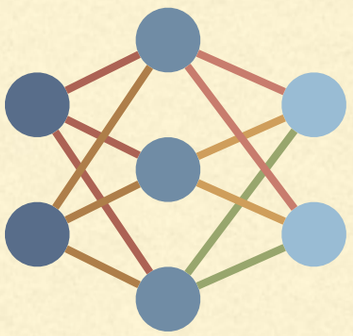
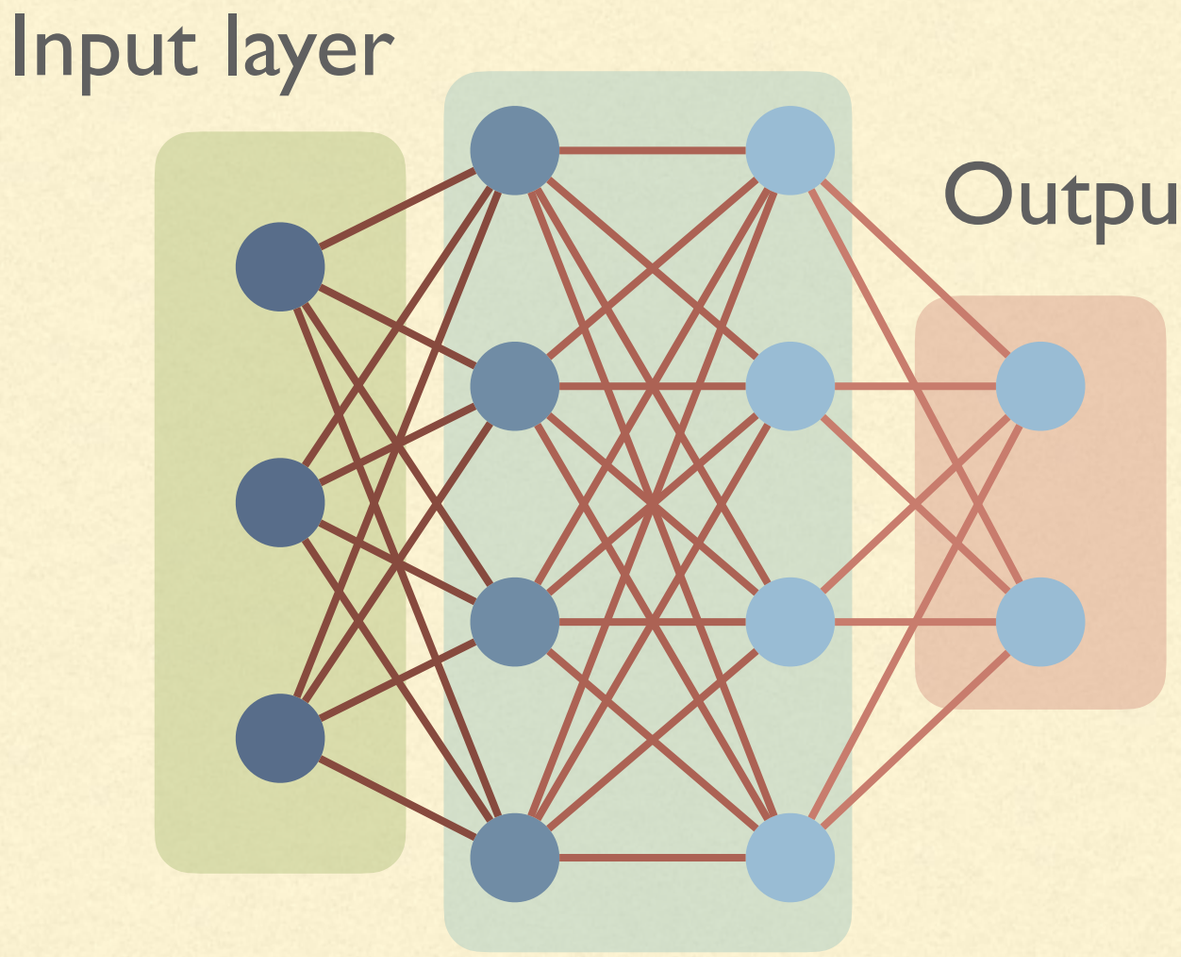
NEUROEVOLUTION

Luca Manzoni



A QUICK AND NOT-TOO-INACCURATE RECAP ON NEURAL NETWORKS



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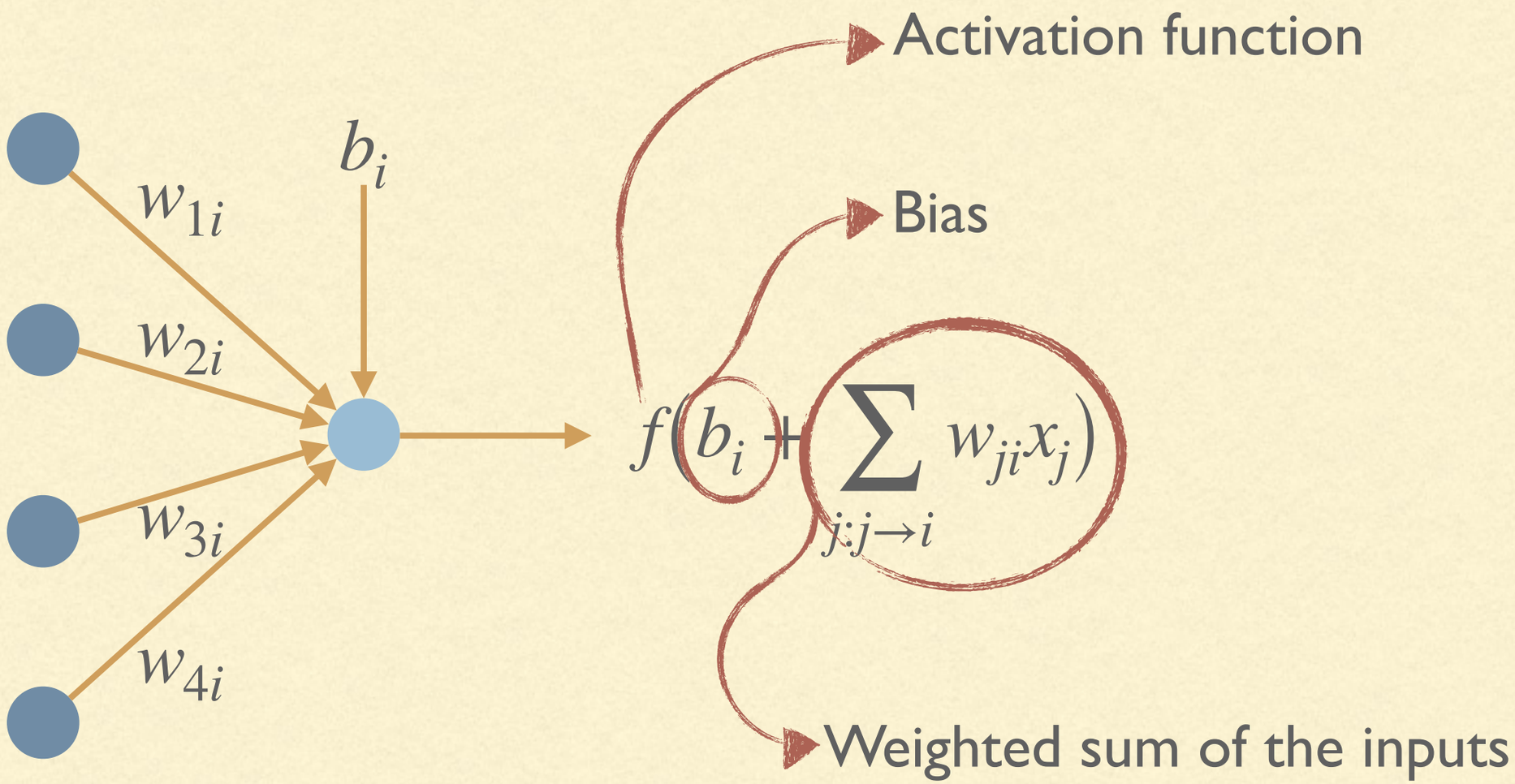


NEURAL NETWORK TRAINING

- Training is usually performed via (stochastic) gradient descend
- Main idea: find in which direction the weights can be modified to reduce the error by differentiating the error w.r.t. the weights
- However, only the weights are learned
- The architecture of the network (i.e., number, size, and type of hidden layers) and the hyperparameters are selected manually

WHAT TO EVOLVE

- Weights (but this can also be done with backpropagation)
- Activation functions
- Hyperparameters (e.g., momentum, learning rate, dropout)
- Architecture (e.g., connections, types of layer)

HISTORY (CLASSIC NEUROEVOLUTION)

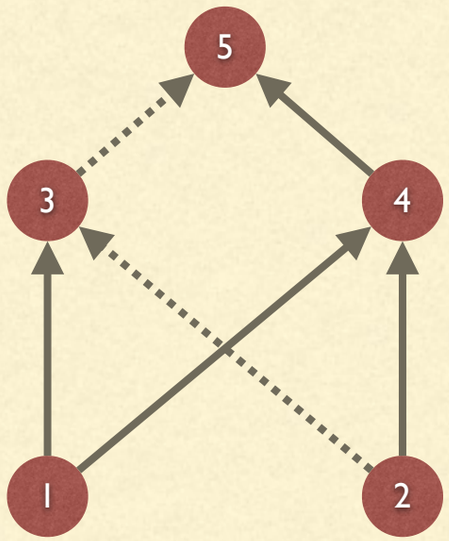
- History: anything before the advent of large/deep networks
- Evolution of weights and topology
- The “unit” was the single neuron/single weight
- Currently unfeasible due to the large number of neurons/weights/layers

ENCODINGS

How a neural network is represented (i.e., the genotype) is important for the kind of operations (mutation and crossover) that can be performed:

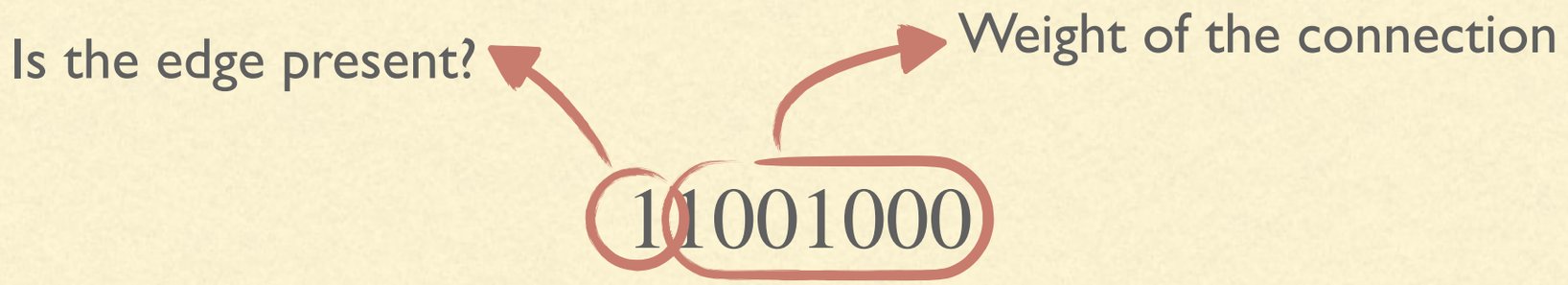
- GENITOR encoding
- Matrix encoding
- Node-based encoding
- Path-based encoding

GENITOR ENCODING



The topology of the network is fixed

Each edge of the network is encoded as a binary string of fixed length:

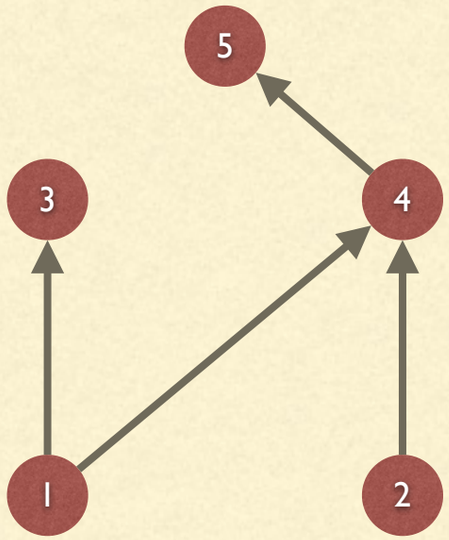


The entire network can be represented as a binary string

MATRIX ENCODING

The connections can be modified…
…but not the number of neurons

The network is represented as a binary matrix



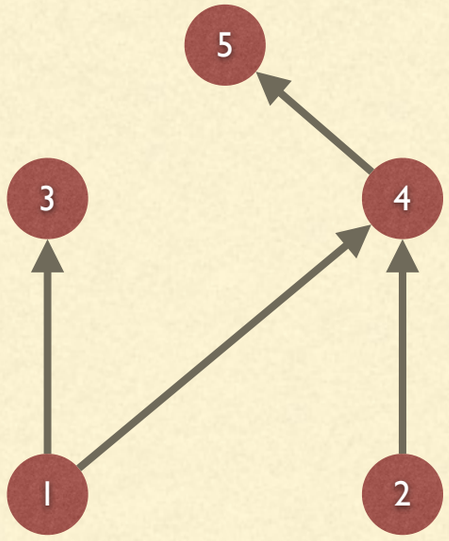
$$\begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Only this part is necessary
if the network is feed-forward

Does not scale even for small networks

NODE-BASED ENCODING

The main "unit" is the node, that also keeps track of the connections and the weights



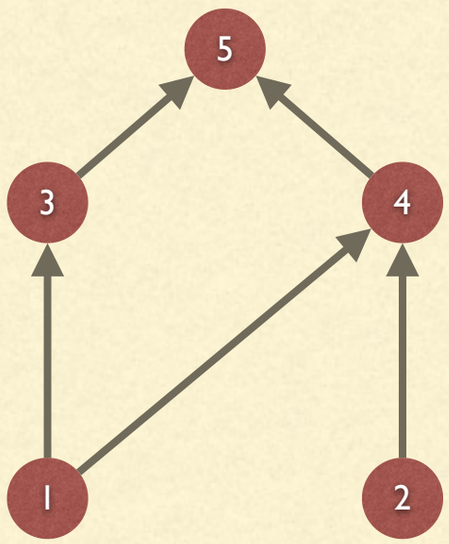
Node 1 Out: [3, 4]	Node 2 Out: [4]	Node 3 Out: []	Node 4 Out: [5]	Node 5 Out: []

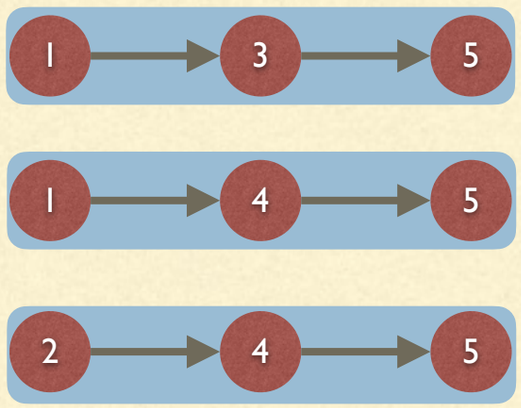
Both new nodes and new connections can be created

A similar encoding is used by NEAT

PATH ENCODING

The network is encoded as a collection of paths from the inputs to the outputs

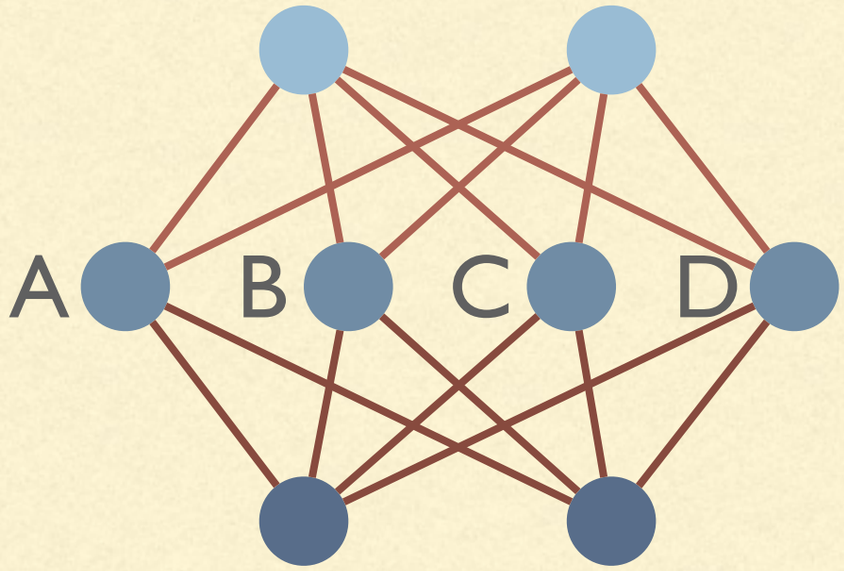


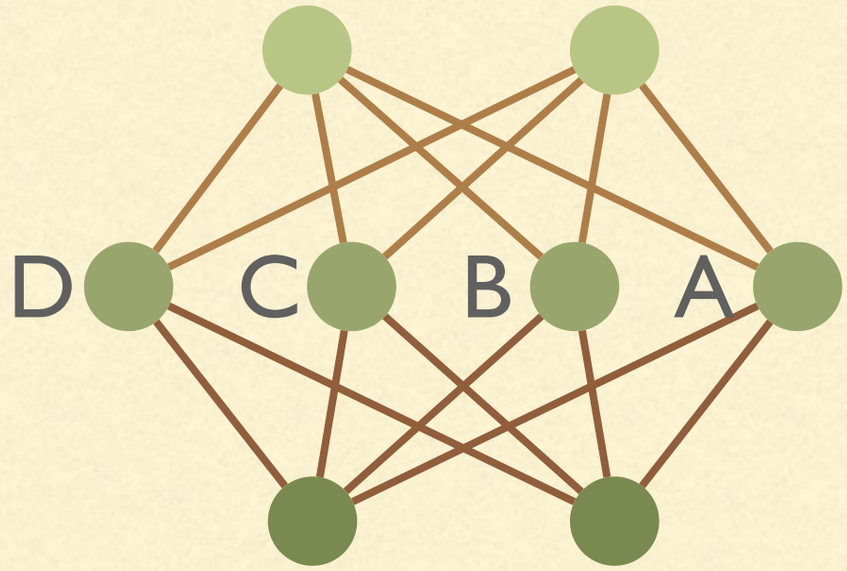


We can reconstruct the network from the paths

Recombination is usually two points
crossover and mutations modify a single path

THE COMPETING CONVENTIONS PROBLEM

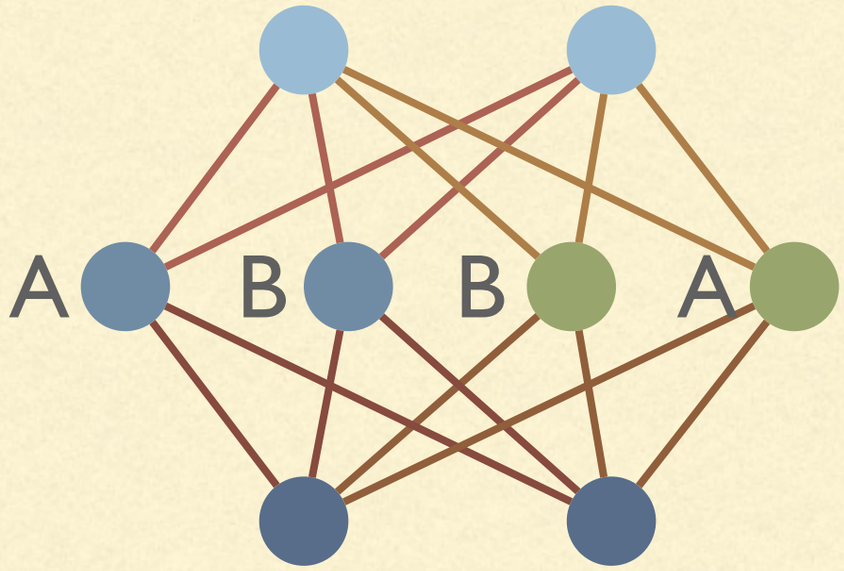


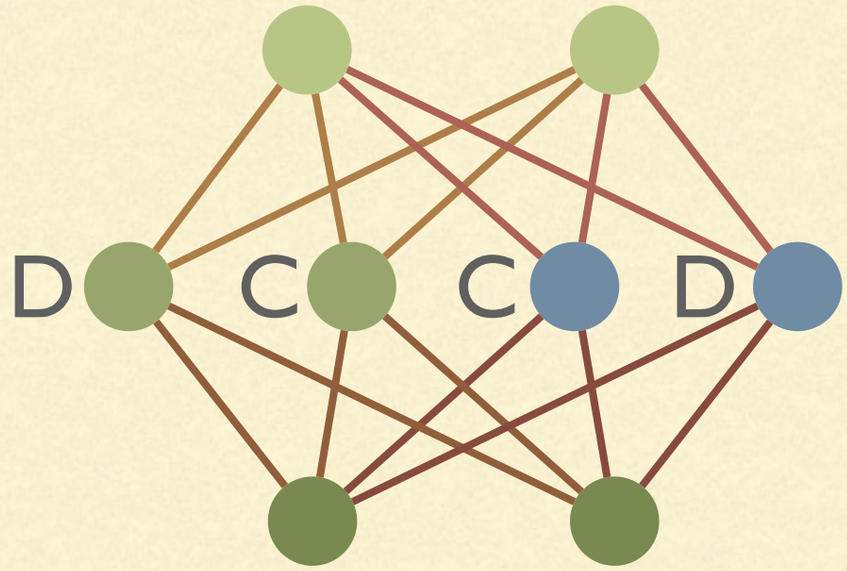


Suppose that each hidden neuron has one of four different functionalities: A, B, C, D.

- Are the two networks different w.r.t. their represented functions?
- What can happen when we perform crossover?

THE COMPETING CONVENTIONS PROBLEM





If crossover is performed without some kind of matching we can end up with two networks that are a lot worse than their parents

NEAT
NEUROEVOLUTION OF AUGMENTING TOPOLOGIES

- Think "direct encoding of a graph structure" where both the structure of the network and the weight are evolved at the same time

- The initial population start "simple" (no hidden nodes). Evolution might add new nodes

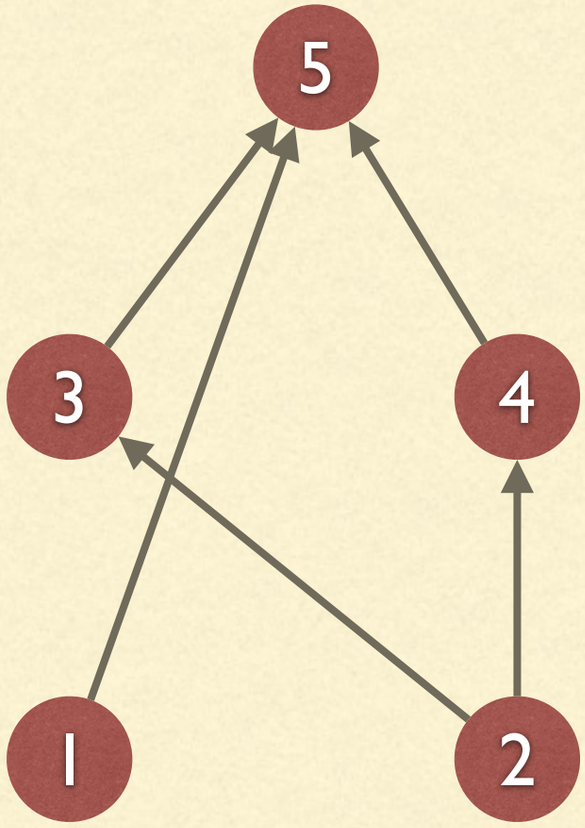
- Each gene has a "birth time" (called innovation number) that tracks when it was introduced. This feature is used to allow crossover

- Features are protected with speciation. That is, at each generation only individuals in the same specie can mate

NEAT: THE GENOME

- **Neuron genes**. These genes encode each neuron by giving to it an ID and a type (e.g., input, output, hidden, bias, etc.).
- **Link genes**. Each link gene contains:
  - The two endpoints of the edge
  - The weight of the edge
  - If the link is enabled or not
  - An *innovation number* used for crossover

NEAT: THE GENOME



Neuron Genes

ID: 1 Type: input	ID: 2 Type: input	ID: 3 Type: hidden	ID: 4 Type: hidden	ID: 5 Type: output

Link Genes

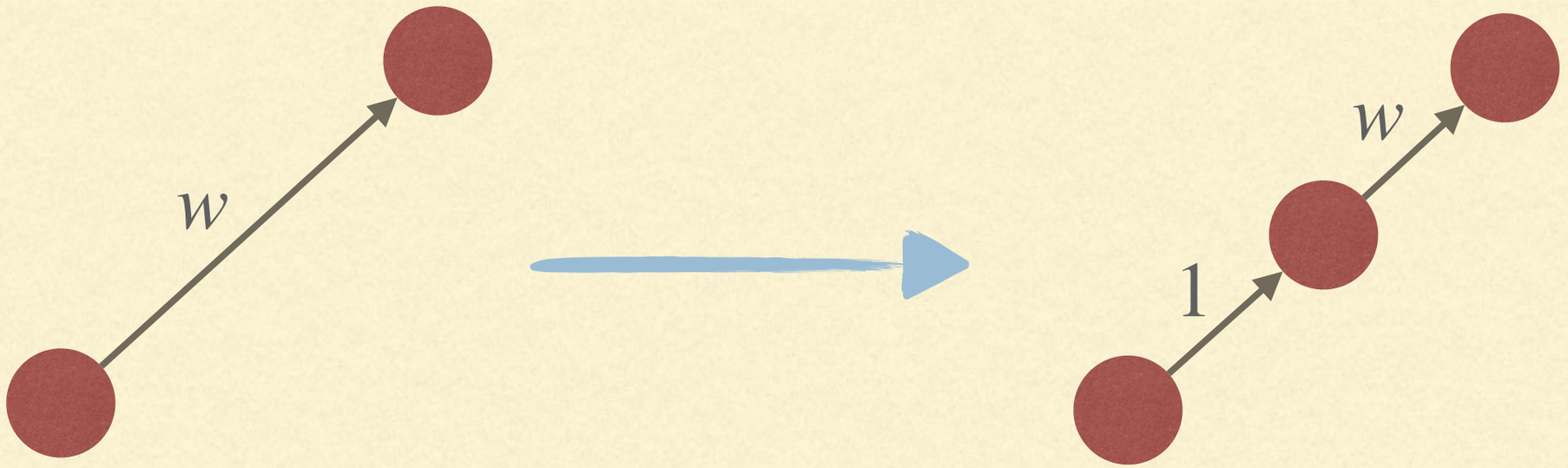
Source: 1 Destination: 5 Weight: 0.4 Enabled: Y Innovation: 3	Source: 2 Destination: 3 Weight: -0.2 Enabled: Y Innovation: 4	Source: 2 Destination: 4 Weight: 1.3 Enabled: Y Innovation: 1	Source: 3 Destination: 5 Weight: -0.9 Enabled: Y Innovation: 7	Source: 4 Destination: 5 Weight: 0.1 Enabled: Y Innovation: 6	Source: 1 Destination: 3 Weight: 1.8 Enabled: N Innovation: 5

Notice that edges might be present in the genome but not enabled!

MUTATION(S)

- There are multiple mutations that are possible and they work on node, edges and weights:
  - Addition of a node (see next slide)
  - Add an edge with a random weight
  - Perform a slight perturbation of a weight
  - Change completely the weight of a connection
  - Enable or disable an edge

MUTATION: ADD NODE



- The addition of a node “splits” an edge with weight w by inserting a node in the middle
- The outgoing edge will have weight w while the incoming one 1

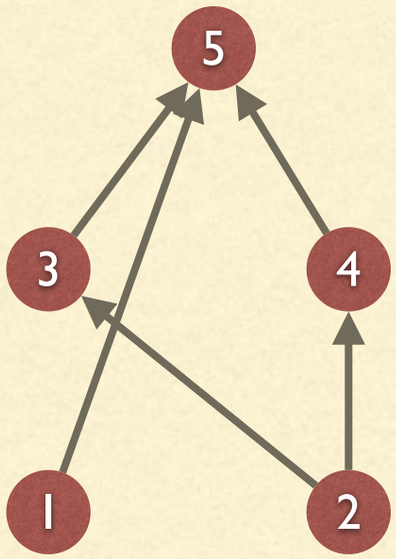
THE INNOVATION NUMBER

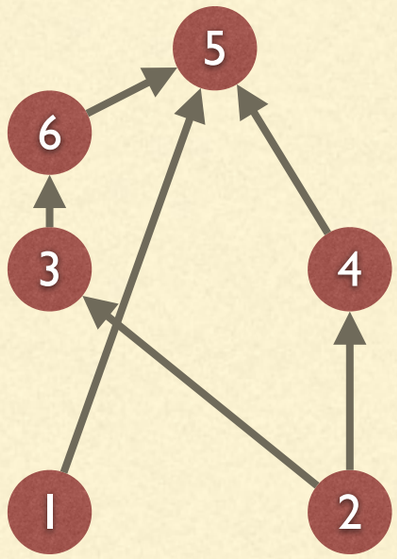
- Each gene inserted by a mutation has an associated **innovation number**, a value that is always incremented and assured to be different for different mutations

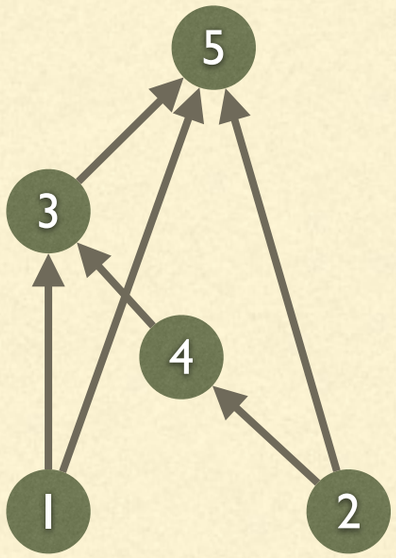
- If the **same mutation** happens multiple time in the same generation (e.g., the addition of a node between node 3 and 4), then it has the same innovation number

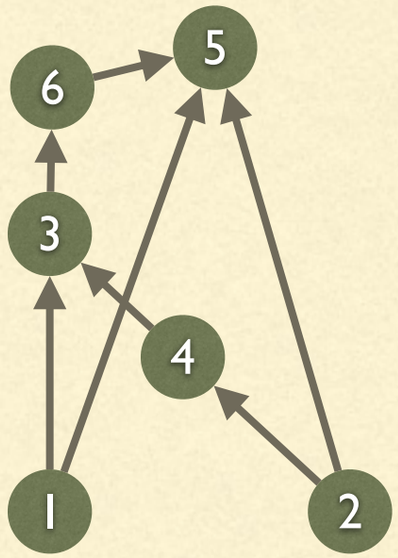
- The innovation number is used during crossover and it is essential to limit the competing conventions problem

THE INNOVATION NUMBER



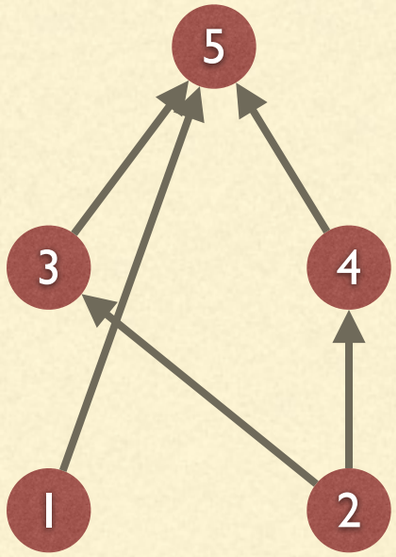






- This is the same mutation in two different individual
- The new edges $3 \to 6$ in both networks will have the same innovation number
- The same also for the new edge $6 \to 5$.

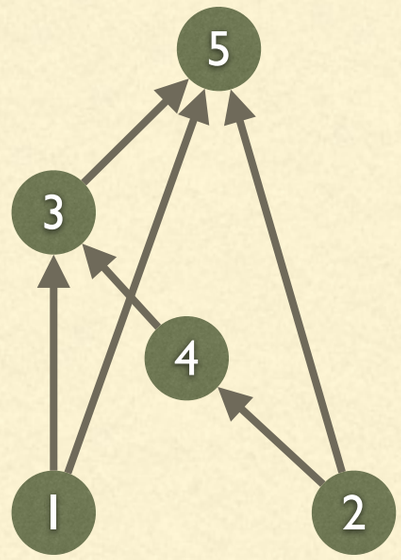
CROSSOVER



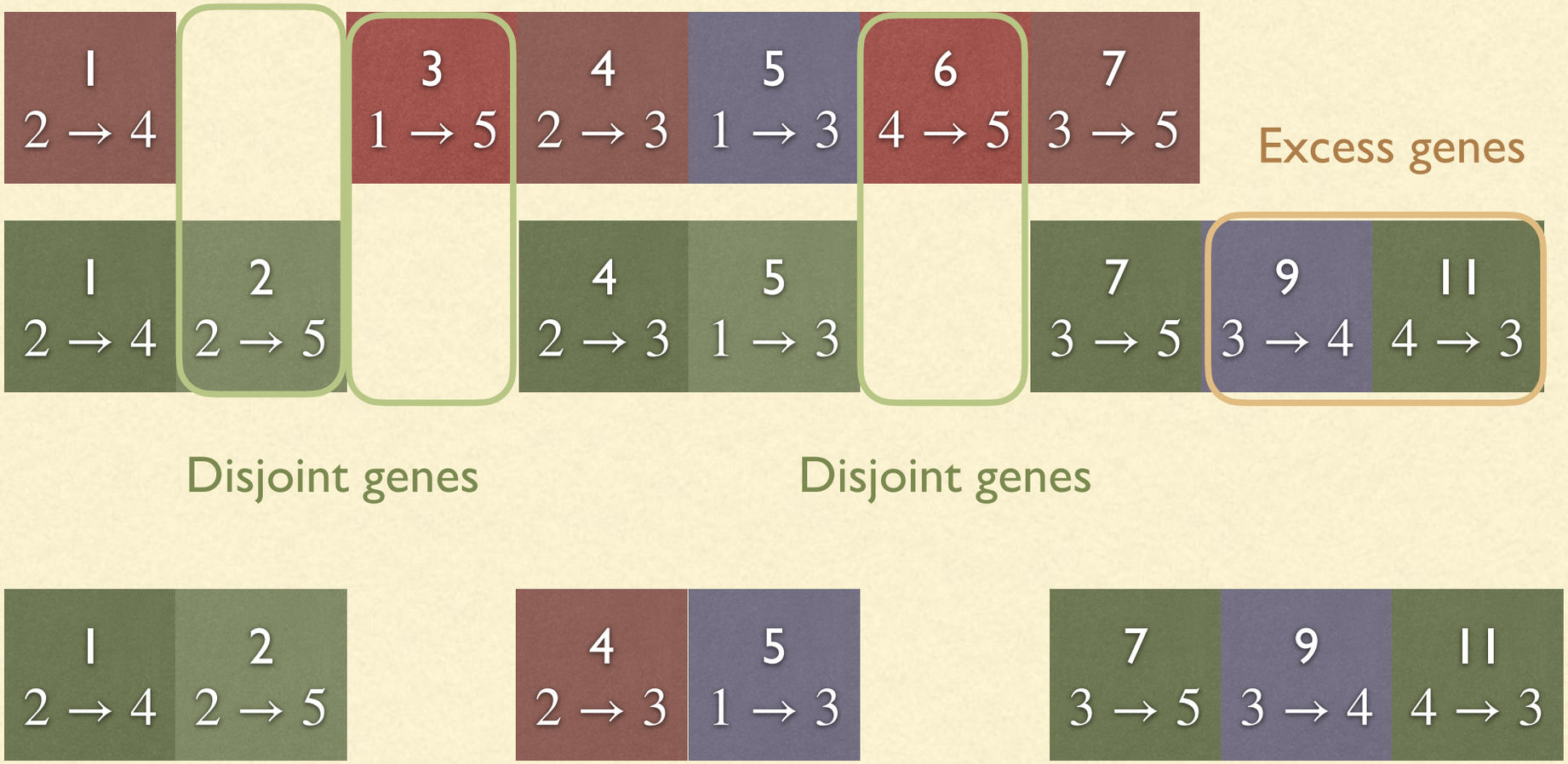
1	3	4	5	6	7
2 → 4	1 → 5	2 → 3	1 → 3	4 → 5	3 → 5

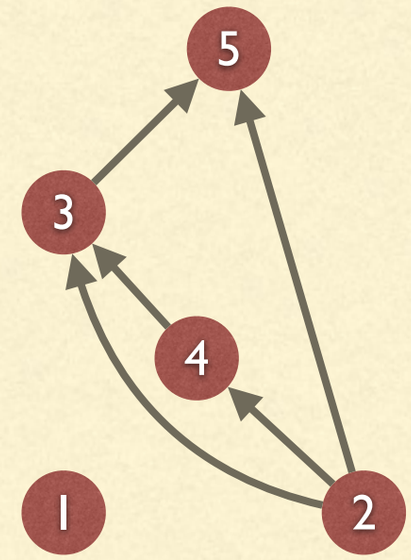
- Let us look at two individuals
- We have sorted the link genes by increasing innovation number
- We can now proceed in aligning the two genomes

1	2	4	5	7	9	11
2 → 4	2 → 5	2 → 3	1 → 3	3 → 5	3 → 4	4 → 3



CROSSOVER





- Genes in common are inherited randomly from one of the two parents
- Disjoint and excess genes are only inherited by the fittest of the parents

SPECIATION

- *A species is a group of populations with similar characteristics that are capable of successfully interbreeding with each other to produce healthy, fertile offspring, but are reproductively isolated from other species.*

- The networks in NEAT are divided into species and crossover can only happen with individuals of the same specie

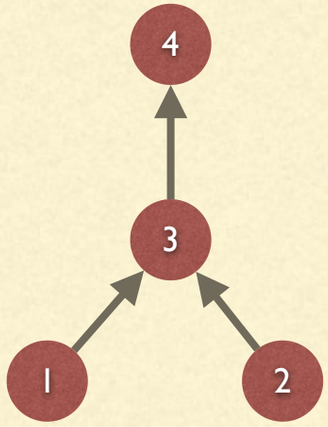
- We need to define two aspects:
  - How new species are created
  - How species compete against each other

INDIRECT ENCODINGS

- Grammar-Based encoding
- Bi-dimensional Growth encoding
- A function giving, for each connection, its weight
- Encoding the hyperparameters of the networks
  in an “aggregate” way.
  E.g., “one fully connected layer with n inputs and m outputs”

GRAMMAR-BASED ENCODING

This is something we had already seen when working on graphs:

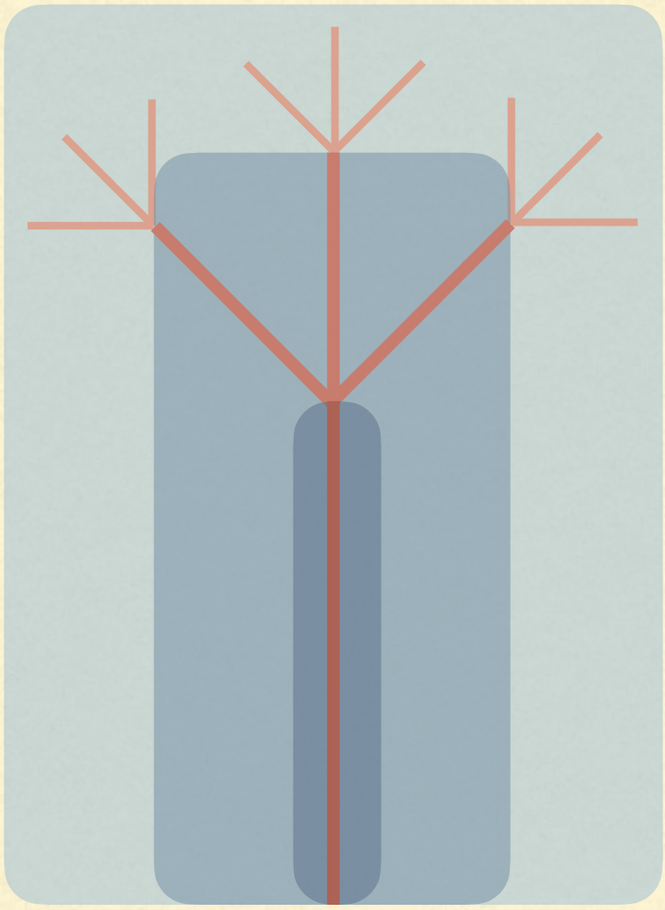


$$S \mapsto \begin{bmatrix} A & B \\ A & C \end{bmatrix} \quad A \mapsto \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \quad B \mapsto \begin{bmatrix} 1 & 0 \\ 1 & 0 \end{bmatrix} \quad C \mapsto \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Starting from a specific *non terminal symbol*, called **axiom**, we derive, by application of production rules, the matrix representing the network

BI-DIMENSIONAL GROWTH ENCODING

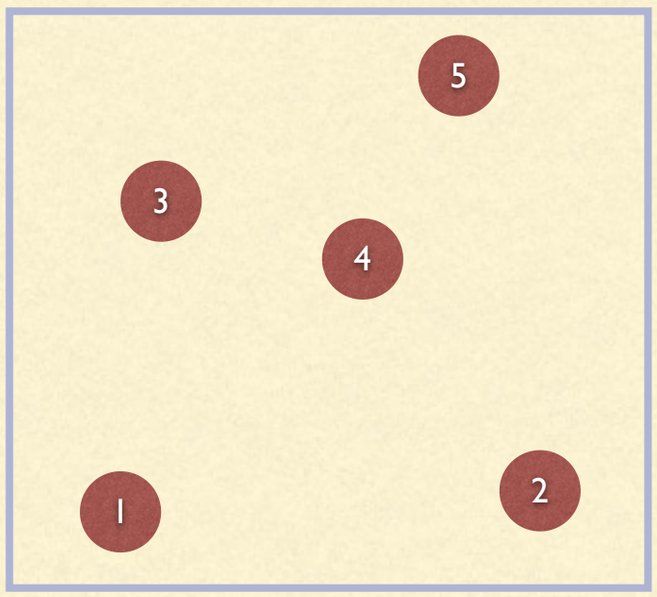
L-Systems

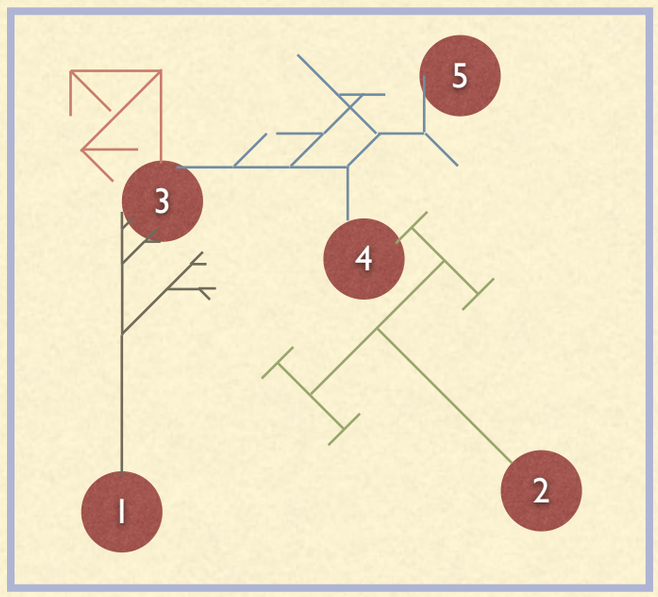


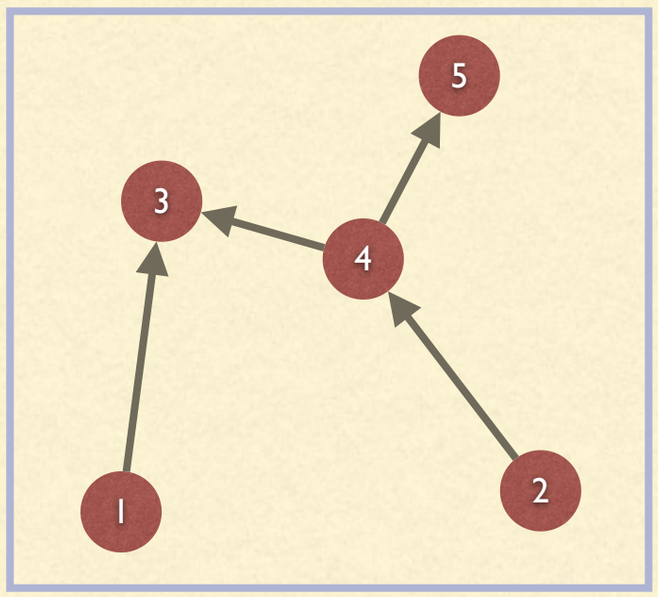
- L-systems are a rewriting systems that can be used to create images recursively
- At each branching point we decide
  - How many branches to create
  - The angle of each branch
  - How long is each branch with respect to the parent branch

BI-DIMENSIONAL GROWTH ENCODING

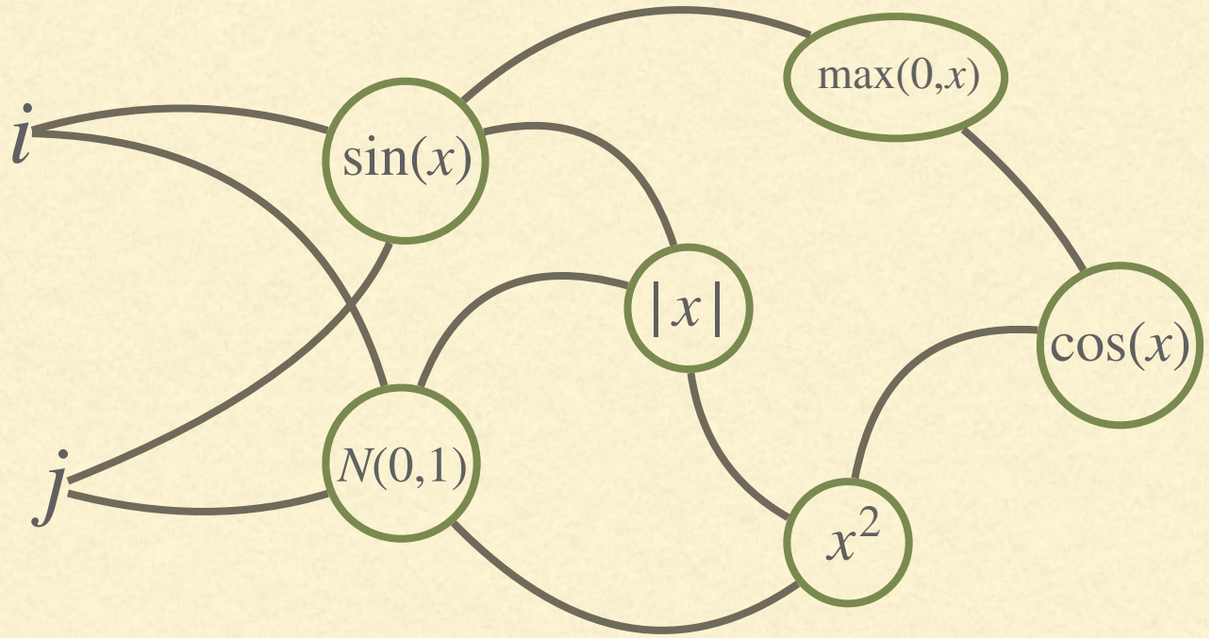
- We associate a L-system to each neuron
- We draw the resulting axons
- We obtain the connections of the network







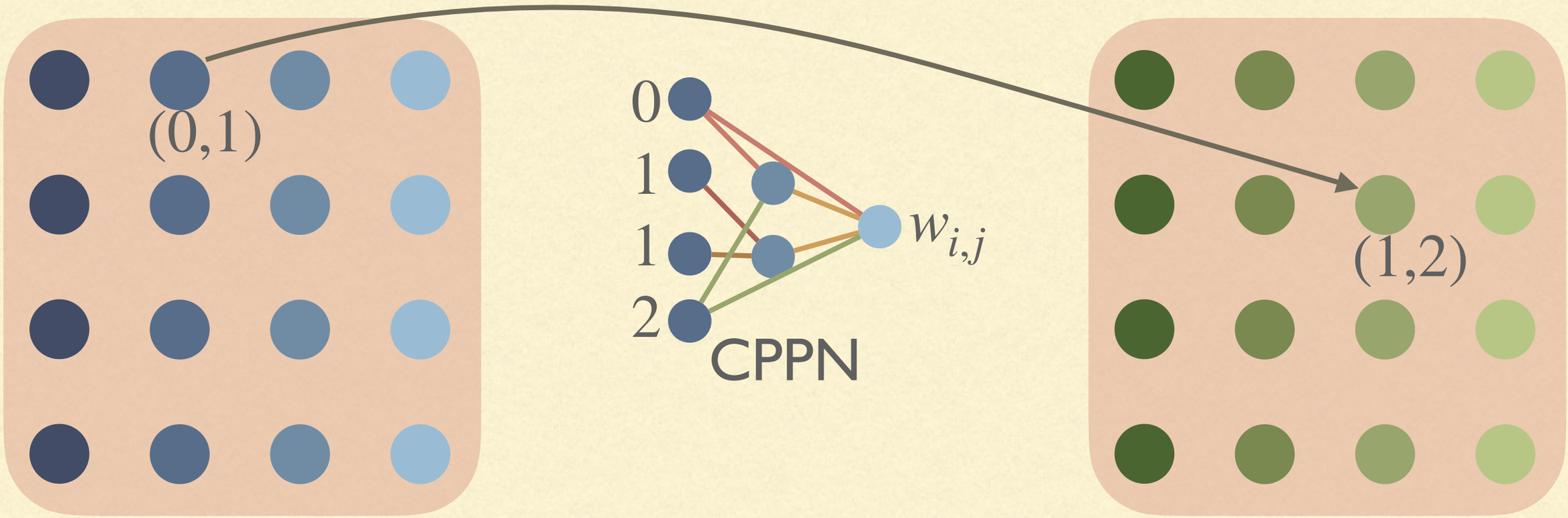
CPPN
COMPOSITIONAL PATTERN-PRODUCING NETWORKS



A "network" of functions that maps a position (i, j) in a 2D plane (more dimensions are possible) to a value

This can be evolved as a "classical" network. E.g., with NEAT.
So, where's the indirect encoding?

HYPERNEAT



Network layer
(2D disposition of neurons)

Network layer
(2D disposition of neurons)

DENSER
DEEP EVOLUTIONARY NETWORK STRUCTURED REPRESENTATION

- A layer-based approach:
  the number, type, and parameters of the layers are evolved

- The weights are obtained via backpropagation

- A two-levels approach:
  - the sequence of layer and a “general” type is encoded by a GA
  - The parameters of each layer are generated by grammatical evolution (GE), in particular dynamic structured GE

- Only the best-performing networks are trained for more than a few epochs