the architecture appears explicitly in the encoding

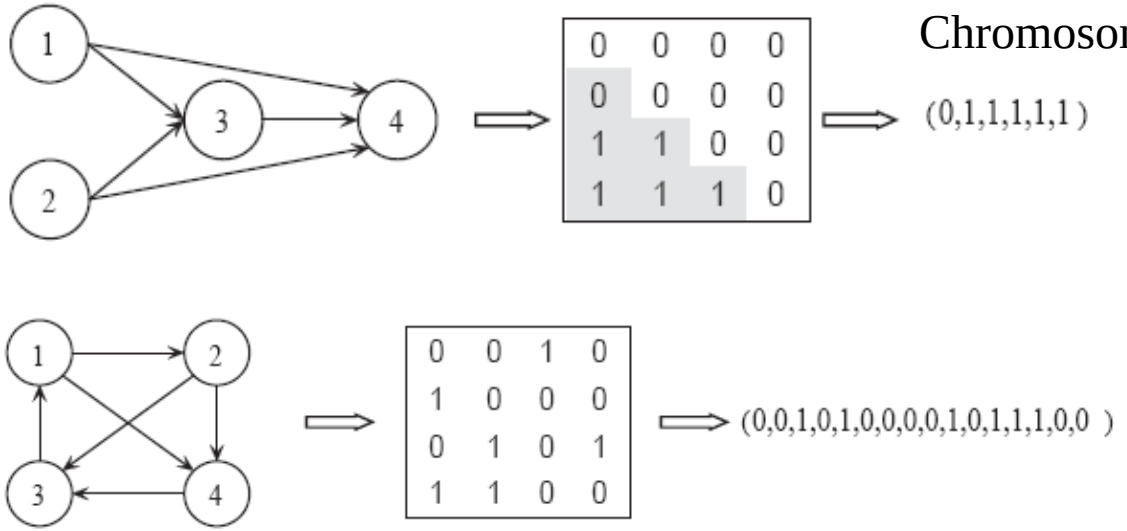
- Network architecture = oriented graph
- The network can be encoded by the adjacency matrix

Rmk. For feedforward networks the units can be numbered such that the unit i receives signals only from units j, such that j<i => inferior triangular matrix

Adjacency matrix

Chromosome

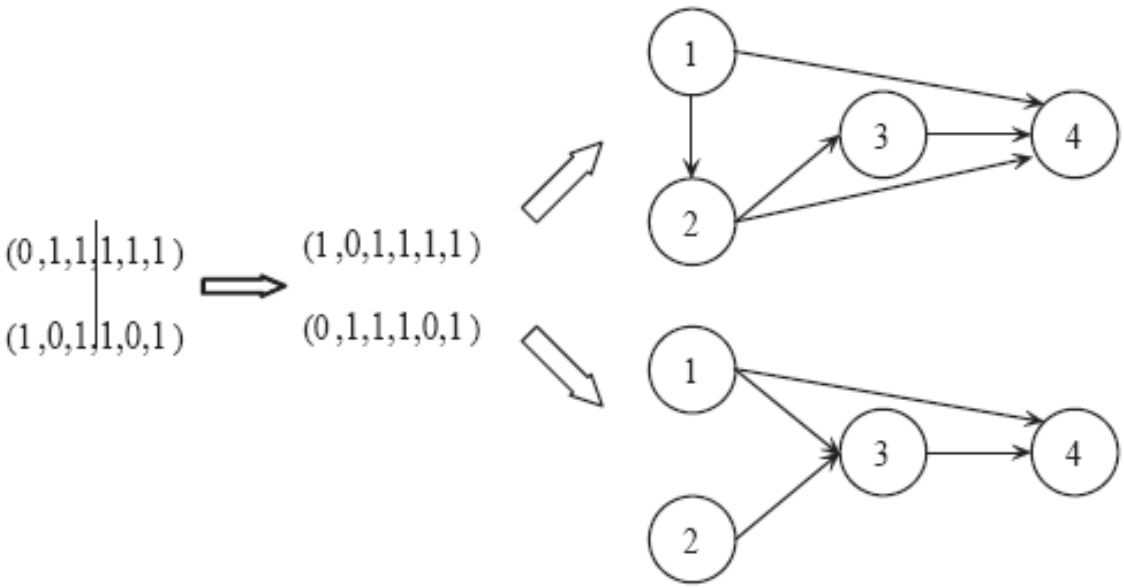
Architecture



Evolving architecture

Operators

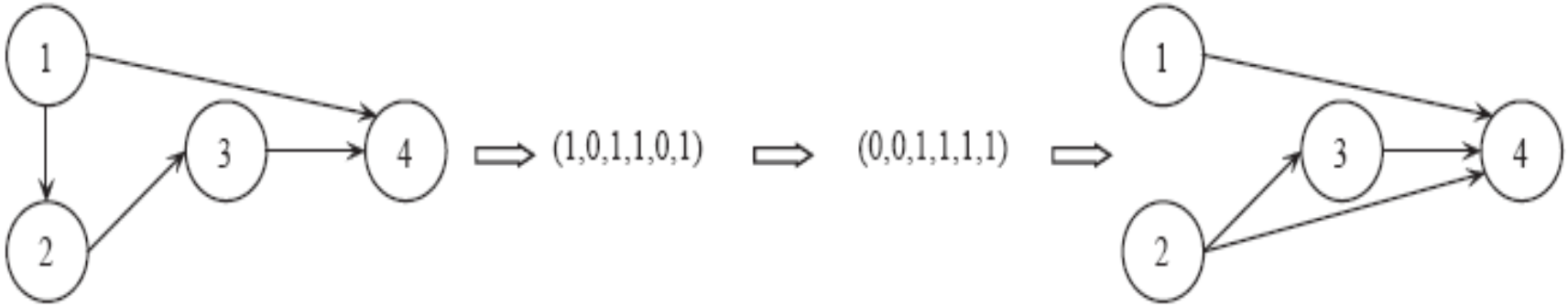
- Crossover similar to that used for genetic algorithms



Evolving architecture

Operators:

- Mutation similar to that used for genetic algorithms



Evolving architecture

Evolve the number of units an connections

Hypothesis: N – maximal number of units

Encoding:

- Binary vector with N elements
  - 0: inactivated unit
  - 1: activ unit
- Adjacency matrix NxN
  - For a zero element in the unit vector the corresponding row and column in the matrix are ignored.

Evolving architecture

Evolving the activation function type:

Encoding :

- Binary vector with N elements
  - 0: inactivated unit
  - 1: active unit with activation function of type 1 (ex: tanh)
  - 2: active unit with activation function of type 2 (ex: logistic)
  - 3: active unit with activation function of type 3 (ex: linear)

Evolution of weights

- The adjacency matrix is replaced with the matrix of weights
  - 0: no coonection
  - <>0: weight value

Evolving architecture

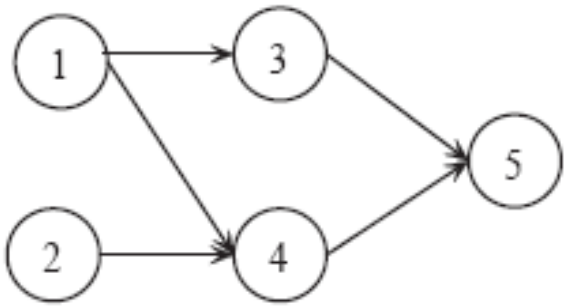
Evaluation:

- The network is trained
- The training error is estimated (E_a)
- The validation error is estimated (E_v)
- The fitness is inverse proportional to:
  - Training error
  - Validation error
  - Network size

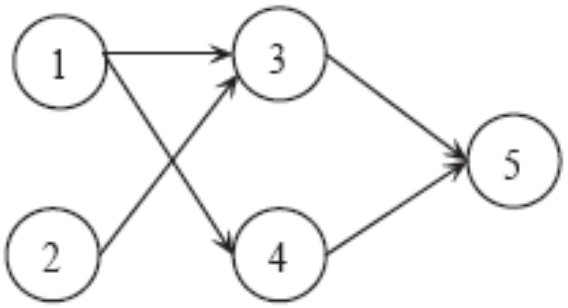
Evolving architecture

Drawbacks of the direct encoding:

- It is not scalable
- Can lead to different representations of the same network (permutation problem)
- It is not appropriate for modular networks



(0,1,0,1,1,0,0,0,1,1)



(0,1,1,1,0,0,0,0,1,1)

Evolving architecture

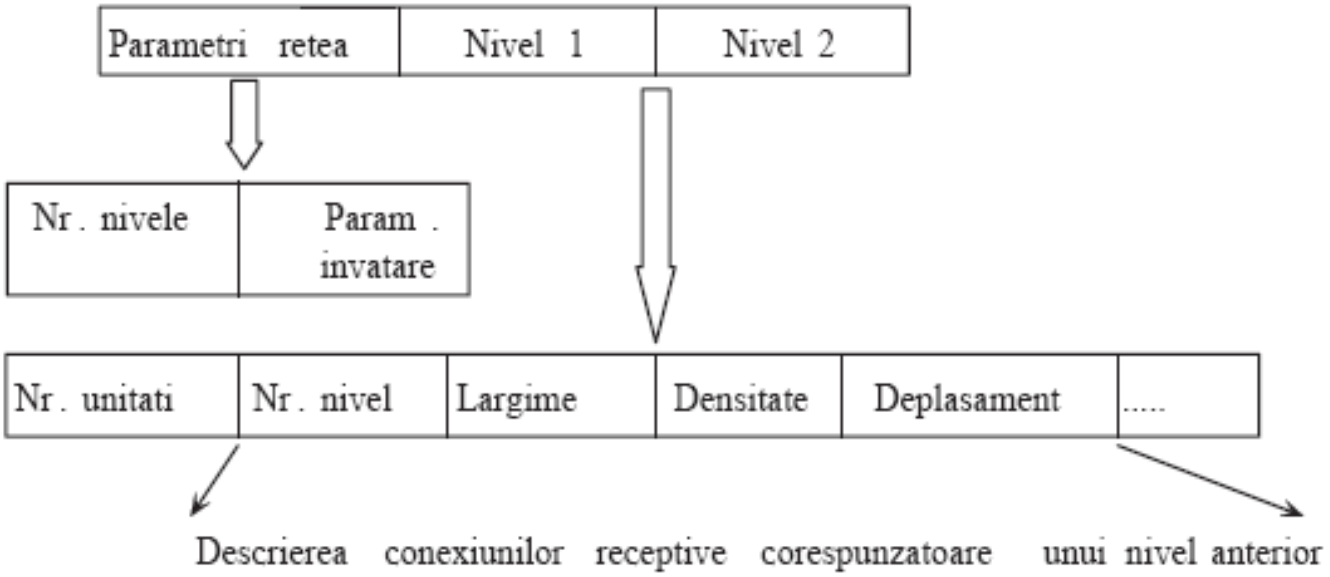
Indirect encoding:

- Biological motivation

- Parametric encoding
  - The network is described by a set of characteristics (fingerprint)
  - Particular case: feedforward network with variable number of hidden units
  - The fingerprint is instantiated in a network only for evaluation
- Rules-based encoding

Evolving architecture

- Parametric encoding



Instantiation: random choice of connections according to the specified characteristics

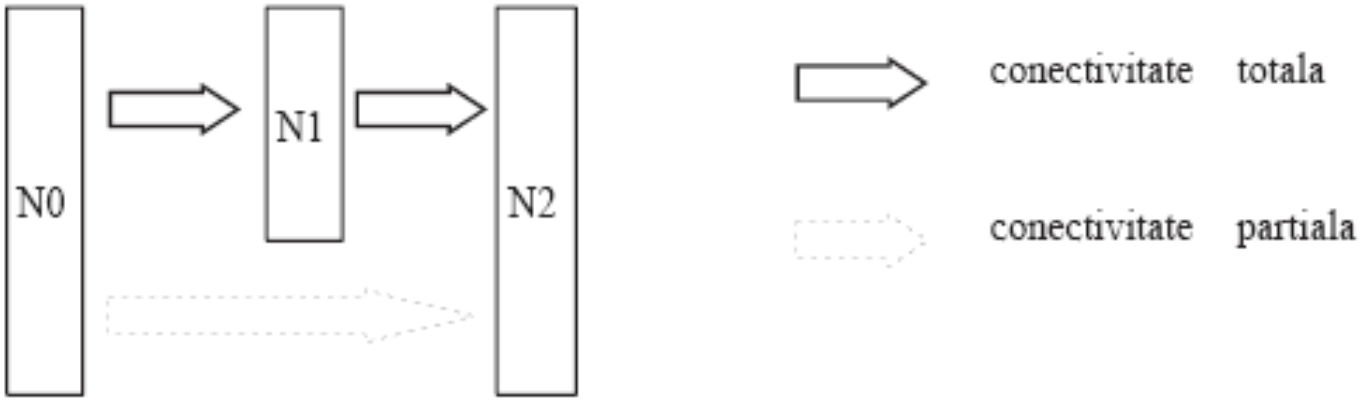
Evolving architecture

Example:

Operators:

Mutation: change the network characteristics

Recombination: combine characteristics of layers



Param. BP

Info. layer 2

2 0.1 0.9 N1 0 100% 100% 0 N2 0 15% 80% 50% 1 100% 100% 0

Info. layer 1

Nr. of layers

Evolving architecture

Rule-based encoding (similar to Grammar Evolution) :

General rule

$$sn \rightarrow \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}$$

Examples:

$$S \rightarrow \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \quad A \rightarrow \begin{pmatrix} a & a \\ a & a \end{pmatrix}, \quad B \rightarrow \begin{pmatrix} b & b \\ b & a \end{pmatrix}, \quad C \rightarrow \begin{pmatrix} b & a \\ a & c \end{pmatrix}, \quad D \rightarrow \begin{pmatrix} a & d \\ a & d \end{pmatrix},$$

$$a \rightarrow \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad b \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad c \rightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad d \rightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Structure of an element:

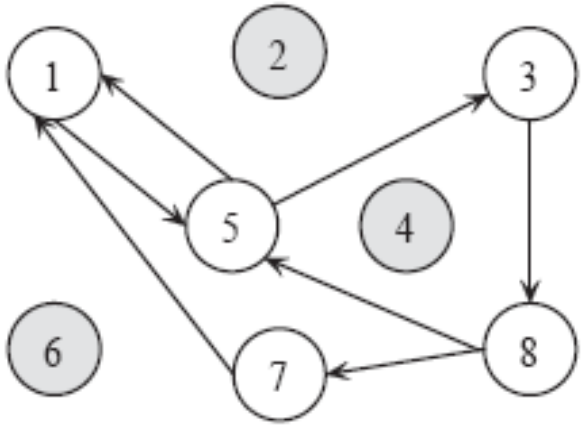
$$(A, B, C, D, a, a, a, a, b, b, b, a, b, a, a, c, a, d, a, d, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0)$$

Evolving architecture

Deriving an architecture:

$$S \rightarrow \begin{pmatrix} A & B \\ C & D \end{pmatrix} \rightarrow \begin{pmatrix} a & a & b & b \\ a & a & b & a \\ b & a & a & d \\ a & c & a & d \end{pmatrix} \rightarrow$$

$$\rightarrow \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$



Evolving architecture

Dezavantaj al evoluției separate a arhitecturii:

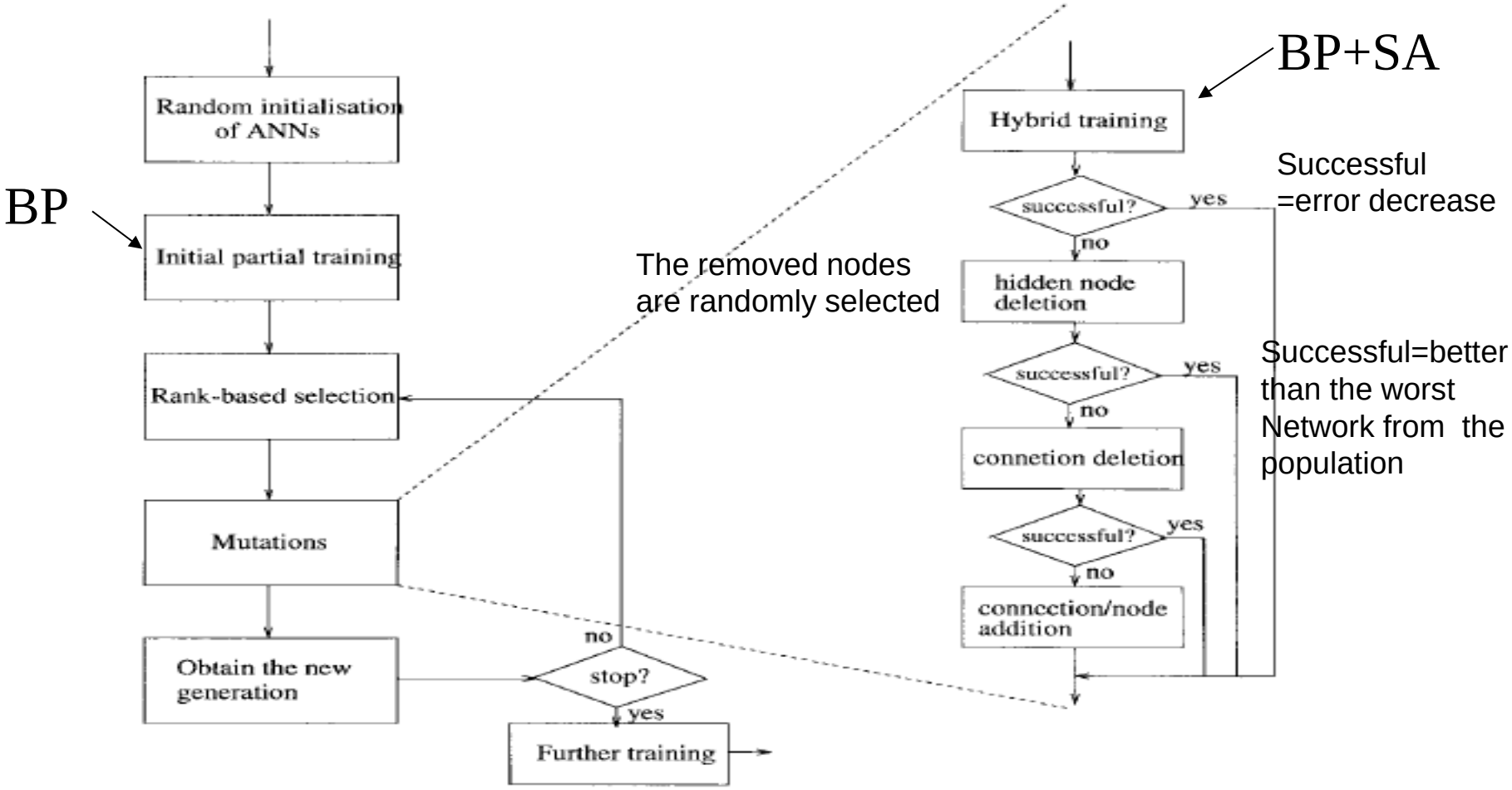
- Ca urmare a antrenării pornind de la valori inițiale aleatoare se obțin estimări afectate de zgomot al fitness-ului corespunzător unei arhitecturi

Soluții:

- Antrenarea de mai multe ori a aceleiași arhitecturi și calculul fitness-ului mediu => costuri mari
- Evoluția simultană a arhitecturii și ponderilor (asigură o corespondență 1 la 1 a genotipului (codificarea arhitecturii) și a fenotipului (rețeaua antrenată))

EPNet

Exemplu: EPNet = evolutionary design of feedforward neural networks using principles of evolutionary proramming [Xin Yao, 1996]

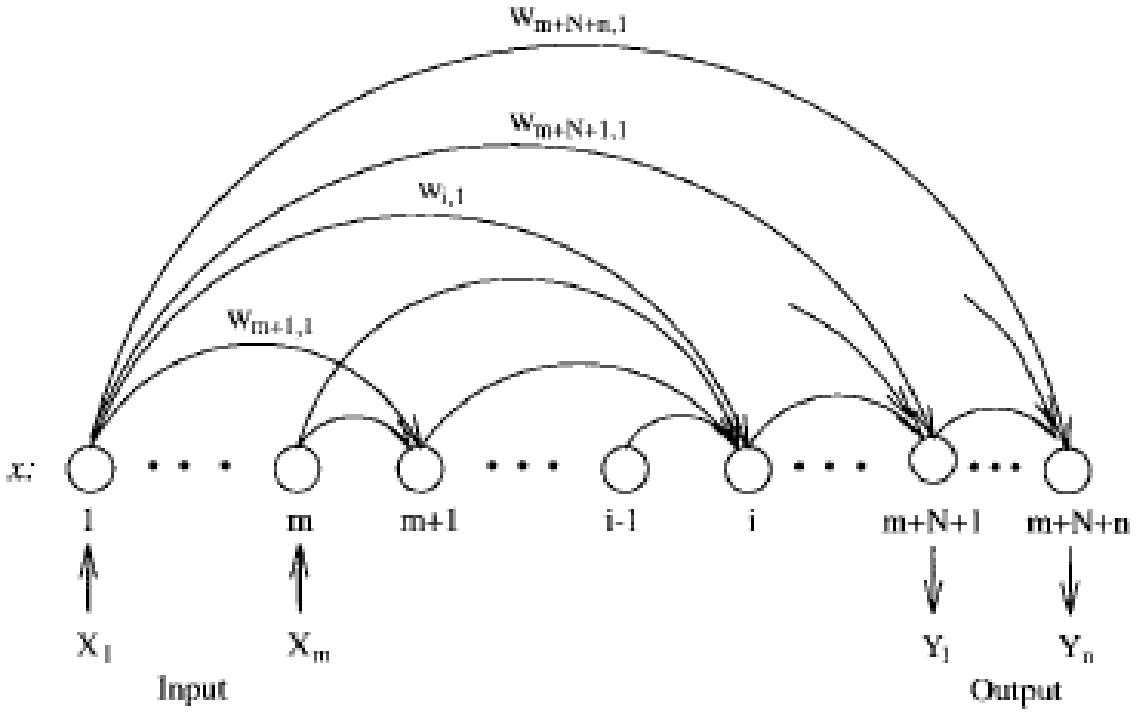


EPNet

Network encoding:

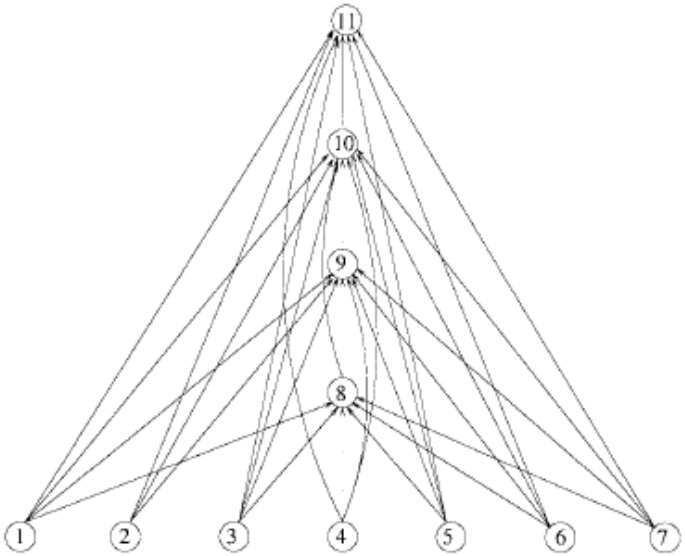
list of hidden units +
Connectivity matrix+
Weight matrix

Example: each neuron (except for the first m which are input neurons) is connected to all previous neurons

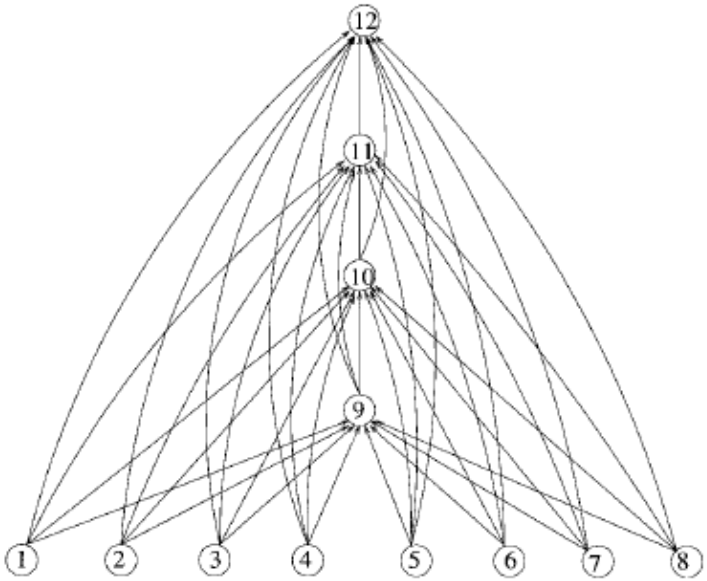


EPNet

Architectures evolved by EPNet for the parity problem



n=7



n=8

NEAT

NEAT = NeuroEvolution of Augmenting Topologies
(http://nn.cs.utexas.edu/?neat)

- Direct encoding:
  - List of nodes (neurons)
    - Type of the nodes: input, hidden, output, bias
  - List of connections; for each connection:
    - In-node
    - Out-node
    - Connection weight
    - Activation bit (0 – active connection, 1- disabled connection)
    - Innovation value

NEAT

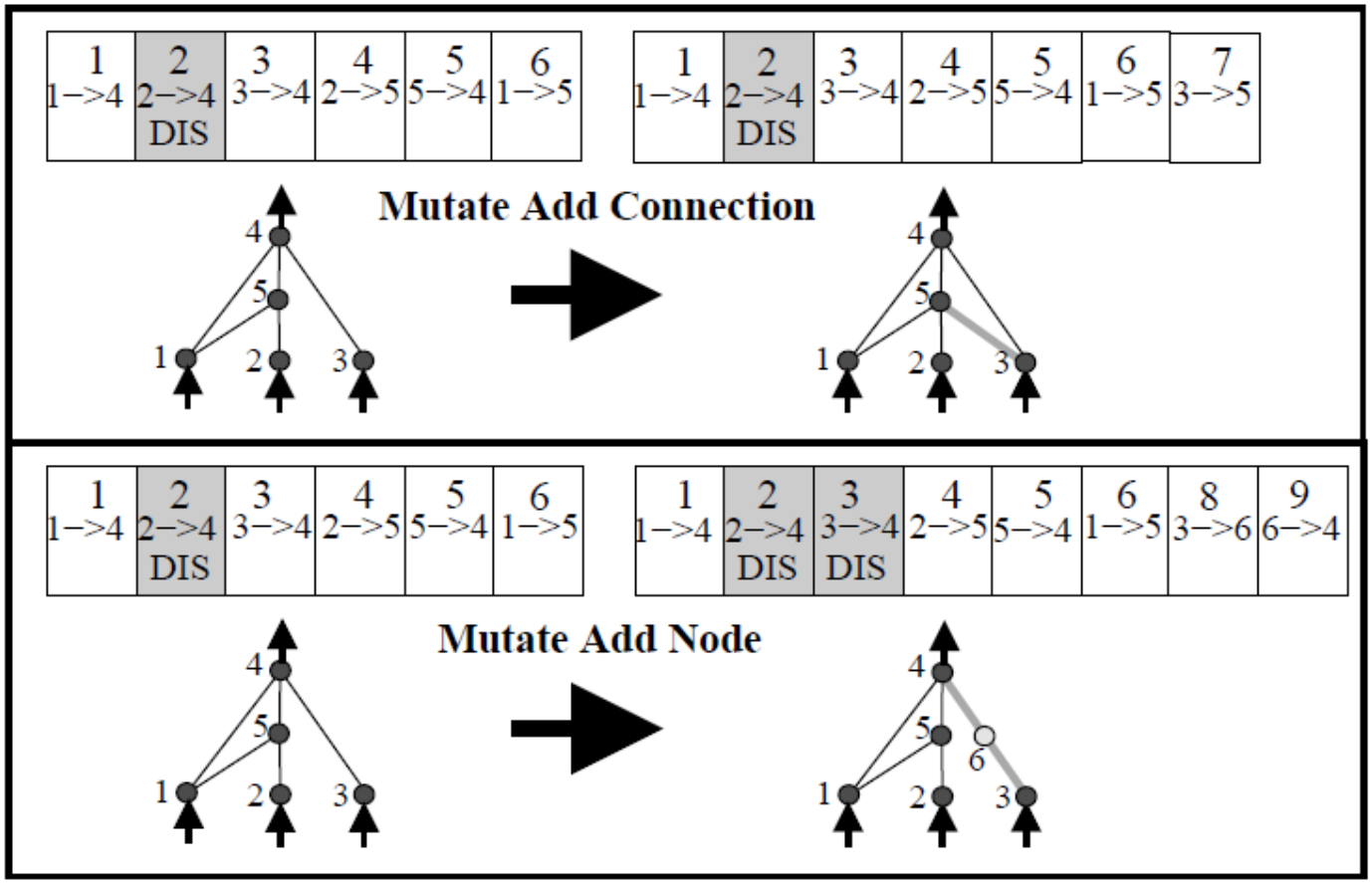
NEAT = NeuroEvolution of Augmenting Topologies
(http://nn.cs.utexas.edu/?neat)

- The initial population consists of simple architectures (only input and output layers)

- Mutation variants:
  - Node adding: insert a new node between two already connected nodes (the old connection is removed and two other connections are added: that entering the new node has the weight=1, that going out from the new node has the weight of the removed connection)
  - Connection adding: a new connection (with a random weight) is added between two previously unconnected nodes

NEAT

Mutation example: (K.Stanley, R. Miikulainen – Evolving Neural Networks through Augmenting Topologies, Evol.Comput. 2002)



NEAT

Crossover:

2 parents ---- 1 offspring

Similar to uniform crossover used in genetic algorithms

Step 1: identify the matching genes from the two parents based on the innovation values

- Two genes match if they have the same innovation value (this values is assigned when the gene is created)
- The non-matching genes are disjoint or in excess genes

NEAT

Crossover:

2 parents ---- 1 offspring

Similar to uniform crossover used in genetic algorithms

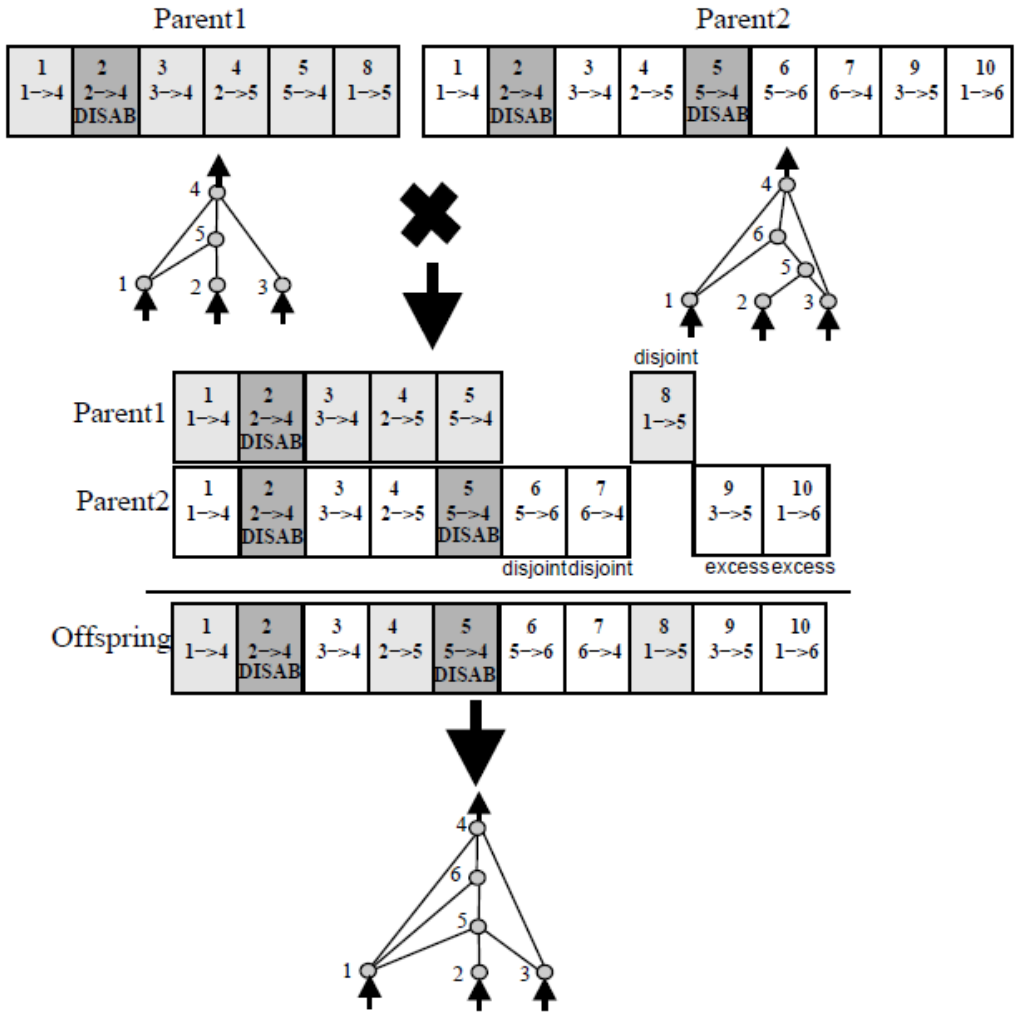
Step 2: offspring construction

- For matching genes the offspring will receive the gene from one of the parents (randomly selected)
- The in excess/disjoint genes are transferred into the ofspring either based on a probabilistic decision or based on the fitness of the parents (the gene its transferred if it belongs to the better parent)

NEAT

Crossover example

(Stanley, Miikulainen, 2002)



Evolving learning rules

General form of a local adjustement rule

$$w_{ij}(k+1) = \varphi(w_{ij}(k), x_i, y_i, x_j, y_j, \delta_i, \delta_j, \alpha)$$

x_i,x_j – input signals

y_i,y_j – output signals

α – control parameters (ex: learning rate)

δ_i,δ_j – error signal

Example: BackPropagation

$$w_{ij}(k+1) = w_{ij}(k) + \eta \delta_i y_j$$

Evolving learning rules

Elements which can be evolved:

- Parameters of the learning process (ex: learning rate, momentum coefficient)
- The adjusting expression (see Genetic Programming)

Evaluation:

- Train networks using the corresponding rule

Drawback: very high cost

Summary

General structure

Levels:

- Weights
- Learning rules
- Architecture