AGH

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MASTER OF SCIENCE THESIS

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IMPROVING POPULATION-BASED ALGORITHMS USED IN GLOBAL OPTIMIZATION WITH FITNESS DETERIORATION TECHNIQUES

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Contents

1. Introduction

> It is impossible for any optimization algorithm to outperform random walks on all possible problems.
>
> ... a conclusion from No Free Lunch Theorem

1.1. A statement of a problem

A Global Optimization Algorithm is defined as optimization algorithm that employs measures that prevent convergence to local optima and increase the probability of finding a global optimum.

Evolutionary algorithms are known as a generic population-based metaheuristics which often perform well approximating solutions to all types of problems because they ideally do not make any assumption about the underlying fitness landscape; this generality is shown to be a great successes in many real-life problems. Evolutionary algorithms have the tendency to lose diversity within their population of feasible solutions and to converge into a single solution. However, there are domains where the global solution may not suffice. Such problems require the location and maintenance of multiple robust local solutions, i.e local solutions whose basins of attraction areproperly wide and deep.

The most common technique in evolutionary algorithm which is used to achieve this goal is to incorporate some sort of niching method like crowding or fitness sharing which promote diversity of population, which in turn delay premature convergence and likely enable the algorithm to find multiple optimal solutions in single population.

Standard niching methods are often inefective and hard to introduce in existing evolutionary algorithms. In this paper we adopt a different approach to multimodal function optimization. Instead of embedding a niching method in the evolutionary algorithm itself we use a hybrid approach in which we perform several runs of a evolutionary algorithm and alter the fitness function in every subsequent run in a way that prevents exploration of basins of attraction which were found in previous runs of the algorithm.

In each iteration we run EA, then cluster received population and based on the assumption that clusters of individuals obtained from the clustering algorithm are located in basins of attraction we interpolate each basin by multidimensional Gaussian function. By combining these functions with current objective function in a proper way we create deteriorated fitness function which will discourages future runs from revisiting the same area.

This work tries to find an effective fitness deterioration technique in high-dimensional domain spaces. We have implemented a general-purpose framework which can be used to test our fitness deterioration techniques in conjunction with various evolutionary algorithms. While our algorithm may be used with many types of EAs it would be the most efficient when used with algorithms which are capable of finding many local solutions in single run. This is why for tests we choose so called Hierarchical Genetic Strategy which performs efficient concurrent search in the optimization landscape by many small populations.

The quality of the deterioration process strongly depends on clustering results. We choose density-based algorithm called OPTICS as with this method we can extract clusters of different densities very efficiently and choose clusters which give the best accuracy of fitness deterioration process.

1.2. Related Work

As mentioned before this work focus on finding solutions for multi-modal optimization tasks. There are many publications which decsribes how to extend EAs to multi-modal optimization. Most of them focuses on *Niching methods* [8, 9, 10] which address this issue by maintaining a population of diverse solutions througout the time and this way they allow parallel convergence into multiple good solutions in multimodal domains.

Our solution works by iterating a simple GA and maintaining the best solution of each run off-line, by detection of basins of attraction and degeneration of fitness landscape. We may consider our algorihtm as a variant of *Sequential niching* approach (throughout this paper we use terms *Sequential niching* and *Fitness deterioration* interchangeably).

At this point it is worth mentioning some of the works of Prof. A. Obuchowicz especially the publication [3] which is the only one I found which use the term *fitness deterioration* explicitly. In [3] he describes ESSS-DOF algorithm (Evolutionary Search with Soft Selection with Deterioration of Objective Function) as an extension to the ESSS method which maintaing population diversity by the following schema:

> When the population converges to local optimum we degenerate the objective function which cause the rapid migration of individuals and enable the population to escape for the local optimum.

The algorithm degenerate the objective function by composing it with Gaussian function which approximate the local optimum. Our deterioration algorithm described in detail in chapter 4 uses Gaussian functions as well (Gaussian function has got many useful properties which makes it well-suited to the fitness deterioration. We describe these characteristics in chapter 4).

Mentined methods are incorporated directly into the basic cycle of evolutionary algorithm which differs from our *Sequential niching* technique. The sequential niching approach has several advantages:

– it is simple to incorporate in existing optimization methods

– it efficiently finds many local solutions

– it provides reasonable stop criterion which in this case is based on the quality of clusters returned by the clustering algorithm

2. Algorithm

2.1. A Hybrid Approach

TODO: algorithm description, pseudo-code description of the remaining chapters

2.2. Pseudocode

while $i < getIterationCount()$ **do**
  $execute(evolutionaryAlgorithm)$
  $population = getPopulation(evolutionaryAlgorithm)$
  $clusters = cluster(population)$
  $detFitness = performCrunching(clusters, currentFitness)$
  if $detFitness = null$ **then**
    $break$
  end if
  $saveClusters(clusters)$
  $updateFitness(detFitness)$
end while
$execute(evolutionaryAlgorithm)$
$extractBestClusters()$

3. Clustering

TODO: cluster extension, set detection (specyfying set of individuals using small set of parameters, e.g center and radius), we make an assumption that clusters are good apprximation of basins of attraction, clustering metrics, clustering as an effective stop criterion (definition of the stop criterion, problems)

Clustering is used as a stand-alone tool to get insight into the distribution of a data set or as a preprocessing step for other algorithms operating on the detected clusters. The latter usecase is used in our deterioration schema.

We have choosen density-base clustering algorihtm called *OPTICS: Ordering Points To Identify the Clustering Structure* [2]. In density clustering clusters are regarded as regions in the data space in which the objects are dense and which are separated by regions of low object density. These regions may have an arbitrary shape and the points inside a region may be arbitrarily distributed.

3.1. Cluster Extension

3.2. Clustering as a Stop Criterion

3.3. OPTICS

TODO: general description, optics ordering, extracting clusters, random samples, clustering, diagrams, reachability plots, why optics is good for further deterioration (describe in the next chapter)

OPTICS is an extendsion to a well-known density clustering algorithm called *DBSCAN*. The basic idea for *DBSCAN* is that for each point of a cluster the neighborhood of a given radius ϵ has to contain at least a minimum number of points $minPts$.

OPTICS works like dbscan but for an infinite number of distance paramters ϵ_i which are smaller than a *generating distance* ϵ. The only difference is that we do not assing cluster memberships. Instead, we store the **order** in which the objects are processed (the main priniple is that we always have to select an object which is density-reachable with respect to the lowest ϵ value to guarantee that clusters with higher density are finished first) and the information which would be used by *DBSCAN* algorithm to assing cluster memberships. This information consists of only two values for each object:

– core-distance - the core-distance of an object p is simply the smallest distance ϵ' between p and an object in its ϵ-neighborhood such that p would be a core object with respect to ϵ' if this neighbor is contained in $N_\epsilon(p)$. Otherwise, the core-distance is *UNDEFINED*

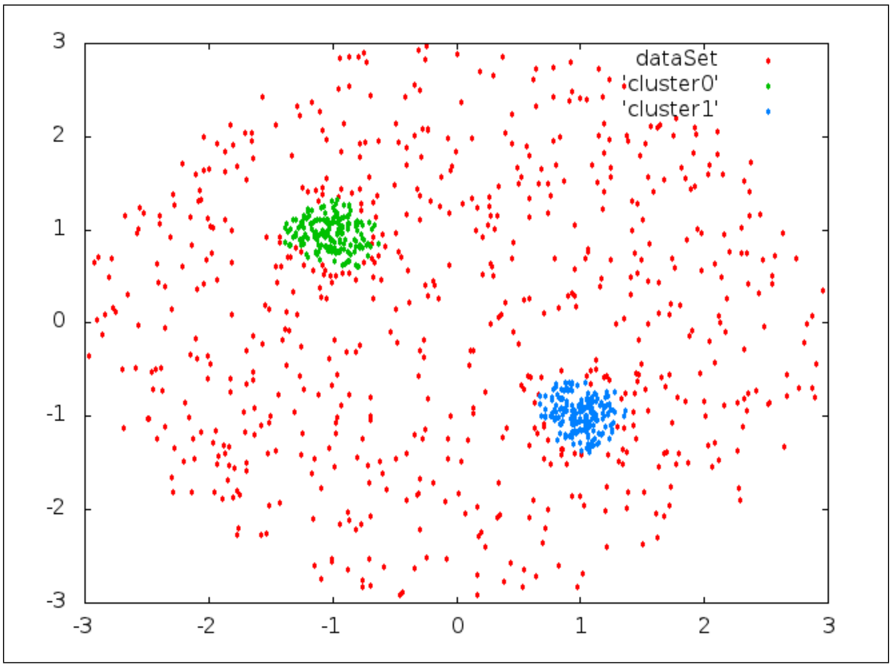

Figure 3.1: Visualization of the DBSCAN algorithm applied to Optics ordering of simple 2-dimensional data set which consists of 1000 points. Optics paramters: $minPts = 20, \epsilon = 1.2$, DBSCAN paramters: $\epsilon' = 0.1$

– reachability-distance - the reachability-distance of an object p with respect to another object o is the smallest distance such that p is directly density-reachable from o if o is a core object

This information is sufficient to extract all density-based clusterings with respect to any distance ϵ' which is smaller that the generating distance ϵ

An advantage of cluster-ordering a data set compared to other clustering methods is that the ordering which might be visualized by *reachability-plot* of ordered points is rather insensitive to the input parameters of the method i.e. the *generating distance* ϵ and the value for $minPts$. Roughly speaking, the values have just to be *large* enough to yield a good result. The concrete values are not crucial because there is a broad range of possible values for which we always can see the clustering structure of a data set when looking at the corresponding *reachability-plot*. Figure 3.1 shows the result of *OPTICS* clustering for a sample set of points. Figure 3.2 shows reachablity plot for various *generating distances* - ϵ.

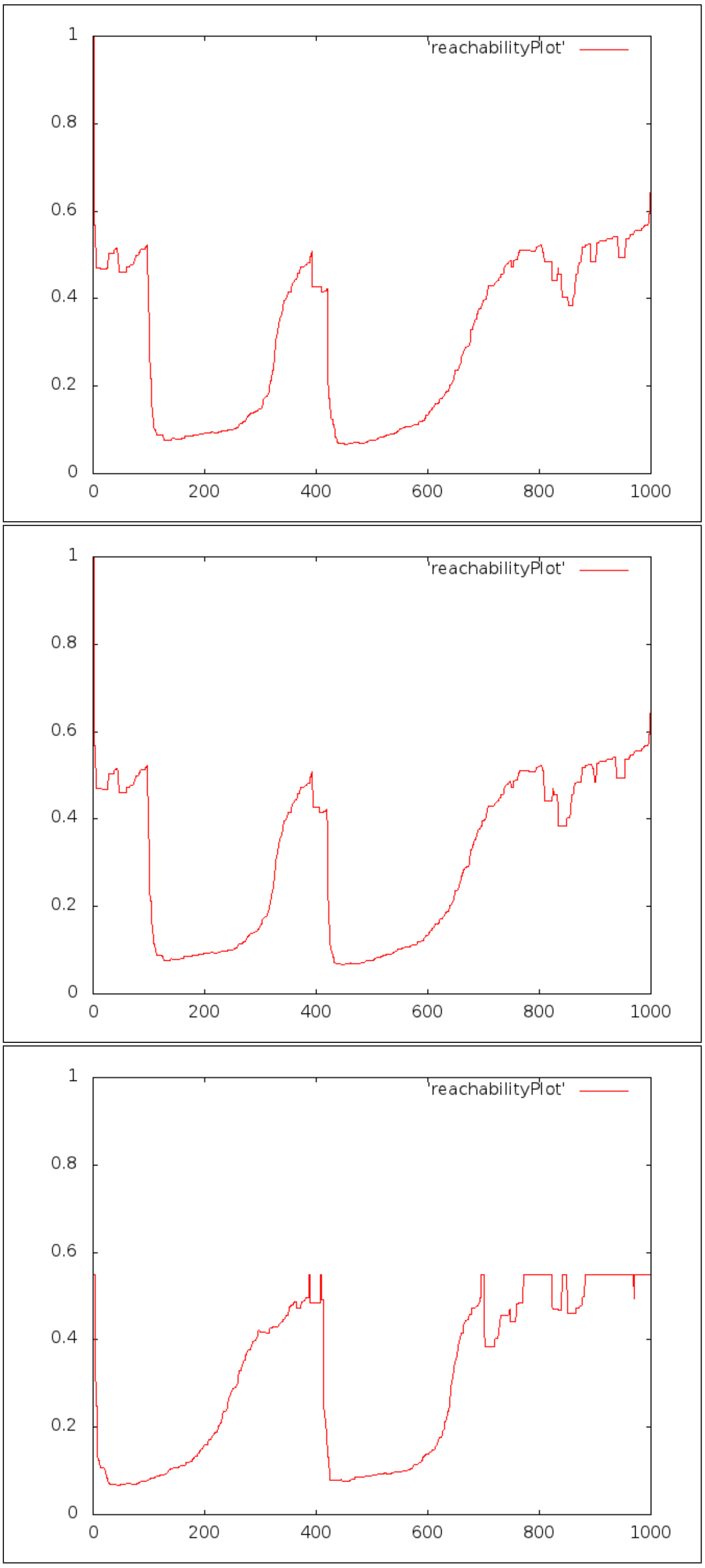

Figure 3.2: Reachability plot for data set presented on figure 3.1. Optics paramters (minPts, ϵ) are: (20, 1.5), (20, 1.0), (20, 0.5) respectively. The two cavities which are visible in each plot depict the two of the clusters on figure 3.1. This proves that there is a large range of values for ϵ for which the appearance of the reachability plot will not change significantly.

4. Fitness Deterioration

TODO: description of the deterioration process, not very computationally intensive, easy to improve in subsequent runs, interpolation accuracy is not crucial, what is most important is to minimize the probability of finding the basins of attraction which was previously explored, use knowledge from clusteres;

4.1. Sequential niching

TODO: basic description of deterioration: when used, what approach, connection with clustering algorithms, advantages of OPTICS algorithm (improving deterioration by extracting clusters wiht different densities, cheapness)

4.1.1. Crunching functions

When degenerating a single basin of attraction represented by a cluster of individuals, we are looking for function with the following properties (TODO: why):

1. cheap (in multi-dimensional spaces)
2. easily adjustable to the shape of the basin of attraction
3. has low impact on the areas of fitness landscape which are distant from the cluster so that we do not introduce unnecesary noise to the fitness landscape in further iterations
4. symmetric

A class of functions which which are suitable for deterioration are so called *(*kernel functions) [16]. Examples of kernels are:

– Triangular $K(u) = (1 - |u|)\,\mathbf{1}_{\{|u| \leq 1\}}$

– Epanechnikov $K(u) = \frac{3}{4}(1 - u^2)\,\mathbf{1}_{\{|u| \leq 1\}}$

– Quartic $K(u) = \frac{15}{16}(1 - u^2)^2\,\mathbf{1}_{\{|u| \leq 1\}}$

– Gaussian $K(u) = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}$

From mentioned function only Gaussian kernel meets all requirements (remaining kernels are defined on some finite intervale, which makes them computationally inefficient in high-dimensional spaces).

4.2. Basic Scheme

The basic version of our fitness crunching algorithm is as follows:
For each cluster generate one or more multi-dimensional Gaussian function:

$$g(x) = -F_k(x_{max})exp(\frac{-1}{2}(x-\mu)'\Sigma^{-1}(x-\mu)) \tag{4.1}$$

where F_k is a fitness function in kth iteration of the algorithm, Σ is an unbiased sample covariance matrix [15] estimated from the cluster population:

$$\Sigma = \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\mu)(x_i-\mu)^T \tag{4.2}$$

Fitness function in $k+1$th iteration is of the form:

$$F_{k+1} = F_k + \sum_{i=1}^{M} g_i \tag{4.3}$$

where M is the number of generated Gaussian functions.

Because of the fast convergence of the HGS subpopulation to the local minimum, clusters sometimes becomes very dense in areas of local optimum and the Gaussian created for such cluster appears to be a high peak which forms a crater inside a basin of attraction (TODO: be more precise). To overcome this issue we developed so called *Covariance Matrix Adjustment(CMA)* algorithm described in section 4.4.

4.3. Adaptive Scheme

TODO: describe in detail
detailed description of adaptive scheme deterioration

4.4. Covariance Matrix Adjustment

We use sample covariance matrix as an estimator [15], which is extremely sensitive to outliers. However we may take this property as our advantage in CMD algorithm. TODO: describe

4.5. Results

Below figures shows the result of our sequential niching algorithm for two simple functions from $f : \mathbb{R}^2 \to \mathbb{R}$, specifically:

- $f(X) = 2e^{-(x^2+y^2)}$, where $X \in \mathbb{R}^2$
- $f(X) = e^{-(x^2+y^2)} + 1.4e^{-((x-1.7)^2+(y-1.7)^2)}$, where $X \in \mathbb{R}^2$

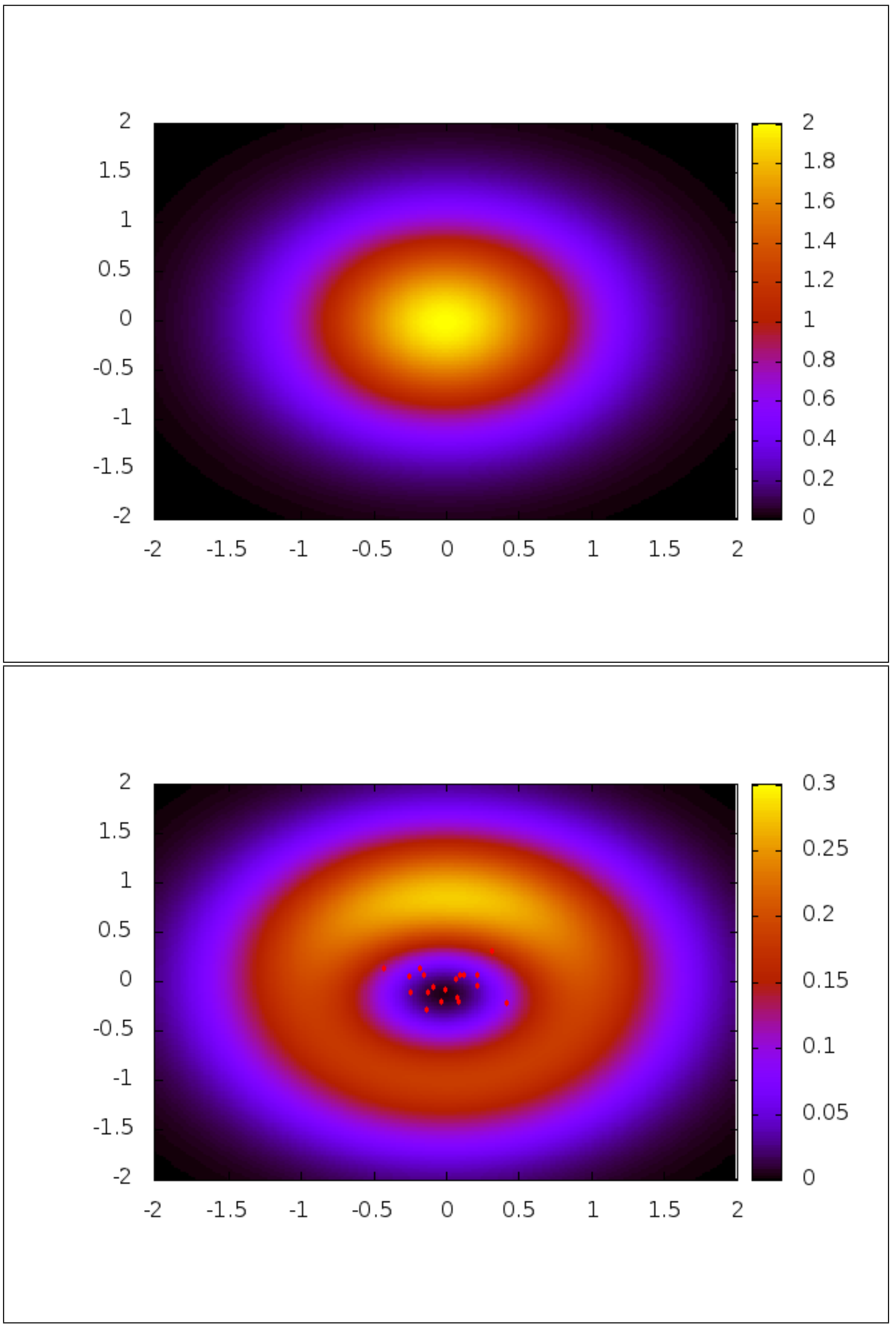

Figure 4.1: The result basic deterioration scheme with CMA applied to unimodal function: $f(X) = 2e^{-(x^2+y^2)}$. Optics paramters: $minPts = 20, \epsilon = 0.4$, algorithm: SGA, iterationCount=1

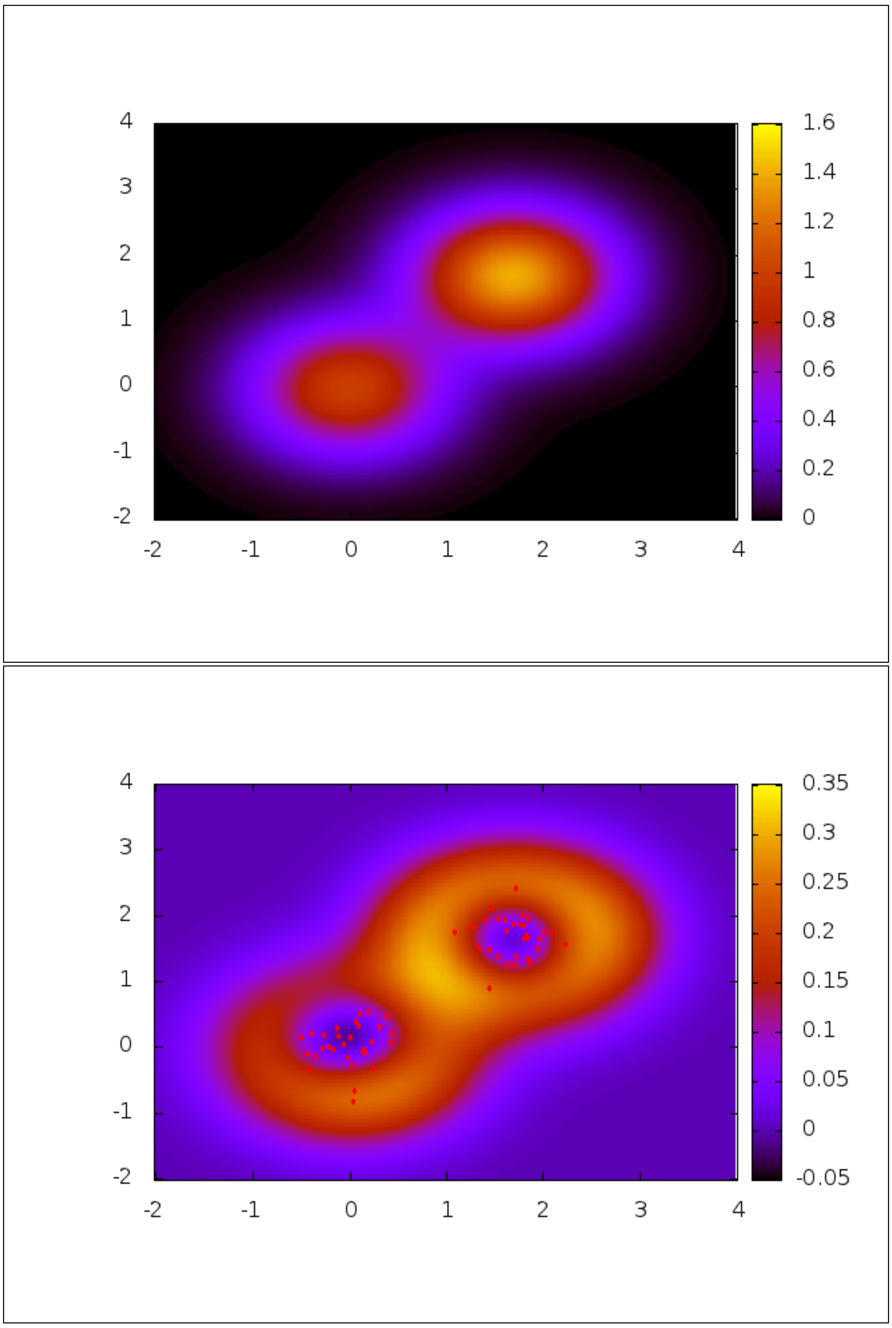

Figure 4.2: The result basic deterioration scheme with CMA applied to bimodal function: $f(X) = e^{-(x^2+y^2)} + 1.4e^{-((x-1.7)^2+(y-1.7)^2)}$. Optics paramters: $minPts = 20, \epsilon = 0.4$, algorithm: SGA, iterationCount=2

5. Tested Algorithms

5.1. HGS

why HGS is well suited to our algorithm (suitable for clustering, fast convergence in leaves)

5.2. Tests

5.2.1. Benchmark functions

uni, bi and multimodal functions

5.2.2. Accuracy measures

how many optimas have been found, diagrams

5.2.3. Efficiency measures

6. Implementation

6.1. Architecture

TODO: architecture details, sample of spring application context, description of a problem domain and fitness function

6.2. Implementation in Java

clean structure, good test coverage, modular architercture, extensible,

6.2.1. Technologies

– Spring [12] - application framework

– Maven [13] - project management and build automation

– Mockito [14] - testing framework

– JAMA [11] - linear algebra package

Spring, Maven, JUnit, Mockito, JAMA, TDD approach

6.2.2. Diagrams

class diagrams, sequence diagrams

Below you may find class diagrams for each of the module implemented in our framework. It shows a general overview of the structure of a system: used classes, their attributes, operations and the relationships between the classes.

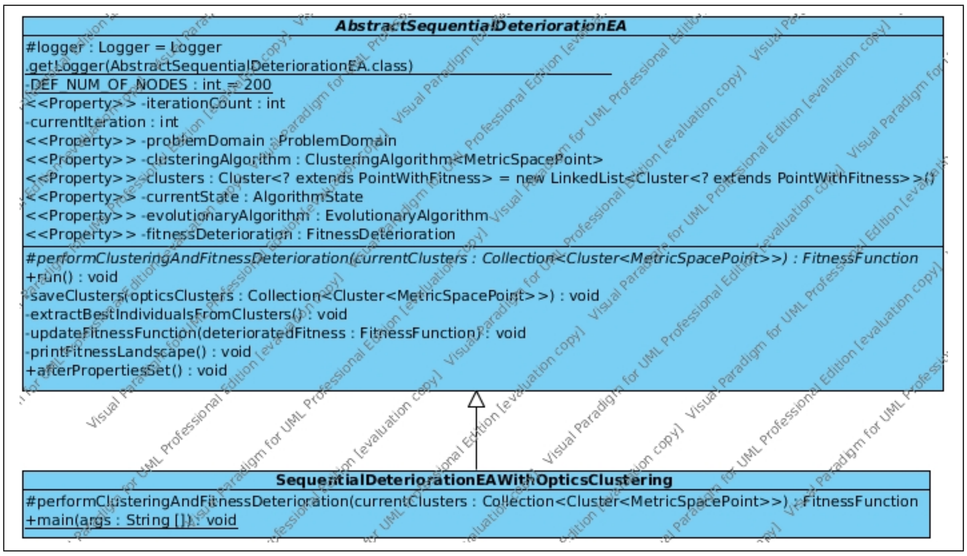

Figure 6.1: Main algorithm package

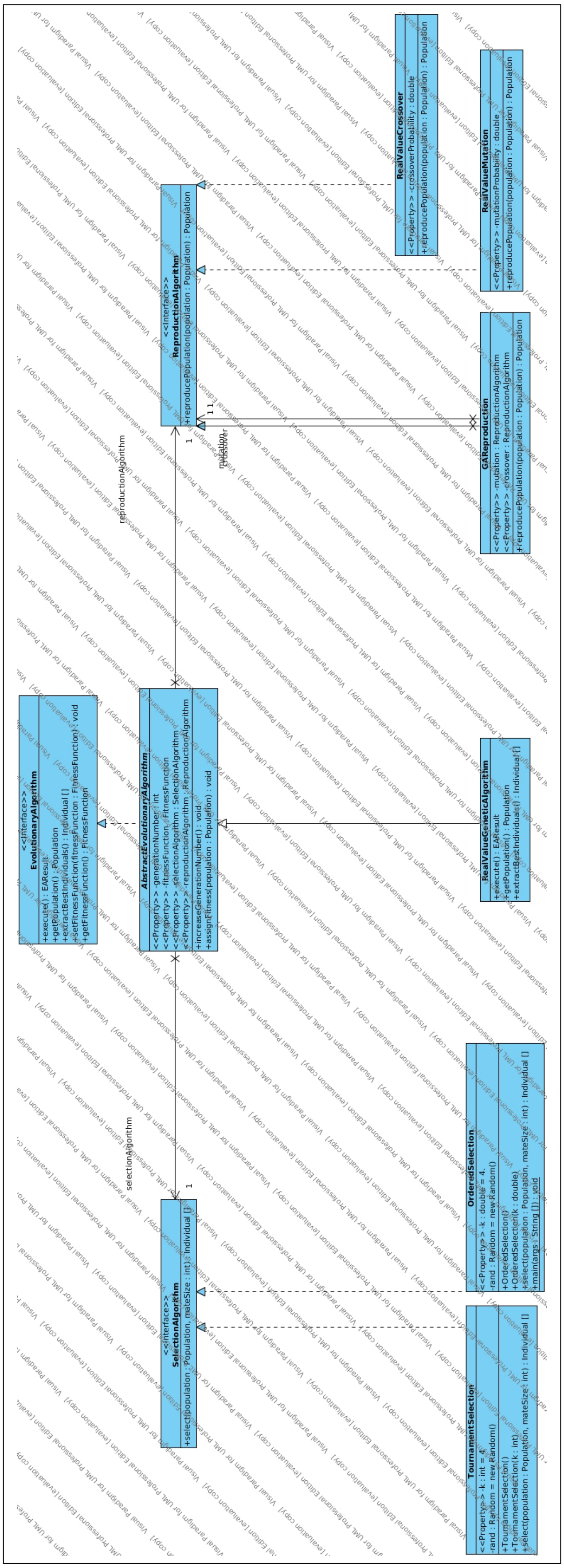

Figure 6.2: Evolutionary algorithms package

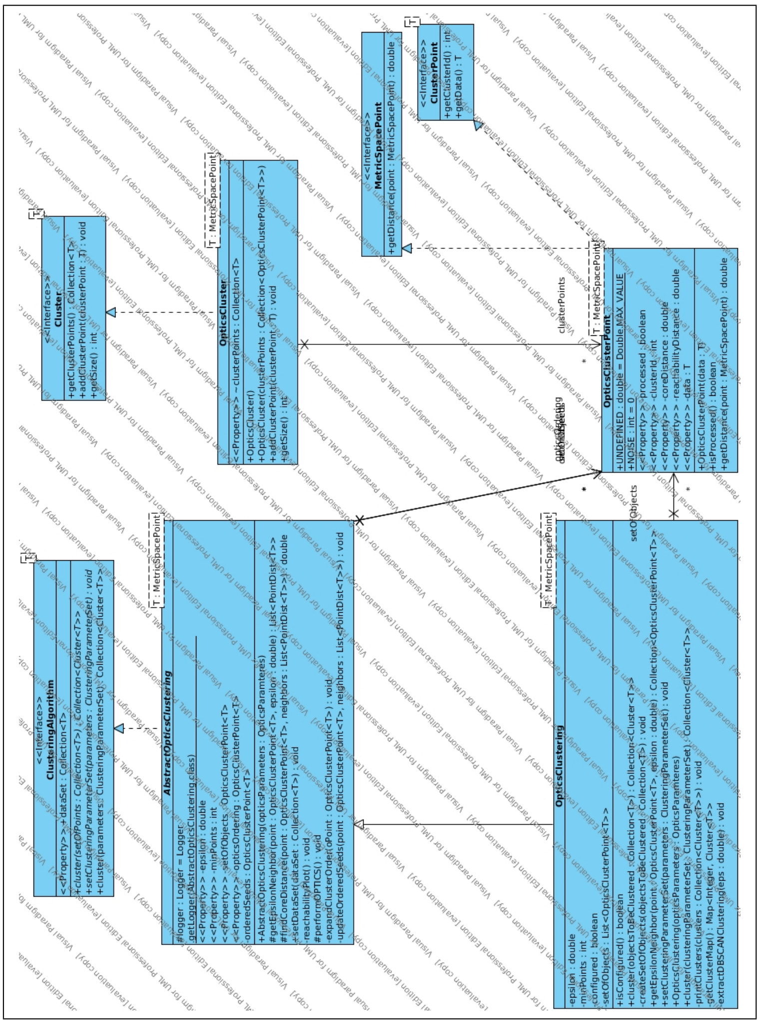

Figure 6.3: Clustering package

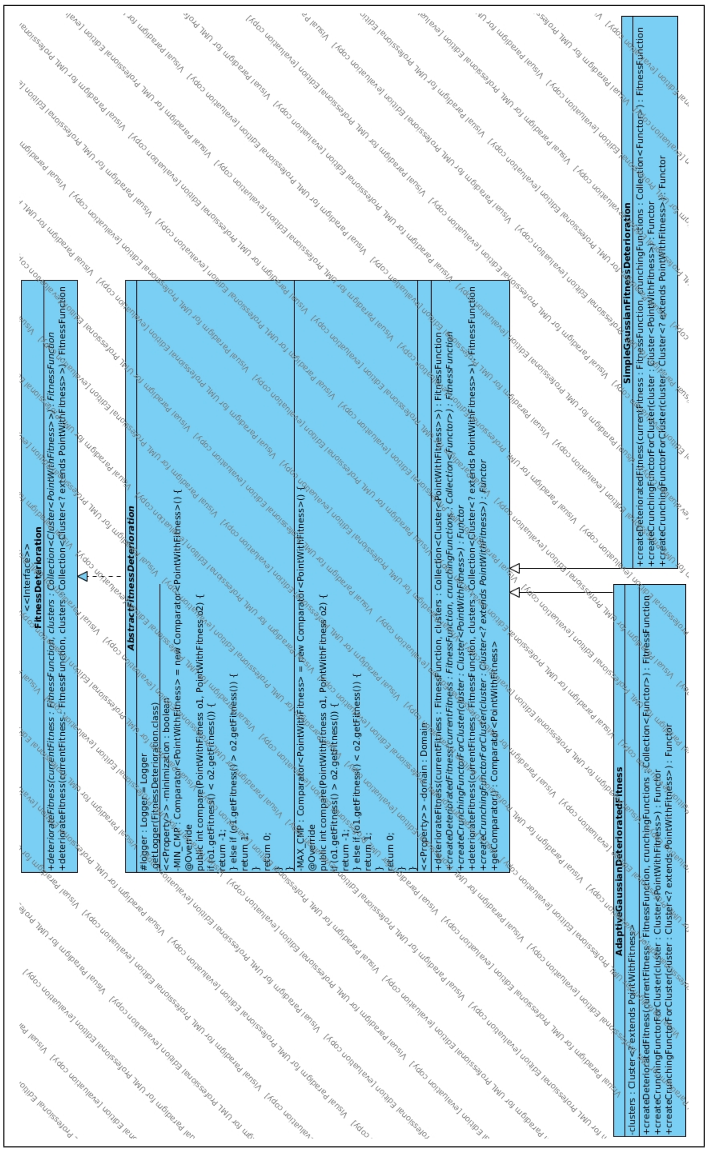

Figure 6.4: Fitness deterioration package

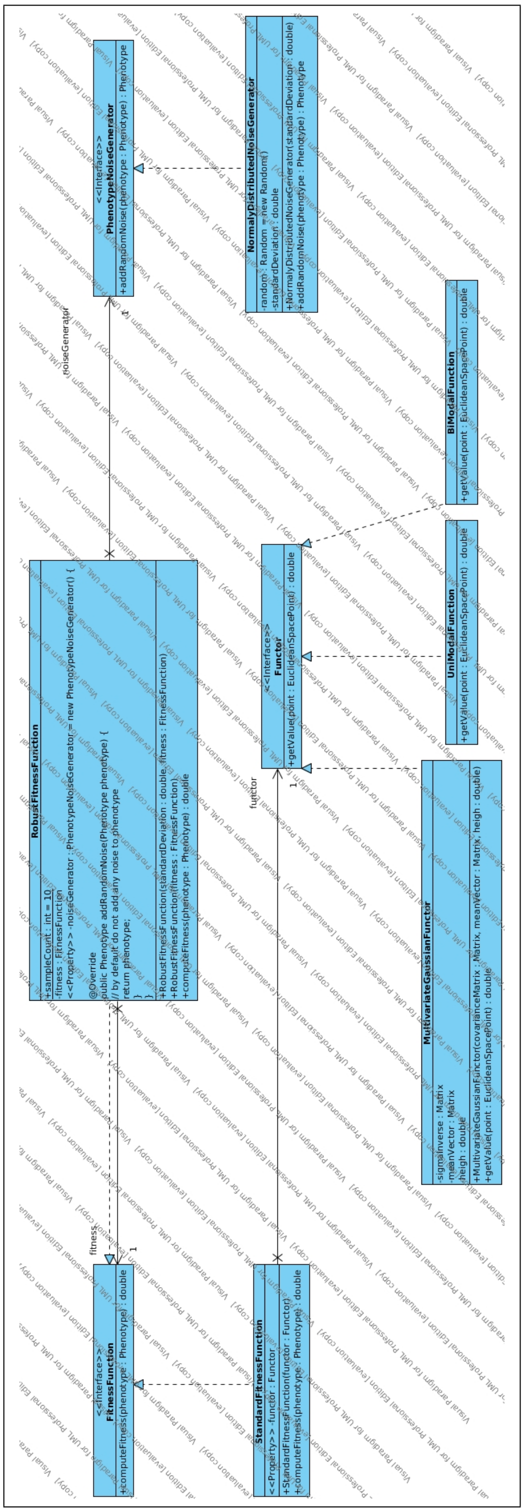

Figure 6.5: Fitness and functors package

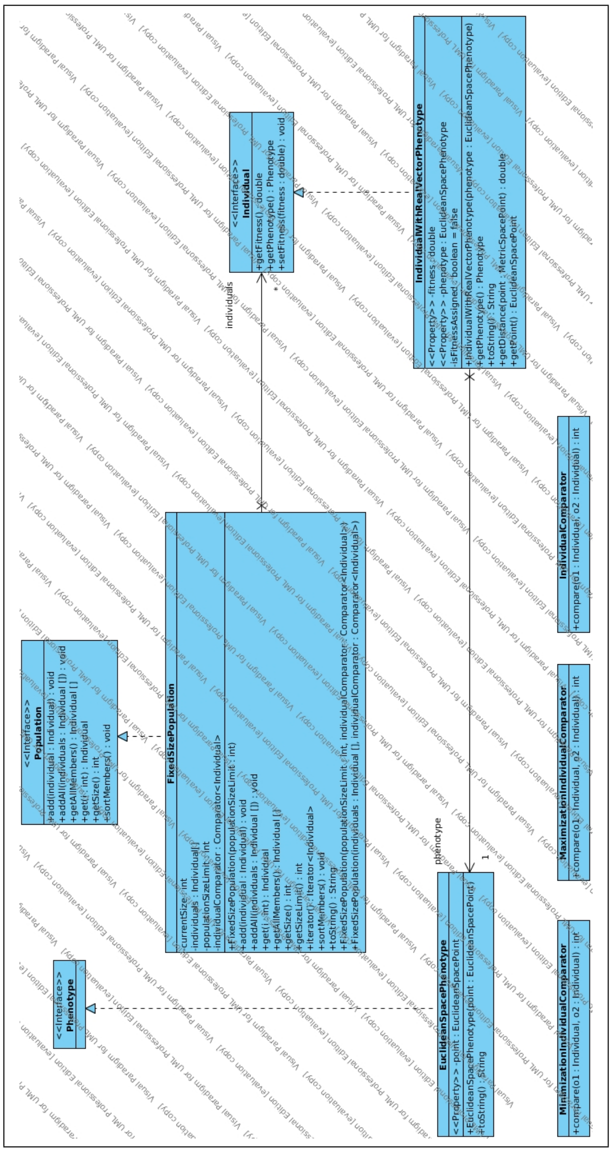

Figure 6.6: Population package

7. Conclusions

7.1. Summary

7.2. Future Research

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