1

Mate Choice in Evolutionary Computation

António Leitão and Penousal Machado

CISUC, Department of Informatics Engineering, University of Coimbra, 3030-290 Coimbra
Coimbra, Portugal `apleitao,machado@dei.uc.pt`

Summary. Darwin considered two major theories that account for the evolution of species. Natural Selection was described as the result of competition within or between species affecting its individuals relative survival ability, while Sexual Selection was described as the result of competition within species affecting its individuals relative rate of reproduction. This theory emerged from Darwin's necessity to explain complex ornamentation and behaviour that while being costly to maintain, bring no apparent survival advantages to individuals. Mate Choice is one of the processes described by Darwin's theory of Sexual Selection as responsible for the emergence of a wide range of characteristics such as the peacock's tail, bright coloration in different species, certain bird singing or extravagant courtship behaviours. As the theory attracted more and more researchers, the role of Mate Choice has been extensively discussed and backed up by supporting evidence, showing how a force which adapts individuals not to their habitat but to each other can have a strong impact on the evolution of species. While Mate Choice is highly regarded in many research fields, its role in Evolutionary Computation (EC) is still far from being explored and understood. Following Darwin's ideas on Mate Choice, as well as Fisher's contributions regarding the heritability of mating preferences, we propose computational models of Mate Choice, which follow three key rules: individuals choose their mating partners based on their perception mechanisms and mating preferences; mating preferences are heritable the same way as any other trait; Mate Choice introduces its own selection pressure but is subjected to selection pressure itself. The use of self-adaptive methods allows individuals to encode their own mating preferences, use them to evaluate mating candidates and pass preferences on to future generations. Self-adaptive Mate Choice also allows evaluation functions to adapt to the problem at hand as well as to the individuals in the population. In this study we show how Genetic Programming (GP) can be used to represent and evolve mating preferences. In our approach the genotype of each individual is composed of two chromosomes encoding: (i) a candidate solution to the problem at hand (ii) a mating partner evaluation function. During the reproduction step of the algorithm, the first parent is chosen based on fitness, as in conventional EC approaches; the mating partner evaluation function encoded on the genotype of this individual is then used to evaluate its potential partners and choose a second parent. Being part of the genotype, the evaluation functions are subjected to evolution and there is an evolutionary pressure to evolve adequate mate evaluation functions. We analyze and discuss the impact of this approach on the evolutionary process, showing how valuable and innovative mate evaluation functions, which would unlikely be designed by humans, arise. We also explain how GP non-terminal and terminal sets can be defined in order to allow the representation of mate selection functions. Finally, we show how self-adaptive Mate Choice can be applied in both academic and real world applications, having achieved encouraging results in both cases. Future venues of research are also proposed such as applications on dynamic environments or multi-objective problems.

1.1 Introduction

Darwin's theory of Natural Selection [4] has been widely accepted and endorsed by the scientific community since its early years. Described as the result of competition within or between species affecting its individuals rate of survival, it has had a deep impact on multiple research field and is at the source of the ideas behind EC. The theory of Sexual Selection [5] was later developed by Darwin to account for a number of traits that were observed in various species, which seemed to have no place in his Natural Selection theory. Darwin described Sexual Selection as the result of the competition between individuals of the same species affecting their relative rate of reproduction, a force capable of shaping traits to high degrees of complexity and responsible for the emergence of rich ornamentation and complex courtship behaviour.

Despite having been discredited by the scientific community at the time, it is now widely regarded as a major influence on evolution theory. Interest arose in the 1970s through the works of Fisher [10, 11] and Zahavi [37] and since then the community as gradually embraced it, having found its place in various research fields. While it has come a long way, Sexual Selection is still far from understood in EC, both regarding possible benefits and behaviour.

Mate Choice was one of the processes of Sexual Selection described by Darwin and that mostly attracted his followers. This chapter describes a nature-inspired self-adaptive Mate Choice setup and covers the design steps necessary for applying it. A two-chromosome scheme where the first chromosome represents a candidate solution and the second chromosome represents mating preferences is proposed. Two approaches for encoding mating preferences are presented and differences discussed. Details on how to apply each of them to problems with different characteristics are given and design choices are discussed. The application of both approaches on different problems is reviewed and the observed behaviour discussed.

Section 1.2 introduces Mate Choice as well as its background, Section 1.3 gives a general overview of Mate Choice in Evolutionary Computation and covers the state of the art through a classification based on adaptation of mating preferences, popular preference choices and the role of genders. The section finally introduces the proposed setup, giving specific details on the ideas behind it and how to apply it. Section 1.4 describes the application of both the proposed approaches to multiple problems and discusses the obtained results and behaviours. Finally, Section 1.5 presents a summary.

1.2 Sexual Selection through Mate Choice

Since his journey on the Beagle, Darwin has thoroughly studied the forces responsible for the evolution of species. The result of competition within or between species affecting their individuals relative rate of survival was named Natural Selection. Since the publication of Darwin's *On the Origin of Species by Means of Natural Selection, or the Preservation of Favoured Races in the Struggle for Life* in 1859 [4], the theory has become widely accepted by the scientific community. This was achieved thanks to the evidence gathered by Darwin, its co-discoverer Alfred Russel Wallace [6] as well as multiple following researchers, ultimately overcoming other competitive ideas [3].

Despite such a success, Darwin battled with gaps in its theory. For instance, Darwin questioned how was it that Natural Selection could account for animal ornamentation or courtship behaviour. He observed a large number of species, where individuals displayed rich and costly ornamentations or complex and risky courtship behaviours that seemed to serve no purpose in survival, sometimes even risking it. These characteristics challenged the theory of Natural Selection and the idea that traits adapted to the environment in a purposeful way. Individuals carrying aimless and costly features should be unfavored in competition, making such features bound to face extinction.

However, as Darwin observed, that was not the case. Ornamentation and courtship behaviour were spread across populations and species, although Natural Selection could not explain their origin. He figured, however, that for these features to emerge they had to bring some kind of competitive advantage. As they didn't fit in Natural Selection, he envisioned the existence of another trait-shaping selection force in nature, one capable of shaping species in complex and diverse ways, by causing traits that help in competing for mates to spread through future generations. These traits were linked to reproduction, as he observed in nature, and brought evolutionary advantages, even when risking survivability. Darwin developed the theory of Sexual Selection [5] to explain this phenomena and described it as the result of competition within species affecting its individuals relative rate of reproduction.

Darwin therefore saw evolution as the interplay between two major forces, Natural Selection as the adaptation of species to their environment, and Sexual Selection as the adaptation of each sex in relation to the other, in a struggle of individuals of one sex for the possession of individuals of the other in order to maximize their reproductive advantages. While the outcome of failing in Natural Selection would be low survivability, the outcome of failing in Sexual Selection would be a low number or no offspring. From an evolutionary perspective, they reach the same outcome with competition in reproductive rates between individuals leading to evolutionary changes across populations.

Unlike his theory of Natural Selection, which easily found support on the scientific community, his theory of Sexual Selection was mostly rebuffed. The scientific community was not keen on Darwin's ideas regarding Sexual Selection, specially his ideas on Female Mate Choice and the impact it could have on evolution. It was clear for them that Natural Selection was the only force capable of adapting species and so a number of theories emerged in order to explain rich displays or courtship behaviour. One of the most avid opponents of Darwin's ideas was Wallace who came up with various reasons for the emergence of traits such as protection through dull colors in females, recognition of individuals of the same species, usage of surplus energy on courtship behaviour or non-selective side effects [3].

The community was better prepared to understand such ideas, which were embraced by various renowned researchers such as Huxley [3]. This lead to a time where Darwin's ideas on Sexual Selection and specially Mate Choice were dismissed as non-important, and its impact to be regarded as a small part of Natural Selection. These ideas remained for over a century, with the exception of a few works by a select few researchers who made important contributions, such as Fisher [10] who explored the origin of mating preferences and runaway sexual selection, Williams [36] who discussed how ornaments should be considered as important as other adaptations or Zahavi [37] who expanded on the role of displays as fitness indicators.

Overtime, the work of these researchers was able to gain some space in the community, eventually reaching more open-minded generations who were also better equipped to test and understand the workings of Sexual Selection and Mate Choice. The resulting discussion has for the past few decades attracted experimental biologists, psychologists and anthropologists that since then have put Darwin's ideas as well as those promoted by his followers to the test, contributing with increasing evidence to back the ideas behind Sexual Selection through Mate Choice. Nowadays, there is active research on various fields and the theory has been widely accepted by the community. Two extensive reviews on Sexual Selection have been published by Helena Cronin [3] and Malte Andersson [1].

Mate Choice is one of the main Sexual Selection processes described by Darwin and where he put much of his effort, as did most of his followers. They aimed to explain the emergence of aesthetic features such as ornamentation or courtship behaviour. One of the pillars of Darwin's theories on evolution was that species went through adaptations because they brought some kind of advantage over time. In this case, these traits emerged because they brought reproductive advantage as a result of preferences when selecting mating partners [5]. Fisher helped explain the relation between mating preferences and traits, and the genetic link between them through his theory of runaway sexual selection. He addressed how displays may arise as a result of positive reinforcement between mental mating preferences and physical traits, through a feedback loop that can lead to extravagant adaptations such as the peacock's tail, colorful appearance or complex courtship behaviour [10, 11].

Fisher's work suggests the inheritance of mating preferences much like any other trait, therefore adapting throughout the generations. This process can be better understood if mate choice is thought of like any other adaptive choice such as food choice [24]. Still, criticism of theses ideas remained, since the evolution of traits through such a runaway process with increasing speed could drastically risk the survival ability of individuals. Zahavi later expanded on this subject, suggesting that aesthetic displays can act as indicators of fitness, health, energy, reproductive potential etc. He argued through his handicap principal [37] that even in the case of costly displays and behaviour, which seemed to have no purpose in Natural Selection, it was in fact their high cost that made them good fitness indicators. As these traits were handicaps, they couldn't be maintained by weak, unfit individuals and that only strong healthy individuals would be able to maintain them and survive. Therefore reinforcement of mating preferences for these traits would be beneficial for females, which would in turn reinforce such physical traits in males as suggested by Fisher [10].

These ideas were explored and discussed by many other researchers, who finally brought Sexual Selection through Mate Choice into the spotlight. Their work corroborated Darwin's ideas and brought new evidence allowing Sexual Selection to be seen as an important force in Evolutionary Theory. The interplay between Natural Selection and Sexual Selection was found to have a deep impact on various traits on many different species, especially among those equipped with complex sensory systems [3]. During the last few decades, Sexual Selection has found its place on various research fields such as Evolutionary Biology, Evolutionary Psychology and Evolutionary Anthropology. On the other hand, it is yet to attract the full attention of the Evolutionary Computation community, despite the publication of several papers over the last couple of decades.

The possible advantages that Sexual Selection, particularly through Mate Choice can bring to the field of Evolutionary Computation have been previously discussed by several researchers, and an extensive discussion on arguably the most relevant ones has been published by Miller and Todd [24]. They find that the addition of Mate Choice to Natural Selection can bring advantages such as i) increased accuracy when mapping from phenotype to fitness, therefore reducing the "error" caused by different forms of Natural Selection; ii) increasing the reproductive variance of populations by distinguishing between individuals with no survival-relevant (fitness) differences; iii) help populations escape from local optima through a directional stochastic process; iv) contribute to the emergence of complex innovations which may eventually contribute to fitness increasing; v) promote sympatric speciation, diversity and parallel evolutionary searches.

1.3 Mate Choice in Evolutionary Computation

Mate Choice has been modeled in Evolutionary Computation by applying more or less the same mechanism. Algorithm 1 succinctly describes the approach. First, parent1 is selected from the population using fitness-based traditional operators. Secondly, a pool of potential mating partners is determined. These could be the whole remaining population, a random subset or a group of individuals selected based on a given characteristic. Thirdly, the mating candidates are evaluated according to a given set of mating preferences. Finally, the candidate that according to the evaluation best matches the first parent is selected as parent2.

To further understand how Mate Choice works, Figs. 1.1 and 1.2 show how traditional approaches and mate choice approaches work respectively. As seen in Fig. 1.1, traditional approaches select each parent independently, based on their fitness alone,

Algorithm 1 Parents Selection using Sexual Selection through Mate Choice

```
proc MateChoice($population$) ≡
    $parent1$ ← parentSelection($population$)
    $candidates$ ← candidatesSelection($population$)
    evaluateCandidates($parent1, candidates$)
    $parent2$ ← selectBest($candidates$)
end
```

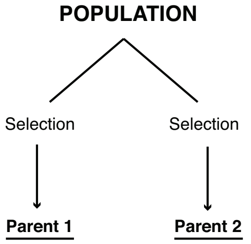

Fig. 1.1. Parents Selection using traditional approaches

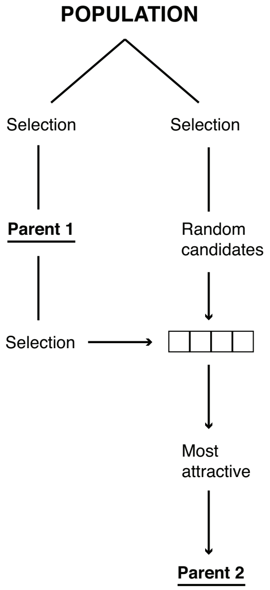

Fig. 1.2. Parents Selection using a Mate Choice approach

meaning that each individual should have reproductive success according to their fitness value. However, these individuals are paired randomly, without any knowledge about their mating partners. In mate choice approaches, as seen in Fig 1.2, individuals selected by traditional approaches are allowed to choose a mating partner based on their own criteria, meaning the pairing is no longer random but happens with a given characteristic in mind. This Mate Choice process is therefore ruled by the mating preferences as they will determine which individuals are good matches and are more likely to achieve reproductive success by producing fit, attractive offspring.

1.3.1 State of the Art

Mating preferences may remain static over the generations or undergo adaptation. In order to address preferences and adaptation mechanisms we will rely on the classification of adaptation of parameters and operators by Hinterding et al. [17]. Afterwards, we will look on different preferences and how they can be used to assess genotypes or phenotypes. Finally we will discuss the use of genders in Mate Choice strategies.

Adaptation of Mate Choice

Various authors rely on guiding the choice of mating partners using pre-established preferences, which remain static over the evolution process. The most widely known strategies are probably those that mate individuals based on similarity measures. Examples found in the literature include using Hamming distances [7, 8, 13, 26, 28, 29, 35], Euclidean distances [13, 29], number of common building blocks [29] or even simply using the fitness value as a distance measure [7, 13, 14, 29, 35]. In some implementations, the first selected parent chooses the candidate that maximizes similarity [9, 16] while in other cases the candidate that minimises the measure is considered the best [35]. Other approaches attribute a probability of selection proportional or inversely proportional to the distance measures [29].

Moreover, some authors don't want to maximize or minimize distances but rather consider an ideal distance and favour mating candidates that have distances closer to that pre-established value. In this case the attractiveness of a candidate is established using bell curves or other functions with a predefined center and width parameters [28].

Other metrics have been applied such as in Hinterding and Michaelwicz's study on constrained optimization [16]. They suggest having the first parent select the mating candidate that in conjunction with itself maximizes the number of constraints satisfied. A second example is the study by Fernandes et al. on vector quantization problems where a problem specific metric is used [9]. Sometimes different metrics are combined in a seduction function. This can be accomplished through the use of rules such as choosing the fittest candidate if two candidates both maximize or minimize the similarity measure or choosing between them randomly if they both also share the same fitness value [35]. A different approach is to combine different metrics using different functions (such as weighted functions) which has been done for instance by Ratford et al. [29].

While fixed parameters and mating preferences can often achieve competitive results and reproduce desired behaviours in Mate Choice algorithms, allowing their online control may be extremely valuable. Such approaches, which allow the Mate Choice strategy to change online without external control, therefore turning it into a dynamic process, can be subdivided into three groups: deterministic, adaptative and self-adaptative.

Deterministic approaches are the least common among the literature. Still, Ratford et al. give a good example [28]. On an aforementioned study they use a function to calculate a candidate's attractiveness which has two variables, centre and depth. It values individuals whose hamming distance from the first parent is closer to the centre of the function. However they complement this study by testing an approach where the centre of the function is adjusted at each generation, so that dissimilar individuals are favoured at the beginning of the run but the opposite happens at the end.

Adaptative approaches are more common and rely on information about the evolution process to adapt parameters or preferences. Fry et al. [12] have applied such a strategy to control which operator is used to select the second parent, either a regular tournament selection or a Mate Choice operator. In their study they choose mating partners by combining fitness with a penalization for similar candidates (different similarity measures are applied). However they use this operator with a given probability which is increased or reduced depending on its relative success in producing enhanced offspring in previous generations. A second example can be found on studies by Sanchez-Velazco and Bullinaria [30, 31]. Mating candidates in this case are evaluated based on a weighted function that combines three metrics: fitness, likelihood of producing enhanced offspring, and age. While age is adapted deterministically at each generation, the second factor represents a feedback on each individual's ability to produce fit offspring in the past.

Self-adaptive approaches better resemble the workings of Mate Choice in nature. By allowing preferences and parameters to be encoded in each individual, self-adaptation allows them to take part in the evolution process and to impact not only the individuals that encode them but the population as a whole. Possibly the simples example of such an approach relies on encoding an index as an extra gene in each individual. When evaluating its mating candidates, each individual will order them from best to worst according to a given metric and select the candidate at the encoded position. Galán and Mengshoel [13] have experimented with this approach using Euclidean distance and fitness to order mating candidates. On the aforementioned study by Fry et al. [12], a second approach was tested, where each individual encodes its own probability of selecting a mating partner using a mate choice operator rather than regular tournament selection. The probability is inherited by the offspring and adapted by comparing their fitness with that of their parents.

More complex mating preferences can be found on self-adaptive approaches. Miller and Todd [25, 34] suggest encoding a reference position on the phenotype space marking each individual's ideal position for a mating candidate. When assessing potential mating partners, the probability of mating varies according to their distance to the reference position. New offspring inherit genetic material from both parents through two-point crossover thus allowing for its self-adaptation throughout the evolutionary process.

Holdener and Tauritz [18] relied on an extra chromosome to encode a list of desired features to look for on mating candidates. They tackle a problem using a binary representation on the first chromosome but rely on a real value representation on the preferences chromosome. This chromosome has the same size as the first chromosome with each gene representing how much an individual wants the corresponding gene to be set to 1. This information is used to evaluate mating candidates by comparing the preferences chromosome with each candidate's potential solution, favouring desired genes. Preference genes are inherited from parents to offspring so that they match the genes they influence and adapt to match the offspring's relative success. On a related study, Guntly and Tauritz [15] proposed a centralized approach in addition to an approach similar to the one described above. The centralized approach relies on two preference vectors common to the whole population: one relative to genes set to 0 and one relative to genes set to 1. These vectors are accessed by individuals when evaluating mating candidates in a similar fashion as in the previous approach. The value of each gene is adapted at each selection step according to the relative success of the offspring.

Smorokdina and Tauritz [32] proposed a different approach where each individual encodes a mate choice function in addition to its own candidate solution to the problem at hand. This function is represented as a tree which is used to select a mating partner. The tree in each individual is initialized using only one terminal node which corresponds to the remaining of the population. As a non-terminal set, a number of selection operators can be used, which compare different metrics between mating candidates. Eventually the tree returns the preferred mating candidate. If the produced offspring shows enhancements then it inherits the tree used for evaluation from its parents, otherwise it inherits the product of recombination between the evaluation trees of both parents.

Mating preferences

As described above, many possible mating preferences have been applied by different researchers. Some of them focus on the similarity between the first parent and each mating candidate. A measure of similarity can be assessed either using genotypic [7, 8, 13, 26, 28, 29, 35] or phenotypic [13, 29] information.

Other metrics focus on characteristics of mating candidates such as previous reproductive success, fitness or age [29]. Characteristics can be compared to those of the first parent in an attempt to find a partner that complements it [16]. Often, when multiple metrics are applied they are combined through rules or functions. In some cases similarity measures are also combined with such metrics [29]. More interestingly are perhaps approaches where the first parent is able to perceive certain genotypic or phenotypic traits on mating candidates and selects the one that best matches its preferences. This is often accomplished by encoding mating preferences in each individual and comparing those preferences with traits displayed by each candidate [18, 25, 32, 34].

Gender roles

In nature, Mate Choice is almost absolutely on the side of females. Due to their high reproductive investment, they are picky when selecting a mating partner, looking for a fit male that can provide good genes. On the other hand males are more willing to mate with as many females as possible in an attempt to increase their number of offspring and benefit the presence of their genes in following generations. Looking back at Algorithm 1, *parent1* takes the female role while the mating candidates and therefore *parent2* take the male role.

There are different approaches in the literature to establish which individuals will take a female role or a male role. For instance, on some approaches a gender is attributed randomly to each individual at the beginning of each generation [14, 30] while in other cases gender is attributed alternatively when offspring are produced [35]. In such cases where each individual has a fixed role, females can be selected from their subpopulation using different strategies. In some cases all females are selected and produce offspring once [14], in other cases traditional selection operators are applied [35]. An alternative approach has each individual participating once as a female and once as a male in the parent selection process [18]. Mating candidates are selected from the males pool, often randomly. In other cases, all individuals in the population have the chance to play either role. In these cases, any individual can be selected as *parent1*, therefore for the role of female, and all the remaining can be selected as mating candidates, or for the role of male. In these cases it is popular to select females through traditional operators and males randomly. If an individual takes the role of female at a selection step, it could be selected as male on the next one and vice-versa.

1.3.2 Designing a nature-inspired Mate Choice approach

When designing Mate Choice approaches we feel that in order to best resemble the natural process, models should follow three nature-inspired rules:

1. individuals must choose who they mate with based on their own mating preferences
2. mating preferences, as mental traits, should be inherited the same way as physical ones
3. mate selection introduces its own selection pressure but is subject to selection pressure itself

We see the evaluation of mating candidates as a complex process, where the relation between observed traits, or their weight on each individual's mate choice mechanism is difficult to establish beforehand. While some traits could be seen as valuable on a mating candidate, others could turn out to be irrelevant or even harmful. The relation between them is also certainly not straightforward as they could be connected in unforeseeable ways. Moreover, certain displayed traits may be very important for survival purposes but hold little value for mate choice, or the other way around. This value can also vary on each selection step, depending on the characteristics of *parent1*, its mating preferences and the mating candidates involved.

This discussion is particularly relevant when we recall the following aspects of Sexual Selection through Mate Choice:

1. each individual has its own characteristics and may benefit differently from reproducing with different mates. Each individual also has its own distinct mating preferences that may value different characteristics in mating candidates. The reproductive success of individuals depends on choosing appropriate mating partners the same way that it depends on how attractive they are to others.
2. the paradigm may result on cases where individuals with poor survival abilities attain a high reproductive success because they display characteristics that are favoured by mating preferences. Their offspring may achieve low fitness values but may contribute to exploration and the emergence of innovation which may eventually turn into ecological opportunities.
3. the handicap principle shows that certain traits may risk the survival ability of individuals while in fact being indicative of good gene quality, thus reducing the accuracy of fitness values. Mate Choice mechanisms may be able to help increase the accuracy of mapping between phenotypes and fitness values and translate that into reproductive success.
4. mating preferences and evolved physical traits have an intrinsic and deep dependence between them which results from the feedback loop described in the theory of runaway sexual selection. The resulting arms race causes mating preferences to evolve in relation to displayed traits and physical traits to adapt in relation to enforced mating preferences. This process can lead traits to a high degree of elaboration.

With these ideas in mind and with the goal of designing mate choice mechanisms that best resemble the natural process, we refrain from establishing what are good or bad mating preferences. Also, we avoid linking each individual's candidate solution with its mating preferences using any pre-established method, such as inheritance rules. We therefore treat genetic material regarding physical traits and mating preferences equally and leave the responsibility of adapting individuals up to the evolutionary process. Inheritance and selection pressure should be able to bring reproductive and survival advantages to individuals carrying genes linked to appropriate phenotypes and mating preferences through the intrinsic relation between Natural Selection and Sexual Selection through Mate Choice.

The following subsections detail how we design Mate Choice approaches that meet the presented rules and aspects.

Representation

We propose a setup where each individual is composed by two chromosomes. The first one encodes a candidate solution to the problem at hand while the second chromosome encodes an individual's mating preferences, which it will use to assess potential mating partners. The first chromosome could use any representation wanted for the problem at hand, be it a Genetic Algorithm (GA) vector, a GP tree or others. We propose representing mating preferences, therefore the second chromosome, as a GP tree.

Mating preferences can be represented using two possible approaches: i) representing an ideal mating partner; ii) representing an evaluation function. The first approach requires that we are able to map GP representations to the phenotype space of the problem at hand. In this case, the terminal and non-terminal sets should be established accordingly, for instance, if we are using a GP representation for the candidate solutions in the first chromosomes, then we can use the same terminal and non-terminal sets. This approach can also be used if we rely on other representations in the first chromosome but there are know GP representations, as long as both representations map to the same phenotype space. The second approach requires that the individuals can extract characteristics from their mating candidates and evaluate them. The terminal set of the GP representation will be the evaluation of such characteristics. The non-terminal set will provide a number of operators that allows the creation of relations between characteristics into complex functions. At the end, in this approach, the second chromosome encodes a GP function that evaluates a number of characteristics on a mating candidate and through a number of operations linking different characteristics, produces an attractiveness value.

Evaluation

The two representation approaches rely on different evaluation mechanisms, however Fig. 1.3 shows a general view of the process. On the first approach, when an individual is assessing a mating candidate, an ideal mating partner according to that individual's preferences is mapped to the phenotype space and compared to the phenotype of the mating candidate. In order to do so, a similarity measure has to be established and used. The mating candidate that best resembles an ideal partner and therefore minimizes the metric used is selected as a mating partner. Notice that this is conceptually different from selecting mating partners so that the distance between parents is minimized or maximized. The behaviour resulting from this approach will be much different but the design effort required is actually quite similar. As long as there is a possible GP representation for the problem at hand, that can be used for the second chromosome and for evaluation to take place, only a similarity measure is required.

The second approach evaluates mating candidates in a different way. Instead of comparing each mating candidate to an ideal mating partner, it will evaluate them according to a number of displayed traits. Therefore, in order to design such an approach, we have to determine a perceptive system, or in other words, what characteristics can each individual observe on others. To do so, researchers have to rely on

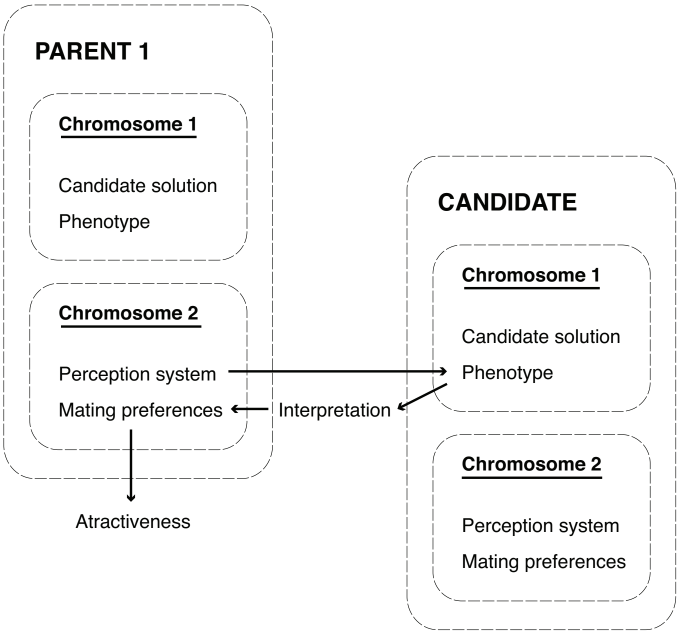

Fig. 1.3. Representation of mating preferences and evaluation of mating candidates

their own knowledge of the problem and determine what may or may not be relevant characteristics. This process often requires the deconstruction of the problem at hand and subdividing it on a set of simpler problems, or assessing simpler objectives that are implicit on the global fitness function. These characteristics will make up the terminal set, so that when an individual is evaluating a candidate, the terminal nodes on the GP tree representing its mating preferences will assume a numeric value representing how the candidate performs on the present characteristics. The operators included on the non-terminal set will determine how these values relate with each other and what weight they have on the mating preferences. Finally, the GP function returns a numeric value which represents the attractiveness of a mating candidate (Fig. 1.4 shows an example of a possible GP tree). The candidate that achieves the highest attractiveness is selected as a mating partner. This approach is more difficult to setup as it requires more knowledge from the person designing the system. However, the choice of relevant characteristics does not have to be perfect, the evolution process will be in charge of determining which are valuable, harmful or irrelevant. It has the advantage of not requiring a GP representation of the problem to be applicable.

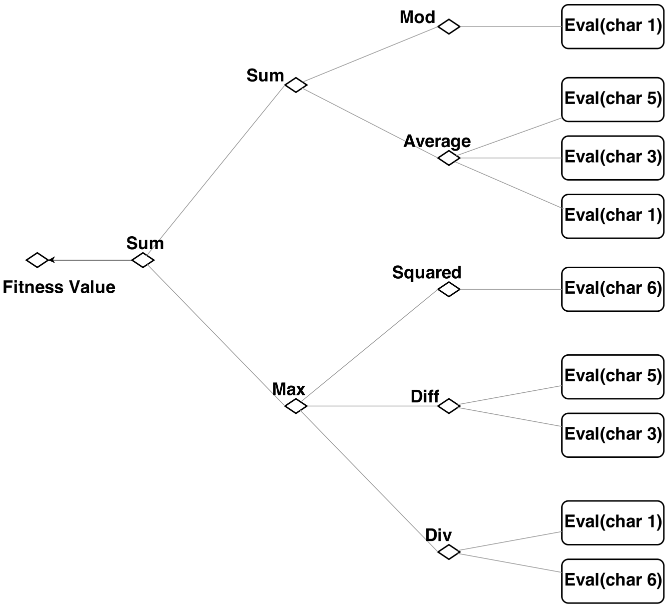

Fig. 1.4. Example of a GP tree combining a different characteristics to evaluate a mating candidate

Operators and Parameters

The Mate Choice mechanism has been mostly described, but a few questions remain. The first one regards selection the first parent and the mating candidates. In our approach we attribute gender roles during selection, meaning that any individual can play the role of female or male. As in many studies, we select females using a traditional operator which may be problem dependent. We usually select male mating candidates using a random operator. This way, any individual even if its survival ability is very low, has the chance of being evaluated by a female and, if attractive enough, may reproduce. All individuals are therefore subject to both natural and sexual selection through mate choice. They both have an impact on the number of offspring that each individual produces. Mate selection pressure is controlled by the size of the mating candidates set. A higher number of mating candidates means that more males will be competing for the same female causing less attractive individuals to have smaller chances of reproducing.

When two parents have been selected, two new offspring are generated by means of reproductive operators. In our setup we apply these operators independently at each chromosome. This decision not only allows different strategies to be applied to each of them, for instance if different representations are used, but also allows operators to be applied with different probabilities and parameters. This is beneficial since the two chromosomes may impact behaviour differently with the same operators and parameters. Regarding the mating preferences chromosome, we suggest applying either crossover or mutation exclusively and with a given probability. This means that new offspring may inherit a combination of the mating preferences of both its parents, a mutated version of the mating preferences of one of its parents, or in case neither crossover or mutation occurs the offspring will inherit the exact mating preferences of one of its parents [19]. Unlike previous studies [18, 32], we don't check the feasibility of new offspring to decide on how their mating preferences will be inherited. Finally, new offspring are inserted into the population of the following generation.

1.4 Applications

The presented Mate Choice setup has been previously applied to different problems, including real-world applications. We have had the chance to test both preference representation approaches and have also compared to a GA representation on a specific problem. The section discusses the obtained results and observed behaviour.

Applying Mate Choice to symbolic regression has probably been the easiest to setup [21]. Using a GP representation to tackle the problem allows us to rely on the same terminal and non-terminal sets on both chromosomes. This way, the first chromosome represents a candidate solution to the target function while the second chromosome represents an ideal mating partner, as described previously. In a nutshell, evaluation of mating candidates is quite similar to the standard evaluation of the phenotype of each individual, but instead of comparing the phenotype with the target function, it's compared to the ideal mating partner represented. The similarity measure applied was the same. The approach was tested on 6 setups with different characteristics, using a Tournament of 5 individuals to select the first parent which chooses its mate from a pool of 5 candidates.

Table 1.1. Mean Best Fitness obtained over 50 runs obtained with a standard, mate choice and random approaches on the symbolic regression of 6 functions

Function	Standard	Mate Choice	Random
Keijzer-1	0.008005462	**0.0059473756**	0.0072442644
Keijzer-2	0.0063776454	**0.0052139161**	0.0062104645
Keijzer-3	0.0071500245	**0.0056003145**	0.0067438776
Keijzer-4	0.0890397335	**0.0833904122**	0.0840754187
Koza-1	**0.0006384168**	0.0014386396	0.0006481816
Nguyen-5	0.0014892713	**0.0004783439**	0.0025763115

Table 1.1 shows the obtained results. The instances where the proposed approach performed statistically better than a standard one or the other way around are shown in bold (A Wilcoxon Mann Whitney test with a significance level of 0.01 was used). The Mate Choice approach was able to outperform the standard approach on all

instances of the problem except for the Koza-1 function. However, the Koza-1 approach is regarded as a particularly easy one [23], where the standard approach is able to convert faster and therefore gain advantage. Also, the Nguyen-5 instance relies on a large population, which may explain why both approaches were able to largely outperform the random approach, with the Mate Choice approach still achieving statistical differences from the standard one.

It is clear by observing the results of the random approach, where the mating candidate is selected randomly, that the evolution process benefits from a lower selection pressure on the problem set. An analysis of the behaviour of each approach, focusing on the Mean Cumulative Destructive Crossovers (MCDC) and Mean Cumulative Neutral Crossovers (MCNC) shows that they behave differently. The Mate Choice approach achieved consistently a smaller number of neutral crossovers (with statistical differences except for the Koza-1 function), which don't contribute to fitness enhancements. At the same time it performed a larger number of destructive crossovers, which reduce the fitness of the offspring when compared with their parents, with statistical differences. This behaviour suggests that Mate Choice focus more on exploration than exploitation in this particular scenario, whereas the standard approach promotes mating between the fittest individuals. This exploration seems to be important for the enhanced results as it helps avoid convergence and turns explored traits into ecological opportunities thus achieving better Mean Best Fitness (MBF) values. The approach also obtains lower MCNC and higher MCDC values consistently when compared with the random approach suggesting that the promoted behaviour is not similar to randomly selecting mating partners. A larger analysis of the behaviour is available [21].

Cluster Geometry Optimization (CGO) consists on finding the geometry of a cluster so that its potential energy is minimized. The problem is a NP-hard task [2] with important applications in Nanoscience, Physics, Chemistry and Biochemistry [38]. The problem provides a number of difficult test instances, from which we have tested the applicability of Mate Choice on Morse clusters ranging from 41 to 80 atoms [20]. We have coupled our setup with an evolutionary algorithm that has previously achieved state of the art results [27]. The initial approach relies on a steady-state population with a substitution mechanism that controls which offspring are allowed into the population. This mechanism is focused on maintaining diversity in the population as this is seen as a key factor when tackling CGO problems.

Each individual encodes the Cartesian coordinates of each particle in the cluster in the 3D space and evolve using GA operators. The Mate Choice setup adds a GP chromosome that allows each individual to evaluate mating candidates on a number of phenotypic features. When tackling the optimization of a Morse Cluster, each individual not only encodes a candidate solution to a N sized cluster but also to all $N-i$ instances. How an individual performs on each of these smaller instances may indicate good, bad or neutral genes, depending on the instance being optimized. It's up to the self-adaptive system to use this information in an appropriate way.

Table 1.2 shows the success rate on finding the putative optima on 30 runs for each instance using a tournament of 5 individuals to select the first parent and 5 mating candidates. A pairwise proportions test was used to test for significant differ-

Table 1.2. Success rate over 30 runs obtained by a standard and mate choice approaches on the cluster geometry optimization of morse 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
Mate Choice	**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
Mate Choice	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

ences [33] with a significance level of 0.01. Overall, out of 40 instances, the Mate Choice approach was able to achieve higher success rates on 20 instances, 4 of them with significant differences. Ties were found on 7 instances as well. A study on the impact of the Mate Choice approach on the behaviour of the algorithm focusing on population diversity as well as on the acceptance rate of the replacement operator has shown relevant differences from a standard approach.

The replacement operator has a powerful role on this problem as it determines which individuals are allowed in the population. If they are structurally similar (according to a distance measure) to one individual of the population, the fittest one is kept. If they are structurally dissimilar from all individuals, the offspring replaces the worst one as long as it has a better fitness. Otherwise the offspring is discarded. Therefore it is foreseeable that mating preferences will adapt so that new offspring can overcome these restrictions.

Results suggest that the algorithm has successfully done so, with an increase in the number of accepted individuals, both similar and dissimilar. Together, there has been an increase of roughly 50% on the cumulative average number of substitutions. While an increase in the acceptance rate of new offspring doesn't necessarily translate into a better performance it does show an adaptation to the replacement strategy. The results in Table 1.2 suggests that such a behaviour contributes to competitive and sometimes better success rates, which is corroborated by average fitness values along the generations.

An analysis of the average population diversity also shows behavioural differences. While the standard approach is able to reach a higher average diversity, the Mate Choice approach is able to maintain it steadier while at the same time conducting a much larger number of substitutions in the population. This effect may indicate that individuals produced by Mate Choice in this scenario have smaller but steadier impact, which seems beneficial on the population level. A more complete analysis on the behaviour of Mate Choice on the optimization of Morse Clusters is available [20].

A third application of our Mate Choice mechanism has been done on the problem of Packing Circles in Squares(CPS). This problem consists on finding the configuration of a set of circles of fixed radius so that they minimize the area of a containing square [22]. In order to represent candidate solutions to this problem, each individual encodes a vector of Cartesian coordinates representing the position of each circle, which is then mapped so that the area of the enclosing square is calculated. Our approach adds a GP chromosome that is used to assess characteristics on other individuals. Similarly to the CGO problem, we have divided the problem into several subproblems, in this case, for the instance of packing N circles, we assess how an individual performs on each $N-i$ instance.

Therefore, the GP functions are initialized using a terminal set composed by such characteristics and a number of arithmetic operators to combine them. Once again, performing well on a given instance may be an indication of either good, bad or neutral genes. The approach was compared to a standard approach, an approach where mating partners are selected randomly from the candidates set and a third approach where the mate evaluation function was encoded using GAs. The GA approach assesses all $N-i$ characteristics on mating candidates and combines them on a weighted sum. Each individual's second chromosome encodes therefore a set of weights, one for each characteristic and representing that characteristic's impact on the Mate Choice process. We expect the algorithm to evolve appropriate weights, either negative, close to zero or positive, according to the weight of each characteristic.

Table 1.3. Mean Best Fitness over 30 runs obtained with a standard, random, mate choice with GA representation and mate choice with GP representation on the packing of N circles in squares

				Mate Choice	
N	Optimal	Standard	Random	GA	GP
2	3.4142	3.4142	3.4142	3.4142	3.4142
3	3.9319	3.9320	3.9320	3.9319	3.9319
4	4.0000	4.0266	4.0001	4.0255	4.0001
5	4.8284	5.0056	4.9911	**4.9250**	**4.9475**
6	5.3282	5.3669	5.3674	5.3685	5.3804
7	5.7321	5.8227	5.8081	5.8296	5.8098
8	5.8637	6.0212	5.9615	5.9913	5.9898
9	6.0000	6.5184	6.4907	6.5401	6.5154
10	6.7474	6.8936	6.8854	6.9110	**6.8536**
11	7.0225	7.1619	7.1764	7.2232	7.1564
12	7.1450	7.3966	7.3565	7.4809	7.3438
13	7.4630	7.8088	7.8167	7.8355	**7.7147**
14	7.7305	8.0705	8.0950	8.1509	**8.0048**
15	7.8637	8.3324	8.4173	8.4345	**8.2581**
16	8.0000	8.7014	8.8632	8.8153	**8.6012**
17	8.5327	8.8765	9.2345	9.0836	8.8665
18	8.6564	9.0996	9.4966	9.2724	9.0984
19	8.9075	9.4442	9.9422	9.6036	**9.3511**
20	8.9781	9.7212	10.2839	9.7641	**9.6030**
21	9.3580	9.9788	10.7402	10.1307	9.9425
22	9.4638	10.2610	11.0512	10.3705	10.2693
23	9.7274	10.5201	11.5476	10.6498	10.5892
24	9.8637	10.7725	11.8382	10.8163	10.8034

Experiments were conducted on problem instances using 2 to 24 circles. The first parent was selected using a tournament of 5 individuals and sets of 5 mating candidates. Table 1.3 shows the MBF over 30 runs obtained by each approach. The GP based approach was able to achieve better results on 18 out of 23 instances, 8 of which with statistical differences (using a Wilcoxon Mann Whitney test with a significance level of 0.05) while the GA based approach performed better on 4 instance, 1 of which with statistical significant differences. The results achieved by the random approach suggest that the algorithm may benefit from a smaller selection pressure on most of the instances. The results obtained by the GA approach were disappointing as it was expected that it would be able to make a better use of the information provided or at least evolve into the original fitness function and therefore achieve results closer to the standard approach.

The results obtained by the GP approach suggest that the approach was able to make good use of the information provided about mating candidates and build appropriate functions to select mating candidates, which are likely to be radically different from the weighted sum designed by us using our knowledge of the problem. We believe that we would unlikely be able to design mating evaluation functions capable of matching the ones evolved by the GP approach. A larger analysis on the application of Mate Choice on the CPS problem is available.

Apart from the presented analysis on performance and behaviour of the Mate Choice setup on the three addressed scenarios, there are a two observations that are transversal and should be discussed. The first one regards the overhead of the setup, which results from the need to evaluate mating candidates using preferences specific to each individual. While on the first approach, based on ideal mating partners, this overhead depends on the metric being used, on the second approach it depends on the characteristics being evaluated. On the first approach, each candidate is evaluated once at each selection step as it is being compared to an ideal mating partner. On the second approach, individuals share what characteristics they can see in mating partners, therefore when a candidate is evaluated on a given characteristics, that process doesn't have to be repeated. The effort also depends on the mating preferences present in the population at each generation. This makes estimating an overhead for the Mate Choice operator a hard task. The second observation regards the complexity of the evolved GP functions, which makes it extremely difficult to assess exactly how individuals are evaluating others, which characteristics they value or not. Figure 1.4 shows what a GP tree representing a mating evaluation function may look like, however they can be much larger in size. Still, the example is enough to show that while we can see what characteristics are present, it is extremely difficult to assess exactly what role they play in the function. Some of them may be extremely relevant while others may be approximately neutral. Moreover, these functions are different from individual to individual and may vary drastically over the evolution process so that certain characteristics can be important at the beginning and others at the end, or may have different importance to each individual. What we can assess however is that we would unlikely be able to design such evaluation functions by hand and that they are radically different from previously used functions. The results suggest that despite how they work, these functions are making a good use of the information that they assess on mating candidates.

1.5 Synthesis

Sexual Selection through Mate Choice has been first proposed by Darwin to explain animal characteristics that didn't seem to fit in his theory of Natural Selection such as extravagant ornamentation and complex courtship behaviour. The theory, while being mostly rejected by the active research community at the time, eventually was able to gain the attention of researchers in multiple fields that have contributed with supporting evidence over the years. Nowadays Sexual Selection through Mate Choice is highly regarded by the scientific community as an important player in the evolution of species.

Despite the success of the theory on other fields, the impact of Mate Choice in the field of Evolutionary Computation is still very small, and a large number of questions remain unanswered regarding its design, implementation, behaviour and potential benefits. Several authors have proposed various approaches inspired by Mate Choice and have tackled multiple problems with more or less success. We have addressed a framework common for Mate Choice approaches and have reviewed important contributions through a classification studies based on their adaptation mechanisms. We have also covered preference choices and gender role attribution mechanisms.

We finally propose a nature-inspired Mate Choice setup. First we discuss relevant aspects of Mate Choice in nature, propose 3 nature-inspired rules and follow up by covering design choices such as representation, evaluation, operators and parameters. The use of an extra chromosome to encode a GP tree to encode mating preferences following two possible approaches was discussed as well as how it can be used to evaluate mating partners and take part of the evolution process.

We present a discussion on the application of Mate Choice on three problems and assess the behaviour of the algorithm. The discussed approaches differ drastically in behaviour from standard selection approaches as well as from an approach where the mating partner is selected randomly. The differences in behaviour impact performance as well as diversity, exploration and exploitation. A comparison with a self-adaptive Mate Choice approach based on a GA representation is also included and the differences discussed. Finally it's argued that assessing the overhead caused by this selection process is a difficult task and that the inner-workings of the evolved Mate Choice functions are very complex, making it extremely difficult to see which are relevant or irrelevant mating preferences. Still, the reported results suggest that the evolved GP functions are able to use the provided information in meaningful and beneficial ways. It is however unlikely that we would be able to design them by hand.

References

1. Malte B Andersson. *Sexual selection.* Princeton University Press, 1994.

2. Longjiu Cheng, Yan Feng, Jie Yang, and Jinlong Yang. Funnel hopping: Searching the cluster potential energy surface over the funnels. *The Journal of chemical physics*, 130(21):214112, 2009.
3. Helena Cronin. *The ant and the peacock: Altruism and sexual selection from Darwin to today*. Cambridge University Press, 1993.
4. C. Darwin. The origin of species, 1859.
5. C. Darwin. *The descent of man and selection in relation to sex*. John Murray London, 1906.
6. Charles Darwin and Alfred Wallace. On the tendency of species to form varieties; and on the perpetuation of varieties and species by natural means of selection. *Journal of the proceedings of the Linnean Society of London. Zoology*, 3(9):45–62, 1858.
7. Susmita De, Sankar K Pal, and Ashish Ghosh. Genotypic and phenotypic assortative mating in genetic algorithm. *Information Sciences*, 105(1):209–226, 1998.
8. Carlos Fernandes and Agostinho Rosa. A study on non-random mating and varying population size in genetic algorithms using a royal road function. In *Evolutionary Computation, 2001. Proceedings of the 2001 Congress on*, volume 1, pages 60–66. IEEE, 2001.
9. Carlos Fernandes, Rui Tavares, Cristian Munteanu, and Agostinho Rosa. Using assortative mating in genetic algorithms for vector quantization problems. In *Proceedings of the 2001 ACM symposium on Applied computing*, pages 361–365. ACM, 2001.
10. R.A. Fisher. The evolution of sexual preference. *The Eugenics Review*, 7(3):184, 1915.
11. R.A. Fisher. The genetical theory of natural selection. 1930.
12. Rodney Fry, Stephen L Smith, and Andy M Tyrrell. A self-adaptive mate selection model for genetic programming. In *Evolutionary Computation, 2005. The 2005 IEEE Congress on*, volume 3, pages 2707–2714. IEEE, 2005.
13. Severino Galan, O Mengshoel, and Rafael Pinter. A novel mating approach for genetic algorithms. *Evolutionary computation*, 21(2):197–229, 2013.
14. Kai Song Goh, Andrew Lim, and Brian Rodrigues. Sexual selection for genetic algorithms. *Artificial Intelligence Review*, 19(2):123–152, 2003.
15. Lisa M Guntly and Daniel R Tauritz. Learning individual mating preferences. In *Proceedings of the 13th annual conference on Genetic and evolutionary computation*, pages 1069–1076. ACM, 2011.
16. Robert Hinterding and Zbigniew Michalewicz. Your brains and my beauty: parent matching for constrained optimisation. In *Evolutionary Computation Proceedings, 1998. IEEE World Congress on Computational Intelligence., The 1998 IEEE International Conference on*, pages 810–815. IEEE, 1998.
17. Robert Hinterding, Zbigniew Michalewicz, and Agoston E Eiben. Adaptation in evolutionary computation: A survey. In *Evolutionary Computation, 1997., IEEE International Conference on*, pages 65–69. IEEE, 1997.
18. Ekaterina A Holdener and Daniel R Tauritz. Learning offspring optimizing mate selection. In *Proceedings of the 10th annual conference on Genetic and evolutionary computation*, pages 1109–1110. ACM, 2008.
19. JohnR. Koza. Genetic programming as a means for programming computers by natural selection. *Statistics and Computing*, 4(2):87–112, 1994.
20. António Leitão and Penousal Machado. Self-adaptive mate choice for cluster geometry optimization. In Christian Blum and Enrique Alba, editors, *Genetic and Evolutionary Computation Conference, GECCO '13, Amsterdam, The Netherlands, July 6-10, 2013*, pages 957–964. ACM, 2013.
21. António Leitão, Jose Carlos Neves, and Penousal Machado. A self-adaptive mate choice model for symbolic regression. In *IEEE Congress on Evolutionary Computation*, pages 8–15, 2013.

22. Penousal Machado and António Leitão. Evolving fitness functions for mating selection. In Sara Silva, James A. Foster, Miguel Nicolau, Penousal Machado, and Mario Giacobini, editors, *Genetic Programming – 14th European Conference, EuroGP 2011, Torino, Italy, April 27-29, 2011. Proceedings*, volume 6621 of *Lecture Notes in Computer Science*, pages 227–238. Springer, 2011.
23. James McDermott, David R White, Sean Luke, Luca Manzoni, Mauro Castelli, Leonardo Vanneschi, Wojciech Jaskowski, Krzysztof Krawiec, Robin Harper, Kenneth De Jong, et al. Genetic programming needs better benchmarks. In *Proceedings of the fourteenth international conference on Genetic and evolutionary computation conference*, pages 791–798. ACM, 2012.
24. Geoffrey F Miller. Exploiting mate choice in evolutionary computation: Sexual selection as a process of search, optimization, and diversification. In *Evolutionary Computing*, pages 65–79. Springer, 1994.
25. Geoffrey F Miller and Peter M Todd. Evolutionary wanderlust: Sexual selection with directional mate preferences. In *From Animals to Animats 2: Proceedings of the Second International Conference on Simulation of Adaptive Behavior*, volume 2, page 21. MIT Press, 1993.
26. Gabriela Ochoa, Christian Mädler-Kron, Ricardo Rodriguez, and Klaus Jaffe. Assortative mating in genetic algorithms for dynamic problems. In *Applications of Evolutionary Computing*, pages 617–622. Springer, 2005.
27. Francisco B Pereira and Jorge MC Marques. A study on diversity for cluster geometry optimization. *Evolutionary Intelligence*, 2(3):121–140, 2009.
28. Michael Ratford, AL Tuson, and Henry Thompson. An investigation of sexual selection as a mechanism for obtaining multiple distinct solutions. *Emerg. Technol*, 1997.
29. Michael Ratford, Andrew Tuson, and Henry Thompson. The single chromosome's guide to dating. In *In Proceedings of the International Conference on Artificial Neural Networks and Genetic Algorithms*. Citeseer, 1996.
30. José Sánchez-Velazco and John A Bullinaria. Gendered selection strategies in genetic algorithms for optimization. *survival*, 8(6):11, 2003.
31. Josīe Sīanchez-Velazco and John A Bullinaria. Sexual selection with competitive/co-operative operators for genetic algorithms. 2003.
32. Ekaterina Smorodkina and Daniel Tauritz. Toward automating ea configuration: the parent selection stage. In *Evolutionary Computation, 2007. CEC 2007. IEEE Congress on*, pages 63–70. IEEE, 2007.
33. Éric D Taillard, Philippe Waelti, and Jacques Zuber. Few statistical tests for proportions comparison. *European Journal of Operational Research*, 185(3):1336–1350, 2008.
34. Peter M Todd and Geoffrey F Miller. Biodiversity through sexual selection. In *Artificial life V: Proceedings of the Fifth International Workshop on the Synthesis and Simulation of living Systems*, volume 5, page 289. MIT Press, 1997.
35. Mohammad Jalali Varnamkhasti and Lai Soon Lee. A genetic algorithm based on sexual selection for the multidimensional 0/1 knapsack problems. In *International Journal of Modern Physics: Conference Series*, volume 9, pages 422–431. World Scientific, 2012.
36. George C Williams and Austin Burt. *Adaptation and natural selection*. na, 1997.
37. A. Zahavi. Mate selection–a selection for a handicap. *Journal of theoretical Biology*, 53(1):205–214, 1975.
38. Jijun Zhao and Rui-Hua Xie. Genetic algorithms for the geometry optimization of atomic and molecular clusters. *Journal of Computational and Theoretical Nanoscience*, 1(2):117–131, 2004.