Evolutionary Design of Neural Networks

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

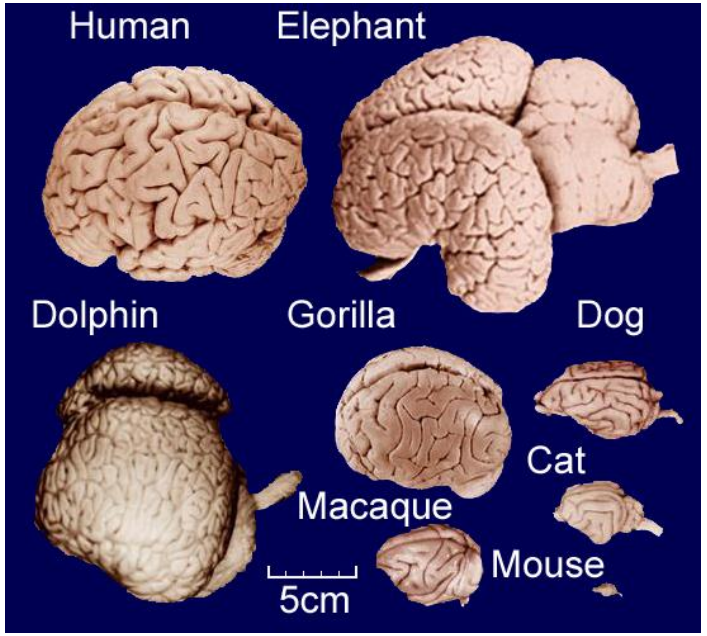
Evolutionary Design of Neural Networks

Neural networks design consists of at least two steps:

- Choice of the architecture (network topology + connectivity)
  - It has an influence on the network ability to solve the problem
  - Usually is a trial-and-error process
- Training of the network
  - It is an optimization problem = find the parameters (weights) which minimize the error on the training set
  - The classical methods (e.g. gradient-based methods as is BackPropagation) have some drawbacks :
    - Risk of getting stuck in local minima
    - They cannot be applied if
      - the activation functions are not differentiable
      - the error function cannot be expressed directly as a function of the parameters (e.g. for recurrent networks)

Evolutionary Design of Neural Networks

Idea: use an evolutionary process



- Inspired by the biological evolution of the brain
- The system is not explicitly 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)

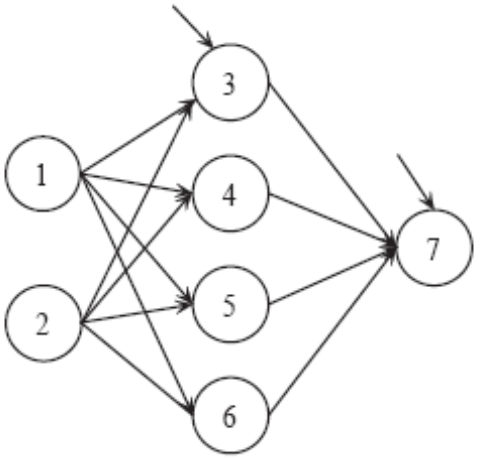
Evolutionary Design of Neural Networks

Variants

- Evolutionary training:
  - Estimate the weights using a global optimization metaheuristic
  - It can be used for networks with discontinuous activation functions and for recurrent networks
- Evolving architecture:
  - Evolve the number of units, types of activation functions, connections
- Evolving the learning process:
  - Evolve adjustment rules in the training process

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

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

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

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

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 or other population-based metaheuristics for global optimization (e.g. particle swarm optimization, differential evolution)
- Evaluation: the quality of an element depends on the mean squared error (MSE) or another loss function computed for the training/validation set; an element is better if the MSE/loss function is smaller

Evolutionary Training

Applications:

- For networks with non-differentiable or non-continuous activation functions
- For recurrent networks (the output value cannot be explicitely computed 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 also 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

Evolutionary Pre-processing

Remarks:

- This technique can be applied also for non neural classifiers (ex: Nearest-Neigbhor)
- It is called “wrapper based attribute selection”
- the optimization problem can be formulated as a multi-objective optimization problem aiming to:
  - Maximize the accuracy
  - Minimize the number of selected features
- Besides GAs, there are various metaheuristics which have been successfully applied for feature selection: PSO, GP, DE, memetic algorithms etc.

[B. Xue et al, A Survey of EC Approaches for Feature Selection, IEEE Trans EC, 2016]

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

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

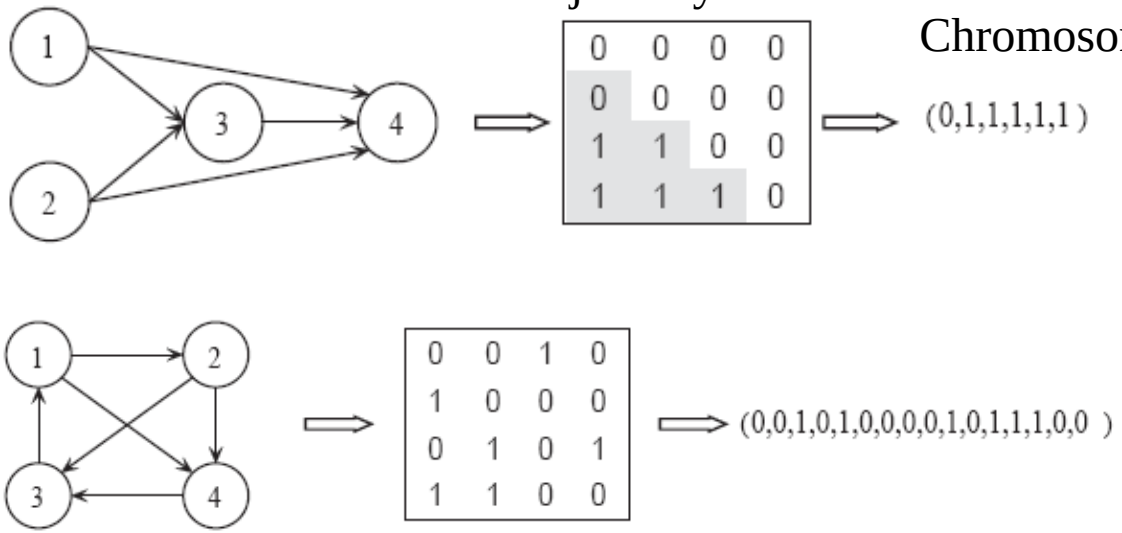
- Network architecture = oriented graph
- The network can be encoded by the adjacency matrix

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

Architecture

Adjacency matrix

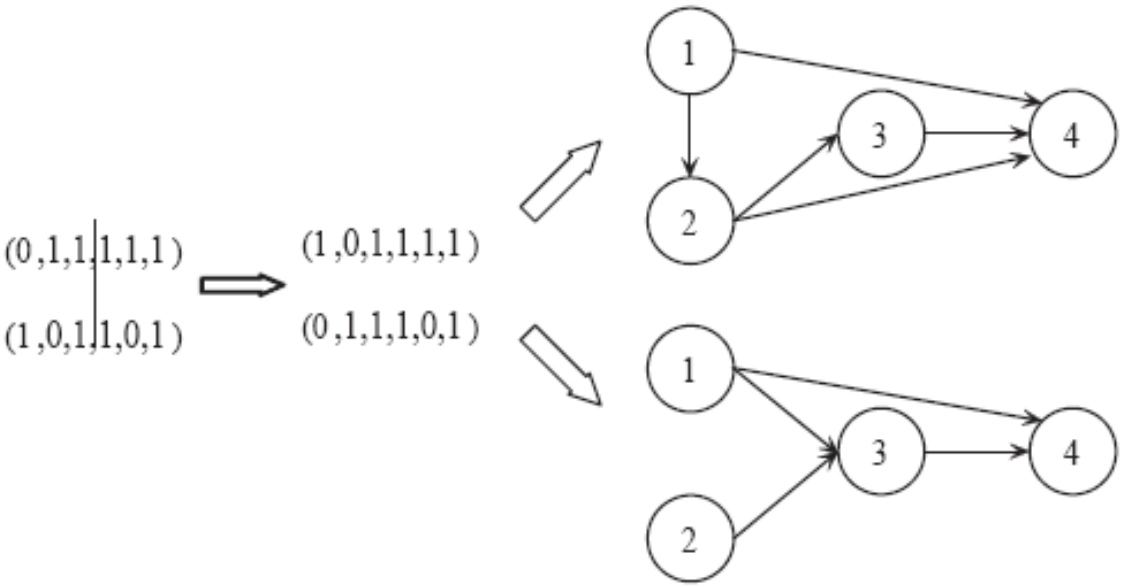
Chromosome



Evolving architecture

Operators

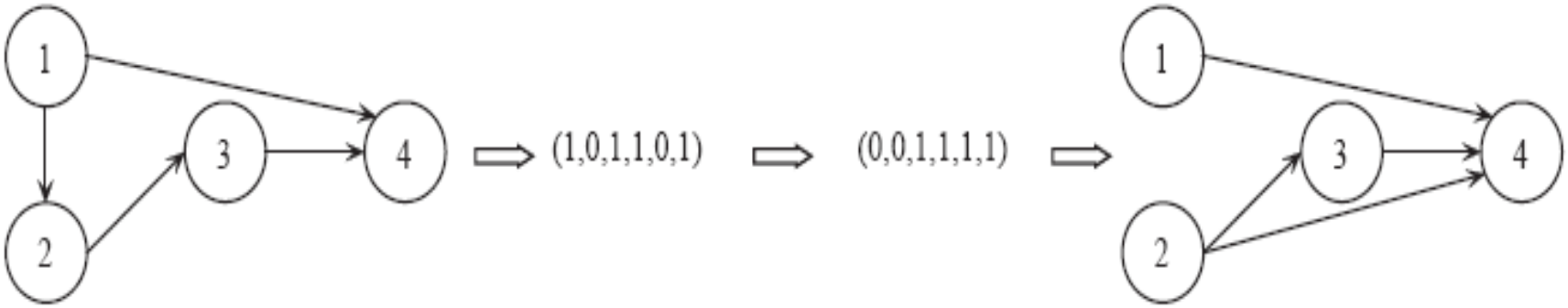
- Crossover similar to that used for genetic algorithms



Evolving architecture

Operators:

- Mutation similar to that used for genetic algorithms



Evolving architecture

Evolve the number of units and 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 in the forward step.

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 connection
  - <>0: weight value

Evolving architecture

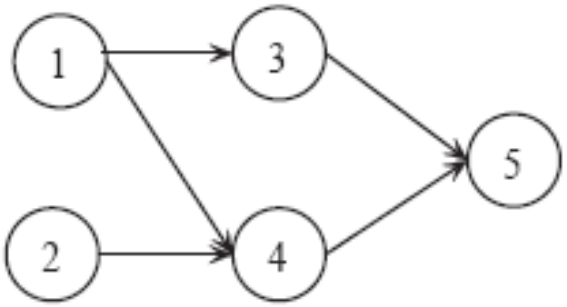
Evaluation:

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

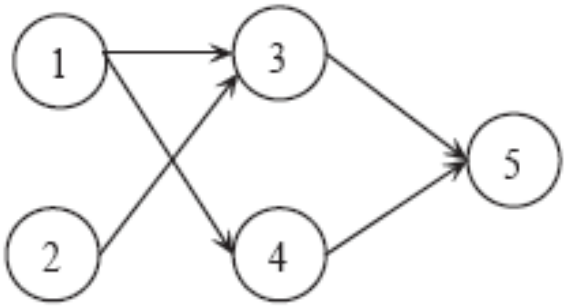
Evolving architecture

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)

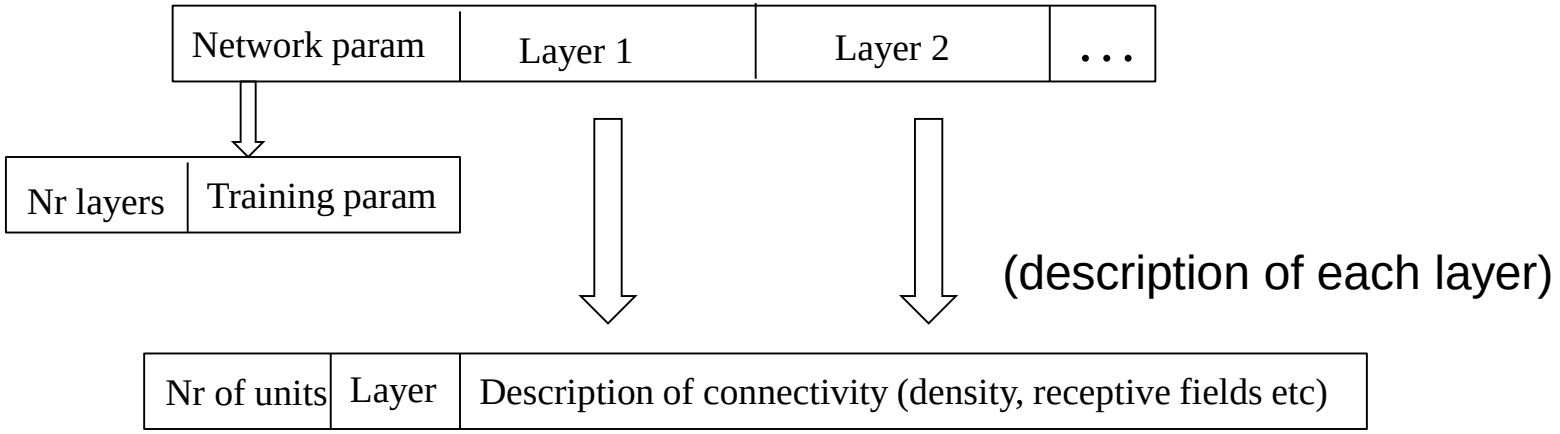
Evolving architecture

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 as a network only during the evaluation stage
- Rules-based encoding

Evolving architecture

- Parametric encoding



Instantiation: random choice of connections according to the specified characteristics

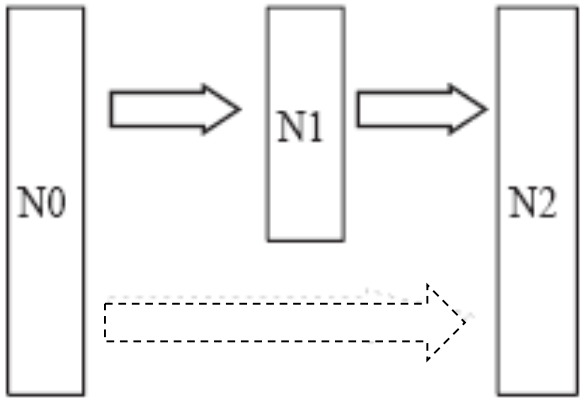
Evolving architecture

Example:

Operators:

Mutation: change the network characteristics

Recombination: combine characteristics of layers



Fully connected layers

Sparsely connected 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

Number 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:

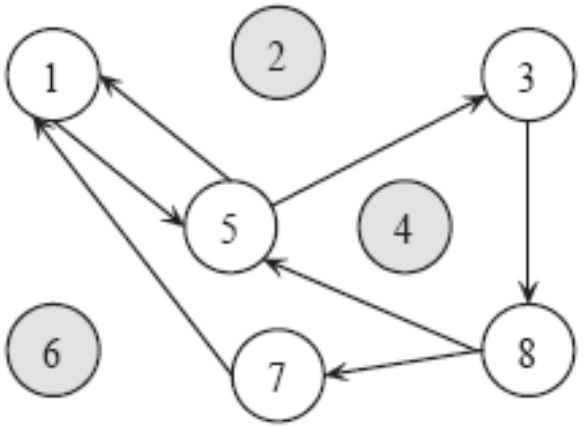
$$(A, B, C, D, a, a, a, a, b, b, b, a, b, a, a, c, a, d, a, d, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0)$$

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

Drawback of separate evolution of the architecture and weights:

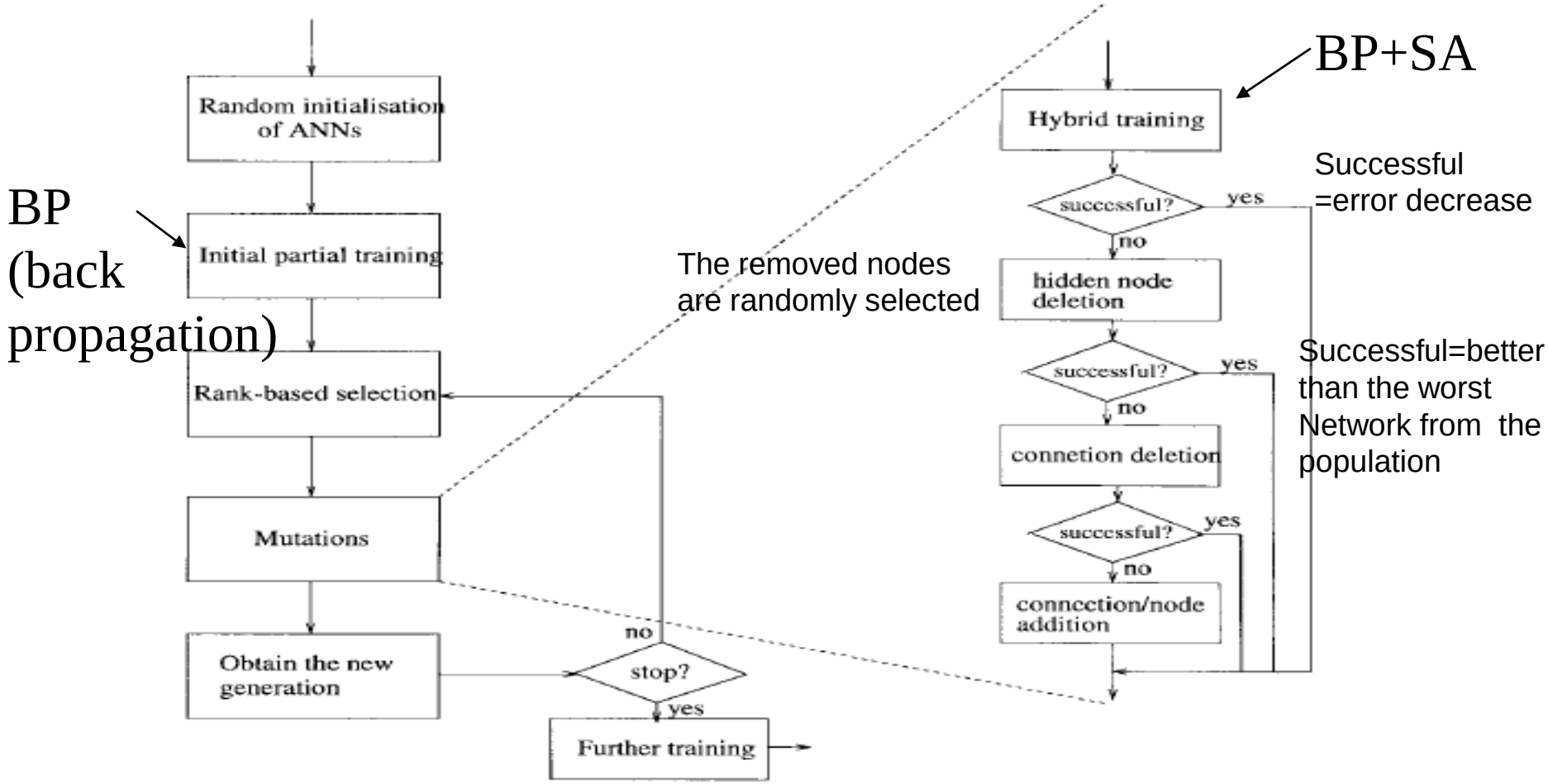
- Since the behaviour of an architecture depends on the weights values, at different evaluations steps, same architecture can have various fitness values (caused by different training processes) - thus the fitness is noisy

Solutions:

- Repeat the training of the same architecture and compute an averaged fitness => high computational costs
- Simultaneous evolution of the architecture and weights (it will ensure a one-to-one mapping between the genotype – the architecture - and the phenotype – the trained network)

EPNet

Exemplu: EPNet = evolutionary design of feedforward neural networks using principles of evolutionary programming [Xin Yao,1999]

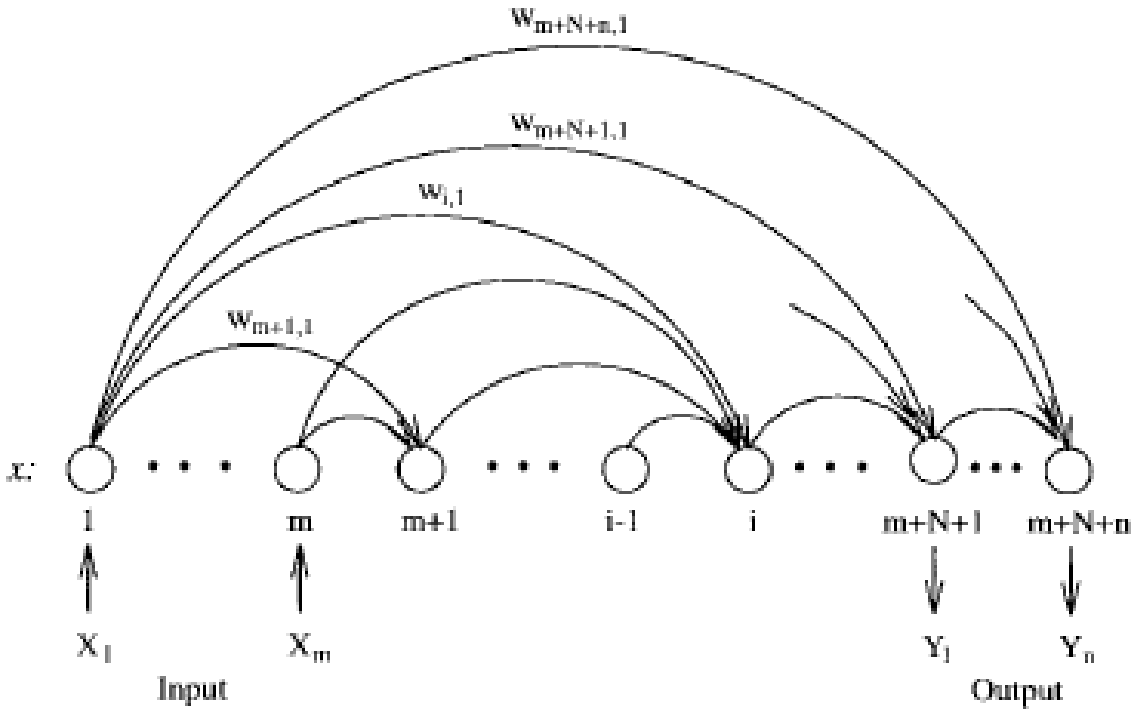


EPNet

Network encoding:

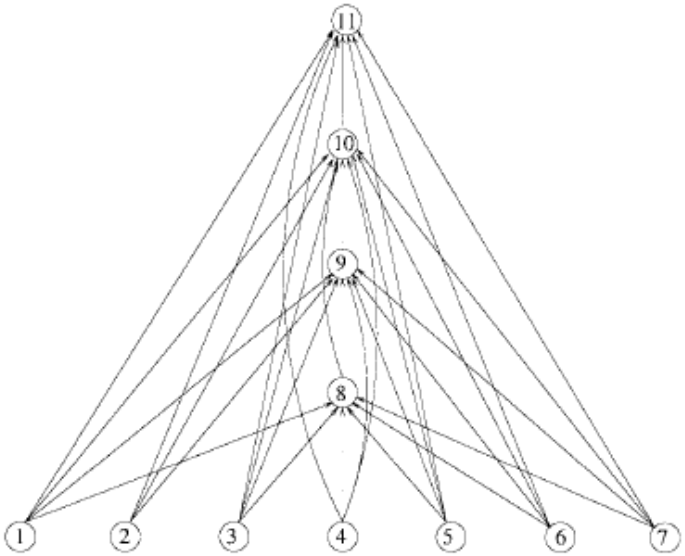
list of hidden units + Connectivity matrix + Weight matrix

Example: each neuron (except for the first m which are input neurons) is connected to all previous neurons [X. Yao – Evolving Artificial Neural Networks, 1999]

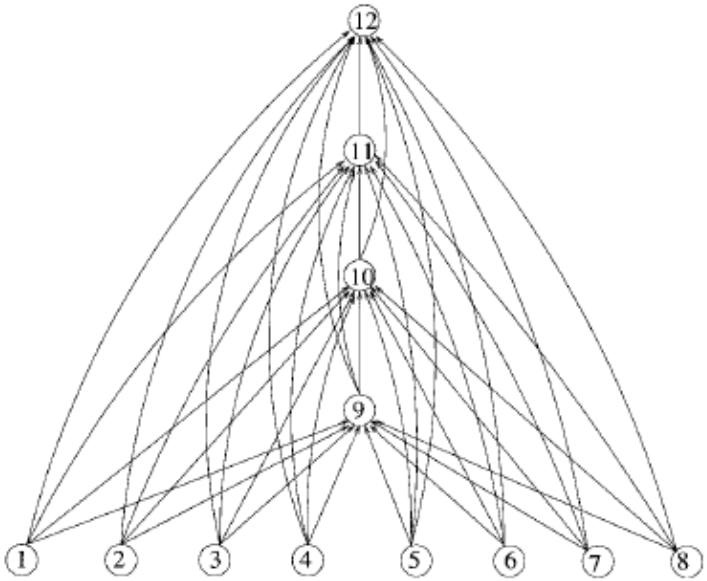


EPNet

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

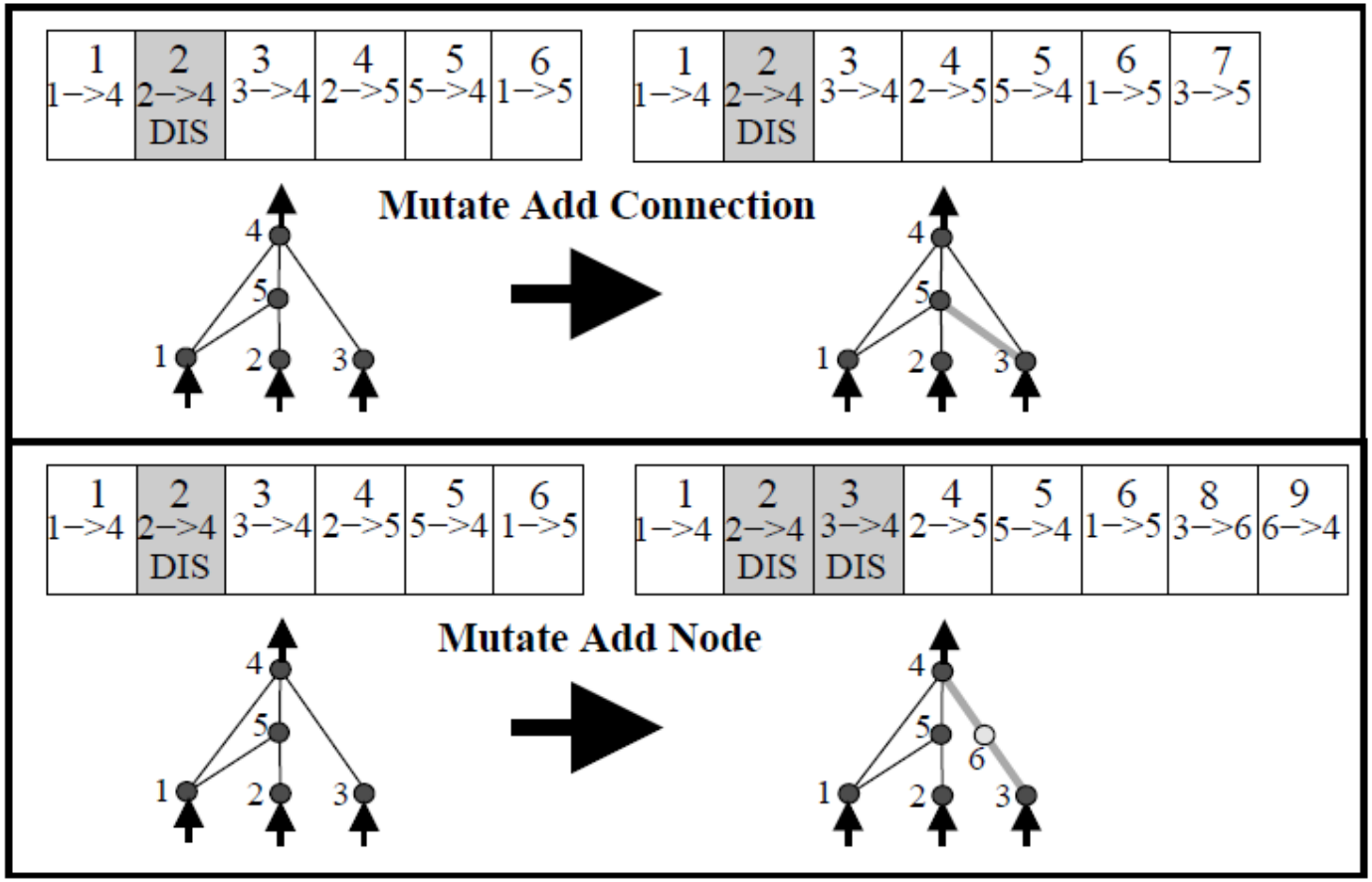
NEAT = NeuroEvolution of Augmenting Topologies
(http://nn.cs.utexas.edu/?neat)

- 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: the connection entering the new node has the weight =1, the connection 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 value is assigned when the gene is created and is specified in the diagram)
- The non-matching genes are disjoint or in excess genes

NEAT

Crossover:

2 parents → 1 offspring

Similar to uniform crossover used in genetic algorithms

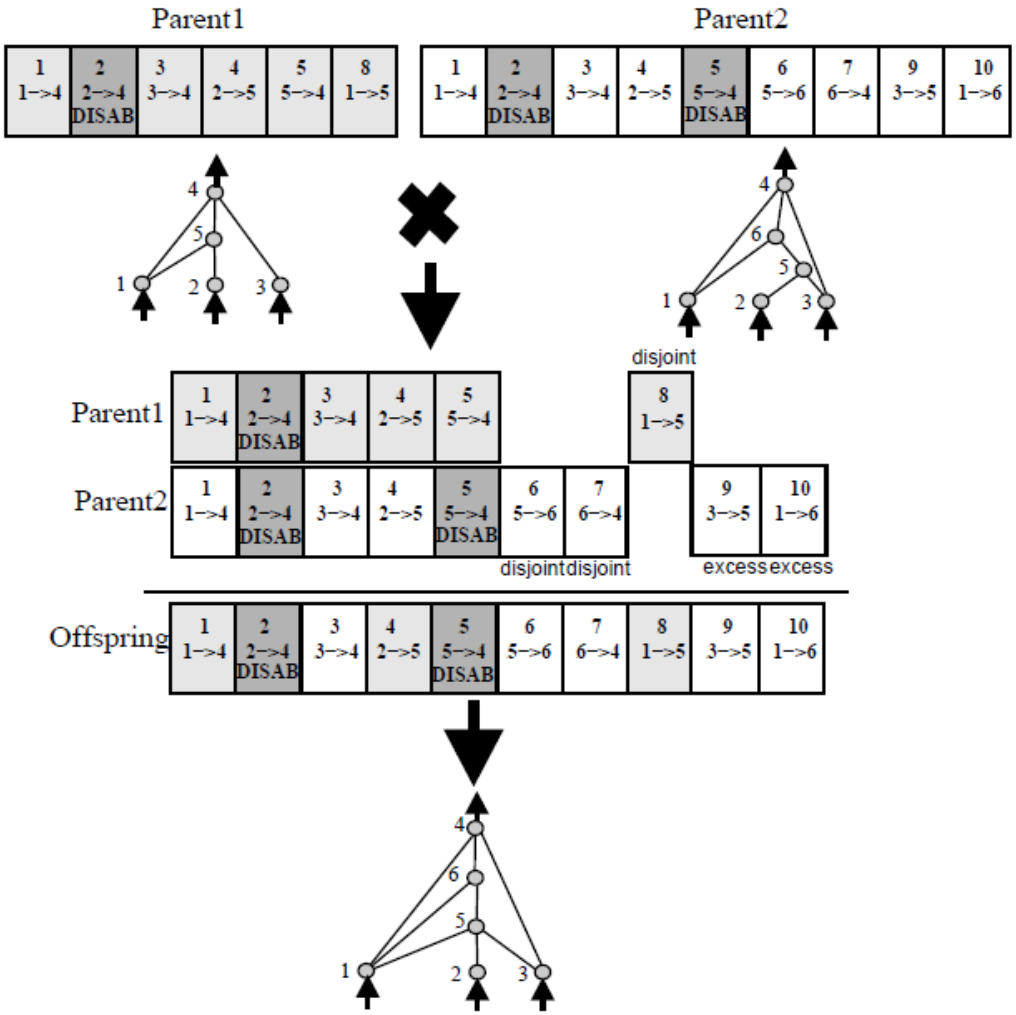
Step 2: offspring construction

- 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

Evolutionary Deep Neural Networks

M.J.Shafiee, A. Mishra, and A. Wong - Deep Learning with Darwin: Evolutionary Synthesis of Deep Neural Networks, 2016

DeepNN = neural networks with many layers

Motivation: evolve efficient Deep NN (instead of trying to compress existing DeepNN in order to make them more efficient

Main ideas:

- the deep neural networks architecture are encoded using synaptic probability models (interpreted as network DNA)
- new networks are synthesized using these probability models which are further trained

Implemented mechanisms: heredity, natural selection, random mutation

Evolutionary Deep Neural Networks

M.J.Shafiee, A. Mishra, and A. Wong - Deep Learning with Darwin: Evolutionary Synthesis of Deep Neural Networks, 2016

Particularities:

- usage of the exponential distribution as probability model for synaptic weights
- Impose constraints on the number of synapses (e.g. an offspring has at most 50% of the synapses of its parent).

Deep Neuroevolution

R. Miikkulainen- Evolving Deep Neural Networks, 2017

- Deep NEAT = extension of NEAT to evolve deep topologies and hyperparameters
  - same idea as in NEAT, i.e. the initial population consists of simple architectures which are further extended through mutation and crossover (new nodes and edges are added)
  - it uses a speciation mechanism: the population is divided into subpopulations (species) based on a similarity metric

- Main difference between NEAT and DeepNEAT
  - In NEAT a node corresponds to a neuron
  - In Deep NEAT a node corresponds to a layer and contains a table of values corresponding to hyperparameters

Deep Neuroevolution

R. Miikkulainen- Evolving Deep Neural Networks, 2017

- Examples of hyperparameters associated to a node (which defines a layer):
  - layer type: convolutional, fully connected, recurrent
  - layer properties: number of neurons, activation function, kernel size, number of filters
  - Remark: the edges in the chromosome do not have associated weights (as in NEAT) but they specify only how are connected the layers
- Examples of global parameters: learning rate, training algorithm, shift and scaling sizes
- Instantiation of a network
  - The chromosome graph is traversed and each node is replaced with the corresponding layer
  - The constructed DNN is then trained
  - The performance of DNN after training is used as fitness value

Deep Neuroevolution

R. Miikkulainen- Evolving Deep Neural Networks, 2017

- Remark: the most successful DNN (e.g. GoogleLeNet, ResNet, AlexNet, SegNet etc) consist of several very similar modules (as structure)

- CoDeepNEAT = Coevolution DeepNEAT = variant of DeepNEAT characterized by:
  - two populations of modules and blueprints are separately evolved
- Remark:
  - each blueprint chromosome is a graph where each node is a reference (pointer) to a particular module species
  - each module chromosome is a graph that represents a small DNN
- During instantiation each node in a blueprint chromosome is replaced with a DNN randomly selected from the species referred by the node

Deep Neuroevolution

R. Miikkulainen- Evolving Deep Neural Networks, 2017

- Evaluation:
  - to each blueprint and module chromosome is associated the average performance score obtained by the DNNs which contain that blueprint or module
  - during evolution the instantiated networks are trained for a small number of epochs (e.g. less than 10)