Niching Techniques: a Study on the Cluster Geometry Optimization Problem

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1. INTRODUCTION
Niching techniques are commonly used in Evolutionary Computation to maintain population diversity and help to explore more efficiently the solutions space. Classic techniques rely on similarity functions to measure the distance between individuals. However, in some optimization problems, the definition of a distance measure between individuals is a serious difficulty.

The cluster geometry optimization is one of these problems. The same cluster structure can be encoded in innumerable ways. A single translation or rotation performed in the cluster can lead to different genotypes for similar structures. A reliable similarity function can be computationally prohibitive or even impossible to define. We analyze the behavior of an alternative technique free of distance measures, the Spatially-Dispersed Genetic Algorithm [1] (sdGA), and its application on the cluster geometry optimization.

2. DESCRIPTION
The energy of Morse clusters, is represented by the *N*-particle pair-wise additive potential defined as

$$V_{Morse} = \varepsilon \sum_{i}^{N-1} \sum_{j>i}^{N} \left[e^{-2\beta(r_{ij} - r_0)} - 2e^{-\beta(r_{ij} - r_0)} \right] \quad (1)$$

where the variable r_{ij} is the Cartesian distance between atoms i and j in the cluster structure. The bond dissociation energy ε, the equilibrium bond length r_o and the range exponent of the potential β are parameters defined for each individual pair-wise Morse interaction. The adopted evolutionary approach, and its main components, is described in [3]. To create and maintain niches, this algorithm was enhanced with the sdGA methods. The sdGA functioning is based on the random distribution of the individuals on a Euclidean space in two specified dimensions. Then, during the evolution cycle, a specified visibility radius for the whole population is used to determine which group of individuals can be selected to mate a first chosen individual. In both selection stages tourney selection is used. Finally, each new individual is placed in a random point on the visibility radius of a randomly selected parent. The mutation operator can also be responsible for slight changes on individuals position. More details can be found in [2].

3. RESULTS
Figure 1 shows the final distribution of the individuals, after the algorithm execution with three different configurations, for the most influent analyzed parameter.

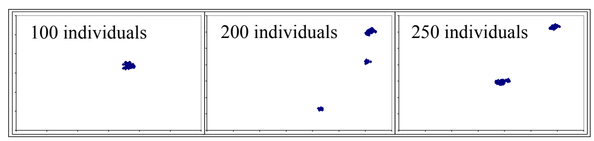

Figure 1

Population size seems to have a great influence in the niching process, although varying other parameters – like tourney sizes, mutation rate or visibility radius – also figured out to have some impact on creating and maintaining niches throughout the algorithm execution. The complete parameter analysis can be found in [2].

The results achieved show that the sdGA architecture is not only capable of creating niches, but also to guide the search into different local optima. It also seems that the sdGA can be used without losing quality on the optimization. More details about this results and its statistical analysis can be found in [2].

4. ACKNOWLEDGMENT
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