Self-adaptive Mate Choice for Cluster Geometry Optimization

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ABSTRACT

Sexual Selection through Mate Choice has, over the past few decades, attracted the attention of researchers from various fields. They have gathered numerous supporting evidence, establishing Mate Choice as a major driving force of evolution, capable of shaping complex traits and behaviours. Despite its wide acceptance and relevance across various research fields, the impact of Mate Choice in Evolutionary Computation is still far from understood, both regarding performance and behaviour.

In this study we describe a nature-inspired self-adaptive mate choice model, relying on a Genetic Programming representation tailored for the optimization of Morse clusters, a relevant and widely accepted problem for benchmarking new algorithms, which provides a set of hard test instances. The model is coupled with a state-of-the-art hybrid steady-state approach and both its performance and behaviour are assessed with a particular interest on the replacement strategy's acceptance rate and diversity handling.

Categories and Subject Descriptors

I.2.8 [**Artificial Intelligence**]: Problem solving, Control Methods, and Search—*Heuristic Methods*

General Terms

Algorithms, Design

Keywords

Evolutionary Algorithms, Genetic Programming, Sexual Selection, Mate Choice, Self-adaption, Cluster Geometry Optimization

1. INTRODUCTION

Darwin has proposed two complementary theories accounting for the evolution of species: Natural Selection [5] and Sexual Selection [6]. Natural Selection was described as the result of competition within or between species affecting its individuals rate of survival, while Sexual Selection resulted from the competition between individuals of the same species affecting their relative rate of reproduction.

While Natural Selection was widely accepted and endorsed by the scientific community, Sexual Selection was discredited as a curiosity rather than an influential theory. However, interest arose in the 1970s through the works of Fisher [9, 10] and Zahavi [30] and an increasing number of researchers have put their efforts on exploring the subject of Sexual Selection. Among the processes that compose Sexual Selection, Darwin was most focused on Mate Choice [6] as were some of his most preeminent followers [9, 10, 30] and many present day researchers. Nowadays, Mate Choice is highly regarded across various research fields and widely accepted as a major force in evolution [1, 2]. While it has come a long way on other research fields, the effects of Mate Choice on Evolutionary Computation are still far from understood, requiring further research on both performance and behaviour.

Cluster geometry optimization (CGO) has important applications in Nanoscience, Physics, Chemistry and Biochemistry [32]. Finding the geometry of a cluster such that its potential energy is minimized is a NP-hard task [4]. Moreover, the problem provides a large set of difficult test instances and has been widely used for benchmarking the efficiency of global optimization algorithms [4, 7, 12, 14, 23, 24, 25]. The most relevant models are Lennard-Jones clusters [17] and Morse clusters [21], mostly because their modeling functions depend solely on the distance between every pair of particles in the cluster. Optimization of Morse clusters is regarded as a particularly tough problem, specially if used to model short range interactions between particles [8].

Evolutionary Algorithms (EA) have been first applied to CGO problems in the early 1990s [14] and are currently considered state-of-the-art approaches. Several breakthroughs have been achieved since then, such as coupling the algorithms with local-search methods to relax individuals into the nearest local optima [7, 12, 14, 25]. The base algorithm adopted in this study has been proposed by Pereira et al. [24], who suggested that maintenance of diversity may be a key-point to efficiency when tackling CGO [23, 24].

In this study we apply Sexual Selection through Mate Choice to the optimization of Morse clusters using an unbiased hybrid steady-state EA combined with a single phase local-search method. The study aims at two goals: assessing performance on a hard optimization problem; getting insight

GECCO'13, July 6–10, 2013, Amsterdam, The Netherlands.

on how Mate Choice affects the behaviour of the algorithm in terms of diversity and acceptance rate.

The following section introduces the subject of Mate Choice, briefly covering its background and reviewing related work in EAs. Section 3 introduces Morse clusters optimization, examines important contributions and describes a hybrid steady-state EA tailored for tackling the problem. It finally describes a Mate Choice approach for the optimization of Morse clusters. Section 4 covers the experimental setup and the results are thoroughly analyzed and discussed. Section 5 presents our conclusions and future work.

2. SEXUAL SELECTION THROUGH MATE CHOICE

Since publishing his theory of Natural Selection, Darwin was intrigued with animal ornamentation and courtship behaviours. Natural Selection would only favor traits that benefit the survivability of individuals and therefore could not explain the emergence of costly and complex traits that he observed across different species and which seemed to make no contribution to survival. He knew however that such traits had to bring evolutionary advantage in order to spread along the generations. Considering that these traits appeared to be related to mating behaviour, Darwin envisioned that there must be a trait-shaping selection feature other than Natural Selection accounting for the emergence of traits that bring advantage in mating rather than survival.

While Natural Selection adapts species to their environment [5], Sexual Selection adapts individuals in relation to others in a competition for mating partners [6]. Failing to find suitable mate(s) results in few or no offspring rather than death. However, from an evolutionary perspective, failing to reproduce or to survive have mostly the same outcome: the long term survivability of the genes is jeopardized.

Darwin described two main processes in Sexual Selection: male competition and female mate choice, the latter being the scope of this study. Darwin's ideas on Mate Choice explained the emergence of traits in males through adaption to female mating preferences [6]. Males that are better adapted to the tastes of females attain a higher reproduction rate. Various contributions followed, the most important arguably by Fisher, who explained how mating preferences evolve and are heritable the same way as physical traits [9, 10]. He also introduced the idea that ornamentations evolve as indicators of fitness (health, energy, etc.), and that females who are able to choose males with good genetic quality will produce healthier offspring that will reinforce both the inherited mating preferences and physical traits [9]. Finally, he showed how mating preferences and physical traits influence each other through a positive feedback loop [10].

Over the years, a number of publications have arisen covering different ideas regarding the design and implementation of Mate Choice in EAs. We are interested in models that follow three nature-inspired rules:

1. individuals must choose who they mate with based on their perception of others and on their own mating preferences;
2. mating preferences are heritable the same way as physical traits;
3. mate selection introduces its own selection pressure but is subject to selection pressure itself [11];

Several publications fall into this scope.

Hinterding and Michalewicz [16] tackle the constrained optimization of a nonlinear programming problem. Instead of relying on traditional methods for constrained optimization, they propose using a Mate Choice approach that promotes the feasibility of individuals. The first parent is selected using a tournament that favors feasible individuals. It will then select a mate from a candidate pool by preferring mates that, in conjunction with itself, violate the least number of constraints. Therefore, individuals that best complement the first parent are promoted in hope of increasing feasibility. The approach was compared with standard constraint optimization methods achieving comparable results.

Smorokdina and Tauritz have proposed a self-adaptive approach where each individual encodes its own Mate selection function in addition to a candidate solution for the working problem [28]. The Mate selection function is represented using Genetic Programming (GP). The terminal nodes of the trees are, exclusively, the remaining individuals in the population. The non-terminals are a set of selection operators such as *tournament selection*, *biggest hamming distance*, etc. Constraints are enforced to make sure the operators are applied correctly. Mate selection functions are inherited from parents to offspring following one of two proposed rules: given that the new offspring show improvements they inherit the function that was actively used; otherwise, the function attributed to new offspring is the result of the recombination of those from both parents. Results on a set of test problems were slightly worse than a traditional approach.

Guntly and Tauritz [13] propose a Learning Individual Mating Preferences (LIMP) approach with two variants: using a centralized mating preferences vector (C-LIMP) and a decentralized approach (D-LIMP). LIMP is tailored for problems with binary representation, using a real-valued preference vector, with the same size as the genotype, to encode in each position how desirable it is that the corresponding gene is set to one. In D-LIMP each individual encodes its own preference vector, used to evaluate others. Offspring inherit their parents' preferences so that they match the genes inherited from each parent. In addition, the preference vectors are updated based on the relative success of the offspring. The C-LIMP uses 2 preference vectors common to the whole population, the first relative to genes set to 0 and the second to genes set to 1. When an individual assess others, it checks either vector based on its own genotype. At each reproduction step, the vectors are updated in a similar way as in D-LIMP. Both approaches were compared with a traditional GA and a variable dissortative mating GA, achieving better results in part of the test set.

Machado and Leitão [20] have addressed self-adaption of mate evaluation functions on the Circle Packing in Squares (CPS) problem. In this problem, candidate solutions to a given instance also encode candidate solutions to smaller instances. How an individual performs on smaller instances of the CPS problem can be used as indicators of genetic quality, carrying information about how they may contribute to healthy offspring. Apart from a candidate solution to the problem, each individual encodes an extra chromosome representing its own mating preferences. Two models were tested either relying on Genetic Algorithms (GA) or GP. The GA mate evaluation function was designed as a weighted sum matching the weights on the first individual with the fitness values obtained by each candidate on smaller instances of the problem and evolving only the weights. The GP approach evolves whole evaluation functions that are built using the fitness values from each candidate on smaller instances as the terminal set and a set of arithmetic operators as the function set. Results achieved by the GA approach were poor when compared to a standard approach. On the other hand, the GP approach was able to improve upon the results obtained with a classical approach.

3. MORSE CLUSTERS OPTIMIZATION

The Morse potential is the N-particle additive function defined by Eq. 1. As in previous studies [22, 24, 4] we have adopted a scaled version of the Morse potential by setting both the bond dissociation energy, ϵ, and the equilibrium bond length, r_0, to 1. The range exponent of the potential, β, has a strong influence on the character of the potential energy surface (PES), the multidimensional function that describes the interactions between the particles in the cluster. As the value of β is increased, the PES is much more likely to assume a multiple-funnel character with an increasing number of local minima [22, 8]. In this study we have set $\beta = 14$ which corresponds to short range interactions [8], regarded as particularly tough. Therefore, r_{ij} is left as the only variable in Eq. 1, resulting on a function that depends only on the distance between particles.

$$\begin{aligned} V_{Morse} \quad = \quad & \epsilon \sum_{i}^{N-1} \sum_{j>i}^{N} \{exp[-2\beta(r_{ij} - r_0)] \\ & - 2exp[-\beta(r_{ij} - r_0)]\} \qquad (1) \end{aligned}$$

3.1 Related Work

This section covers key achievements on CGO. An overview of EA approaches has been published by Hartke [15].

Morse clusters optimization was first tackled by Doyes and Wales [22] who applied a basin-hopping algorithm and report finding all but 12 putative optima on clusters ranging up to 80 atoms. Roberts et al. [27] applied an EA which combined a real-valued representation [31] with a Cut and Splice crossover operator (C&S) [7] and Lamarckian local optimization [7]. They achieved most of the putative optima on Morse clusters consisting of 19 to 50 atoms.

Locatelli and Schoen proposed using a two-phase local search algorithm designed to tackle multi-funnel charactered PESs [19]. Their algorithm would on a first phase perform local optimization on a modified potential function combining knowledge from the true PES and the geometric structure of the putative solution thus biasing the search toward local optima with specific proprieties and helping search on the true PES during the second step. The algorithm was coupled with a basin-hopping approach and applied to Morse clusters [8], finding all putative optima on clusters ranging from 41 to 80 atoms. The two-phase algorithm has also been combined with a population-based algorithm [12].

Despite the success of these approaches, they depend on a number of parameters that need to be set a priori and that rely on information regarding the target solution. This raises questions concerning bias and their performance when such information is unknown. Two self-adaptive approaches have been proposed to overcome this setback. Cassioli et al. [3] presented a population basin-hopping algorithm where the required parameters are encoded in each individual as weight factors that undergo self-adaptation. Pereira and Marques [23] proposed encoding in each individual the parameters to be applied in their own local-search method, starting with random values that adjust online. These approaches successfully remove the need of setting the parameters beforehand despite causing a reduction on the success rate when applied to Morse clusters ranging up to 80 atoms.

On the same study, Pereira and Marques discussed that the success of their approach was mostly the result of an increased diversity induced by the self-adaption of parameters. A later study by Pereira et al. [24] applied an unbiased hybrid steady-state EA coupled with an unbiased single-phase local optimization procedure and reports finding all putative optima on Morse clusters consisting from 41 to 80 atoms. They show that an unbiased hybrid EA can successfully tackle such problems and that maintenance of diversity is a key-factor in doing so.

3.2 A hybrid steady-state EA for Morse clusters optimization

The aforementioned study by Pereira et al. [24] introduced the base algorithm of this research. The Mate Choice approach applied in this study introduces however some changes as it relies on individuals composed of two chromosomes. The first chromosome encodes a candidate solution for the optimization of Morse Clusters while the second chromosome represents each individual's function for assessing mating candidates. The remaining of this section relates to the first chromosome and other components of the algorithm. Specifics of the Mate Choice approach and the second chromosome are introduced in Sect. 3.3.

3.2.1 Representation

A cluster with N atoms on the *3D* space is represented as a $3 \times N$ real valued array that encodes the Cartesian coordinates of the particles. Each gene ranges between *0* and $N^{1/3}$ which is widely accepted to allow the correct scaling of the cluster volume with N [24, 31]. Restrictions are enforced on the distance between each pair of particles during initialization and when genetic operators are applied as to avoid excessively repulsive potentials that result from too small distances. Only solutions where distances are larger than a pre-specified parameter, $\delta = 0.5$, are allowed.

3.2.2 Genetic operators

Both crossover and mutation operators specifically tailored for CGO are applied. A generalized C&S operator, proposed by Pereira et al. [26] ensures that parents contribute with particles that are placed close together while sigma mutation [26], applied to offspring, acts on one particle at each time. The new location is obtained by disrupting its coordinates on the *3D* space with values sampled from a Normal distribution with mean *0* and standard deviation σ.

3.2.3 Local optimization

The limited memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) method, which relies on first order derivative information, guides individuals into the nearest local optimum. The generic element n of the Morse potential gradient is obtained through Eq. 2 where x_{ni} represents the difference between the Cartesian coordinates of particles n and i, $x_{ni} = x_n - x_i$. Similar expressions apply to the y and z axis. L-BFGS is applied to every generated individual prior to evaluation and executes until it finds a local optimum or until it reaches a maximum number of iterations, the Local Search Length (LSL). The accuracy of the method as been set to $1.0E-8$.

$$g_n = -2\beta\epsilon \sum_{i \neq n}^{N} \left(\frac{x_{ni}}{r_{ni}}\right) \{exp[-2\beta(r_{ni}-r_0)] - exp[-\beta(r_{ni}-r_0)]\} \quad (2)$$

3.2.4 *The population*

Individuals evolve as a steady-state model where two offspring are generated at each step and compete with the remaining individuals for a place in the population. This procedure is repeated until a termination criterion is met. Such a model requires a replacement strategy that controls which offspring are allowed in the population and which individuals perish in return. The one applied in this study is a fitness-based strategy that includes mechanisms which aim at maintaining diversity [18]. Briefly, given an individual X already locally optimized and evaluated, if the population contains an individual Y that is closer to X than a predefined value d_{min}, then only the best one is kept. Otherwise, X is different from all other solutions and will replace the worst one, given that X is better. In order to perceive if individuals are close, a distance measure $d(X,Y)$ is required, reflecting the similarity between individuals.

3.2.5 *The diversity measure*

This study relies on a measure based on the distances of particles to the cluster's center of mass, as first proposed by Grosso et al. [12], which expresses the structural dissimilarity between individuals. The choice was made based on the analysis by Pereira et al. [24]. Briefly, for each cluster, the distances from the particles to the center of mass are ordered in a vector in a non-decreasing fashion. Given two clusters and the respective ordered vectors Ord_X and Ord_Y, $d(X,Y)$ is given by Eq. 3. To estimate d_{min}, information provided by the initial population is used according to Eq. 4 where *Pop* represents the size of the population, $d(X,Y)$ the distance between individuals X and Y and ζ corresponds to the proportion among the average distance calculated with a set of randomly generated individuals and the minimum allowed distance between each pair. ζ has been set to 0.25.

$$d_{ord}(X,Y) = \frac{1}{10}\sum_{i=1}^{N} |(Ord_X(i) - Ord_Y(i))|^3 \quad (3)$$

$$d_{min} = \zeta \times \frac{\sum_{X=1}^{Pop-1}\sum_{Y=X+1}^{Pop} d(X,Y)}{\frac{1}{2}(Pop^2 - Pop)} \quad (4)$$

3.3 A mate choice approach to the optimization of Morse Clusters

As introduced in Sect. 3.2.1, each individual is composed of two chromosomes. The first is a GA vector that represents a candidate solution to the optimization of Morse clusters. The second is a GP tree that represents the function used by each individual to assess its mating candidates. The selection process is succinctly described in Alg. 1. *Parent 1* is selected using a fitness based tournament selection ad a set of mating candidates is selected randomly. *Parent 1* evaluates each of the candidates using its own evaluation function. The candidate that seems the most attractive, i.e. the one for which the GP tree of *Parent 1* returns the lowest value, is selected for mating. Since CGO is a minimization problem, we have opted to select the candidate with the lowest attractiveness value as the best one. When reproduction occurs, offspring inherit genetic material from both parents, resulting from GA operators acting on the first chromosomes and GP operators acting on the second ones.

Algorithm 1 Parent selection using Sexual Selection through Mate Choice

```
mate selection {
    parent1 = parent_selection(Pop)
    candidates = mating_candidates_selection(Pop)
    evaluate_mating_candidates(parent1,candidates)
    parent2 = select_best(candidates)
}
```

In order for individuals to assess others, they perceive problem-specific information regarding their phenotype. As described in sect. 3.2, when tackling the optimization of clusters of size *N*, individuals encode the positions of *N* particles, meaning that they also encode candidate solutions to each $N-1$ smaller clusters. How an individual performs on each of these clusters is an indicator of gene quality, showing how they may contribute to the optimization of *N* sized clusters. However, optimal solutions to clusters with different sizes can correspond to different geometric motifs. Thus, performing well on a $N-i$ sized cluster does not necessarily translate into good genes for the optimization of the *N* sized cluster. Without access to the cluster motifs it is difficult to build a function that uses this information in an appropriate way. We expect to self-adapt functions that do so in a meaningful way for the purpose of selecting mating partners.

Coupling a self-adaptive Mate Choice approach with a steady-state EA raises an interesting discussion point. Both mating preferences and physical traits evolve in a feedback loop, promoting those that bring reproductive advantage and causing individuals to continuously adapt to each other. The replacement strategy will however discard individuals that do not meet its constraints. Mating preferences that are unable to select adequate mating partners and produce offspring that are accepted into the population will therefore be incapable of spreading and gaining evolutionary advantage. On the other hand, accepted individuals will inherit and successfully promote both mating preferences and physical traits. Ultimately, the replacement strategy guides the evolution process. We expect mate evaluation functions to evolve accordingly and promote offspring that successfully integrate the population, therefore contributing to progress.

4. EXPERIMENTAL RESULTS

This section firstly describes the test setup applied in this study, followed by an analysis of both behaviour and performance.

4.1 Experimental Setup

The standard approach evolves a population of 100 individuals for 5.000.000 evaluations. Each iteration of the L-BFGS method counts as one evaluation. LSL is set to

1.000. Selection of both parents is done through a tournament of size 5, followed by crossover, applied with a rate of 70%, and mutation, applied with a rate of 5% [24]. Also $\sigma = 0.05 \times N^{1/3}$. Experiments were repeated 30 times for Morse clusters ranging from 41 to 80 particles. Finally, for analysis purposes, for every 100 individuals bred a generation counter is incremented.

In the Mate Choice approach, the first parent is selected through a tournament of 5 individuals. Then, a pool of 5 mating candidates is randomly selected from the population and the second parent is chosen following Alg. 1. Reproduction occurs by means of operators applied independently to each chromosome. The operators described in sect. 3.2.2 are applied to the first chromosome and crossover and mutation are applied to the second chromosome with the rates of 85% and 5% respectively. The terminal set of the GP trees is composed by the constants $\{-1, 2\}$ and 5 dynamic terminals. These dynamic terminals correspond to smaller instances of the target cluster so that they are equally spaced in the interval $[1, N-1]$. When a mating candidate is assessed, the dynamic terminals in the active function translate to the fitness obtained by the candidate on the corresponding instance. The non-terminal set consists on the following arithmetic functions: $\{+, -, *, /\}$. Experiments were repeated 30 times for Morse clusters ranging from 41 to 80 particles.

Performance of state-of-the-art approaches for tackling CGO problems is often measured based on the success rate of the runs [24, 8, 12], therefore, we register the number of runs where the putative optima was found for each instance of the problem. Also, in order to analyze the behaviour of our approach, the following elements were registered on each run: best fitness, average fitness, number of substitutions and average dissimilarity between individuals.

4.2 Analysis and Results

The success rates obtained by the studied approaches can be found in Table 1, where the label *Sexual Sel.* corresponds to our approach and the label *Standard* corresponds to the results reported in the study by Pereira et al. [24]. Our approach was able to find all putative optima on Morse clusters ranging from 41 to 80 atoms as well as outperform the Standard approach in 20 instances of the problem. On the other hand it achieved smaller rates in 13 instances and 7 ties. The pairwise proportions test proposed by Taillard et al. [29] was conducted with a significance level of *0.01* and significant differences were found on 4 instances which have been emphasized in Table 1. There is an obvious evolutionary overhead introduced by the evolution of Mate Choice functions: unless good mating choice functions are found, the ability of individuals to select appropriate mates is hindered, which could significantly delay evolution. While no significant differences were found on the majority of the instances, the proposed approach was able to attain competitive and sometimes better results than the standard approach, which indicates that the algorithm, in spite of the aforementioned overhead, is able to evolve mate choice functions that assess individuals in meaningful and advantageous ways.

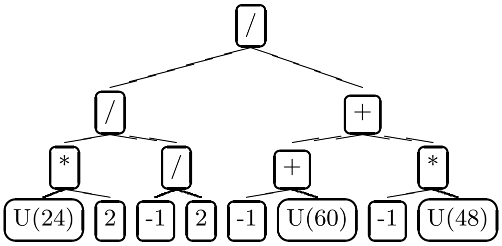

Figure 1: Example of a GP tree evolved for mating selection

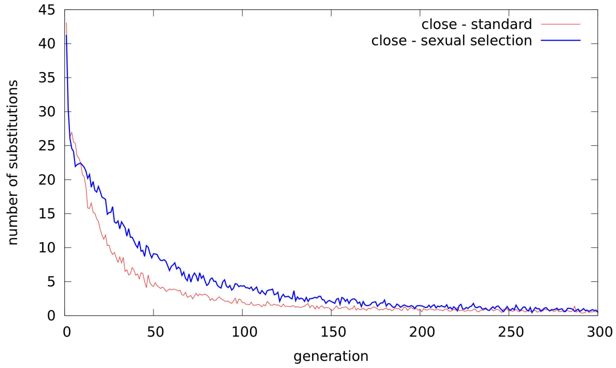

Figure 2: Average substitution rate from 30 runs with clusters of size 61, where *close* corresponds to individuals replacing a similar one in the population.

The means by which the algorithm is able to take advantage of the mate choice process are not straightforward to analyze. Figure 1 shows an example of a GP tree evolved for the purpose of selecting mating partners. While the algorithm has evolved much larger trees, the presented one still serves the purpose of showing that interpreting the meanings of the evolved trees is not an easy task. An analysis of the example in Fig. 1 leads us to conjecture that how individuals perform on the optimization of clusters sizing 24, 48 and 60 atoms is relevant for the individual owning this tree. However, how these terminals relate with each other and how much they weigh in the process of choosing a mate depends on how non-terminals act on them, which often prevents us from attributing meaning to the terminals. This makes the analysis of the evolved mate selection functions an often frustrating task, specially on larger trees. Still, we can draw two conclusions from the obtained results and tree analysis: the provided terminal and non-terminal sets can be combined in useful ways for mate selection; evolved functions allow individuals to choose their partners in unforeseeable ways which we would unlikely be able to design on our own.

While the inner workings of Mate Choice are difficult to analyze, its impact on the behaviour of the algorithm is quite noticeable. Experiments were conducted in order to measure the impact of Mate Choice on the acceptance rate as well as on the structural diversity of the population, two relevant aspects on the Standard approach. The following discussion will focus on Morse clusters consisting of 61 atoms, an instance that is considered particularly tough [8, 12].

Figures 2 and 3 compare the acceptance rates of individuals on both approaches. The replacement strategy has a powerful role in the steady-state model since it determines which of the offspring are allowed in the population. Ultimately, the progress of the evolution process is determined by how well it is able to adapt to the restrictions imposed by the replacement strategy and its capabilities to continuously produce offspring that are included in the population. Fur-

Table 1: Success rate obtained by the Standard and the Mate Choice approaches on clusters of size *N*

N	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60
Sexual Sel.	**24**	**21**	18	**18**	12	14	6	16	16	2	2	9	4	7	7	11	9	5	3	**7**
Standard	15	12	14	7	5	9	2	14	18	5	7	6	5	12	6	11	8	4	2	0

N	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80
Sexual Sel.	1	6	8	8	9	10	5	3	6	6	6	3	6	5	5	3	3	4	2	5
Standard	1	12	6	11	8	8	5	4	6	8	6	7	6	1	2	4	7	3	6	5

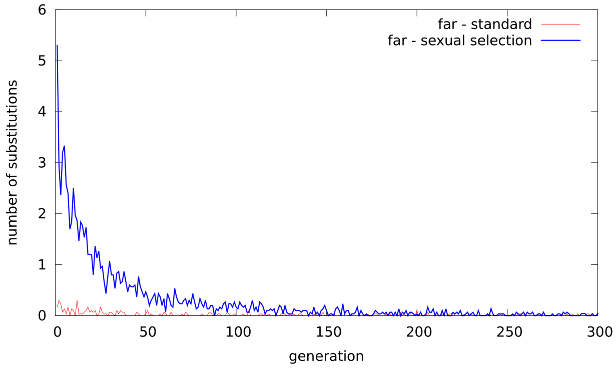

Figure 3: Average substitution rate from 30 runs with clusters of size 61, where *far* corresponds to individuals replacing worst one in the population.

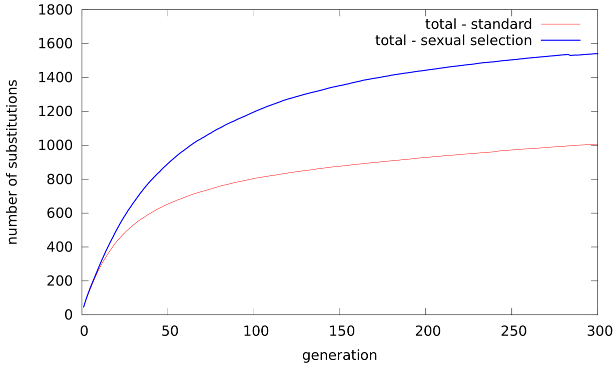

Figure 4: Cumulative average number of substitutions obtained in 30 runs with clusters of size 61.

thermore, on the proposed model, the replacement strategy not only controls what genes are allowed to spread through the population of candidate solutions but also which mating preferences will disseminate.

Figure 2 shows that the Mate Choice approach is able to successfully contribute with offspring that are better than the most structurally similar individuals in the population. Also, it does so at a fairly higher average rate than the Standard approach since the early stages of the runs. A similar behaviour is displayed in Fig. 3 regarding offspring that while being structurally different from the individuals in the population, are better than the worst one. These substitution rates are much lower, than the ones of Fig. 2 since the algorithms are more likely to produce offspring similar to individuals in the population, an effect that seems more pronounced in this particular instance. Still, differences between the two approaches are quite visible.

Although an increase in the acceptance rate doesn't necessarily translate into a better performance, it does show an aptitude to adapt to the replacement strategy. While the Standard approach is bound to give advantage to fittest individuals, the Mate Choice approach, despite selecting one of the parents through a tournament operator, may adopt different strategies to select the second one. Also, these strategies vary and self-adapt on the individual level. Adaption occurs as the replacement strategy discards unfit offspring, therefore giving an advantage not only to individuals that are fit but also to those that are able to select mating partners that contribute positively to the quality of their offspring. By means of inheritance, good mating evaluation functions are bound to spread through the population and further contribute to an increase of the acceptance rate observed in Figs. 2 and 3. Results in Table 1 suggest that such an increase in the acceptance rate contributes to competitive and sometimes better success rates.

A possible setback on the application of our mate choice approach is the extra computational overhead created by the evaluation of mating candidates. While this is not the scope of the study, it is relevant to note that such an analysis is not straightforward due to a number of reasons. Firstly, mating candidates do not undergo local optimization while being evaluated on smaller instances of the problem, which is responsible for the largest part of the computational effort required for evaluating individuals. Secondly, the effort needed to calculate the potential energy of a cluster varies with its size. Thirdly, mechanisms may be easily included in the algorithm to ensure that individuals are not repeatedly evaluated on the same instances of the problem, which is particularly relevant on steady-state models where individuals may have a considerably long life. Fourthly, which individuals are evaluated and on what instances is highly dependent on the mating preferences present in the population, which are subject to adaptation along the run. Finally, as Fig. 4 shows, the Mate Choice approach produces an increase of roughly 50% on the cumulative average number of substitution, reaching the average number of substitutions attained by the Standard approach still early in the evolution process. By reducing periods of stasis, our approach may reach the putative optima on a smaller number of generations thus reducing the number of required evaluations.

Even though the Mate Choice approach results on a much larger number of substitutions along the evolution process, their impact is quite different from those on the Standard approach. Figure 5 shows the average distance between individuals and how it is influenced by substitutions in each approach. The measure is calculated through Eq. 3 and evaluates the structural dissimilarity between individuals in

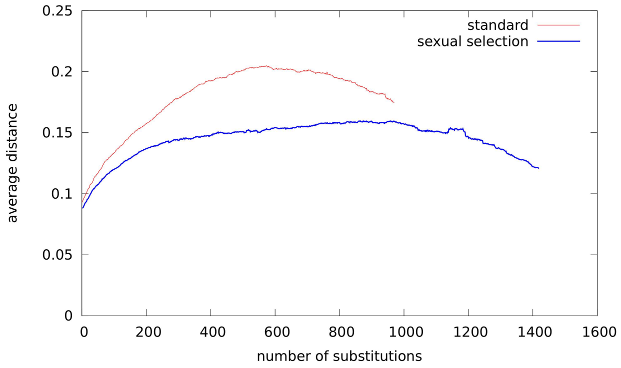

Figure 5: Average distance between individuals obtained from 30 runs with clusters of size 61.

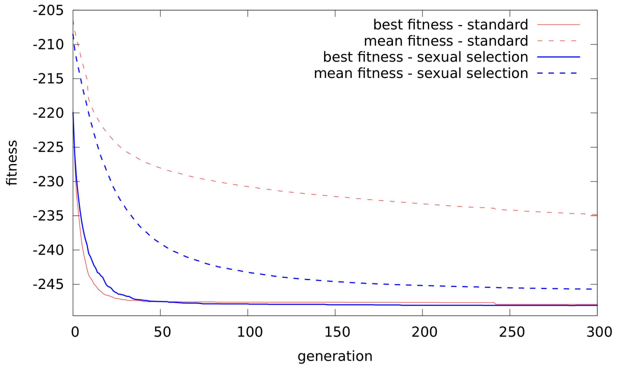

Figure 6: Average fitness obtained from 30 runs with clusters of size 61.

the population. Both approaches start with nearly the same dissimilarity value, however, the Standard approach, while producing a smaller number of offspring, is able to introduce new individuals in the population that have a much stronger impact on its average dissimilarity. These results may appear contradictory with the ones reported in Fig. 3, which shows that Mate Choice generates more replacements by dissimilar individuals. This can be explained as follows: the number of substitutions resulting from the introduction of dissimilar individuals is low in both strategies and hence unnoticeable in terms of average distance.

Our approach shares some characteristics with the Standard one, with a period where the average dissimilarity between individuals increases, followed by stagnation and a period where it slowly downfalls. There are however inherent differences between the impact of new individuals. While unable to reach an average dissimilarity as high as the Standard approach, Mate Choice causes a slower yet longer increase in the population's dissimilarity, suggesting that offspring cause a smaller but steadier impact on the progress of the evolution process. Nonetheless, despite the gradual decrease of dissimilarity toward the end of the run, both approaches are able to keep diversity above initial levels, promoting a good mixture of individuals along each run.

Based on the number of substitutions in Figs. 2 and 3 as well as on the impact new individuals have on the population as reported in Fig. 5, Mate Choice seems to produce offspring that share a higher structural similarity with individuals in the population. Such an effect is most likely the result of how mating preferences evolve along the run, suggesting that they adapt in a way that favours reproduction between structurally similar individuals, thus producing offspring that have less impact on the average dissimilarity of the population while still being valuable to the evolution process. However, as Fig. 3 shows, this does not prevent the discovery of individuals that are structurally dissimilar and, yet, reasonably fit – in the sense that they are at least better than the worst individual of the population. Thus, even when generating dissimilar individuals the Mate Choice approach behaves more robustly than the Standard approach, eventually leading to a higher number of substitutions by both similar and dissimilar individuals. This indicates that individuals tend to chose "compatible" mating partners.

The promotion of structurally similar individuals shown by Fig. 2 and the resulting impact on the average dissimilarity between individuals illustrated by Fig. 5 may indicate that the higher rate of substitutions caused by the evolved mating evaluation functions contributes to a slower search for the optimal solution as Mate Choice generates individuals that cause a smaller impact and possibly smaller gains in performance. However, Fig. 6 seems to contradict this assumption, showing that Mate Choice actively contributes to performance gains, a behaviour that is repeatedly found on the other instances of the problem.

5. CONCLUSIONS

This study proposes a Mate Choice approach to the optimization of Morse clusters. Major breakthroughs on CGO are reviewed and a hybrid steady-state EA coupled with a local-search method is thoroughly described. Mate Choice is introduced and state of the art approaches applied to a variety of problems are presented. A Mate Choice model for Morse clusters optimization is described and coupled with the aforementioned EA.

Morse clusters ranging from 41 to 80 atoms are tackled, the results compared and discussed with a particular interest on diversity handling as well as on the replacement strategy's acceptance rate. The results show a significant increase on the success rate on 4 instances of the problem and a slightly more robust behaviour on the global level. It is discussed that the evolved mating functions are difficult to analyze and seem to evolve in unforeseeable yet useful ways. The acceptance rate is analyzed and it is suggested that the Mate Choice approach is able to produce valuable individuals at an higher rate than the Standard approach, showing an adaption to the replacement strategy. Also, the analysis of diversity handling suggests that the Mate Choice model promotes mating between structurally similar individuals, therefore producing offspring that have a smaller yet longer impact on the population's diversity, and that individuals appear to choose compatible mating partners. It is also shown that the model is able to contribute to performance gains in the population. Finally, difficulties in studying the overhead caused by Mate Choice are discussed.

Future work may include applying Mate Choice to a set of Morse clusters ranging up to 160 atoms as well as studying how different mating preferences, representations, and varying mutation and crossover probabilities affect the behaviour and performance of Mate Choice on hybrid steady-state approaches to CGO.

6. ACKNOWLEDGMENTS

This work was partially funded by the Portuguese Foundation for Science and Technology (FCT) under project INO164-PTDC/EIA-EIA/102212/2008, High-Performance Computing over the Large-Scale Internet.

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