A Clustering-based Visual Analysis Tool for Genetic Algorithm

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Abstract: While Genetic Algorithm (GA) is a powerful tool for combinatorial optimization, the vast population of candidate solutions it typically deploys and algorithm's intrinsic randomness lead to difficulty in understanding its search behavior. We discuss in this paper a clustering-based visualization tool for GA that attempts to mediate this problem. GA population across its entire generations are clustered, and each cluster and its individuals are mapped to a visual symbol. The tool enables a GA researcher or user to understand better the behavior of a GA run, specifically the local searches it performs in its global exploration to go from one generation to another.

1 INTRODUCTION

Genetic Algorithm (GA), initially conceived by John Holland (Holland, 1975), is among the most popular meta-heuristics for combinatorial optimization problems these days. GA typically generates a huge number of candidate solutions (individuals) to a problem in a search process inspired by Darwinian natural evolution, involving concepts such as selection, crossover and mutation. While a powerful paradigm, the vast amount of data semi-randomly evolved by GA eludes an intuitive interpretation, leading to difficulty in understanding its search behavior.

The main approach pursued in this paper to address the above-mentioned problem is visualization. The mainstay of big data analysis (Fan and Bifet, 2013), visualization can serve users with different levels of expertise (Gelman and Unwin, 2013). Applied to GA, it can potentially be used to analyze its inner working (Hart and Ross, 2001).

Specifically, this paper describes a clustering-based visualization tool for GA. The proposed tool performs an offline visualization on the GA data. The clustering structures the population visited by GA across its generations, allowing a GA researcher to make sense of the local searches performed by GA in its global exploration. Individuals within a cluster are mapped in a certain way to a certain symbol, allowing the researcher to make statements about the way in which the GA has been progressing.

While there have been various tools for the visualization of GA, the one proposed in this paper is unique due to its emphasis. Prior work in general focuses on the visualization of high-dimensional individuals in GA, while our proposed tool concerns more on visualizing the dynamics of cluster formations in GA. In particular, this tool enables us:

1. To study the search space explored by GA and analyze the behavior of the operators and parameters deployed for the search.
2. To obtain useful information that can be used later by the GA researcher to interactively manipulate the search space.

The rest of this paper is organized as follows: In section 2, work related to the visualization of GA is reviewed. The details of the visualization implemented in our proposed tool is elaborated in section 3. An example analysis is presented in section 4, followed by a comparison with the existent tools in section 5. Finally in section 6, the conclusion is drawn along with suggestions for future work.

2 RELATED WORK

In the following, existent tools and methods for offline visualization of GA are reviewed. Early works in the 90s were mostly published by Collins. In (Collins, 1996), Collins proposed a mapping method called *Genotypic-Space Mapping* based on the direct linear two-way relationship between high-dimensional

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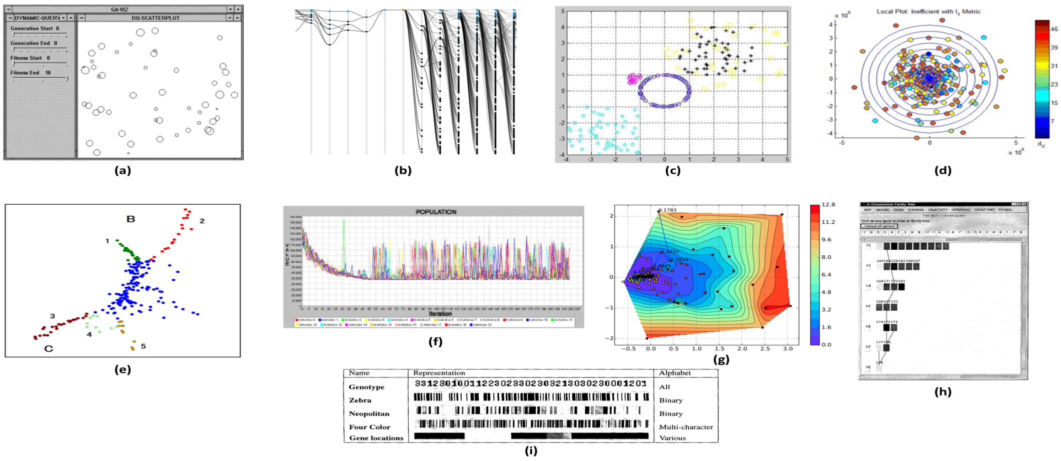


Figure 1: (a) Tool developed by Collins; (b) ELICIT tool; (c) Tool developed by He and Yen; (d) Tool developed by Craven and Jimbo; (e) Tool developed by Kudo and Yoshikawa; (f) FOM tool; (g) Tool developed by Kramer and Luckehe; (h) GAVEL tool; (i) VIS tool.

strings and two or three dimensional co-ordinates for visualization of GA population. Although this was the first dedicated work on visualization of high-dimensional individuals, it only offers a single view into the GA population and also insufficient level of user interactivity.

A tool developed by Wu *et al.* (Wu et al., 1999) called *VIS* to analyze the details of an Evolutionary Algorithm (EA) run. For visualization of individuals, five different graphical representations are offered by this tool, namely: *Genotype*, *Zebra*, *Neapolitan*, *Four Color*, and *Gene Location*, each of which is suitable for a specific chromosome representation. Also, it offers a view named *Family Format* to show the parents and offspring of a particular individual. However, it does not provide any view for the visualization of individuals in objective space, and also for individuals phenotype.

GAVEL introduced by Hart and Ross (Hart and Ross, 2001), is another analysis tool for GA. The main idea of this tool is to start from the best solution found at the end of a GA run and trace back its evolution by finding the parents and parents of parents, etc., all the way back to the initial generation of individuals. The aim of this process is to produce a complete ancestry tree of the best solution. Moreover, this tool tracks the history of every single gene in the best individual's chromosome to find the individual it originated in. *GAVEL* visualizes the individuals using three graphical representations, namely: *Alleles Values*, *Gene Origins*, and *Operator Origins*. Like the *VIS* tool, this tool has the disadvantage of not providing any view for the individuals phenotype.

Parejo *et al.* (Parejo et al., 2003) developed a framework for meta-heuristic optimization called FOM. This tool includes the implementation of several meta-heuristics such as *Steepest Descent*, *Iterative Steepest Descent*, *Tabu Search*, *Simulated Annealing*, *GRASP*, *Variable Neighbourhood Search* and *GA*. FOM provides visualization and some statistical information of the individuals fitness values. However, no view is provided for representing individuals in parameter space and also for individuals phenotype.

Kudo and Yoshikawa (Kudo and Yoshikawa, 2012) proposed a visualization method using an idea of Isomap. They applied the proposed method to data came from a Multi-Objective Genetic Algorithm (MOGA), which was used to solve a problem in engineering design field, i.e. conceptual design optimization problem of hybrid rocket engine. The focus of this method is to analyze the distribution of Pareto individuals by visualizing the manifold embedded in the high dimensional objective space, and in fact, this is the only view provided by this method.

Craven and Jimbo (Craven and Jimbo, 2014) introduced a hybrid visualization scheme to determine the stability of an EA with regards to changes of its control parameters. In this method, the EA stability is measured according to two perturbation metrics, and will result a different visual representation of local neighborhoods in parameter space for each metric. However, the visualization using this method is limited to parameter space, and objective space is not considered.

Kramer and Luckehe (Kramer and Lückehe, 2015) presented a visualization approach for contínues evolutionary runs, using isometric mapping (ISOMAP) for mapping high-dimensional individuals to a two-dimensional representation. By performing some experiments, they claimed that ISOMAP results equally or better locally linear embedding than

Principal Component Analysis (PCA) in maintaining neighborhoods of high-dimensional individuals.

A tool called *ELICIT* was developed by Cruz and Machado (Cruz et al., 2015) to enable the visual exploration of evolutionary computation algorithms. Two levels of view is provided by ELICIT, namely *General View* to cover the whole population, and *Individual View* to cover a particular individual. For an individual, both genotype and phenotype can be visualized. However, this tool lacks in providing enough statistical information beside the visualizations.

In a recent effort, He and Yen (He and Yen, 2016) proposed a new method to visualize the population of Many-Objective Evolutionary Algorithms (MaOEAs) in high-dimensional objective space. They claimed that their proposed method maps individuals from a high-dimensional objective space into a 2D polar coordinate graph while preserving Pareto dominance relationship, retaining shape and location of the Pareto front, and maintaining distribution of individuals. Although effective in visualizing the high-dimensional objective space, this tool only provides a single view into the EA population which might not be sufficient for gaining a comprehensive insight.

A screenshot from each of the reviewed works is presented in Fig. 1. Although all these works have their own strengths and weaknesses which some are already mentioned, each of them has at least one of the following limitations:

- Poor level of user-interactivity.
- Expert knowledge required on the context in order to digest the visualization result, which makes it unsuitable for users with less knowledge in evolutionary computation.

In contrast, by taking into consideration the above limitations, the tool proposed in this paper provides the user with a high level of interactivity in a 3-D environment to move inside and in between views with different levels of granularity. However, it is noteworthy that the 3-D environment is merely used to organize the information space, and the third dimension itself contains no information.

3 VISUALIZATION APPROACH

3.1 Overview

The data produced by the evolutionary process of GA including all the individuals genotypes and their objective values will be given to the visualizer as input. The process pipeline includes a clustering algorithm to perform a (global) clustering across all generations of a GA run based on the distribution (similarity) of individuals in parameter space. Then, clusters will pass through a symbol mapping process, to be described in subsections to follow. Finally, all the clusters and their mapped symbols will be passed to an interactive visualization interface. Since the information to be visualized is over multiple generations, clusters and sub-clusters, the visualization interface contains square-walls to ease the organization, partitioning and positioning of this information. Symbols to be used in the elaboration are listed below:

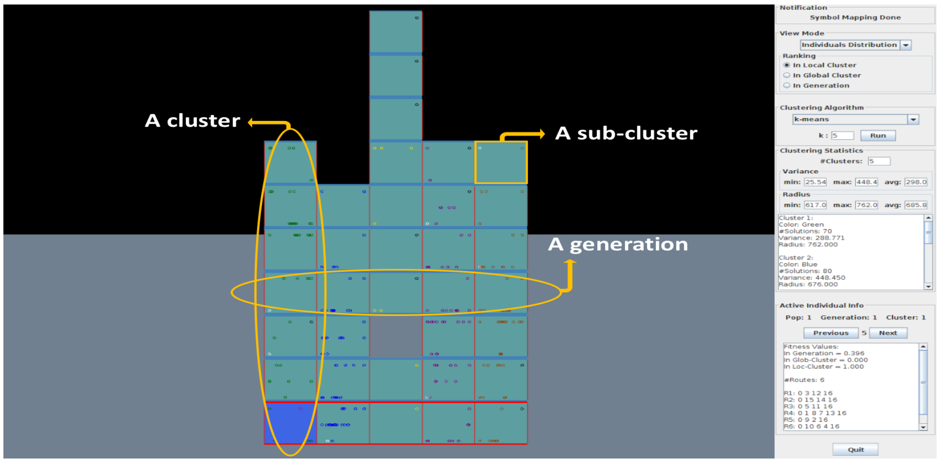
- N: total number of individuals in all generations of a GA run
- M: number of generations
- K: number of clusters
- $I = \{\, i_n \mid 1 < n <= N \,\}$ is the set of all individuals
- $C_k,\ 1 < k <= K, C_k \subseteq I$ is a cluster of individuals across all generations
- $C = \{C_1, C_2, C_3, ..., C_K\}$ is the set of all clusters
- $c_{km},\ 1 < k <= K,\ 1 < m <= M,\ c_{km} \subseteq C_k$ is a part of cluster C_k in generation m (sub-cluster)

Fig. 2 gives a bird's-eye view of the visualization interface where the whole population of N individuals are placed on a tower, with each column representing a cluster, each row representing a generation and each square-wall representing a sub-cluster.

There is a control panel at right side of the interface (Fig. 2), which not only provides some statistics of clustering and information about the individuals, but also enables the user to choose between three options from different families of clustering algorithms, set their associated parameters and re-run the clustering (i.e. restart the whole process pipeline). The options for clustering algorithm are as follows:

- Centroid-based: k-means
- Density-based: DBSCAN
- Connectivity-based: Hierarchical agglomerative

The user is able to move the camera in six directions to have a look from an arbitrary angle. Moreover, different walls, floors and towers (multiple towers in case of multi-population visualization) can be chosen by a mouse click to get the related statistics in the control panel. As shown in Fig. 2, the wall on down-left corner of the tower is currently being activated. In fact, blue color indicates the active wall (sub-cluster) and red border indicates the active floor (generation). The "Next" and "Previous" buttons in the control panel can be used to navigate through individuals of the active wall to see their gene values,



Notification
Symbol Mapping Done

View Mode
Individuals Distribution
Ranking
● In Local Cluster
○ In Global Cluster
○ In Generation

Clustering Algorithm
k-means
k : 5 Run

Clustering Statistics
#Clusters: 5
Variance
min: 25.54 max: 448.4 avg: 298.0
Radius
min: 617.0 max: 762.0 avg: 685.8

```
Cluster 1:
Color: Green
#Solutions: 70
Variance: 288.771
Radius: 762.000

Cluster 2:
Color: Blue
#Solutions: 80
Variance: 448.450
Radius: 676.000
```

Active Individual Info
Pop: 1 Generation: 1 Cluster: 1
Previous 5 Next

```
Fitness Values:
In Generation = 0.396
In Glob-Cluster = 0.000
In Loc-Cluster = 1.000

#Routes: 6

R1: 0 3 12 16
R2: 0 15 14 16
R3: 0 5 11 16
R4: 0 1 8 7 13 16
R5: 0 9 2 16
R6: 0 10 6 4 16
```

Quit

Figure 2: A bird's-eye view of the visualization interface.

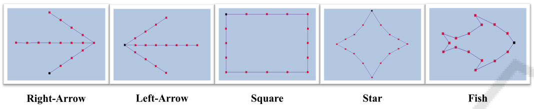


Figure 3: An example set of reference shapes with 16 vertices in their graph structures.

scaled aggregate fitness values and objective scores. The active individual is always presented by a red color. To gain a rich insight, the visualization interface provides three levels of view into the GA population which are described in the following.

3.2 Symbol-view

This is a high-level view in which a unique visual symbol is assigned to each cluster. Then, a representative individual from each sub-cluster is mapped to the symbol of the cluster it belongs to, so that shape transformation of the symbol in each generation depicts the evolution of the representative individual. Fig. 3 shows a set of five shapes drawn by our simple shape-drawer program to be used as symbols. Each of these shapes will be used as symbol of a particular cluster. Two methods of symbol mapping are presented here. First, is Isomorphic Graph-Mapping which is a genotypic-based method and is mainly useful in case of combinatorial problems. Second, is Polygon-Morphing which is a fitness-based method and can be used for any kind of problem given to GA.

3.2.1 Isomorphic Graph-mapping

Let G={V, E} and G′ = {V′, E′} be graphs. G and G′ are said to be isomorphic (G ≅ G′) if there is a bijection φ = V → V′ which preserves adjacency and nonadjacency (with $xy \in E \Leftrightarrow \varphi(x)\varphi(y) \in E'$ for all $x, y \in V$) (Diestel, 2000). Such a mapping φ is called an isomorphism. Although two isomorphic graphs might have different shapes, their structures are exactly the same.

Algorithm 1 describes the assignment of a symbol to each cluster, using Isomorphic Graph-Mapping. In step 4 of the algorithm, we are facing with an optimization problem to find the best mapping from the graph produced by the representative individual (e.g. in the case of Vehicle Routing Problem (VRP), the graph includes customer nodes as its vertices and vehicle routes as its edges) to the graph of its corresponding symbol. A genetic algorithm is used here to handle the optimization problem. The GA being used tries to find the best mapping from the vertex-set of the representative individual to the vertex-set of its symbol. In order to measure the quality of mappings found by the GA chromosomes, Hausdorff distance is being used in the fitness function. This distance measures the extent to which each point of a model set lies near some point of another set and vice versa (Huttenlocher et al., 1993). The Hausdorff distance is presented as the function in Algorithm 2.

After assigning a symbol to each cluster (step 2 to 5 of Algorithm 1), each sub-cluster is taken to map its representative to the symbol of the cluster it belongs to, based on the mapping found in step 4.

3.2.2 Polygon-morphing

This method uses fitness values to assign symbols, hence it is neither dependent on the type of problem nor the representation of individuals. Basically, it generates a range of morphed shapes for each symbol. The process begins by generating a random mapping of vertex-list for the original symbol to get an ugly instance of it. Then, the generated shape will be mor-

Algorithm 1: Assigning symbols based on Isomorphic Graph-Mapping.

```
procedure ASSIGN_ISO_SYMBOLS($C, shapes$)
    for $k \leftarrow 1$ to $K$ do
        $ClRepIndv \leftarrow get\_rep\_indiv(C_k)$
        $\varphi_k \leftarrow best\_mapping(ClRepIndv, shapes_k)$

    end for
    for $m \leftarrow 1$ to $M$ do
        for $k \leftarrow 1$ to $K$ do
            $SubClRepIndv \leftarrow get\_rep\_indv(c_{km})$
            $map(SubClRepIndv,\ shapes_k,\ \varphi_k)$
        end for
    end for
end procedure
```

Algorithm 2: Finding Hausdorff distance between two graphs G and G'.

```
function HAUSDORFF_DIST($G, G'$)
    $hausDist \leftarrow 0$
    for each vertex ($v\ in\ G\ and\ \varphi(v)\ in\ G'$) do
        $longestDist \leftarrow 0$
        for each neighbor $n\ of\ v\ in\ G$ do
            $shortestDist \leftarrow +\infty$
            for each neighbor $n'\ of\ \varphi(v)\ in\ G'$ do
                $d \leftarrow euclidean\_Dist(n, n')$
                if $d < shortestDist$ then
                    $shortestDist \leftarrow d$
                end if
            end for
            if $shortestDist > longestDist$ then
                $longestDist \leftarrow shortestDist$
            end if
        end for
        $hausDist \leftarrow hausDist + longestDist$
    end for
    return $hausDist$
end function
```

phed towards the original shape in multiple steps. The number of steps depends on defined length of the morphing range by the user. Obviously, longer length of the range results in a more accurate mapping while needing more computational time and resources. Again by using Hausdorff distance, each morphed shape will be compared to its original shape and given a similarity score. Finally, representatives of each sub-cluster will be associated with one of the morphed shapes based on the closeness of their aggregate fitness values to the similarity score of the morphed shapes.

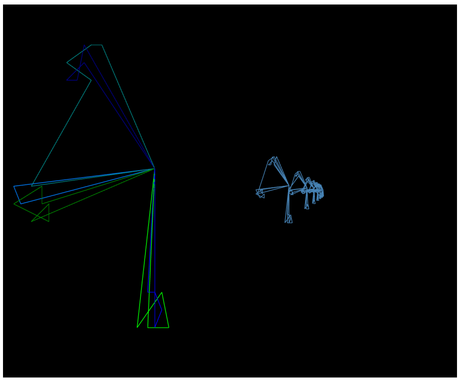


Figure 4: Phenotype-View.

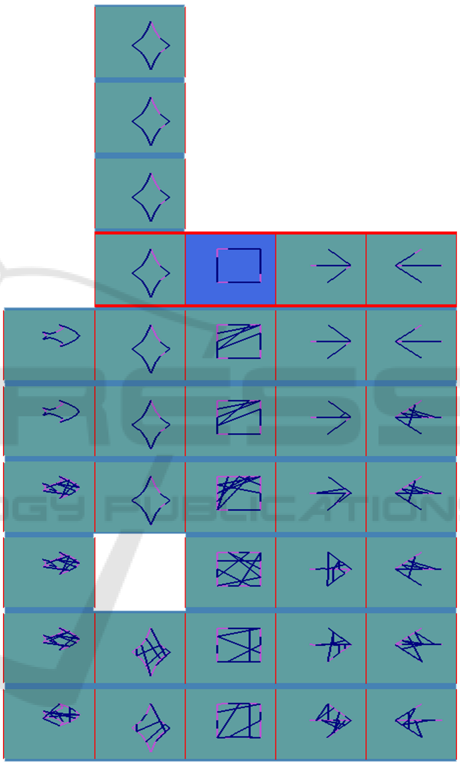


Figure 5: Result of Isomorphic Graph-Mapping.

3.3 Individual-distribution View

This is a middle-level view which shows the distribution of individuals in clusters by placing circles (as individuals) on a square-wall. While a unique color (for the circles) is assigned to each cluster, the positioning of individuals on 2-D walls is based on their scaled objective scores. The control panel enables the user to choose between three options of individual ranking that results different positioning on the walls: in sub-cluster, in cluster, and in generation.

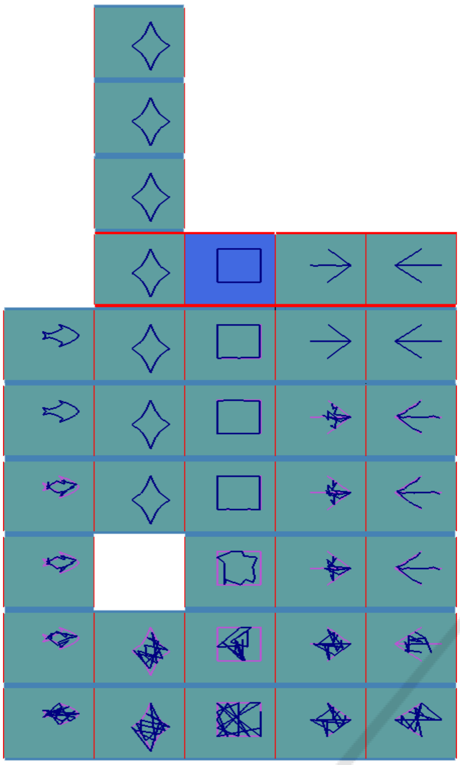


Figure 6: Result of Polygon-Morphing.

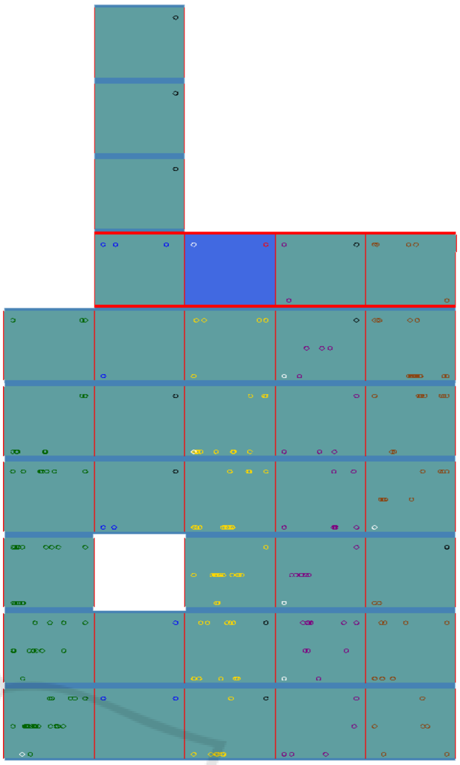


Figure 7: Result of Individual-Distribution View.

3.4 Phenotype-view

The lowest-level view of the visualizer provides phenotype of the individuals in a sub-cluster chosen by the user (Fig. 4). The individuals are sorted from highest to lowest aggregate fitness in a row. The camera is placed on the 45-degree angle from the individuals to provide a more dominant view of the whole row, so the user is able to compare the most-front individual with some of those behind in one look. Nevertheless, the active individual is always highlighted by a different color. In addition, the control panel includes a checkbox which enables the user to link the camera to the active individual, so each time the user switch to another individual, camera will automatically be placed at a close position to the active individual.

4 EXAMPLE ANALYSIS

A test application of the proposed approach is performed in the following context: We applied Non-dominated Sorting Genetic Algorithm II (NSGA-II) (Deb et al., 2002) to an instance of VRP. The VRP instance being used is a smaller version (15 customer nodes) of C101 instance from Solomon's benchmarks. The maximum number of generations for GA was set to 10 (which proved to be enough for a good convergence as C101 has a clustered structure) with 50 individuals per generations.

Fig. 5 shows the result when Isomorphic Graph-Mapping is chosen to map the symbols. In the first few generations down there, all the symbols are seen to be messy that is a proper representation of the weak individuals. By each generational step, symbols tend to be more similar to the perfect shape. For instance, the left-most cluster with a fish as its symbol lasts until sixth generation and it had no improvement from fifth to sixth generation, because its symbols at these generations are identical. However, second cluster with a star symbol, despite of being absent in generation 3, lasts up to the end of evolutionary process which obviously represents the place in fitness landscape where GA is converged in. The reason that second cluster with a star symbol disappears in generation 3 is due to the fact that none of its individuals belongs to this generation. In other words, GA left this cluster in generation 3 and went back to it in generation 4 onward. Same goes to empty sub-clusters in Fig. 2, Fig. 6 and Fig. 7.

Fig. 6 illustrates the results for the Polygon-Morphing method of mapping symbols. Unlike the previous method which takes care of similarity in

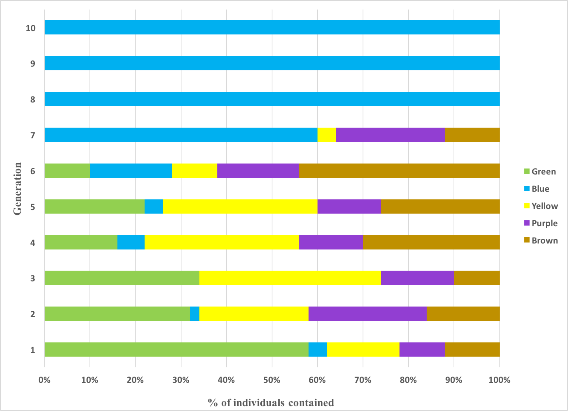


Figure 8: Number of individuals in different clusters during each generation.

parameter space, Polygon-Morphing visualizes the changes in objective space. As an example, the square-symbol cluster on the middle of tower experienced two jumps in its fitness from first generation to third, but form generation 4 onwards, the changes are little.

Moving one level deeper, the Individual-Distribution View is experimented with. One of the useful insights given by this view is the diversity level of the population. In Fig. 7, individuals are placed on the walls based on their scaled objective scores in sub-cluster for total traveled distance (horizontal axes, left to right) and number of routes (vertical axes, down to up). Further, at each floor, the best and worst individuals in generation are presented with black and white color respectively. When comparing blue cluster with yellow, it can be seen that yellow is much more diverse while blue is the one which contains the best-in-generation individual for half of the generations. Fig. 8 illustrates how GA converges in the blue cluster. By referring to statistics given by our visualization tool, we see that the variance of the blue cluster is almost 28, which is the minimum among all, together with the chart in Fig. 8, one can conclude that GA tries to gradually find and climb the global optima (i.e. the blue cluster) in the fitness landscape while at the same time tests different places (i.e. other clusters that might be around local optima). In other words, by having a holistic look at the tower, it is clear that GA tends to globally explore the fitness landscape by hanging around different optima and trying to evolve them using its local searches. Also, it shows that at each generational step, depending on competitiveness of the local optima compared to others, GA might clone more individuals around it or conversely, take out (some) individuals from there.

Last but not least, lowest-level view of the visualizer is presented in Fig. 4, which provides a close look at the individual's phenotype. As can be seen, the active individual is presented with a different color, which in the case of VRP, each route has a unique color. By traversing the individuals in the row, it can be seen that fitter individuals are less colorful due to their superiority in the number of routes objective.

5 COMPARISON WITH OTHER TOOLS

This section presents a comparison between the features offered by our proposed tool and the tools previously discussed in section 2. The choice of the characteristics for this comparison was based on three main factors: the ability to visualize the evolutionary process and individuals from various perspectives, the suitability for users with different levels of expertise, and the level of user-interactivity. This comparison is shown in Table 1. As we can observe, the ability of visualizing cluster formations in GA evolutionary process is offered by none of the tools except our proposed tool. Moreover, all other features provided by the existent tools are also offered by our tool with the exception of the feature to visualize many-objective problems. This feature is planned to be integrated into the current tool in the near future.

6 CONCLUSION AND FUTURE WORK

A clustering-based visualization tool for GA has been presented in this paper. The tool has the potential of providing useful information on the dynamics of cluster formations in GA. Since cluster formations correspond to local searches performed by the GA, it can provide insight on how effectively the GA is behaving in its search effort. The proposed tool particularly enables us to analyze the behavior of GA operators and parameters, and also obtain useful information that can be used later to interactively manipulate the search space.

More work of course remains to be done to enhance the usefulness or usability of the tool and its underlying paradigm. In the near term, we intend to investigate the following:

- Full analysis of the clusters found by different clustering algorithms.
- Using different distance measures for clustering to possibly get different insights into the fitness landscape.

Table 1: A comparison between the features provided by the existent tools and our proposed tool.

Name of the Tool/Author	Cluster Formations Vis.	Many-Objective Vis.	Parameter Space Vis.	Objective Space Vis.	Phenotype Vis.	Providing Statistics	User Interaction	Multi-Level Views
Our proposed tool	x		x	x	x	x	x	x
He and Yen		x	x	x				
ELICIT			x	x	x		x	x
Kramer and Luckehe		x	x	x				x
Craven and Jimbo			x					x
Kudo and Yoshikawa		x	x	x				
FOM				x		x		
GAVEL			x	x		x	x	x
VIS			x			x	x	x
Collins		x	x	x			x	

- Incorporating dimensionality reduction techniques into the visualizer to handle the case of problems with many objectives.

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