Behavioral Locality in Genetic Programming

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Abstract: Locality is a key concept affecting exploration and exploitation in evolutionary computation systems. Genotype to phenotype mapping has locality if the neighborhood is preserved under that mapping. Unfortunately, assessment of the locality in Genetic Programming is dependent on the distance metric used to compare program trees. Furthermore, there is no distinction between genotype and phenotype in GP. As such the definition of locality in GP was studied only in the context of genotype-fitness mapping. In this work we propose a different family of similarity measures, graph kernels, as alternatives to the traditional family of distance metrics in use, that is edit distance. Traditional tree edit distance is compared to the Weisfeiler-Lehman Subtree Kernel, which is considered to be the state-of-the-art method in graph classification. Additionally, we extend the definition of the locality of GP, by studying the relationship between genotypes and behaviors. In this paper, we consider a mutation-based GP system applied to two basic benchmark problems: artificial ant (multimodal deceptive landscape) and even parity (highly neutral landscape).

INTRODUCTION

1

The most important question in Evolutionary Computation (EC) field is: "How to characterize, study and predict EC search?" Various approaches were employed to answer this question. These are Microscopic Dynamical System Models, Component Analysis, Schema Theories, and Fitness Landscape.

Fitness Landscape is a metaphor used to visualize problems and is also most commonly used to define a problem difficulty. In the simplest form, a fitness landscape can be represented as a two-dimensional plot of an individual against its fitness. Furthermore, if the genotype can be visualized in two dimensions, the plot can be seen as a three-dimensional map with peaks, valleys, hills, and plateaus. This representation of a search space incorporates the concept of neighbors (Langdon and Poli, 2013). To properly understand the features of the landscape and exploit it, we need to understand how a neighborhood of a point looks like. Additionally, to understand how an evolutionary algorithm explores and exploits such a landscape, it is necessary to understand the locality of representations and operators used during the evolutionary process.

In an abstract sense, the locality of an operator (of

a mapping) refers to how well such an operator preserves the neighborhood of a point. In the context of evolutionary algorithms, small changes in genotype space should correspond to small changes in phenotype space. The most extensive work on the topic of locality in EC has been presented in (Rothlauf, 2006), which has analyzed the importance of locality in performing an effective search over a given landscape. However, studies on locality in tree-based GP are still very rare (Poli et al., 2008). A study of genotype to fitness mapping was proposed in (Galván-López et al., 2010b) as an alternative to standard genotypephenotype mapping, which cannot be simply used for typical GP. That is, there is no distinction between genotypes and phenotypes in GP. However, it is more natural to consider mapping from genotype to some kind of phenotype, an intermediate form between genotype and its fitness.

Therefore in this work, we are interested in investigating the locality of genotype-behavior mapping. That is, we want to study the locality present in GP for behaviors of evolved individuals. For this purpose, we use three basic mutation operators (subtree, structural, and one-point (Koza, 1992)), and study their behavior using two distance measures defined on tree structures. In addition to traditionally used Tree Edit Distance (TED), we also propose using a new family of

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similarity measures, referred to as Graph Kernels. Localities of these operators are studied for artificial ant problem (with multimodal landscape (Langdon et al., 1998)) and even parity problem (with neutral landscape (Galvan-Lopez, 2009)).

2 PRELIMINARIES

2.1 Locality

The locality is an essential concept in EC, which affects how an algorithm explores and exploits the search space. In the sense of EC, a genotype to phenotype mapping has locality if the neighborhood is preserved under that mapping. The study of locality is important for two reasons: (i) locality can be used as an indicator of problem difficulty; (ii) to successfully search the space, a small change in genotype should result in a small change of fitness.

In (Rothlauf, 2006) definition of locality assumes that a distance measure exists on both genotype and phenotype spaces. Additionally, it should be possible to define the neighborhood in terms of minimum distance. There are two types of locality: low and high. A representation is said to have a high locality if neighboring genotypes correspond to neighboring phenotypes. Conversely, in representation with a low locality, neighboring genotypes do not correspond to neighboring phenotypes. According to (Galván-López et al., 2010b), representations with high localities are more efficient at evolutionary search. That is, any search operator has the same effect in both the genotype and phenotype space. In this case, the problem difficulty is unchanged.

On the other hand when the locality is low, (Jones et al., 1995) considers three categories:

- 1. easy, fitness is positively correlated with the distance to the global optimum,
- 2. difficult, there is no correlation between fitness and distance from the global optimum,
- 3. misleading, fitness is negatively correlated with the distance to the global optimum.

If a given problem is easy, then the low locality representation will make it harder, that is, will convert the problem type to difficult. This is the result of the uncorrelated fitness landscape of the low locality representations, which randomizes the search. If a problem is difficult, then the difficulty is unchanged. In rare cases, there are representations that can convert a problem from difficult to easy. Finally, if the problem is of the third category, a low locality representation will convert it to a difficult problem. That is, the problem becomes easier because the search is more random.

In Genetic Programming, there is no distinction between genotypes and phenotypes, therefore, the locality in GP was studied in terms of genotypefitness mapping instead (Galván-López et al., 2010a; Galván-López et al., 2010b).

2.2 Distance Metrics

For evolutionary algorithms with simple genotypes, such as genetic algorithms with binary representation, distance can be evaluated using Hamming distance (Belea et al., 2004). On the other hand, when the genotype becomes more complex, e.g. trees in GP, then more sophisticated methods are necessary. The most commonly used dissimilarity measures in EC belong to the family of edit distances (Gustafson and Vanneschi, 2008).

Another set of methods that are used in evaluating distance between trees are various tests for isomorphism. In (Burke et al., 2004), they are referred to as pseudo-isomorphisms, which were found by defining a three-tuple of \langle terminals, non-terminals, depth \rangle . Approaches, such as genetic markers (Burks and Punch, 2015) and hybrid methods (Kelly et al., 2019), belong to this group of methods. In this setting, two trees are the same if and only if their respective tuples are the same. These methods are used because exact tests for isomorphism were, and in some cases still are, too computationally expensive.

Lastly, a new class of algorithms for graph comparisons have been proposed and improved over time. These methods are referred to as graph kernels and are widely used in fields such as chemoinformatics, bioinformatics, and natural language processing (Nikolentzos et al., 2019). While these methods were developed for use with more complex graphs, they can also be used for simpler structures. In this context, GP syntax trees can be defined as connected acyclic graphs, therefore, graph kernels can be used as a distance metric.

The following subsections provide a brief introduction to the topics of (i) edit distance; (ii) kernel methods; and (iii) graph kernel methods.

2.2.1 Edit Distance

Edit distance is a family of distance metrics defined on non-vectorial data, such as strings, trees, and graphs. The Levenshtein distance is a well-known edit distance method, which is used to measure the distance between two sequences, for example, strings. The distance between two strings is given by the minimum number of operations, insertion, deletion, or substitution, required to transform one string to another.

Generalization of the edit distance for more complex data structures, namely trees, was introduced in (Tai, 1979) and was later referred to as Tree Edit Distance (TED). Edit distance was introduced to the field of EC as a distance metric in (O'Reilly, 1997), to measure the degree of dissimilarity between two tree-like structures. More formally, let *G* and *G'* be two rooted trees where each vertex is assigned a label from alphabet Σ . The edit distance between these two trees is the minimum cost of transforming *G* into *G'* using a sequence of operations (single operation per node): (i) substitution of a node *v*, that is, change its label; (ii) deletion of the node *v* and resetting the children as the children of *v*'s parent; and (iii) insertion of a node *v*, as a reverse of the deletion operation.

2.2.2 Graph Kernel Methods

Classical learning algorithms use instances, e.g. x, x'in non-empty set X, through an inner product $\langle x, x' \rangle$. This can be interpreted as a distance, or similarity between instances x and x'. The biggest advantage of kernel methods is that they can operate on any type of data. The input space X is not restricted to vector space, and it can be applied to structured domains, such as strings or graphs. Kernels can be used on structured data as long as an appropriate mapping to RKHS \mathscr{H} can be found, that is $\phi : X \to \mathscr{H}$. However, the structure of the graph is invariant to permutations of its representations. That is, the ordering of the nodes and edges does not change the structure of the graph. Therefore, similarity measures also have to take into account this property. Various paradigms were proposed to evaluate similarity in such a way. These methods can be roughly divided into following subgroups: neighborhood aggregation methods, assignment kernels, matching-based kernels, walks and paths based kernels, and finally subgraph patternbased kernels (Kriege et al., 2020). The last paradigm seems to be the most natural way to define kernel methods on structured data. This class of functions is based on the decomposition of the object into substructures, e.g. subgraphs or vertices, which are then compared by applying existing kernels. Such kernels are referred to as \mathcal{R} -convolution kernels.

2.2.3 Weisfeiler-Lehman Framework

The Weisfeiler-Lehman algorithm/framework was inspired by the Weisfeiler-Lehman's graph isomorphism test, also known as "naive vertex refinement". This framework can be applied to any graph kernel, such as the shortest path or subtree kernel (Shervashidze et al., 2011). Among those, the Weisfeiler-Lehman subtree kernel is considered to be the stateof-the-art algorithm in graph classification. The key idea of this algorithm is to augment labels of each node with so-called multiset label consisting of the original label of the vertex and sorted labels of its neighborhood. This newly created multiset is then compressed, resulting in a new and short label (shown in Figure 1). Relabeling procedure is repeated for hiterations, and two nodes from different graphs will match if and only if they have identical multiset labels. Formally, the Weisfeiler-Lehman Framework can be defined as follows:

Definition 1. (Weisfeiler-Lehman Framework) (*Nikolentzos et al., 2019*)

Let k be any kernel for graphs, that we will call the base kernel. Then the Weisfeiler-Lehman kernel with h iterations with the base kernel k between two graphs G and G' is defined as:

$$k_{WL}(G,G') = k(G_0,G'_0) + k(G_1,G'_1) + \dots + k(G_h,G'_h)$$
(1)

where h is the number of Weisfeiler-Lehman iterations, and $\{G_0, G_1, \ldots, G_h\}$ and $\{G'_0, G'_1, \ldots, G'_h\}$ are the Weisfeiler-Lehman sequences of G and G', respectively.

The above definition states, that any graph kernel which considers graphs with discrete node labels can take advantage of the Weisfeiler-Lehman framework. Furthermore, if the base kernel compares subtrees of two graphs G and G', then the method is referred to as the Weisfeiler-Lehman Subtree Kernel. For further information (on both theory and implementation), see (Nikolentzos et al., 2019) and (Kriege et al., 2020).

3 EXPERIMENTAL SETUP

Many studies try to improve GP, by incorporating semantic information during exploration and exploitation of the search space (Vanneschi et al., 2014). Unfortunately, most studies are purely empirical with no theoretical backing. Most of the works are based on experience rather than mathematics. To solve this issue, a lot of work was done to understand how the locality of both representations and genetic operators affect the problem difficulty. This approach, while being straightforward for simple structures used in GAs, is troublesome when applied to tree-based GP. Genotype to phenotype mapping cannot be simply studied, as there is no clear distinction between representation (genotype) and solution (phenotype). Therefore, most works consider genotype-fitness mapping. However, it is more natural to consider mapping from genotype



Figure 1: Illustration of the relabeling process used in the Weisfeiler-Lehman subtree kernel for h = 1 for two trees G and G^0 . In the Genetic Programming setting, node labels are first relabeled from mathematical operations into simpler representation, e.g. integers (top). In the following step, node labels are augmented with multiset labels, which consist of the original label of the node and sorted labels of its neighborhood (a tree with multiset labels is presented in the bottom left). Created multiset is compressed by relabeling it with a new label, which did not exist in the original set of labels. Relabeling scheme is presented in the bottom middle, and relabeled trees are shown in the bottom right.

to some intermediate form, such as the behavior of an individual. In this work, we study the locality of genotype to behavior mapping for three basic mutation operators: subtree, structural, and one-point. This is examined for two benchmark problems: (i) Artificial Ant; and (ii) Even-*n*-Parity.

Artificial Ant is often used as a GP benchmark problem. It consists of finding a program that can successfully navigate an artificial ant along a path on a 32×32 toroidal grid. The most commonly used trail (called Santa Fe trail) consists of 89 pellets of food, and the number of pellets eaten by an ant is its fitness. Standard set of non-terminals $F = \{$ IfFoodAhead, prog2, prog3 $\}$ and terminals T ={Move, Right, Left} is used. In this study we consider the behavior of the artificial ant to be its sequence of moves and positions. That is, each individual in population is associated with a vectors of the form (x, y, dir), where x, y are positions in space and dir is the direction faced by an ant with values: {north, east, south, west}. Program times-out after 600 steps, thus, behavioral differences between the individuals can be determined by simply comparing these vectors.

The goal of the boolean Even-*n*-Parity problem is to evolve a function that returns true if an even number of the inputs evaluates to true, and false otherwise. GP uses set of terminals (n = 6 inputs), and non-terminals $F = \{NOT, OR, AND\}$. Fitness of a program is the number of successfull parity evaluations, thus, the maximum fitness is $2^6 = 64$. The behavior of a program can be defined in terms of the out-

Table 1: Common GP parameters.

Parameters	Values	
Population size	500	
Initialization	Ramped half and half	
Max depth	6	
Selection	Tournament	
Size	7	
Generations	50_ATIONS	
Runs	50	
Crossover rate	70%	
Mutation rate	30%	
Max depth	2	
Static tree height limit	20	

puts it produces. Outputs are recorded as sequences of binary values for each of the test cases used during fitness evaluations. Behavioral differences between the individuals can be calculated by comparing sequences of outputs.

Parameters of the GP used to solve artificial ant and even-6-parity problems are presented in Table 1. Population size was set to 500 and was initialized with ramped half and half method (Koza, 1992). The initial population consists of trees with heights from 1 to 6. Programs were evolved for 50 generations. Crossover rate was set to 70% and parents were selected using tournament selection of size 7. Additionally, individuals were mutated with the probability of 30% using one of the three mutation operators: (i) subtree, replaces a randomly selected subtree with randomly created subtree; (ii) structural, either inflates or deflates the individual; or (iii) one-point, replaces a single node in the individual. Subtree mutation was restricted to generating subtrees with a maximum height of 2. To avoid excessive bloat of the trees, a static height limit of 20 was set for a crossover operator. That is, if crossover operation resulted in an offspring with a height greater than 20, then the offspring was replaced by one of the parents at random. However, this limit does not affect mutation operators, as they are limited in the growth of the trees. This GP run was repeated 50 times to collect the appropriate amount of statistical data. A set of experiments was conducted to examine proposed approaches.

Before proceeding with investigating the behavioral locality of mutation operators, we have to determine the differences between two distance measures used in this study.

A conventional distance measure, Tree Edit Distance considers the distance between the trees to be the minimum amount of edits needed to transform one tree to another. Thus, it takes into account only local properties. This approach provides us with a finegrained distance (a measure of dissimilarity) between the individuals, in the form of an integer with the maximum distance being $|G_1| + |G_2|$, where $|G_1|$ and $|G_2|$ are the number of nodes of compared trees G_1 and G_2 . Zhang and Shasha's dynamic programming implementation of TED (Zhang and Shasha, 1989) was applied in this study.

On the other hand, the Weisfeiler-Lehman Subtree Kernel is a method of evaluating the similarity between the trees. Similarly to TED, this method returns an integer value. However, this value defines the closeness of individuals. That is, the higher the value, the more similarities are shared between individuals. To compare this method to TED it is necessary to convert similarity value to dissimilarity by first normalizing similarity ($\frac{k(G,G')}{k(G,G)+k(G',G')}$), and then subtracting it from 1.

These methods were compared by calculating the average dissimilarity of an individual to the rest of the population. This is done by creating a matrix consisting of pairwise distances, which is further summed for one of the axes. A vector of values received in this way represents the distribution of average dissimilarities and is plotted against indices used to label individuals. This comparison was executed for the population in the last generation of GP run, which was repeated 50 times, to examine an average difference in behaviors of these two methods.

After the initial investigation of differences between distance measures, we proceeded with the investigation of the behavioral locality of mutation operators. To have sufficient statistical data, we have created 1,250,000 individuals. This was achieved by recording all individuals created during the evolution of GP with parameters as defined in the Table 1. All three mutation operators were used in the evolutionary process, to avoid bias in data. Gathered individuals were mutated using subtree, structural and onepoint mutations. Finally, data created in such a way was divided into parts consisting of positive, neutral, and negative mutations, that is, mutations which increased, did not change, and decreased fitness of an individual, respectively.

In the first set of results, this data was used to present occurrences of individuals with positive, neutral, and negative mutations for subtree, structural and one-point mutations. These results are necessary to determine what kind of distribution was created by our experimental setup, thus, allowing us to directly compare these results with past investigations.

The second set of results present distributions of fitness and behavior distance with respect to the frequency of such a mutation occurring. In this case, we plotted an absolute fitness distance, as it is not important if the change was positive or negative. We are interested in how often fitness and behavior distance of 1 occurred. That is, the most frequently occurring mutation operator can be said to be of the highest locality.

Finally, this work presents fitness distance, behavior distance, tree edit distance, and WL-Subtree Kernel distance plotted against the fitness of an individual before mutation (referred to as original fitness). This subset of results is presented in the form of a 3×4 grid, with rows corresponding to mutation operators. Three super-sets of results are presented for positive, neutral, and negative mutations. Due to space restrictions, this result is shown only for an artificial ant problem. This representation should allow us to see an average structural change (in terms of TED and WL-Subtree Kernel) introduced by mutation operators. At the same time, the use of the same *x*-axis allows us to see how this structural change relates to fitness and behavioral changes.

4 RESULTS AND DISCUSSION

A comparison between TED and WL-Subtree Kernel is presented in Figure 2. Individuals in the population were sorted with respect to their sizes (number of nodes in the tree). That is, individuals on the left side (closer to 0) consist of fewer nodes than individuals to the right (closer to 500). For all tested cases, TED (depicted with orange lines) returns higher average distances than WL-Subtree Kernel (shown as blue lines). On the other hand, differences between those



Figure 2: Distribution of average dissimilarity vs label of an individual for artificial ant (left) and even-6-parity (right).



Figure 3: Occurrences of individuals after applying subtree (left), structural (middle), and one-point mutation (right). Results for artificial ant problem (top) and even-6-parity (bottom).

Table 2: Frequencies of subtree, structural and one-point mutations leading to fitness and behavior distance to be 1.

	Artificial Ant		Even-6-Parity	
	Fitness	Behavior	Fitness	Behavior
Subtree	$2.86 \cdot 10^{-2}$	$6.17 \cdot 10^{-5}$	$1.75 \cdot 10^{-2}$	$9.06 \cdot 10^{-3}$
Structural	$2.96 \cdot 10^{-2}$	$4.25 \cdot 10^{-5}$	$1.33\cdot10^{-2}$	$7.10 \cdot 10^{-3}$
One-Point	$1.65 \cdot 10^{-2}$	$1.85\cdot 10^{-5}$	$1.19 \cdot 10^{-2}$	$6.57 \cdot 10^{-3}$

two values are fairly stable (green line). This is the difference in dissimilarity evaluation between TED, which computes dissimilarity by considering only local differences, and WL-Subtree kernel, which considers both local and global properties of the trees. WL-Subtree kernel calculates the similarity by taking into account several feature vectors, created through the relabeling procedure, as shown in Figure 1. As an effect, it "dilutes" small differences, thus considers trees to be more similar. This is more visible for bigger individuals, where the difference between the two methods is increasing (seen as a rise in values presented by the green line).

Figure 3 shows the occurrences of individuals after applying three mutation operators. For artificial ant problem, we can observe various peaks of neutral



Figure 4: Distribution of fitness distance (top) and behavior distance (bottom) vs frequency. Results for the artificial ant problem (left) and even-6-parity (right) using subtree, structural, and one-point mutation.



Figure 5: Results after applying subtree (top), structural (middle), and one-point mutation (bottom) for an artificial ant problem. Original fitness vs positive fitness (first column), original fitness vs behavior distance (second column), and structural distance metrics using edit distance (third column) and Weisfeiler-Lehman Subtree Kernel (fourth column).

and negative mutations in the fitness range. The first set of peaks can be observed for low fitness values (< 15). This is consistent with results given in (Langdon and Poli, 2013), where it was shown that the number of individuals with low fitnesses (regardless

of their size) is always high in artificial ant problem. However, similarly high peaks can also be observed in the fitness range of [50, 70]. However, these peaks appear in the distribution of fitness values in the search space, thus are unique to the problem rather than to



Figure 6: Results after applying subtree (top), structural (middle), and one-point mutation (bottom) for an artificial ant problem. Original fitness vs neutral fitness (first column), original fitness vs behavior distance (second column), and structural distance metrics using edit distance (third column) and Weisfeiler-Lehman Subtree Kernel (fourth column).



Figure 7: Results after applying subtree (top), structural (middle), and one-point mutation (bottom) for an artificial ant problem. Original fitness vs negative fitness (first column), original fitness vs behavior distance (second column), and structural distance metrics using edit distance (third column) and Weisfeiler-Lehman Subtree Kernel (fourth column).

the genetic operators (Galván-López et al., 2010b). In our case, there is also an additional peak for a fitness value of 89. This peak is the result of our static bloat control, which simply discarded all offspring created using crossover, which resulted in trees with heights higher than 20. This resulted in the replication of highly fit (and possibly bloated) individuals in the latter stage of the evolutionary process, thus, it is the result of our sampling method. It is interesting to see that for subtree and structural mutations, neutral mutations dominate in low fitness range. This changes above fitness value of 20, where suddenly most of the mutations have negative effects. In the latter fitness range, neutral and negative mutations occur at a similar rate. On the other hand, when the one-point mutation is applied, most of the mutations are neutral for fitness values lower than 45. Positive mutations act similarly for all mutation operators. These occur most frequently in low fitness range and are very rare for individuals with high fitnesses. Reversed behavior can be observed for even-6parity problems. In this case, most of the mutations appear for programs with high fitness values (above half of the maximum fitness, i.e. 32 for even-6parity). In this range, neutral and negative mutations dominate and occur at similar rates. On the other hand, positive mutations are as frequent as neutral mutations in the lower half of fitness values. Similar results were reported in (Galván-López et al., 2010b). This means that bloat control, which changed the distribution of fitness values for an artificial ant problem, did not affect outcomes for even-6-parity problem.

The locality of mutation operators is shown in Figure 4. Let us start an analysis of the locality of a mutation operator in a genotype-fitness mapping (top part of Figure 4). First of all the highest frequency can be observed for neutral mutations (fitness distance of 0), regardless of mutation operator. For artificial ant problem, we can see that it is substantially less common for mutation operator to introduce big fitness change. This tendency can also be observed for even parity problem. However, it is far more common for mutation operation to drastically change the fitness of the individual in even parity problem. This is related to the neutral landscape of even parity problem, for which even small changes of the genotype can be detrimental for the program.

The locality of mutation operators in genotypebehavior mapping can be seen in the bottom part of Figure 4. For even parity problem, the distribution of behavior distance to the frequency of it occurring, looks pretty much the same as the distribution of fitness distance. On the other hand, genotype-behavior mapping presents a completely different view of an artificial ant problem. Even in this picture, neutral mutations are most common, however, small behavioral differences are very rare (frequencies at the level of 10^{-5}). Conversely, big behavioral changes (behavior distances close to 600) are very common (around 10^{-2}). Frequencies, when fitness distance and behavior distance are 1, are presented in Table 2. Presented values show that subtree mutation presents the highest locality, with the one-point mutation having the lowest locality. This result is counter-intuitive. The one-point mutation is the simplest mutation, which replaces a single node of a tree, thus should have the highest locality. On the other hand, subtree mutation is capable of introducing drastic genotypic changes. This finding is a little bit different from the results reported in (Galván-López et al., 2010b), in which structural mutation is shown to have the highest locality.

Finally, we have to analyze the relation between fitness and behavior distance to genotypic change in-

troduced through mutations. Cases for positive, neutral, and negative mutations are analysed separately, and are shown in Figures 5, 6, and 7, respectively. Due to space restrictions, only results for an artificial ant problem are presented.

Let us first focus on the results for positive mutations (Figure 5). We can see that on average, the biggest fitness change is introduced to individuals with original fitness of around 10. After this point, the average improvement of an individual's fitness decreases, thus becoming harder to improve programs. The biggest change can be seen for original fitness values above 60, where suddenly the distribution becomes rugged. These are local optima, which cannot be easily escaped. It is known that an artificial ant problem has a highly multimodal landscape, with many plateaus split by deep valleys (Langdon et al., 1998). This means that bigger genotypic, as well as behavioral changes, are required to escape such optima. Similar ruggedness of the landscape can be observed in the following plots for behavioral and structural distances. In the case of behavior, we can see that overall behavioral changes (corresponding to fitness improvements) are high, but they also decrease after the original fitness of 10. This behavior is fairly natural, that is, to improve individuals with high fitnesses we have to optimize their behaviors. However, when optimal solutions are found (fitnesses > 60), it is necessary to introduce big changes to the behavior (similar to fitness and genotypic changes) to improve an individual. Similar behavior can be observed for structural changes, which are relatively low for the whole spectrum of fitness values. However, this relation becomes rugged in the same region as for fitness and behavior changes. In the case of tree edit distance, this relation is harder to see, because it takes into account only how many edits are necessary to change one tree into another. According to TED, big behavioral changes are accompanied by small genotypic changes (only a small subset of nodes was changed). On the other hand, WL-Subtree kernel claims that the introduced changes are far greater (on par with changes introduced for individuals with low fitnesses).

For neutral mutations, we can observe that big behavioral changes are recorded for individuals with low fitness values. These behavioral changes are accompanied by relatively high genotypic changes as shown by both distance measures. On the other hand, individuals with high original fitnesses, experience small or no behavioral changes, even for relatively high genotypic mutations, as given by WL-Subtree kernel. That is, a highly fit individual cannot drastically change its behavior if it wants to keep its fitness value unchanged. It is worth mentioning, that these genotypic changes are smaller than the ones observed for positive mutations (according to WL-Subtree kernel: < 0.2 for neutral and > 0.2 for positive mutations). That is, these changes are small enough not to escape local optima, as well as, they are not big enough to enter valleys.

Finally, in the case of negative mutations, we see that the most detrimental changes can be observed for individuals with high original fitnesses (> 70). From the behavioral perspective, all individuals experience very high changes to their behaviors. This landscape is stable in comparison to the behavior changes observed for positive mutations. It is interesting to see that for negative mutations, structural changes are overall higher than the ones observed for neutral mutations, but are lower than for positive mutations.

5 CONCLUSIONS

Two contributions of this paper are: (i) extending the definition of GP by considering genotype to behavior mapping; and (ii) proposed to use the family of similarity measures, Graph Kernels, as a way to calculate genotypic distance. Our proposals were tested on two benchmark problems, artificial ant and even parity problem.

First of all, traditionally used Tree Edit Distance (TED) was compared to the Weisfeiler-Lehman Subtree Kernel. This comparison showed that TED considers trees to be significantly more different than WL-Subtree kernel. This is due to the way, the dissimilarity between the trees is calculated, that is WL-Subtree kernel considers both local (node level) and global (neighborhoods) properties of trees. This means that the WL-Subtree kernel uses both syntactic (structural) and semantic (behavioral) information, to evaluate dissimilarity.

Investigations on the locality of three basic mutation operators: subtree, structural, and one-point mutations, showed that subtree mutation has the highest locality. This result is counter-intuitive because subtree mutation changes subtrees (and possibly whole tree). This result is common for both genotype to fitness and genotype to behavior mappings. However, for the artificial ant problem, all three mutation operators have low locality in genotype to behavior mapping. That is, the frequency of a highly local change to occur is much less common than a low locality change to happen (frequencies at the level of 10^5 vs 10^2 , respectively). In the case of even-6-parity, distributions of fitness, and behavior distances were approximately the same. Finally, our results showed that all mutations are detrimental to the original behavior of an individual, regardless of its original fitness and the size of introduced genotypic change. Three considered mutation operators are of low behavioral locality, that is, they rarely preserve behaviors of programs. Therefore, even small changes in the genotype, drastically change an individual's behavior, thus resulting in slight improvements or considerable deterioration of the fitness of an individual. Small behavioral changes were also recorded, however, these did not change the fitness of programs.

This work can be extended in several ways. First of all, it could be applied to a wider variety of problems, e.g. symbolic regression (both benchmark and real-world problems), maze navigation, image processing, and scheduling. Furthermore, this work applied the Weisfeiler-Lehman Subtree kernel as a dissimilarity measure, however, various methods could also be used, such as, Shortest Path, Random Walk, Graphlet Sampling, and Laplacian kernels. Finally, it may be worthwhile to investigate how different reperesentations of intermediate phenotypes (e.g. binary decision diagrams) affect the fitness landscape.

REFERENCES

- Belea, R., Caraman, S., and Palade, V. (2004). Diagnosing the population state in a genetic algorithm using hamming distance. In *International Conference* on Knowledge-Based and Intelligent Information and Engineering Systems, pages 246–255. Springer.
- Burke, E. K., Gustafson, S., and Kendall, G. (2004). Diversity in genetic programming: An analysis of measures and correlation with fitness. *IEEE Transactions on Evolutionary Computation*, 8(1):47–62.
- Burks, A. R. and Punch, W. F. (2015). An efficient structural diversity technique for genetic programming. In Proceedings of the 2015 Annual Conference on Genetic and Evolutionary Computation, pages 991–998.
- Galvan-Lopez, E. (2009). An analysis of the effects of neutrality on problem hardness for evolutionary algorithms. PhD thesis, University of Essex.
- Galván-López, E., McDermott, J., O'Neill, M., and Brabazon, A. (2010a). Defining locality in genetic programming to predict performance. In *IEEE Congress on Evolutionary Computation*, pages 1–8. IEEE.
- Galván-López, E., McDermott, J., O'Neill, M., and Brabazon, A. (2010b). Towards an understanding of locality in genetic programming. In *Proceedings of the 12th annual conference on Genetic and evolutionary computation*, pages 901–908.
- Gustafson, S. and Vanneschi, L. (2008). Crossover-based tree distance in genetic programming. *IEEE Transactions on Evolutionary Computation*, 12(4):506–524.

- Jones, T. et al. (1995). Evolutionary algorithms, fitness landscapes and search. PhD thesis, Citeseer.
- Kelly, J., Hemberg, E., and O'Reilly, U.-M. (2019). Improving genetic programming with novel explorationexploitation control. In *European Conference on Genetic Programming*, pages 64–80. Springer.
- Koza, J. R. (1992). Genetic programming: on the programming of computers by means of natural selection, volume 1. MIT press.
- Kriege, N. M., Johansson, F. D., and Morris, C. (2020). A survey on graph kernels. *Applied Network Science*, 5(1):1–42.
- Langdon, W. B. and Poli, R. (2013). Foundations of genetic programming. Springer Science & Business Media.
- Langdon, W. B., Poli, R., et al. (1998). Why ants are hard.
- Nikolentzos, G., Siglidis, G., and Vazirgiannis, M. (2019). Graph kernels: A survey. *arXiv preprint arXiv:1904.12218*.
- O'Reilly, U.-M. (1997). Using a distance metric on genetic programs to understand genetic operators. In 1997 IEEE International Conference on Systems, Man, and Cybernetics. Computational Cybernetics and Simulation, volume 5, pages 4092–4097. IEEE.
- Poli, R., Langdon, W. B., McPhee, N. F., and Koza, J. R. (2008). *A field guide to genetic programming*. Lulu. com.
- Rothlauf, F. (2006). Representations for genetic and evolutionary algorithms. In *Representations for Genetic* and Evolutionary Algorithms, pages 9–32. Springer.
- Shervashidze, N., Schweitzer, P., Leeuwen, E. J. v., Mehlhorn, K., and Borgwardt, K. M. (2011). Weisfeiler-lehman graph kernels. *Journal of Machine Learning Research*, 12(Sep):2539–2561.
- Tai, K.-C. (1979). The tree-to-tree correction problem. *Journal of the ACM (JACM)*, 26(3):422–433.
- Vanneschi, L., Castelli, M., and Silva, S. (2014). A survey of semantic methods in genetic programming. *Genetic Programming and Evolvable Machines*, 15(2):195– 214.
- Zhang, K. and Shasha, D. (1989). Simple fast algorithms for the editing distance between trees and related problems. SIAM journal on computing, 18(6):1245–1262.