Chapter 3

NeuroEvolution of Augmenting Topologies (NEAT)

An efficient system capable of evolving complex structures at the same time as weights should be based upon the three principles discussed in the background: The system should implement a method of detecting homology between genes, it should protect innovation, and it should minimize structure in order to minimize the number of dimensions being searched. The NEAT approach follows these principles. Historical markings are used as a way of identifying homology, speciation accomplishes the protection of innovation, and minimizing structure is accomplished by starting out with a population of networks with no hidden nodes.

This section begins with an overview of the genetic encoding used in NEAT. Using the genetic encoding, structural mutations are introduced to make it clear how genomes grow in NEAT. Historical markings, which are applied whenever a genome grows, are then explained in detail. Crossover, which uses historical markings to allowing disparate topologies to be combined, is discussed next. NEAT's approach to speciation using fitness sharing is introduced as a way to protect innovation, and the last section explains growth from a minimal starting point.

3.1 Genetic Encoding

Evolving structure requires a flexible genetic encoding. In order to allow structures to complexify, their representations must be dynamic and expandable. Each genome in NEAT includes a list of *connection genes*, each of which refers to two *node genes* being connected (Figure 3.1). Each connection gene specifies the in-node, the out-node, the weight of the connection, whether or not the connection gene is expressed (an enable bit), and an *innovation number*, which allows finding corresponding genes during crossover.

Mutation in NEAT can change both connection weights and network structures. Connection weights mutate as in any NE system; each connection weight is perturbed with a fixed probability by

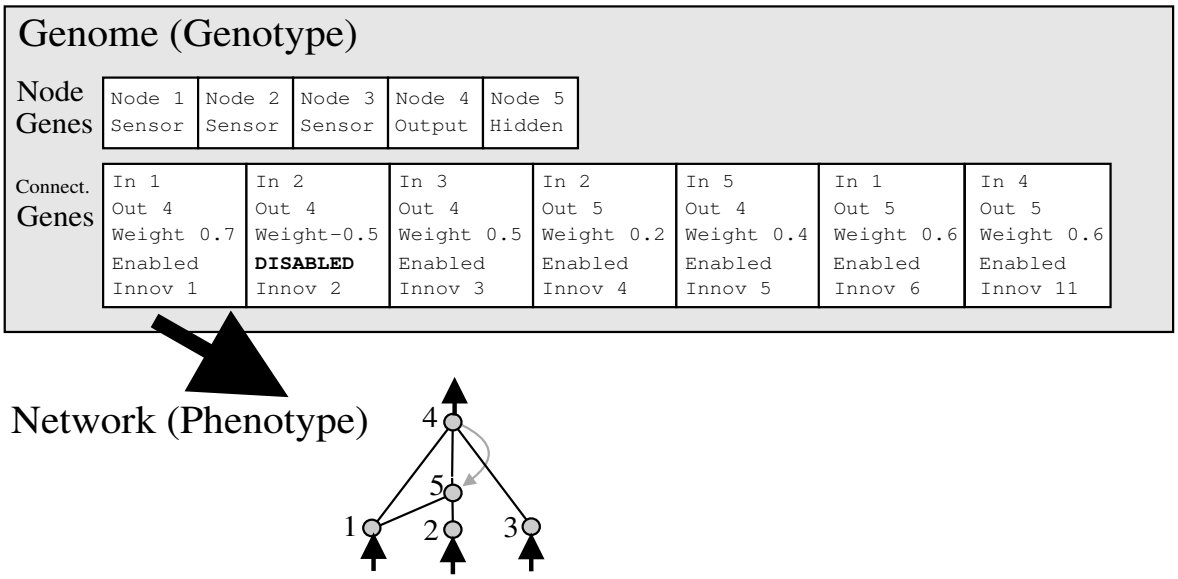

Figure 3.1: **A NEAT genotype to phenotype mapping example.** A genotype is depicted that produces the shown phenotype. There are 3 input nodes, one hidden, one output node, and seven connection definitions, one of which is recurrent. The second gene is disabled, so the connection that it specifies (between nodes 2 and 4) is not expressed in the phenotype. In order to allow complexification, genome length is unbounded.

adding a floating point number chosen from a uniform distribution of positive and negative values. Structural mutations, which form the basis of complexification, occur in two ways (Figure 3.2). Each mutation expands the size of the genome by adding genes. In the *add connection* mutation, a single new connection gene is added connecting two previously unconnected nodes. In the *add node* mutation, an existing connection is split and the new node placed where the old connection used to be. The old connection is disabled and two new connections are added to the genome. The connection between the first node in the chain and the new node is given a weight of one, and the connection between the new node and the last node in the chain is given the same weight as the connection being split. Splitting the connection in this way introduces a nonlinearity (i.e. sigmoid function) where there was none before. Because the new node is immediately integrated into the network, its effect on fitness can be evaluated right away. Preexisting network structure is not destroyed and performs the same function, while the new structure provides an opportunity to elaborate on the original behaviors.

Through mutation, the genomes in NEAT will gradually get larger. Genomes of varying sizes will result, sometimes with different connections at the same positions. Crossover must be able to recombine networks with differing topologies, which can be difficult (Radcliffe 1993). The next section explains how NEAT approaches this problem.

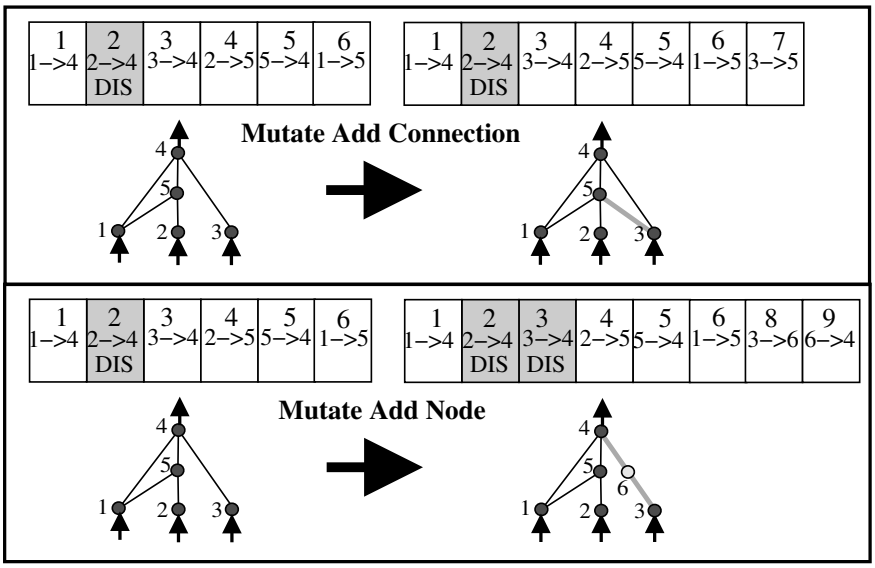

Figure 3.2: **The two types of structural mutation in NEAT.** Both types, adding a connection and adding a node, are illustrated with the genes above their phenotypes. The top number in each genome is the *innovation number* of that gene. The bottom two numbers denote the two nodes connected by that gene. The weight of the connection, also encoded in the gene, is not shown. The symbol DIS means that the gene is disabled, and therefore not expressed in the network. The figure shows how connection genes are appended to the genome when a new connection and a new node is added to the network. Assuming the depicted mutations occurred one after the other, the genes would be assigned increasing innovation numbers as the figure illustrates, thereby allowing NEAT to keep an implicit history of the origin of every gene in the population.

3.2 Tracking Genes through Historical Markings

It turns out that the historical origin of each gene can be used to tell us exactly which genes match up between *any* individuals in the population. Two genes with the same historical origin represent the same structure (although possibly with different weights), since they were both derived from the same ancestral gene at some point in the past. Thus, all a system needs to do is to keep track of the historical origin of every gene in the system.

Tracking the historical origins requires very little computation. Whenever a new gene appears (through structural mutation), a *global innovation number* is incremented and assigned to that gene. The innovation numbers thus represent a chronology of every gene in the system. As an example, let us say the two mutations in Figure 3.2 occurred one after another in the system. The new connection gene created in the first mutation is assigned the number 7, and the two new connection genes added during the new node mutation are assigned the numbers 8 and 9. In the future, whenever these genomes cross over, the offspring will inherit the same innovation numbers on each gene. Thus, the historical origin of every gene in the system is known throughout evolution.

A possible problem is that the same structural innovation will receive different innovation

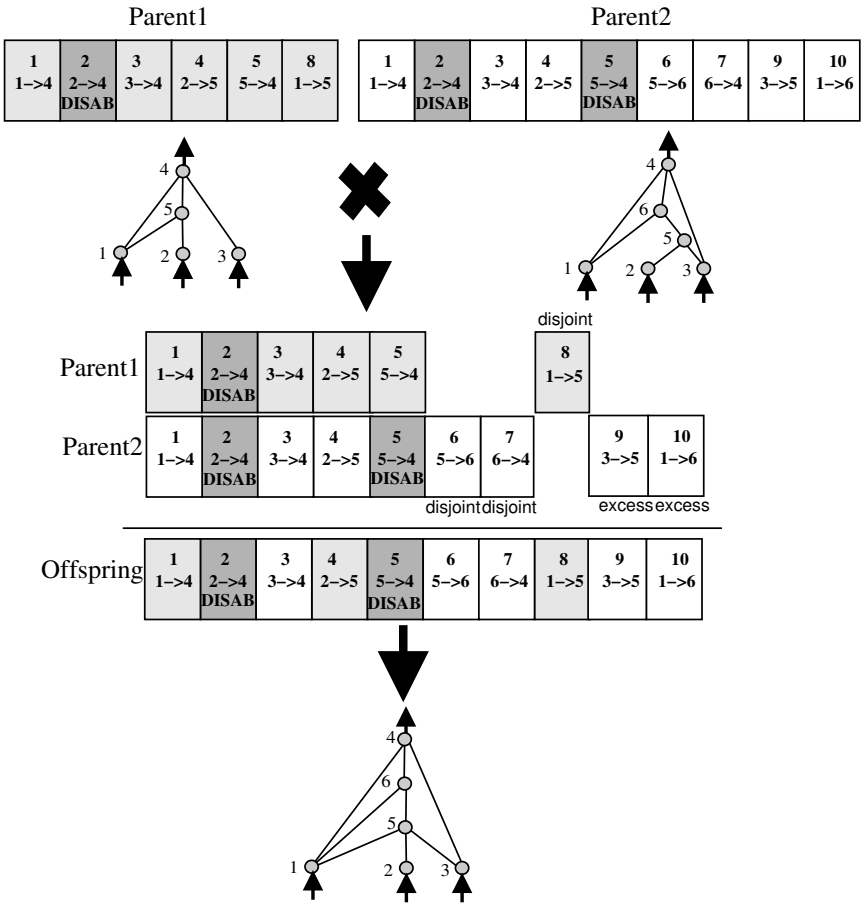

Figure 3.3: **Matching up genomes for different network topologies using innovation numbers.** Although Parent 1 and Parent 2 look different, their innovation numbers (shown at the top of each gene) tell us that several of their genes match up even without topological analysis. A new structure that combines the overlapping parts of the two parents as well as their different parts can be created in crossover. In this case, equal fitnesses are assumed, so each disjoint and excess gene is inherited from either parent randomly. Otherwise the genes would be inherited from the more fit parent. The disabled genes may become enabled again in future generations: There is a preset chance that an inherited gene is enabled if it is disabled in either parent.

numbers in the same generation if it occurs by chance more than once. However, by keeping a list of the innovations that occurred in the current generation, it is possible to ensure that when the same structure arises more than once through independent mutations in the same generation, each identical mutation is assigned the same innovation number. Extensive experimentation established that resetting the list every generation as opposed to keeping a growing list of mutations throughout evolution is sufficient to prevent innovation numbers from exploding.

Through innovation numbers, the system now knows exactly which genes match up with

which (Figure 3.3). Genes that do not share the same historical marking as any gene in other other parent genome are *disjoint*. Genes that appeared in one parent later in evolution than any genes in the other parent are *excess*. When crossing over, the genes with the same innovation numbers are lined up and crossed over in one of two ways. In the first method, matching genes are randomly chosen for the offspring genome. Alternatively, the connection weights of matching genes can be averaged (Wright (1991) reviews both types of crossover and their merits). NEAT uses both types of crossover. Disjoint and excess genes are inherited from the more fit parent, or if they are equally fit, each gene is inherited from either parent randomly. Disabled genes have a chance of being reenabled during crossover, allowing networks to make use of older genes once again.

Historical markings allow NEAT to perform crossover without analyzing topologies. Genomes of different organizations and sizes stay compatible throughout evolution. This methodology allows NEAT to complexify structure while different networks still remain compatible. However, it turns out that it is difficult for a population of varying topologies to support new innovations that add structure to existing networks, Because smaller structures optimize faster than larger structures, and adding nodes and connections usually initially decreases the fitness of the network, recently augmented structures have little hope of surviving more than one generation even though the innovations they represent might be crucial towards solving the task in the long run. The solution is to protect innovation by speciating the population, as explained in the next section.

3.3 Protecting Innovation through Speciation

NEAT speciates the population so that individuals compete primarily within their own niches instead of with the population at large. This way, topological innovations are protected and have time to optimize their structure before they have to compete with other niches in the population. In addition, speciation prevents bloating of genomes: Species with smaller genomes survive as long as their fitness is competitive, ensuring that small networks are not replaced by larger ones unnecessarily. Protecting innovation through speciation follows the philosophy that new ideas must be given time to reach their potential before they are eliminated.

Using historical markings, the system can determine how much history is shared among different genomes and use that information to divide the population into species. The distance δ between two network encodings can be measured as a linear combination of the number of excess (E) and disjoint (D) genes, as well as the average weight differences of matching genes ($\overline{W}$):

$$\delta = \frac{c_1 E}{N} + \frac{c_2 D}{N} + c_3 \cdot \overline{W}. \tag{3.1}$$

The coefficients c_1, c_2, and c_3 adjust the importance of the three factors, and the factor N, the number of genes in the larger genome, normalizes for genome size (N can be set to 1 unless both genomes are excessively large).

Throughout evolution, NEAT maintains a list of species numbered in the order they appeared. In the first generation, since there are no preexisting species, NEAT begins by creating species 1 and placing the first genome into that species. All other genomes are placed into species as follows: A random member of each existing species is chosen as its permanent *representative*. Genomes are tested one at a time; if a genome's distance to the representative of any existing species is less than δ_t, a compatibility threshold, it is placed into this species. Otherwise, if it is not compatible with any existing species, a new species is created and given a new number. After the first generation, genomes are first compared with species from the *previous generation* so that the same species numbers can be used to identify species throughout the run. Keeping the same set of species from one generation to the next allows NEAT to remove stagnant species, i.e. species that have not improved for too many generations. In general, because structure is added slowly and only useful innovations survive in the long run, throughout evolution topologies within the same species in the same generation tend to be similar. The problem of choosing the best value for δ_t can be avoided by making δ_t *dynamic*; that is, given a target number of species, the system can slightly raise δ_t if there are too many species, and lower δ_t if there are too few.

Let P be the entire population. The algorithm for clustering genomes into species follows:

- The Genome Loop:
  - Take next genome g from P
  - The Species Loop:
    - If all species in S have been checked, create new species s_{new} and place g in it
    - Else
      - get next species s from S
      - If g is compatible with s, add g to s
    - If g has not been placed, Species Loop
  - If not all genomes in G have been placed, Genome Loop
  - Else STOP

As the reproduction mechanism, NEAT uses *explicit fitness sharing* (Goldberg and Richardson 1987), where organisms in the same species must share the fitness of their niche. Thus, a species cannot afford to become too big even if many of its organisms perform well. Therefore, any one species is unlikely to take over the entire population, which is crucial for speciated evolution to support a variety of topologies. The adjusted fitness f'_i for organism i is calculated according to its distance δ from every other organism j in the population:

$$f'_i = \frac{f_i}{\sum_{j=1}^{n} \mathrm{sh}(\delta(i,j))}. \tag{3.2}$$

The sharing function sh is set to 0 when distance $\delta(i,j)$ is above the threshold δ_t; otherwise, $\mathrm{sh}(\delta(i,j))$ is set to 1 (Spears 1995). Thus, $\sum_{j=1}^{n} \mathrm{sh}(\delta(i,j))$ reduces to the number of organisms in the same species as organism i. This reduction is natural since species are already clustered by compatibility using the threshold δ_t. Every species is assigned a potentially different number of offspring in proportion to the sum of adjusted fitnesses f'_i of its member organisms. The net effect of fitness sharing in NEAT can be summarized as follows. Let $\overline{F_k}$ be the average fitness of species k and $|P|$ be the size of the population. Let $\overline{F}_{tot} = \sum_k \overline{F_k}$ be the total of all species fitness averages. The number of offspring n_k allotted to species k is:

$$n_k = \frac{\overline{F_k}}{\overline{F}_{tot}}|P|. \tag{3.3}$$

The lowest performing fraction of each species is eliminated. The parents to produce the next generation are chosen randomly among the remaining individuals (uniform distribution with replacement). The highest performing individual in each species, i.e. the *species champions*, carries over from each generation. Otherwise the next generation completely replaces the one before.

The net effect of speciating the population is that structural innovation is protected. The final goal of the system, then, is to perform the search for a solution as efficiently as possible. This goal is achieved through complexification from a simple starting structure, as detailed in the next section.

3.4 Minimizing Dimensionality through Complexification

Unlike other systems that evolve network topologies and weights (Angeline et al. 1993; Gruau et al. 1996; Yao 1999; Zhang and Muhlenbein 1993), all the networks in the first generation in NEAT have the same small topology: All the inputs are directly connected to every output, and there are no hidden nodes. These first generation networks differ only in their initial random weights. Speciation protects new innovations, allowing diverse topologies to gradually accumulate over evolution. Thus, because NEAT protects innovation using speciation, it can start in this manner, minimally, and grow new structure over generations.

New structure is introduced incrementally as structural mutations occur, and only those structures survive that are found to be useful through fitness evaluations. This way, NEAT searches through a minimal number of weight dimensions, significantly reducing the number of generations necessary to find a solution, and ensuring that networks become no more complex than necessary. This gradual increase in complexity over generations is *complexification*. In other words, NEAT searches for the optimal topology by incrementally complexifying existing structure.

The process of complexification and its benefits can be summarized as follows. The system is initially searching a very low-dimensional parameter space with very few connections. Solutions are optimized in this low-dimensional space. The space may not be expressive enough to solve the problem, but locally optimal solutions appear. The system then increases the dimensionality

of the search space by adding new topology through structural mutations. This causes a shift into a new space. However, it is likely that the position of the new genome in the new space is on a promising hill, because most of its connections are already optimized to perform a useful function. The new connections, representing extra dimensions of search, can be optimized to coordinate with the older connections, which themselves may change somewhat in order to adapt to the new higher-dimensional space. Many different innovations happen at the same time, in the same generation, so NEAT is searching many different dimensional search spaces simultaneously. These different spaces are each represented by a species. Each search space is a branch off of a smaller space that was already somewhat optimized. Because solutions tend to start out in larger spaces already near their goal, much of the work of searching has been accomplished in a lower dimensional space, which means less parameters needed to be optimized simultaneously, which allows searching in higher-dimensional space than would otherwise be possible.

3.5 Conclusion

NEAT is based on three principles that work together to efficiently evolve network topologies and weights. The first principle is homology: NEAT encodes each node and connection in a network with a gene. Whenever a structural mutation results in a new gene, that gene receives a historical marking. Historical markings are used to match up homologous genes during crossover, and to define a compatibility operator.

The second principle is protecting innovation. A compatibility operator is used to speciate the population, which protects innovative solutions and prevents incompatible genomes from crossing over.

Finally, NEAT follows the philosophy that search should begin in as small a space as possible and expand gradually. Evolution in NEAT always begins with a population of minimal structures. Structural mutations add new connections and nodes to networks in the population, leading to incremental growth. Topological innovations have a chance to realize their potential because they are protected from the rest of the population by speciation. Because only useful structural additions tend to survive in the long term, the structures being optimized tend to be the minimum necessary to solve the problem.

NEAT's approach allows fast search because the number of dimensions being searched is minimized. The next two chapters demonstrate the power of this process.