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Abstract

We propose a phenotypic diversity measurement in genetic algorithms with neural networks as individuals, called Neural Network Trait Diversity (NNTD). It is an extension of Simpsons Diversity Index, known from ecology.

Avoiding low diversity in a genetic algorithm's population is crucial for finding a global optimum. When diversity is overlooked, premature convergence is the consequence, possibly leading to a local optimum.

Experiments are conducted to compare NNTD to the genotypic diversity measure of Hamming distance, and a phenotypic fitness-based diversity measure. We argue why both of these measures have weaknesses that NNTD overcomes.

Our experiments show that NNTD consistently mirrors the intuition of how diversity in populations develop for various replacement rules, better than that of the Hamming distance and fitness-based diversity measurement methods, which seem less predictable.

Interestingly, the experiments also show that there might be a connection between the genetic construction of an individual and its phenotypic behaviour.

1. Introduction

For many problems in computer science, a greedy strategy will not always lead to the best result. A greedy strategy chooses the next step by considering how promising each step is at that given moment. As an example, if a mountain climber wants to reach the highest peak in the Himalayas: Mount Everest, a greedy strategy would be to move in any direction he think is the best, as long as he climbs upwards and never downwards. Using this strategy, he is definitely able to climb up somewhere, but once he reaches a peak, he might discover an even greater peak he could not see before. Unfortunately, his strategy is to never back down, so now he is stuck at what we call a local optimum. What he wanted was the global optimum: Mount Everest.

Genetic algorithms (GAs) can be used to search for a global optimum in many types of problems, such as optimization problems. A GA manages a number of individuals, which constitute a population. Each of the individuals represents a candidate solution to the same problem. Neural networks are often chosen as individuals. A Neural network takes a number of inputs, do some internal calculations, and then yield a number of outputs. The neural network as its whole can be interpreted as a solution to the problem. For instance, for the particular problem of adding two integers, the neural network can take two integers s and t as input, and output a single value, which ideally should equal $s+t$. Most often, the individuals in a GA do not solve the problem in question adequately. However, different individuals may have good solutions to different aspects of the problem. Ideally, the GA will make individuals procreate to form offspring that combines the best traits from both its parents. Intuitively, the combination of these traits constitutes a better solution to the given problem. The fitness value of an individual indicates how adequately it solves the problem in question.

To identify a constructive combination of traits, a diverse set of individuals is required. If diversity is not maintained, only a local optimum of the population's available traits will be explored, and a global optimum might never be found [17].

We believe it is essential that a diversity measure reflects the difference in traits among individuals. By concentrating on neural networks as individuals, we develop a new diversity measure that, as we will see, is not affected by pitfalls in traditional diversity measures.

Since a *trait* is a rather vague term, we introduce a clear definition of traits among neural networks: "*two neural networks have different traits, if they for some input produce different outputs*". We now argue why we think that neither fitness-based nor genotypic diversity measures catch a diversity among traits, or the *trait diversity*.

Consider two individuals who try to find the highest peak on an elevation map, where the fitness of each individual is based on the height of the peak they return. The two individuals might have completely different strategies causing them to get stuck on two different peaks. If both peaks happen to have the same height, the two individuals will have the same fitness, and hence a fitness-based diversity measure will return a low diversity, even though the two individuals have different traits.

Two individuals of different genotypes can have the same behaviour, which means they yield the same output on any input. An example of such two neural networks is shown in fig. 1. No matter what input they receive, their output will always be the same. They are genotypically diverse, because their bit strings are different, but they are not trait diverse at all. We develop a new method for measuring phenotypic diversity in GAs using neural networks as individuals. We claim that our method better reflects different traits among the individuals. Furthermore, we use our method to explore how different replacement rules affect the diversity of a population.

Section 2 introduces the concepts used in our diversity measure, and can be skipped if the reader knows about genetic algorithms and neural networks. Section 3 describes our diversity measure, which is experimentally evaluated and compared to other measures in section 4. In section 5 we evaluate NNTD.

1.1. Related work

Concepts and applications of GAs are described in [3,5,10,16,17,18,20,22]. The use of diversity maintenance in GAs is discussed in [2,4,6,23], and measures of population diversity are described in [11,15]. Combining GAs and neural networks is described in [8].

2. Preliminaries

In this section we present the concepts used in this paper. We begin with an introduction of artificial neural networks, followed by an introduction of genetic algorithms (GAs).

2.1. Artificial Neural Network

An artificial neural network is a finite directed graph that, from the outside, can be seen as a black box, which given the values $x_1, x_2, \ldots, x_n$, outputs the values $y_1, y_2, \ldots, y_m$. With the right internal structure, a neural network can be used for a variety of applications, e.g. recognition of handwriting [21], where the intensities of different pixels in an image are used as input, and a set of output values are produced, where each output could correspond to a symbol. The highest output value gives the prediction of the network. We now describe the structure and inner workings of neural networks to understand how these output values are calculated based on input values.

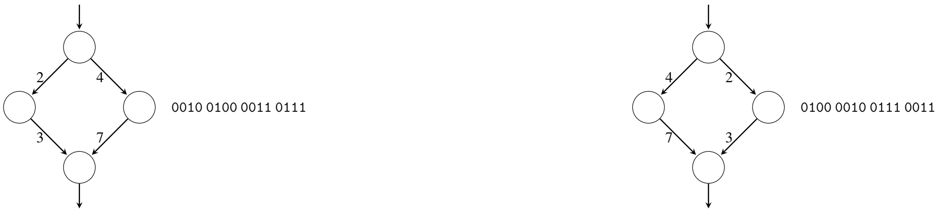
Neurons. Nodes in the graph of a neural network are called neurons. Three types of neurons exist: input, hidden, and output. Each input neuron receives one of the input values $x_1, x_2, \ldots, x_n$ and forward the same value to each neuron in the first hidden layer. Hidden and output neurons take a number of values as input from edges exiting other neurons, applies a weight to each value, sums them, and then applies a function to produce a single output value. The function applied is called the transfer function, and is the same for all hidden and output neurons in the network. The output value of neuron i is recursively expressed by

$$y_i = \begin{cases} x_i & \text{if } i \text{ is an input neuron} \\ \theta\left(\sum_{j=1}^{n} w_{ji} y_j\right) & \text{otherwise} \end{cases}$$

where x_i is the ith input, n is the amount of neurons, y_i is the output value of neuron i, w_{ji} is the weight of the edge from neuron j to i (0 if no connection exists), and θ is the transfer function, typically defined to be the sigmoid function

$$\theta(t) = \frac{1}{1+e^{-t}}$$

In a feed-forward network, neurons are placed in one or more layers in an acyclic directed graph, where each neuron in layer i is connected to every neuron in layer $i+1$. The value(s) output by the last layer, or the output layer, becomes the output of the neural network. Figure 2 illustrates the generic graph structure of a feed-forward neural network with a single hidden layer. If a neuron is given the value 0 on all of its inputs, most transfer functions will only allow that neuron to output 0 as well. This is not desirable for all applications, and is often overcome by giving each neuron a bias value. The bias value of a neuron is added to the sum of inputs it receives, before finally applying the transfer function. Thus, if a neuron receives only 0's as input, it will output



(a) An artificial neural network with connections and weights.

(b) An artificial neural network equivalent to fig. 1a.

Figure 1: Networks with same phenotype, but different genotypes. Each weight is represented by four bits.

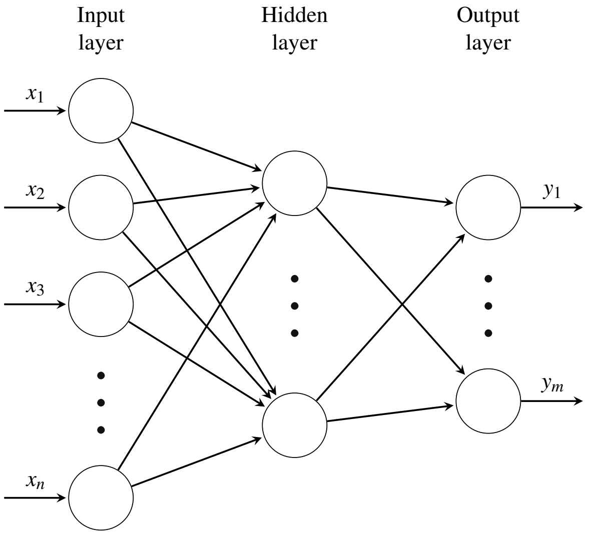


Figure 2: Structure of a neural network.

the value obtained by applying the transfer function to its bias value.

Training a Neural Network. Any application of a neural network requires a suitable number of layers, neurons, biases, and weights between neurons, to adequately solve a given problem. How many hidden neurons and layers to have is a highly debated subject, see [13].

The weights on edges connecting neurons and bias neurons are decided by a process called training. Training processes are categorised into supervised and unsupervised learning. When the desired output of a given problem is known beforehand, supervised learning can be used. An error term is calculated, which affects how the weights between neurons are changed [9]. Consider training an artificially intelligent (AI) player for a computer game. Given a state of the game, it might not be able to tell whether a particular action is good or bad due to the complexity of the game, and hence supervised learning cannot calculate an error term and update the weights accordingly. Instead a genetic algorithm (GA) can be used to search for an optimal AI player, which is an unsupervised learning method.

2.2. Genetic algorithms

Genetic algorithms are optimization algorithms which imitate the process of natural selection in the search of a global optimum.

Individuals and chromosomes. Genetic algorithms (GA) maintain a list of *individuals*, which together form a *population*. Each individual represents a possible solution to the optimization problem in question and has a fitness value, which denotes how adequately the individual can solve the optimization problem. An individual is encoded by its *chromosome*, which is typically represented by a bit string. We refer to encoded individuals chromosomes and bit strings synonymously. Therefore, using a GA requires a way of decoding an individuals chromosome into a solution to the optimization problem.

The population used by a GA typically has a fixed number of individuals, each initialized with a random chromosome when the GA is run. That is, the bit string representing the chromosome is initialized with random bits. As the GA iterates, new individuals are made by combining and modifying chromosomes from existing individuals of the population. In steady state GAs, some of the new individuals will replace older individuals according to some replacement rule. In contrast, a generational GA will choose only from offspring when forming the next generation [16, 18, 20]. We will focus on steady state GAs, using the term *generation* G_n to denote the content of the population after $n-1$ iterations.

Individuals. Individuals in GAs have a set of traits and behaviours which define each individual. They can take on any form of data structure, as long as they wholly represent a possible solution to the problem.

Neural networks as individuals. Neural networks can be used to solve many types of problems, e.g. classification and decision making. Before we can be use neural networks as individuals in a GA, we must define a method for encoding a neural network as a bit string, which will be manipulated by the GA. For any GA we will consider, every individual in its population will have the same architecture. That is, the number of neurons, the size of each layer, and how neurons are connected is the same.

Thus, neural networks differ only in their weights between neurons and the bias of each neuron. Each individual is therefore represented only in terms of the weights and biases. For each GA, any weight and bias is encoded with a fixed number of bits *n* and *m*, respectively. The bit string is constructed in an ordered manner, such that the first *n* bits represent the weight of the connection between the first input neuron and the first hidden neuron, the next *n* bits represent the weight of the connection between the first input neuron and the second hidden neuron, and so forth. Figure 1 shows an example of two neural networks and the bit string that encodes each of them. If biases are used by the GA, these are encoded right after the weights, and ordered such that the first *m* bits encode the bias of the first neuron, the next *m* bits encode the bias of the second neuron, and so forth. In this way we encode a neural network, which is manipulated by different GA operators.

If two chromosomes have different bit strings, we say that they have different genotypes. If the neural network they encode produces a different output for some input, we say they have different phenotypes.

Crossovers and mutations. In natural evolution, a pair of individuals come together to produce one or more new children, each having genes from both of its parents. In GAs, the process of procreation is done by performing a *crossover* of the two parent individuals' chromosomes. Parts of each parent's bit strings are used to create the child individual.

Mutations can also occur randomly at any point in time upon creating a child individual. If genes are encoded as bit strings, then a mutation arbitrarily toggles one or more bits. This ensures that new genes not previously present in the population can be made.

Fitness functions. A *fitness function* must be defined to calculate the desirability for each individual. This function is used to define the most fit individuals in a population. By giving more fit individuals a greater chance of reproducing, the intuition is that more fit individuals will be created, having the best traits from each of their parents.

2.3. Crowding

Methods to overcome decreasing diversity in a population include inserting random immigrants (randomly initialized individuals) [3], using complex population structures to lower the gene flow, and the use of special selection procedures [5, 17], known as crowding. How a particular crowding method works is commonly described by a replacement rule.

The replacement rule determines which individuals of the *i*th generation G_i, and their offspring β_i are selected to form the next generation G_{i+1}.

Greedy. Common descriptions of GAs that do not try to account for premature convergence, construct generation G_i from the n most fit individuals from $G_{i-1} \cup \beta_{i-1}$, where n is a fixed population size. We will refer to this as the *Greedy replacement rule* [8].

Ancestor Elitism. The ancestor elitism replacement rule is similar to $(\mu + \lambda)$ and generation gap algorithms, but we developed it independently of these algorithms [10, p. 34, p. 50].

Generation G_{i+1} is made from generation G_i as follows: every individual from G_i is put into G_{i+1}. Any offspring individual in β_i who only has a single parent (made from mutation) and is more fit than its parent, will replace that parent in G_{i+1}. Any individual in β_i who has two parents (made from crossover) and is more fit than both of its parents, will replace both parents in G_{i+1} by itself and a random immigrant. Finally, the 50 % least fit individuals in G_{i+1} are replaced by random immigrants.

Single Parent Elitism. Single Parent Elitism is similar to Restricted Tournament Selection, but we developed it independently of that method [10, p. 132].

G_{i+1} is made from G_i as follows: every individual from G_i is put into G_{i+1}. Any individual in β_i who only has a single parent (made from mutation) and is more fit than its parent, will replace that parent in G_{i+1}. Any individual in β_i who has two parents (made from crossover), and is more fit than a randomly chosen parent, will replace its parent in G_{i+1} by itself.

Mass Extinction Explore Exploit. Inspired by the changes between exploration and exploitation phases used by Ursem [17], we introduce the following replacement rule, which we will refer to as the *Mass Extinction Explore Exploit* (MEEE) replacement rule. The MEEE replacement rule is equivalent to Single Parent Elitism, except that it additionally performs a mass extinction when the diversity drops below a threshold. In any generation G_i, if $d(G_i) < \alpha$, we replace the $\frac{n}{2}$ least fit individuals from G_i by random immigrants, where $n = |G_i|$,

$d(G)$ denotes the diversity of a generation, and α is a threshold ratio. Then *Single Parent Elitism* replacement rule is performed on (G_i, β_i).

2.4. Diversity measures

It is often argued that the weakness of GAs is the fall in diversity over generations, often resulting in premature convergence [2,6,23].

Here, we summarise key points regarding genotypic and phenotypic diversity measures.

Genotypic diversity measures. The genotypic diversity of a set of individuals is determined by how different their genetic structures are. To measure this type of diversity, methods to compute the distance between any two individuals' encoded bit strings are required.

The diversity between a set of bit strings can then be expressed as the average distance between any two bit strings. Summation can also be used instead of averaging, which is merely a convenient optimization.

The *Hamming distance* between two bit strings A and B of equal length is the number of indexes i, such that $A[i] \neq B[i]$. The *Levenshtein distance* between these two bit strings is the number of bits that must be inserted, deleted, or substituted to change A into B.

As shown in fig. 1, two networks of different genotypes may have the exact same behaviour. One can argue that the two genotypes shown in fig. 1 are in fact not that different, since only two bits are different in each substring. The Levenshtein distance measure catches this intuition better than Hamming distance. For example, the distance between between the bit strings

$$01010101 \tag{1}$$

$$10101010 \tag{2}$$

is 8 when using Hamming distance, and 2 when using Levenshtein distance, because transforming eq. (1) into eq. (2) is done by deleting the first bit and prepending a 0, totalling 2 operations [22].

If we define F to be a set of neural networks, the complexity of calculating h_{ij}, where h_{ij} is the Hamming distance between two neural networks $f_i, f_j \in F$ is $\mathrm{O}(l)$, which is linear in the length of an encoded network's bit string l. The complexity of computing Hamming distance for all $f \in F$ is thus $\mathrm{O}\left(|F|^2 \cdot l\right)$.

The complexity of calculating v_{ij}, where v_{ij} is the Levenshtein distance between two neural networks $f_i, f_j \in F$ is $\mathrm{O}\left(l^2\right)$ [7]. Therefore, computing the Levenshtein distance between all individuals in F yields the complexity $\mathrm{O}\left(|F|^2 \cdot l^2\right)$.

Phenotypic diversity measures. A *phenotypic diversity* measure is concerned with the individuals' behavioural differences, and can be calculated based on their fitness values. Such diversity measures include computing the standard deviation of fitness values, the average number of unique fitness values in a population, and entropy-based methods, see [2,22].

One advantage of fitness-based diversity measures is that no extra computations are associated with calculating the diversity, because the fitness values already have been calculated by the GA to assess how fit each individual is [11].

Taking the precomputation of fitness values into account gives these diversity measures an advantage when it comes to complexity. To calculate the number of distinct individuals, we can use a hash table. If we assume it unlikely to have a clash between hash values and choose to ignore this, we can achieve a complexity linear in the size of the population, or $\mathrm{O}(|F|)$ for fitness-based diversity measures.

Other measurements. Some diversity measures exist that are neither genotypic nor phenotypic. For instance the *Ancestral ID* method, which assigns a unique ID to each individual in the initial population. Every mutated individual receives a new unique ID while every child gets the ID of one of its parents. The diversity is then based on the uniqueness of IDs in a population [22].

3. Neural Network Trait Diversity

In the following, we propose a method for measuring trait diversity, which we call *Neural Network Trait Diversity* (NNTD). NNTD aims to reflect the diversity of different traits among individuals.

3.1. Algorithm

NNTD is based on Simpsons Diversity Index (SDI), which is a diversity measure used in ecology to quantify the biodiversity of a habitat [15]. SDI is the probability that two randomly chosen individuals belong to different species [19].

Let $F = \{f_1, f_2, \ldots, f_a\}$ denote the set of neural networks contained in a population, all with the same architecture of n input and m output neurons. NNTD is calculated with respect to a number of random inputs $R = \{r_1, r_2, \ldots, r_b\}$, where each r_k for $1 \leq k \leq b$ is an n-tuple of randomly chosen input values—one for each input neuron in the neural network architecture used. Since one is typically interested in how different the neural networks behave in the environment they are intended to operate in, we suggest that a random value for each input neuron is chosen according to the probability of receiving that value as input in the intended environment. For each input r_x, SDI is calculated with respect to that input. Calculating SDI requires a distribution of individuals into a number of species. We now define how each neural network is assigned to a single species given an input r_x.

Let $b_m b_{m-1} \ldots b_1$ be the binary representation of a number i. We define the species $S_i(r)$ to contain any individual $f \in F$, that given $r \in R$ as input satisfies

$$\forall j,h \in \{1,2,\ldots,m\}\,(b_j \to (o_j \geq o_h)) \tag{3}$$

where $o_k \in O$ is the value of the kth output neuron of neural network f. As an example, assume that we have a neural network with six output neurons. If the third output neuron has the highest output when given r_x as input, the neural network will belong to species S_4, because the `1`s in `00100` (the binary representation of 4) matches the indices of the output neurons with the highest value. If multiple output neurons have the highest value, say the first and third output neuron, the neural network will belong to species S_5 since `000101` in binary is 5 in decimal. If all output neurons have the same value, the neural network belongs to species S_{63} since `111111` in binary is 63 in decimal.

Since we only want to be concerned with non-empty species, we define this as a set, which is also defined with respect to a random input

$$Q_x = \{S_i(r_x) \mid S_i(r_x) \neq \emptyset\}$$

Diversity for random input r_x is then defined using the formula for SDI [19]

$$D_x = 1 - \frac{\sum_{q \in Q_x} (|q|\,(|q|-1))}{|F|\,(|F|-1)}$$

The NNTD D (that is, the actual diversity) is then calculated as the average of all D_x values

$$D = \frac{\sum_{x=1}^{|R|} D_x}{|R|} \tag{4}$$

One disadvantage of NNTD is that it relies on random inputs, which means that fewer random inputs implies less statistical significance.

Due to the nature of NNTD, it is not suitable for continuous problems. Consider for instance two neural networks f_1 and f_2, used for approximating a function g, where f_1 and f_2 both have only a single output neuron. To tell how different f_1 and f_2 behave, it is necessary to distinguish between different values of each neural network's output neuron. Since NNTD defines species based on the output neuron with the highest value, and we in this case only have a single output neuron in f_1 and f_2, the two neural networks will always belong to the same species $S_1(r)$ for all $r \in R$, yielding a diversity of 0.

3.2. Complexity

Computations associated with NNTD are split into two halves. The first half distributes neural networks into a number of species for each random input corresponding to eq. (3). These species are then used in the second half, where SDI is calculated for each random input, corresponding to eq. (4).

The first part of computation is carried out as follows. For each random input $r \in R$, every neural network $f \in F$ must calculate an output based on random input r. Each output neuron $o \in O$ belonging to f is now considered once to calculate the particular species f belongs to. The complexity of the first part is thus $\mathrm{O}(|R| \cdot |F| \cdot (t + |O|))$, where t is the time required to calculate the output of a neural network given any input. When calculating the output of a neural network, every neuron in the network must be considered. Therefore, t is an upper bound of $|O|$. This allows us to reduce the complexity to $\mathrm{O}(|R| \cdot |F| \cdot t)$ for the first half of NNTD.

In the second part, we note that SDI considers every species once for every random input, and hence this part has complexity $\mathrm{O}(|R| \cdot |Q|)$, where Q is the largest set of non-empty species for all random inputs R. Since each neural network is put in only one species, $|F|$ is an upper bound of $|Q|$, yielding the complexity $\mathrm{O}(|R| \cdot |F|)$ for the second half.

Combining both halves results in a total complexity of $\mathrm{O}(|R| \cdot |F| \cdot t + |R| \cdot |F|)$, which is reduced to $\mathrm{O}(|R| \cdot |F| \cdot t)$.

3.3. Complexity comparison

Out of all diversity measures, the linear complexity of fitness-based measures is difficult to compete with.

Comparing the complexities of Hamming distance and NNTD allows some interesting reductions and assumptions. Upon comparison, we can remove the common factor F in both of two complexities $\mathrm{O}(|R| \cdot |F| \cdot t)$ of NNTD and $\mathrm{O}\left(|F|^2 \cdot l\right)$ of Hamming distance resulting in $\mathrm{O}(|R| \cdot t)$ and $\mathrm{O}(|F| \cdot l)$, respectively.

Additionally, we can make an assumption about how the length of a bit string l is related to the value t, which is the number of steps required to calculate the output of a neural network given an arbitrarily input. Let E denote the set of edges in a neural network. Each weight must be considered only once when the output of a neural network is calculated. Applying the activation function one time can be considered a constant amount of work. In the extreme case, every neuron will only have a single input connection, hence the activation function will be calculated at most $|E|$ times. Therefore, we have that $t = \theta(|E|)$. If we assume that $|E| = \theta(l)$, we also get that $t = \theta(l)$. This assumption is reasonable, since it is fulfilled if the weight of each edge is separately encoded in the bit string. With this assumption, we can simplify the complexity comparison of NNTD and Hamming distance to a comparison of the complexities $\mathrm{O}(|R|)$ and $\mathrm{O}(|F|)$, respectively.

In this manner, we can conclude that the complexity of NNTD and Hamming distance is asymptotically the same whenever $|R| = c \cdot |F|$ for some constant c. That is, whenever the number of random inputs chosen for NNTD is a constant times the population size.

4. Experiments

In this section, we evaluate our proposed diversity measurement (NNTD) by using it to measure diversity of a population in two different environments.

In the first environment, which we refer to as the static environment, the GA does not iterate. For the three maximization problems introduced in section 4.2, we create an initial population using a constrain c, and a significance α. We choose c such that we have an intuition about how the behavioural diversity of individuals are dependent on α. By experiments, we see if it is likely that NNTD catches this dependency.

In the second environment, which we refer to as the dynamic environment, the GA runs for a number of iterations on each of the three problems. For each problem, we perform a test using each of the four replacement rules introduced in section 2.3. During all of the tests, we measure the diversity using NNTD as well as each of the diversity measures described in section 2.4.

By these experiments we can conclude whether the diversities returned by NNTD better match the expected behavioural differences of the test cases, compared to the other diversity measures.

4.1. Parameter settings

We use a population size of 100 individuals. For each iteration, 100 new offspring individuals are created. Half of the offspring is cloned from a random parent. These are found by using a rank-based selection, and then mutated. The other half is made by performing crossover between two random parents, also using rank-based selection. These settings are presented in table 1.

Three crossover methods are used: one-point crossover, two-point crossover, and uniform crossover. When a new individual is chosen for creation using crossover, there is an equal chance for any of the crossover methods to be used. Each offspring created by crossover has a 10 % chance to be mutated. When mutating an individual, each bit in its bit string has a 5 % chance to be assigned a random boolean value. For specific implementation details, we refer to the source code [12].

Parameter		Specification
Number of runs		100
Generations per run	snake	2000
	XOR	2000
	leaf	500
Population size		100
Selection method		rank-based

Table 1: GA parameters used throughout experimenting.

4.2. Problems under study

We hereby explain the three discrete problems we perform our experiments on. The first problem of approximating the XOR function is interesting, since it is the simplest boolean function that is not linearly separable. This fact has made it quite popular in neural network research communities [8]. Next is the classification of leaves from a dataset in the UCI Machine Learning Repository is interesting, because it is radically different from the XOR problem. XOR is a simple and well defined function, whereas classifying leaves is more complex and depends on observations in nature, which may contain noise. The Snake game differs in that it is an agent decision problem, where not just a single, but a sequence of decisions determines the outcome, where each decision changes the intermediate state.

XOR. We use a neural network to approximate the XOR between two 8-bit strings. To evaluate the fitness of an individual solving this problem, we calculate the XOR of 1000 random two 8-bit strings. For each instance, we determine how many bits the individual calculates correctly. The fitness is then defined as the average number of bits correctly calculated. For the 8-bit XOR problem, any fitness value will thus be a real number in the range $[0, 8]$. The XOR between two bits of random values has equal probability of yielding the value 0 or 1. Therefore, randomly guessing a solution to the XOR between two bit strings of length 8 is expected to yield a fitness of 4.

The network has 16 input neurons, 16 hidden neurons, 8 output neurons, 2 bits per weight, and 1 bit per bias for each hidden and output neuron. We represent the two 8-bit strings as being side by side. So, any output neuron i represents the XOR between the two input neurons i and $i+8$.

We have used as few neurons and bits to represent weights and biases as possible, while still being able to verify that the maximum fitness value of 8 is achievable. The same random seed is always used for generating the 1000 problem instances.

Leaf classification. We use a neural network to classify the Leaf data set [1, 14]. The neural network is given 16 properties about an unknown leaf and has to decide which of 40 types of leaves it is. Fitness is evaluated based on how many instances out of the entire data set the neural network correctly classifies. The implementation consists of 16 input neurons, 10 hidden and 40 output neurons. The output neuron with the highest value decides the classification. Each weight is encoded by 9 bits and neurons have no bias.

Snake. Snake is a game found on old Nokia cell phones, where the player controls a snake around a grid to pick up pieces of food. Every time a piece of food is collected, both the length of the snake and your score increases by 1. You lose if the snake head hits its body or one of the edges of the grid. At all times, the grid contains only a single piece of food. The game becomes harder as the length of the snake increases, and as the snake is constantly moving, the challenge in not trapping oneself gets tougher.

We use a neural network to play a game of Snake in a 10×10 grid with an initial snake length of 5 units. We have defined the fitness of a neural network to be

$$\rho + \frac{\rho}{s/1000}$$

where ρ is the amount of collected food, and s is the total number of steps the snake is alive. The game is constrained such that the snake can only change its direction 90° per step. The neural network has 6 input neurons, each receiving a bit of information about the game state. The first two inputs are relative to the snake's head. So, if the food is vertically and horizontally aligned with the head, then these two input values are 0

1. $\{-1,0,1\}$ food is left of, verti. aligned, or right of
2. $\{-1,0,1\}$ food is above, hori. aligned, or below
3. $\{0,1\}$ death upon moving up
4. $\{0,1\}$ death upon moving down
5. $\{0,1\}$ death upon moving right
6. $\{0,1\}$ death upon moving left

The neural network has 4 output neurons, one for each direction to choose. The neuron with the highest value determines which direction the snake moves. The neural network uses 5 hidden neurons, 9 bits per weight and neurons have no bias. For every game of Snake, we always use the same random seed to decide the positions where pieces of food will spawn.

4.3. Static experiments

We perform two different static experiments, which differ in the way they constrain the initially generated population.

Initial similarity. In the first test, we introduce the variable *initial similarity*, which is a real value in the range $[0,1]$. When making an initial population, an initial similarity of α means that α of the individuals in the population will have the exact same genotype, and $(1-\alpha)$ of the individuals are completely random. An initial similarity of 1 means that all genotypes are the same, and hence the behaviour of all individuals is the same, as well. In this case, we expect the lowest diversity possible. As initial similarity increases, more genotypes will be identical, and hence more individuals will behave the same. We therefore expect the diversity to decrease as initial similarity is increased. An initial similarity of 0 means that all genotypes are random, and hence we expect the most diverse behaviour among individuals to be found here.

Initial mutation. In the second test, we introduce the variable *initial mutation*, which is a real value in the range $[0,1]$. When making an initial population, an initial mutation of α affects the population in the following way. A random genotype is created and given to every individual in the population, such that all individuals have an identical, randomly chosen genotype. Now, the bit string of each individual is mutated. Each bit will with probability α be set to a random boolean value. We expect to see an increase in the difference in behaviour, as a result of mutating bit strings.

Results of initial similarity The results of various initial similarity values shown in fig. 3 play along with our intuition. For each of the problems, each diversity measure's diversity output gradually falls upon increasing the amount of similar individuals in the population. Interestingly enough, at an initial similarity of 0, we expect all diversity measures to output maximum diversity. Here, NNTD outputs the maximum possible diversity of 1, whereas Hamming distance outputs a diversity that is only half of its maximum. It seems that NNTD captures the chaotic nature of a completely random population better than the other two measures, with a larger fall in diversity over time. One could naively assume that you could just double Hamming distance's diversity, but it is actually possible for the Hamming distance measure to output 1 if each bit in two individuals is different.

Results of initial mutation By changing the initial mutation in a population with the results shown in fig. 4, we notice a larger difference between diversity measures. At an initial mutation rate of a mere 1 %, NNTD takes a great leap compared to the other two measures. For Hamming distance, it is obvious that changing only a few bits in the genotypes will only cause a small change in diversity. This is because Hamming distance measures diversity based on genotypes.

For the fitness-based diversity measure, it must be noted that the fitness values are dependent on the particular problem in question and how one chooses to define the fitness function. Consider for instance the problem of making an AI for the game Snake. We have experienced that if we define the fitness only in terms of how many pieces of food a snake collects, then about 98 % of all random individuals get a fitness value of 0. This is the reason why we chose a fitness function that also takes into account the number of steps a snake is alive. Despite yielding more diverse fitness values, it also increased the fitness values obtained after just 100 iterations, notably. This does not mean that a fitness function cannot reflect behavioural differences, but it shows that how one defines the fitness function is crucial, if one wishes to catch the behavioural differences of individuals.

4.4. Dynamic experiments

Our main goal with the experiments we perform is to see how diversity progresses throughout the many iterations of a GA. Furthermore, we must see if there are any significant differences between different diversity measures and replacement rules. To measure diversity, we use a fitness-based measurement, Hamming distance, and our own measure NNTD. The four replacement rules are: Greedy Replacement, Ancestor Elitism, Single Parent Elitism, and MEEE, described in section 2.3. We run the experiments four times, one with each of the replacement rules.

For the snake and XOR problems, we measured the average diversity of 100 runs over 2000 iterations, meaning each run initializes an entirely new population, and each population goes through 2000 iterations of procreation in the search for optimal solutions. After each iteration, diversity of the population is measured for each diversity measure. We then take the average diversity for each generation of the 100 runs. For the leaf data set, we ran the same experiment only through 500 generations, because it is a smaller data set consisting of only 340 instances. This is due to the fact that we saw no improvement in the population beyond this number of iterations.

Results. The results are presented in figures 5 through 7. The experiments performed on the leaf data set are presented in fig. 5, the XOR experiments are presented in fig. 6, and the Snake game results are presented in fig. 7. Each of these three figures contain four plots. The first three of these subfigures illustrate each diversity measure, with the fourth subfigure illustrating the average fitness for the four replacement rules throughout the iterations.

Results of Leaf By comparing the first three graphs in fig. 5, we see that each replacement rule has somewhat the same curve fit for each diversity measure. Each diversity measure captures the intuition of the replacement rules. An interesting observation is the irregular spike in diversity for the fitness-based measure around generation 50. Why this happens is hard to say, due to the stochastic nature of GAs.

NNTD and Hamming distance measures look very similar for this data set. We can argue that NNTD better illustrates how diverse the traits of the individuals are, because with the Hamming distance, we do not see diversity ever rise over 0.5, even for the Ancestor Elitism replacement rule, which consistently introduces many randomly initialized individuals.

Results of XOR The results of each diversity measure presented in fig. 6 are very similar to the Leaf data set above. Once again, we see the irregular spike in the graph presenting the fitness-based measure.

Results of Snake The results shown in fig. 7, once again show a constant difference between the NNTD and Hamming distance measures. The fitness-based measure is again very irregular, this time for the Ancestor Elitism replacement rule. Here, the plot falls and rises before it stabilises.

The big picture If we compare experiments run on each data set illustrated in fig. 5 through fig. 7, we see that the fitness-based diversity measure stands out from the other two in each of the experiments. For example, the fitness-based graphs have some irregular curves, which are not easily explained. Because of this, combined with the fact that multiple individuals can have the same fitness yet behave very differently, we argue that fitness-based diversity does not represent the actual diversity very accurately. This measure is simple and

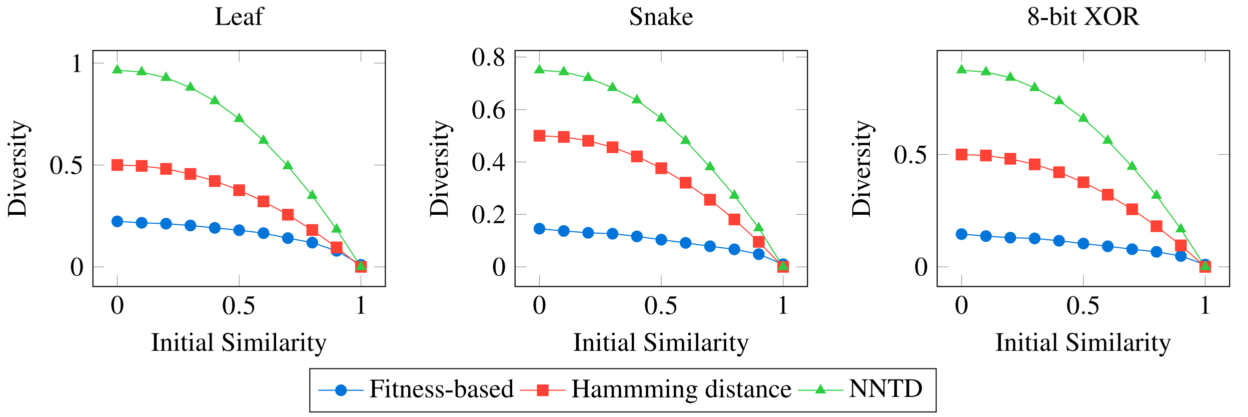


Figure 3: Average over 100 runs for each diversity measure on data sets over intervals of initial similarity. Each point represents the average of 100.

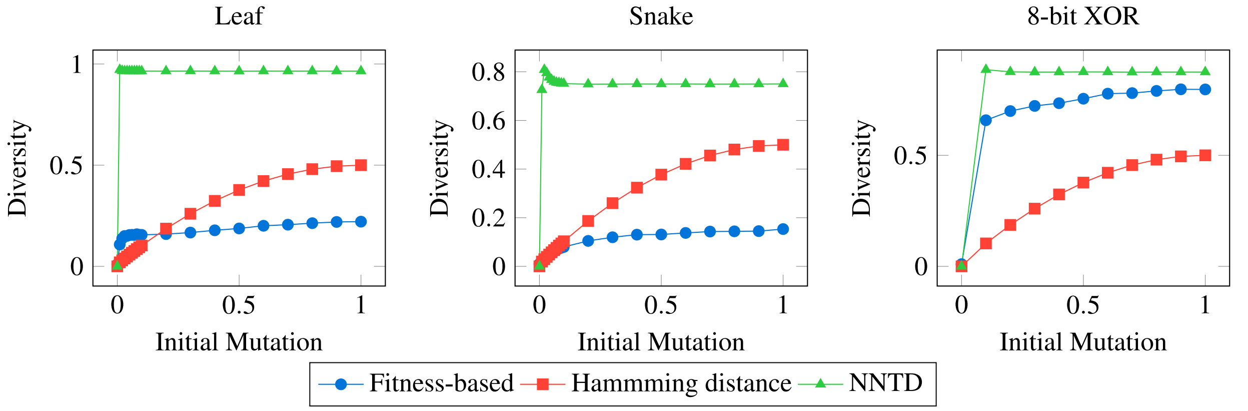


Figure 4: Diversity meaures for each interval of an initially mutated population. Each point represents the average of 100 runs.

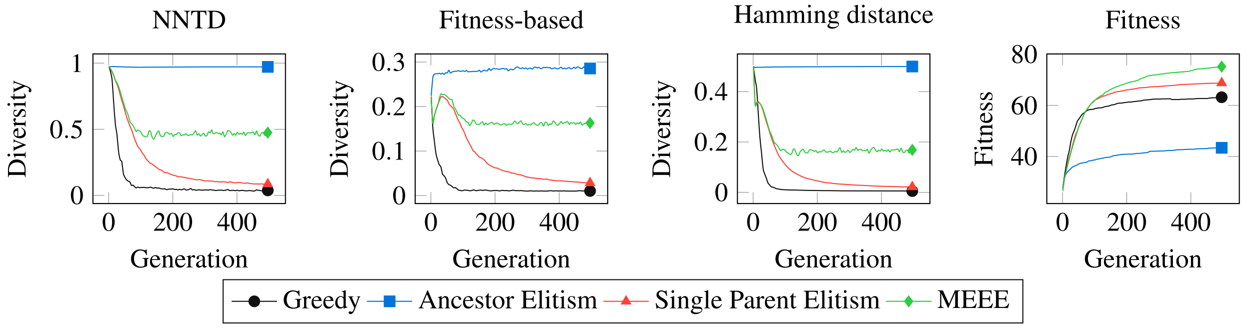


Figure 5: Average over 100 runs for each diversity measure on the leaf data set.

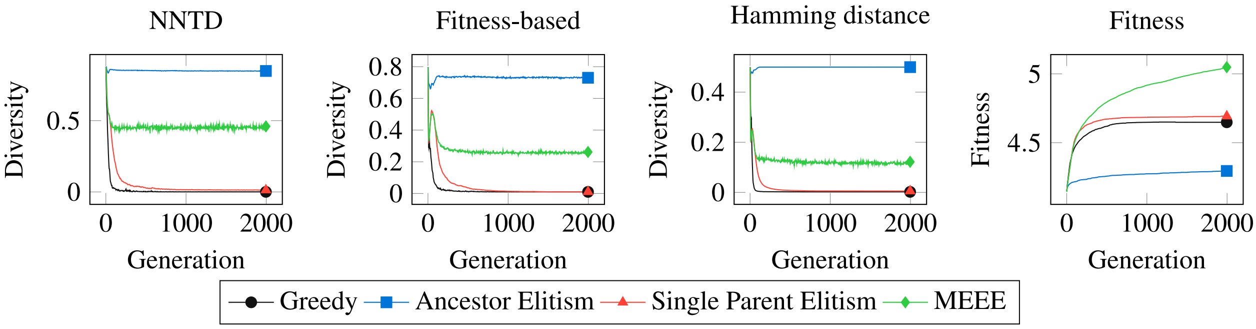


Figure 6: Average over 100 runs for each diversity measure on approximating an 8-bit XOR gate.

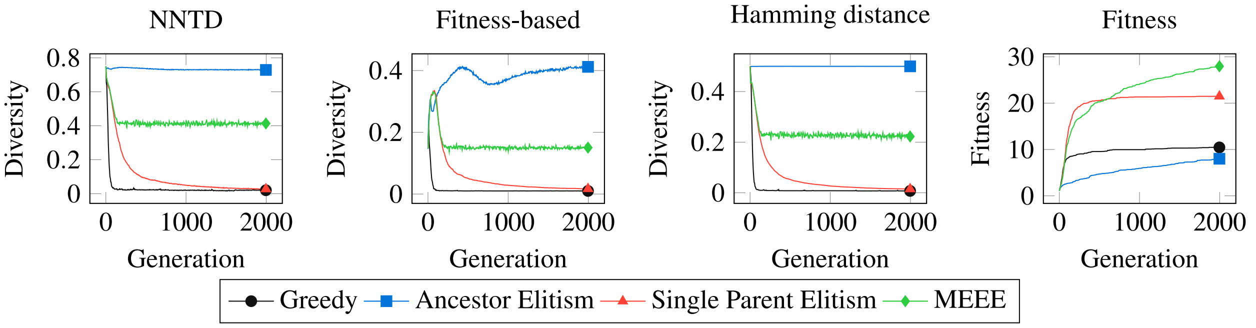


Figure 7: Average over 100 runs for each diversity measure on the snake data set.

does not need any extra computations, but it is not suitable for every problem.

Another observation from the three experiments is that NNTD and Hamming distance do not vary much between the different problems. Each replacement rule is always around the same interval for these two measures. Fitness-based diversity is much more dependent on the problem, as its results are not regular. In each figure presenting the dynamic experiments, the graph presenting the fitness-based measurement is notably different from the two other graphs, presenting NNTD and Hamming distance.

The experiments show that there might be a correspondence between the phenotypic NNTD diversity measure and the genotypic Hamming distance diversity measure. If we take a closer look at the graphs illustrating NNTD and Hamming distance, we can see that they are scaled with a constant, compared to each other. The Hamming distance is always below the NNTD measurement.

When it comes to the fitness of the three experiments, it is clear to see that fitness is at its best when using the MEEE replacement rule. This rule does not have the most diverse population, but as we see, this is not necessarily a bad thing. This indicates that it is not the best solution to aim for a 100 % diverse population, as stated in [4]. One must find a balanced solution and take advantage of the fact that it is possible to switch between maintaining a high diversity and not doing so, which is in correspondance with the results presented in [4].

5. Conclusion

We have argued that fitness-based diversity measurements do not always catch behavioural differences, since two different individuals can have the same fitness, and yet behave differently. The opposite is the case for genotypic diversity measures, for instance Hamming distance. Here we have shown how two individuals of different genotypes can have the exact same behaviour.

We have performed and compared a number of experiments to test our own diversity measure, which we call Neural Network Trait Diversity (NNTD). For each diversity measure, we performed a test using each of the four replacement rules, the Greedy replacement rule, Ancestor Elitism, Single Parent Elitism, and MEEE. These experiments indicate that fitness-based diversity measures are unpredictable.

When it comes to NNTD, which is a phenotypic measure, and Hamming distance, which is a genotypic measure, we observe something interesting. It seems like these two measures follow each other in a manner. This only holds for tests performed in a dynamic environment though. In real world applications, like those investigated in the dynamic tests, there might be some connection between Hamming distance and NNTD.

From tests performed in a static environment, we saw that even a slight mutation among chromosomes of identical individuals caused a major peak in NNTD, but only a small change in Hamming distance. We think it makes sense that even a small change in an individual's genotype can cause a significant change in its behaviour. Consider for instance changing just a single bit of a chromosome. This bit could be a sign bit that causes a significant change to the neural network's behaviour, or it could cause no change at all. Hamming distance neglects this fact and produces the same diversity measure regardless of whether the bit caused a behavioural change of the individual or not. It is also important to be aware of the fact that the Hamming distance measure never exceeded a diversity of 0.5 during our tests, which is obvious, due to the fact that two random bits have the probability 0.5 of being identical. A Hamming distance above 0.5 is indeed possible, but neither during static nor dynamic tests, did this happen.

Based on our experiments and observations, we can conclude that it is reasonable to believe that we have succeeded in creating a diversity measure that better reflects different traits among individuals of a population.

It is interesting, that for each of the three problems under study, the MEEE replacement rule produced the best fitness values. Furthermore, it was the only replacement rule for which it seems that performing more iterations would yield even greater fitness values. The MEEE replacement rule actively uses a diversity measure. Therefore, it is important to have a diversity measure that can capture the concept of a population being diverse.

We have found that NNTD seems to better catch different behaviour of the individuals compared to the two other measures in the data sets we used, which may be more favourable compared to measuring diversity based on genotypes or fitness values.

The complexity of the fitness-based diversity measure is indeed cheaper than that of NNTD and Hamming distance, yet also yielding the most stochastic results. Comparing the complexity of NNTD and Hamming distance depends on the population size and how many random inputs one chooses to use for NNTD. If the number of random inputs is just a constant times the population size, the two diversity measures will have the same complexity, asymptotically speaking.

6. Future work

The number and domain of random inputs used for NNTD will surely affect the reliability of the diversity returned. It is beyond the scope of this article, but indeed crucial to determine how the amount of random inputs can be chosen to produce a reliable result. Despite the amount of random inputs used, it is also interesting to investigate how each random input should be chosen. We chose to assign a random value v to an input neuron x based on the probability that x receives v in a real application. However, other methods can also be used for determining these random values. The impact of other methods can be investigated in the future.

We have shown how NNTD can be used to measure the diversity among neural networks for discrete problems. In the future, we would find it interesting to investigate how the concepts of NNTD can be applied to continuous problems as well. Another idea is to split each output neuron o_i into a set of new output neurons O_i, and a set of ranges Z_i, such that no ranges in Z_i overlap. The value of each output neuron O_i is then defined to be 1 if the value of o_i is in the range Z_i and 0 otherwise. Experiments must be performed to reason about how these ranges should be chosen, as well as the number of ranges used.

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