Multimodal Optimization by Means of a Topological Species Conservation Algorithm

Catalin Stoean, *Member, IEEE,* Mike Preuss, *Member, IEEE,* Ruxandra Stoean, *Member, IEEE,* and D. Dumitrescu

***Abstract*—Any evolutionary technique for multimodal optimization must answer two crucial questions in order to guarantee some success on a given task: How to most unboundedly distinguish between the different attraction basins and how to most accurately safeguard the consequently discovered solutions. This paper thus aims to present a novel technique that integrates the conservation of the best successive local individuals (as in the species conserving genetic algorithm) with a topological subpopulations separation (as in the multinational genetic algorithm) instead of the common but problematic radius-triggered manner. A special treatment for offspring integration, a more rigorous control on the allowed number and uniqueness of the resulting seeds, and a more efficient fitness evaluations budget management further augment a previously suggested naïve combination of the two algorithms. Experiments have been performed on a series of benchmark test functions, including a problem from engineering design. Comparison is primarily conducted to show the significant performance difference to the naïve combination; also the related radius-dependent conserving algorithm is subsequently addressed. Additionally, three more multimodal evolutionary methods, being either conceptually close, competitive as radius-based strategies, or recent state-of-the-art are also taken into account. We detect a clear advantage of three of the six algorithms that, in the case of our method, probably comes from the proper topological separation into subpopulations according to the existing attraction basins, independent of their locations in the function landscape. Additionally, an investigation of the parameter independence of the method as compared to the radius-compelled algorithms is systematically accomplished.**

***Index Terms*—Evolutionary algorithms, function optimization, landscape detection, multimodal optimization, species conservation.**

I. Introduction

MOST OF THE black-box real-world problems considered to be difficult are multimodal. Hence, any optimization technique applied in this area should be able to discover several solutions, namely located in a number of basins of attraction. This enables decision makers to choose from multiple distinct solutions to a problem and, at the same time, increases confidence to have attained the global optimum. Canonical evolutionary algorithms (EA)—despite usually being population-based—have the property of converging to a population that contains only one solution and small variations of it (genetic drift) [1], [2]. In the best case, the fittest obtained solution represents the global optimum, but it may also happen that it only refers to a local optimum in which the search process is confined. In order to achieve an explorative search, EAs that perform multimodal optimization have to either apply multistart techniques or maintain a high diversity in the population with the purpose of searching within many different locations in parallel. Every multimodal optimization method has to consequently satisfy two partly conflicting tasks: to locate the global optimum out of multiple local peaks and to find a set of several good solutions for variety and insights into the problem space.

There have been several attempts for transforming EAs so that they could deal with multimodal fitness landscapes (e.g., [1], [3]–[11]). However, when tailoring such an EA, there are a number of issues to be tackled: 1) how to divide the population into subpopulations; 2) how to preserve these subpopulations in order to avoid the genetic drift; and 3) how to eventually connect them to the existing optima within the fitness landscape. Most techniques for the detection of multiple attraction basins (niching) form subpopulations by appointing a radius such that all individuals within the same species lie at a distance from each other that is lower than the given threshold (they are highly similar). The value that has to be selected for the radius directly depends on the fitness landscape, i.e., on the problem to be solved, whereas its proper choice is crucial in assuring accurate results. Deb and Goldberg [12] proposed a very precise approximation for this parameter, however, especially for real-world applications, the information on the fitness landscape required by the formula is not available beforehand and, therefore, in such situations, it cannot be used. Additionally, it makes the assumption of equally sized, roughly spherically shaped basins of attraction.

In this respect, the present paper proposes a novel evolutionary method for multimodal optimization that does not employ a radius for distinguishing between different species. In order to detect if two individuals belong to the same subpopulation, the approach makes use of their fitness evaluations and of those of some intermediary assigned candidates to provide an overview on their position. More importantly, this alternative

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C. Stoean and R. Stoean are with the Department of Computer Science, Faculty of Mathematics and Computer Science, University of Craiova, Craiova 200585, Romania (e-mail: catalin.stoean@inf.ucv.ro; ruxandra.stoean@inf.ucv.ro).

AQ:1 M. Preuss is with the Department of Computer Science, Dortmund University of Technology, Dortmund 44227, Germany (e-mail: mike.preuss@cs.uni-dortmund.de).

D. Dumitrescu is with the Department of Computer Science, Babes-Bolyai University, Cluj-Napoca 400084, Romania (e-mail: ddumitr@cs.ubbcluj.ro).

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triggers flexibility as regards the formation of the species within attraction basins of different sizes. Multiple optima maintenance is conducted through the preservation of several distinct solutions. Each species is concentrated on a seed, which represents the fittest individual of the species. The seeds from all species are copied from one generation to another so that no important regions are lost through selection and variation operators. The species masters are then updated at each cycle, by once more appointing their fittest inner individuals.

The manner of detecting whether two individuals follow different peaks or not was initially proposed in [5] and [13], within the multinational genetic algorithm (MGA), but the complete mechanism proved to be very expensive as regards the number of fitness evaluations necessary to converge to the solution [14]. On the other hand, the idea of species conservation first appeared in [6], however, subpopulation differentiation is powered by a radius.

A first attempt to unite the seed preservation and the fitness landscape inspection through a straight integration was the topological species conservation (TSC) approach in [14]. However, the method presented here (TSC2) is significantly improved as it reconsiders the species management to save precious evaluations and accelerate convergence into the basins. Experimentation finally demonstrates its superiority over the initial naïve combination.

The comparison is conducted on several functions that have at least two variables—in order to observe how the optimal peaks are disposed within the landscape—and up to 20, as most real-world problems are multidimensional. The multimodality conditions range from one optimum (the method must still not fail to perform well in the unimodal case) to many global or local peaks environments. Also, a multimodal problem that bears relationship to a generalized real-world application of engineering design is chosen as a test instance. In order to achieve an objective validation, the results obtained by the novel technique are put against those of two other related and recently proposed multimodal EAs [6], [7], the outcomes of a niching strategy [15], and those of a crowding (thus nonradius-based) approach [11]. To demonstrate the important differences to the preliminary integration in [14], TSC2 is also compared to the original TSC.

The paper is organized as follows. The next section briefly describes some of the traditional evolutionary approaches for multimodal optimization and several new ones that are relevant from the point of view of the design and objectives of proposed technique. The novel method TSC2 is presented in detail in Section III, also highlighting the differences to TSC. Section IV reports on the experimental results comparing to the algorithms named above, and Section V concludes the paper.

II. Evolutionary Speciation Techniques for Multimodal Optimization

In nature, an ecosystem is usually composed of regions (niches) that exhibit different characteristics and allow the formation and maintenance of different types of species. Commonly, the individuals in a species share similar biological features that allow them to coexist in their niches, capable of interbreeding among themselves, but unable to breed with individuals from different species. Each niche is usually populated by a number of individuals that directly depends on the amount of resources the niche provides.

Analogously, in an artificial system, each niche is related to an optimum of the fitness landscape and the resident species contains, in the best case, only individuals being located in the basin of attraction of that peak. In this respect, niching or speciation methods have been proposed for the simultaneous evolution of subpopulations.

A. Radius-Based

The best known niching method is the sharing approach that was initially introduced by Holland [8] and subsequently improved by Goldberg and Richardson [4]. The population is split into several species by taking into account the similarity between individuals. A sharing function modifies the fitness of an individual to be dependent on the number of potential solutions that exist within the same subpopulation. Within the species conserving genetic algorithm (SCGA) in [6], the fittest individuals that are more distant from each other than a predefined radius are set as seeds of their subpopulations. All other individuals (that are not seeds) are each appointed to belong to the subpopulation of the fittest individual that is found within the given radius. The seeds are conserved from one generation to another in order to avoid the risk of extinction following the application of variation operators and they are updated every generation. The SCGA elitist idea of transferring the seeds of each subpopulation from one generation to another is also adopted in the technique proposed herein.

Dynamic fitness sharing (DFS) is introduced in [7]. The technique uses a radius for separating the population into species, allows for a fixed minimum value (of two individuals) for the size of a subpopulation and has, like in the case of SCGA, a dominating individual called the *species master*. This is considered to be the member of the species that has the highest raw fitness value. Within DFS, the subpopulations are identified in each generation using the distance between individuals, while comparing it to the radius threshold. Fitness sharing is employed to compute the weighted fitness of each individual. A species elitist strategy is employed to ensure the conservation of the most prolific individual in each subpopulation from a generation to the other.

The niching variant of the covariance matrix adaptation-evolution strategy (CMA-ES) of Hansen and Ostermeier [16] was introduced by Shir and Bäck [17]. Using a fixed given radius, the population is split into species by means of a technique named dynamic peak identification, so that a predefined number of q niches is generated. This largely resembles a parallel execution of several independent hillclimbers at different locations, separated by a distance of at least the given radius. On recommendation of the authors of [10] who also provided source code for the method, a niching CMA-ES based on q separate $(1+10)$-CMA-ES is employed. These have been proposed by Igel *et al.* [18], are extremely simple and cope well with populations of only one parent individual. The CMA-ES parameters have been shown to be very robust toward many forms of distortion of the optimized function, e.g., rotation (see the invariance discussion in [19]). However, no investigation of the niching parameters is found in literature. Note that the abbreviation niching covariance matrix adaptation-evolution strategy (NCMA-ES) or simply NCMA will be used for this algorithm in the following references as it has not been labeled by the authors.

B. Radius Determination

As already mentioned earlier, Deb and Goldberg [12] suggested a way of computing the value for the σ_{share} radius in charge of subpopulations differentiation, which has been afterwards embraced by most of the researchers dealing with such parameters. It uses the radius of the smallest hypersphere containing feasible space, which is given as

$$r = \frac{1}{2}\sqrt{\sum_{i=1}^{D}(x_i^u - x_i^l)^2}. \quad (1)$$

In (1), D represents the number of dimensions of the problem at hand and x_i^u and x_i^l are the upper and lower bounds of the ith dimension. Knowing the number of existing global optima N_G and being aware that each niche is enclosed by a D-dimensional hypersphere of radius r, the niche radius σ_{share} can be estimated as

$$\sigma_{\text{share}} = \frac{r}{\sqrt[D]{N_G}}. \quad (2)$$

The main drawback in using (2) for obtaining a suitable radius value is that it is practically impossible to know in advance the number of optima that exist within the fitness landscape. Moreover, if their attraction basins have different sizes and are irregularly disposed within the fitness landscape, then one fixed value for the radius, even if accurately determined, is not sufficient for finding and maintaining the different optima.

C. Nonradius-Based

Cavicchio's dissertation [9] was one of the first attempts to use niching within genetic algorithms, by introducing a procedure called *preselection*. This presumed that each obtained offspring had to fight for survival with the weakest parent. Five years later, De Jong generalized Cavicchio's work by creating *crowding* [3]. A subset of the current population is chosen for every offspring, which subsequently replaces its most similar individual within the selected subpopulation. Variants like deterministic crowding [20] or probabilistic crowding [21] followed. The main difference between them lies in the way the replacement of the closest individual is performed, either in a deterministic or probabilistic fashion. Crowding was integrated within various evolutionary approaches with the aim of maintaining population diversity, for instance as a part of differential evolution in [11], where a very competitive approach for multimodal optimization was obtained.

Within other approaches like the island or cellular models [1], the main idea is to simply separate subsets of individuals from the population as impelled by selection and variation operators. Having several subpopulations that evolve in parallel without any connectivity between them is equivalent to running the same EA several times, i.e., the search process could be driven to a different location in the search space each time. This is the reason why, within the island model, different subpopulations exchange individuals after a certain number of generations. In a cellular model, the population is split into a number of subregions (or neighborhoods) that are distributed within algorithmic space. This is achieved by considering that each individual lies on a different point on a grid and selection and recombination take place only between neighbors. Note that search space topology and grid topology are generally entirely distinct as no measures are taken to generate a certain covering of the search space. Approaches like the island or cellular models keep population diversity for a longer period than others, but have the main disadvantage that recombination may take place between very different genotypes. It is for this reason that the commonly employed evolutionary techniques, like niching or crowding and other variations of them, take into consideration distance within the genotypic space for establishing reproduction areas.

An original approach that does not make use of a radius and distances between genotypes when separating individuals into subpopulations was developed by Ursem [5], [13]. The MGA detects if two individuals track the same optimum by considering a set of additional candidate solutions in-between and testing if any of these is weaker than the chosen pair. If this is true, a valley between the individuals is assumed and consequently, they are supposed to follow different peaks and will be distributed into different subpopulations. The hill-valley detector unburdens the EA of using a radius and gains precision and ability to overcome the irregularities in basin formation within the fitness landscape. However, in practice, the overall MGA is a high *consumer* of fitness evaluations [14].

A final interesting alternative to radius-based paradigms is brought by the cultural algorithms [22]. They determine multimodality by establishing dual populations in which a belief space supports contributions and in turn influences future populations of individuals, which are parallelized by fuzzy clustering means [23].

III. Topological Species Conservation Version 2

Our modified algorithm, TSC2, inherits the ideas of SCGA of establishing and conserving a dominating individual (seed) for every species. At the same time, subpopulations differentiation is performed through the use of the MGA component to distinguish between basins of attraction. Seed dynamics are furthermore controlled, both as replication and exploration are concerned, but also with respect to the economy of fitness evaluations that are caused by the inner workings. A naïve integration was introduced in [14] as the TSC and provides the starting point for improvements described herein. Although an experimentally confirmed competitive multimodality detector in the field, TSC lacks computational efficiency. Therefore, the current TSC2 aims to become a method for species differentiation based on the fitness landscape topology that uses fitness evaluations much more economical.

A. Motivation

The efficiency of the SCGA method lies in its elitism. Subpopulations cannot be completely lost, even if selection may leave out all individuals within one species or they may disappear because of recombination and mutation. Conservation of the seeds in the found species prevents them from going extinct. However, SCGA uses no particular mating selection mechanism and thus, after some generations, most of the individuals belong to those subpopulations that are connected to the fittest regions in the search space. The local optima are very likely to be followed exclusively by species containing solely the seed, which is basically conserved from one generation to another. Therefore, the seeds stagnate near local optima, without further improvement. In order to avoid this situation, TSC2 employs a shared fitness for mating selection and, as a consequence, each optimum possesses a subpopulation size proportional to its fitness.

The radius-dependent trigger to differentiate subpopulations has been abandoned in favor of an approach that employs fitness discrepancies (as in MGA) mainly for two reasons.

1) We get rid of a crucial parameter whose proper value is very difficult to set, especially in higher dimensional problems.
2) A more flexible technique is obtained that fits the subpopulations better to the attraction basins of different sizes. Less performant individuals that are merely different enough from the others are not put into distinct species. This is obvious especially for vast plateaus contained in the fitness landscape or for optima that have very large basins of attraction. While the SCGA method would form a great number of subpopulations, depending on the value for the radius, the MGA module detects only one peak to follow.

However, the expensive behavior of the original MGA while detecting distinct basins of attraction is avoided. By incorporating the preservation of diversity through seed conservation and efficiently keeping track of each individuals subpopulation during evolution, TSC2 can deal with a much smaller budget of fitness evaluations.

Consequently, it borrows strength, while simultaneously solves inefficiencies from both these powerful methods. The SCGA has the weakness in the use of a radius, whereas the MGA has a very expensive underlying idea, if fitness evaluation calls are counted.

In TSC2, distance computations between individuals now replace several expensive fitness calls. The number of seeds is restricted to a percentage of the population within TSC2, a restraint that did not appear either within the early integration, or in SCGA. This is very important for the highly multimodal functions, where an increased number of seeds is formed even from the early stages of the EA. If such a limit for the potential number of subpopulations were not imposed, the entire population could be transformed into seeds and thus the search blocks into local optima. Finally, TSC2 forbids the existence of clone seeds, and descendants are allowed to form their own species, adding more explorative power to the search, as opposed to TSC.

B. Mechanics

Within the TSC2 technique, the main characteristics of a species become the following.

1) An individual can belong to only one species.
2) In the ideal case, all individuals within one species lie in the basin of attraction of the same optimum. This certitude very much depends on the number of intermediary individuals that are considered for the verification of multimodality.
3) Each species has a seed, which is represented by the fittest individual of that subpopulation.
4) For each species, i.e., for all individuals it contains, a unique positive integer value is assigned as ID (i.e., identification). The purpose of the ID is to avoid the repetition of the multimodal verification over the generations.

The method does not employ a radius for separating subpopulations, however, at certain times it makes use of the dissimilarity between individuals, with the purpose of reducing the number of consumed fitness evaluations. In order to further outline the formation of subpopulations, the mechanisms of the *detect-multimodal* component need to be explained first.

1) *Detect-Multimodal Method:* The verification of whether two points in the search space track the same optimum or not is performed through an approach that was originally referred to as the *hill-valley* mechanism [5], but which, for reasons of clarity, is herein renamed to *detect-multimodal*. The function takes two individuals (points) as arguments and returns whether there is a valley between them in the fitness landscape or not, i.e., they follow different peaks or on the contrary. In the following, maximization is assumed, but the method may be easily changed into one dealing with minimization problems.

In order to reach a decision, a set of interior points between the two given as arguments is generated. The interior points are chosen based on user-defined gradations in the (0, 1) interval. If the fitness values of all interior points are higher than the minimal fitness of the two tested individuals, then it is concluded that they track the same optimum. On the other hand, if there exists such a point whose fitness is smaller than the minimal fitness of the two, then it is assessed that they follow different peaks. The mechanism is described in Algorithm 1. $f(x)$ denotes the fitness evaluation of individual x and it is supposed that it has to be maximized.

In conclusion, *detect-multimodal* returns true if the two points follow different optima and false if they track the same peak.

The value for the *number of gradations* variable in Algorithm 1 actually coincides with the number of interior points that are considered. The vector $gradation_j$ contains equally distant values in the (0, 1) interval. If an individual with a fitness evaluation value that is smaller than the minimal performance of the two initial points is found, the method stops and returns *true* (lines 7–9). As a consequence, the interior points are all evaluated only if the individuals follow the same peak or when it is only the final point that has the evaluation smaller than the minimal fitness of the two.

Algorithm 1 Detect-Multimodal Mechanism Between Two Individuals x and y

$i = 1$;
found = FALSE;
while $i <$ *number of gradations* and not *found* **do**
  for $j = 1$ to D **do**
    $interior_j = x_j + (y_j - x_j) \cdot gradation_j$;
  end for
  if $f(interior) < min\{f(x), f(y)\}$ **then**
    found = TRUE;
  end if
  $i = i + 1$;
end while
return *found*;

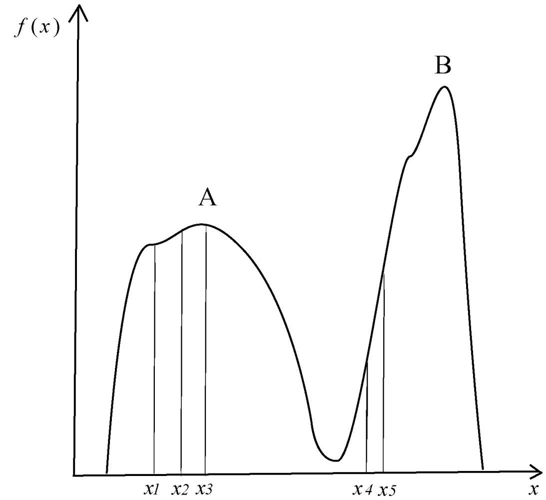


Fig. 1. Valuable individuals could vanish if not conserved.

Although robust, this mechanism makes an algorithm more expensive in terms of the number of fitness evaluations, as observed in MGA and TSC [14]. To counteract its effect, a free individual is checked against the seeds in increasing distance order to minimize the number of calls to the *detect-multimodal* procedure.

An important advantage of this manner of detecting multimodality is that it avoids the existence of several subpopulations assigned to follow a certain optimum, as it happens when the radius-based mechanism of species conservation is used. Instead, it assumes the connection of a subpopulation to only one peak, regardless of the size of the basin of attraction of that optimum.

Conversely, when TSC2 deals with a spiny function, with large increments followed by small decrements before rising again, the currently inflicted upper bound for the number of seeds prevents the entire population from being transformed (blocked) into species masters. This blockage would appear as a result of *detect-multimodal* being in charge of establishing them. But, with this limit, only a small part of the population is chosen as seeds. If other good solutions are subsequently found, each is assigned to the closest existing seed (according to the genotype) and, if fitter than the latter, it becomes the current species seed in the next generation.

2) *Conservation—Is It Necessary?:* In every generation, there are a certain number of species, each having its dominating individual and following a different peak. On the one hand, a weighted mating selection is employed, resulting that the fitness of each individual is divided by the size of the species it belongs to. This gives a greater chance to escape extinction to species that have only few individuals, just like in Goldberg and Richardson's fitness sharing [4].

On the other hand, this precaution measure is not always sufficient, as there may exist subpopulations with few individuals that are situated just at the base of an optimum, as it is the case with points x_4 and x_5 in Fig. 1. They may not be selected for recombination at all, or, if affirmative, might recombine with individuals from different species. In this way, they produce fitter offspring in other regions of the search space, which would eventually replace them. Therefore, for every subpopulation detected so far, the best individual it contains is retained in the next generation. However, before copying such an individual, it is checked whether its instance does not already exist in the population. It could have been chosen through mating selection and remained unaltered in the population. The insertion of these dominating individuals thus happens only when they are not members of the next generation, with the aim of avoiding the introduction of identical prototypes in the population.

Concerning the preservation of the species, the new imposition that the niches are kept occupied by a number of individuals proportional to their resources, which is achieved both within the earlier TSC and the new TSC2, by means of weighted mating selection, represents a mechanism that is not integrated within SCGA. Within the complementary MGA [5], however, it is claimed that the selection mechanism has influence upon the number of found peaks and, as a consequence, two types of selection are chosen. One is the global weighted selection and the other one is the local selection within each subpopulation (nation). In the previous TSC [14], both selection types are employed with the aim of keeping the population properly distributed. No important influence was observed as concerns the results and consequently the more direct option, i.e., global weighted selection, is herein adopted.

As regards the annulment of multiple instances for a seed, this is a very important difference of the novel TSC2 in comparison to the corresponding procedure within either the initial TSC or SCGA.

3) *Determining the Species:* Before referring to subpopulations detection, the way the seeds are found must be indicated, as species are formed through the gathering of individuals around these dominating instances. The first generation is the most expensive one as regards the used number of fitness evaluations. This is the time when the *detect-multimodal* method is applied for establishing the starting subpopulations. In the next generations, until the end of the evolutionary process, the species IDs are further used to reflect membership wherever needed and possible. Algorithm 2 describes the manner in which the seeds are selected and, at the same time, the subpopulations are created around them. We denoted by n

Algorithm 2 Seeds Selection Procedure Within TSC2

Require: The current population P
Ensure: The seeds

1: **begin**
2: Sort population P decreasingly according to the fitness;
3: $Seeds = \{P_1\}$; (fittest individual is a seed)
4: **if** not(first generation) **then**
5: $P_{1_{previousID}} = P_{1_{ID}}$; ($previousID$ = the ID in the former generation)
6: **end if**
7: $P_{1_{ID}} = 1$; (the ID of the first seed)
8: $currentID = 2$; ($currentID$ incremented)
9: **for** $i = 2$ to n **do**
10: **if** first generation **then**
11: Find the closest seed s in *Seeds* for which detect-multimodal(P_i, s) = *false*;
12: **else**
13: Find the closest seed s in *Seeds* for which $P_{i_{ID}} = s_{previousID}$;
14: **end if**
15: **if** there exists such a seed s **then**
16: $P_{i_{ID}} = s_{ID}$; (P_i belongs to the species dominated by s)
17: **else**
18: **if** $Seeds$.length $< MAX_{\text{Seeds}}$ **then**
19: $Seeds = Seeds \cup \{P_i\}$; ($P_i$ is a seed)
20: **if** not(first generation) **then**
21: $P_{i_{previousID}} = P_{i_{ID}}$;
22: **end if**
23: $P_{i_{ID}} = currentID$;
24: $currentID = currentID + 1$;
25: **else**
26: Find the closest seed s in *Seeds* for P_i;
27: $P_{i_{ID}} = s_{ID}$; (integrate the individual to closest seed species)
28: **end if**
29: **end if**
30: **end for**
31: **return** the *Seeds* set
32: **end**

the population size and by P_i the ith individual in the current population P.

The set *Seeds* is constructed by considering all individuals, in decreasing order of their fitness. The fittest individual represents the first seed that is added to the set (lines 2 and 3). In the first generation, when an individual is taken into consideration in its turn, it is checked against the other existing seeds using the *detect-multimodal* mechanism, to see whether it follows the same peak or not. In order to save some fitness evaluations, TSC2 tries to avoid unnecessary applications of the detector and chooses the seeds by starting from the one closest to the current individual. The species dominated by this seed is, naturally, the most likely one to follow the same peak as the current individual. If this is not the case, the individual is checked against the next closest seed and so on (lines 10 and 11).

The seeds for all species are updated at every generation. As the entire population is ordered decreasingly every iteration, the IDs of the subpopulations do not remain identical from one evolutionary cycle to another. The ranking of individuals naturally changes, therefore, the IDs are rearranged around the fittest ones. The IDs start over (from 1 up to the number of seeds) from the fittest individual (first seed) to the least fit one that still represents a species master. Hence, the need to retain the previous IDs for the newly set seeds (lines 4–6 and 20–22), so that the individuals that belong to their species could be identified (line 13) and have their IDs updated (line 16). Thus, after the first generation, when an individual is verified whether it is a seed or belongs to a certain species, it is no longer the *detect-multimodal* procedure that checks if it follows the same peak with any of the already-found seeds or not. Instead, its seed ID is compared to those attributed to the currently detected seeds in the previous generation specifically for this purpose. When the number of seeds already reaches the maximum allowed value, the newly found fit individuals that follow different peaks are assigned to their closest seeds in the search space (lines 26 and 27). It is by MAX_{Seeds} that the actual maximum number of seeds that may exist at a time is denoted.

Although within TSC the species were already referred through their IDs with the aim of saving an important amount of fitness evaluations, TSC2 goes further in that direction by comparing the individuals with the seeds that are most likely to follow the same optima.

When the function has a large number of local optima, the *detect-multimodal* method might generate a number of seeds that is too big. That would further on block the population into seeds that would only be copied from one generation to another. This represents an important drawback of TSC that TSC2 resolves through the limitation of the maximum number of seeds to a percent of the population, fact that also counts as another difference to SCGA.

Obviously, it cannot happen that all species are detected from the first generation and kept until the end of the evolutionary process, but new subpopulations can be discovered and added to the existing ones at each iteration. The evolutionary process continues with the weighted mating selection and then the variation operators are applied. When mutation operates on an individual, the offspring does not belong to any of the existing species, i.e., it does not have a value for the ID. These candidate solutions are further referred as *free individuals*. In case of recombination, if both parents belong to the same species, the offspring inherits the ID from the parents. Otherwise, the descendants will be free individuals, just like in the case of the offspring resulting from mutation. The conservation of the species seeds follows immediately afterwards and the newly created individuals with no assigned ID are subsequently integrated.

4) *Seeds Conservation:* The conservation of the seeds is described in Algorithm 3. Once again, f denotes the fitness function to be maximized. For each seed, be that it does not already have an instance in the population (line 4), it is searched for the worst individual of its species, i.e., the least fit individual that has the same ID value (line 5); ties are handled by taking the first instance of a worst individual. If the seed has a better fitness value than that individual, it enters the population instead of it (lines 6–9). In case there is no such individual in the population belonging to the same species, the seed is introduced instead of the worst, unmarked individual in the entire population (lines 10–13). The marking process is necessary in order to avoid the deletion of already introduced seeds.

Algorithm 3 Seeds Conservation Procedure Within TSC2

Require: The current population P
Ensure: The population that contains the seeds
1: **begin**
2: Mark all individuals in P as unprocessed;
3: **for** every s in *Seeds* **do**
4: **if** s does not already exist in P **then**
5: Take worst unprocessed w from P, such that $s_{ID} = w_{ID}$;
6: **if** w exists **then**
7: **if** $f(w) < f(s)$ **then**
8: $w = s$;
9: **end if**
10: **else**
11: Take worst unprocessed w in P;
12: $w = s$;
13: **end if**
14: Mark w as processed;
15: **end if**
16: **end for**
17: **return** the population with the integrated seeds
18: **end**

After detailing the TSC2 conservation mechanism, two differences can be identified relative to the corresponding procedure in the SCGA. The first modification is that no radius-related distance is used, since TSC2 (and the previous TSC, as well) verifies whether the species IDs coincide with those of the individuals that are to be replaced by the seeds. The second distinction, and also an enhancement in contrast to the TSC version, is made by the condition that, before inserting the seeds into the population, the algorithm checks whether a copy of their instance already exists, in order to prevent having duplicate individuals.

5) *Free Individuals Integration:* The approach to integrating the free individuals is described in Algorithm 4. Compared to the original TSC, the new procedure differs in two aspects. In order to avoid the inherent formation of too many species, which may happen only when the optimization function is highly multimodal, the limit for the allowed number of seeds is considered again. Second, it is the treatment of the free individuals as possible species seeds that is changed from the TSC way of collecting them all in a "Tower of Babel" species.

The first choice for the integration of the individuals outside a species is to test whether they belong to any of the already existing ones. Thus, through the application of the *detect-multimodal* procedure for each free individual it is checked whether it follows the same peak as any of the established seeds. With the aim to prevent the excessive use of the detector, the seeds are tested in ascending distance order to the current individual as it more likely belongs to nearer seeds. If a seed that follows the same peak as the present individual is found, then the latter is set to belong to that seed species, takes its ID and is no longer *free* (lines 2–7).

If individuals that do not belong to any of the existing species remain, then they build their own species in which they represent the seeds. That is done by sorting all these individuals in decreasing order in terms of fitness and then establishing the fittest one as a new seed with the ID incremented from the last species ID (lines 9–12). The next individual is then verified for possible membership to the same newly created species. If so, it will have the same ID assigned, otherwise, it will be a new seed as well, having the next ID value. The process continues for all individuals by checking them only against the newly added seeds (lines 13–22).

If free individuals still exist, they are simply assigned to the seeds closest to them (lines 23–28). This happens when the maximum number of seeds has been reached. Thus, in case MAX_{Seeds} species are formed at a certain point and a better solution than the existing ones is found, it enters in the closest seed subpopulation that exists in the genotypic space. In the next generation, this solution is chosen as the seed of the species if fitter than the rest from that subpopulation. This

Algorithm 4 Integration of the *Free Individuals* Within TSC2

Require: A set of free individuals
Ensure: The population and *Seeds* set with the integrated (formerly free) individuals
1: **begin**
2: **for** each free individual x **do**
3: Find the closest seed s to x for which detect-multimodal(x, s) = *false*;
4: **if** s exists **then**
5: $x_{ID} = s_{ID}$;
6: **end if**
7: **end for**
8: **if** *Seeds*.length $< MAX_{\text{Seeds}}$ **then**
9: *currentID* = *Seeds*.length + 1;
10: Find the fittest free individual x;
11: *Seeds* = *Seeds* $\cup \{x\}$; (x is a new seed)
12: $x_{ID} = currentID$;
13: **while** there are still free individuals and $currentID < MAX_{\text{Seeds}}$ **do**
14: For the fittest free individual x find the closest newly added seed s for which *detect-multimodal*(x, s) = *false*;
15: **if** s exists **then**
16: $x_{ID} = s_{ID}$;
17: **else**
18: $currentID = currentID + 1$;
19: *Seeds* = *Seeds* $\cup \{x\}$;
20: $x_{ID} = currentID$;
21: **end if**
22: **end while**
23: **else**
24: **for** each free individual x **do**
25: Find the closest seed s to x;
26: $x_{ID} = s_{ID}$; (integrate the free individual to closest seed species)
27: **end for**
28: **end if**
29: **return** the population and *Seeds* set with the integrated (formerly free) individuals
30: **end**

Algorithm 5 Structure of TSC2

Require: A search/optimization problem
Ensure: The set of seeds

```
begin
  Initialize population;
  while stop condition is not met do
    Identify species seeds; (seeds selection algorithm)
    Apply weighted mating selection;
    Apply recombination;
    Apply mutation;
    Integrate the seeds into current population; (seeds conservation algorithm)
    Integrate free individuals;
  end while
  return the set of seeds
end
```

way, it is conserved from one generation to another and the risk of extinction is eliminated.

6) *Topological Species Conservation Algorithm:* After previously describing the main steps that are followed by TSC2, these are now altogether integrated in Algorithm 5. At each generation, before mating selection is applied, the species are identified and the IDs of all individuals are updated. A weighted mating selection is chosen in order to keep a good proportion between each niche resources and the individuals it contains. Individuals from different subpopulations are allowed to recombine, as their descendants may appear in unexplored regions of the search space and, in case an optimum lies there, they may produce new species. Conversely, when recombination takes place between individuals from the same species, as an intermediate scheme was experimentally chosen, the offspring is considered to belong to the same subpopulation as its parents, i.e., it inherits their ID. The seeds that had been retained in the *Seeds* set before the variation operators were applied are then integrated into the population. Finally, the assimilation of the descendants that do not yet belong to any species takes place.

7) *Extensions Beyond the Initial Integration:* TSC2 differs from the original TSC framework [14] in the following ways.

1) To save fitness evaluations by preventing frequent use of the *detect-multimodal* procedure, it is compared to existing species seeds in Euclidean distance order, starting with the nearest.
2) The free individuals are separately treated (and not during seed conservation). Their independent integration has the advantages that any free individual may form a new species and, when there exist other free individuals that follow the same peak, they will join the same subpopulation. In the previous TSC version, if not members of an existing species, they were all included in a newly created, diverse subpopulation. This nonhomogeneous species was able to give birth to interesting solutions but, at the same time, many promising individuals were not prevented from vanishing during the evolutionary iterations. Within TSC2, these individuals are better controlled, i.e., they create their own species or, if the number of subpopulations reaches the upper bound, they are each assigned to the species that resembles them the most.
3) The introduction of duplicate individuals when seeds conservation takes place is avoided.
4) An upper bound is set for the number of seeds, a fact of major importance when targeting functions with spiny landscapes.

These differences are expected to produce a major impact on the obtained performance of TSC2. The initial TSC version of [14] is, therefore, also considered for comparison in the experiments in order to illustrate the effect of the changes.

8) *Distinctions From Species Conservation:* As compared to the related SCGA, there are first the major differences and improvements: speciation does not make use of a radius whose value is experimentally hard to be set and the computation of a high number of distances in order to identify the species together with their seeds is avoided. Besides these, TSC2 does not require a mechanism for achieving the final output. All the seeds provided by the currently proposed approach in the end of a run represent the set of solutions, in case the aim is to find several global and/or local optima. This is due to the fact that, within TSC2, all individuals that follow a certain optimum are grouped into one species and the case that different species follow the same optimum is extremely unlikely. Finally, what is more, the parameter that gives the number of interior points (gradations) to be considered for TSC2 is a positive integer and is presumably easier to be tuned than the positive real-valued radius within SCGA. However, in the experiments section, direct comparison of how dependent the two connected models are on these specific parameters is thoroughly conducted.

IV. Experimental Comparison

In the following set of experiments, we investigate how differences in modality (one, few, and many optima), search space size and the number of variables, among others, impact the algorithm's performance relative to existing ones such as TSC and SCGA. In order to address relatively difficult problems even with a low number of dimensions, the easiest presumed case regards the optimization of functions with two variables. The reason for the choices of functions in the test suite was correlated with the aim to perform a deep empirical study on several aspects of multimodal optimization. The goals are thus to test the ability of such a technique to still be able to tackle a unimodal problem, to validate its capacity to detect all the global/local peaks of a function and to check the skill to reach the global optimum/optima in an environment with close (even spinal) local peaks.

All the five functions considered by the MGA [5] are included in the experiments of the current paper, i.e., $F1$ (Waves), $F2$ (Six-Hump Camel Back), $F11$, $F12$, and $F13$. $F7$ (Branin RCOS) and $F8$ (Shubert function) are acquired from the SCGA experimentation [6]. AQ:2 The selection of hard multimodal problems is extended by several functions that are included in [11], namely $F9$ (Ackley), and $F10$ (Michalewicz). The previous $F11$, $F12$, and $F13$ are further called by the same designations as in [11]. In addition to

TABLE I

CONSIDERED BENCHMARK FUNCTIONS AND THE NUMBER OF DIMENSIONS D FOR WHICH THEY ARE TESTED

Common Name and Dimensions D	Function	Optima
Waves, 2 dimensions	$F1(x,y) = (0.3x)^3 - (y^2 - 4.5y^2)xy - 4.7\cos(3x - y^2(2+x))\sin(2.5\Pi x))$ $-0.9 \le x \le 1.2, -1.2 \le y \le 1.2$	10
Six-Hump Camel Back, 2 dimensions	$F2(x,y) = -((4 - 2.1x^2 + \frac{x^4}{3})x^2 + xy + (-4 + 4y^2)y^2)$ $-1.9 \le x \le 1.9, -1.1 \le y \le 1.1$	6
Sphere, 2, 10 dimensions	$F3(\overrightarrow{x}) = \sum_{i=1}^{D}(-x_i^2) \qquad -5.12 \le x_i \le 5.12$	1
Shifted Rastrigin, 2, 10 dimensions	$F4(\overrightarrow{x}) = \sum_{i=1}^{D}(x_i^2 - 10\cos(2\Pi x_i) + 10) + f\_bias$ $-5 \le x_i \le 5$	1/many
Rotated Hybrid Composition function, 2, 10 dimensions	$F5$ corresponds to function $F21$ in [25]	1/many
Rescaled Six-hump, 2 dimensions	$F6(x,y) = -((4 - 2.1x^2 + \frac{x^4}{3})x^2 + 10xy + (-4 + 4(10y)^2)(10y)^2)$ $-1.9 \le x \le 1.9, -0.11 \le y \le 0.11$	6
Branin RCOS, 2 dimensions	$F7(x,y) = (y - \frac{5.1}{4\pi^2}x^2 + \frac{5}{\pi}x - 6)^2 + 10(1 - \frac{1}{8\pi})\cos(x) + 10$ $-5 \le x \le 10, 0 \le y \le 15$	3
Shubert, 2 dimensions	$F8(x,y) = \sum_{i=1}^{5} icos[(i+1)x + i] \cdot \sum_{i=1}^{5} icos[(i+1)y + i]$ $-10 \le x, y \le 10$	18/many
Ackley, 2 dimensions	$F9(x,y) = 20 + e - 20e^{-0.2\sqrt{\frac{x^2+y^2}{2}}} - e^{\frac{\cos(2\pi x)+\cos(2\pi y)}{2}}$ $-30 \le x, y \le 30$	1/many
Michalewicz, 2 dimensions	$F10(x,y) = \sin(x)\sin^{20}(\frac{x^2}{\pi}) + \sin(y)\sin^{20}(\frac{2y^2}{\pi})$ $0 \le x, y \le \pi$	2
Ursem F1 in [5], 2 dimensions	$F11(x,y) = \sin(2x - 0.5\pi) + 3\cos(y) + 0.5x$ $-2.5 \le x \le 3, -2 \le y \le 2$	2
Ursem F3 in [5], 2 dimensions	$F12(x,y) = \sin(2.2\pi x + 0.5\pi) \cdot \frac{2-\lvert y\rvert}{2} \cdot \frac{3-\lvert x\rvert}{2} +$ $\sin(0.5\pi y^2 + 0.5\pi) \cdot \frac{2-\lvert y\rvert}{2} \cdot \frac{2-\lvert x\rvert}{2}, -2.5 \le x \le 3, -2 \le y \le 2$	5
Ursem F4 in [5], 2 dimensions	$F13(x,y) = 3\sin(0.5\pi x + 0.5\pi) \cdot \frac{2-\sqrt{x^2+y^2}}{4}, -2 \le x, y \le 2$	5
Keane's Bump Problem, 20 dimensions	$F14(\overrightarrow{x}) = \frac{\lvert\sum_{i=1}^{D}\cos^4(x_i) - 2 * \prod_{i=1}^{D}\cos^2(x_i)\rvert}{\sqrt{\sum_{i=1}^{D} i * {x_i}^2}}$ $0 \le x_i \le 10$, subject to $\prod_{i=1}^{D} x_i > 0.75$ and $\sum_{i=1}^{D} x_i < \frac{15 * D}{2}$	1/many

TABLE II

CONSIDERED PARAMETER VALUES FOR ALL EVOLUTIONARY METHODS EXCEPT THE NCMA-ES

Population Size	$p_r/p_m/$ Scaling Factor	Radius/Mutation Strength				No. of Gradations
		[0, 5]	[0, 15]	[0, 30]	[0, 80]	
{2, 3, ..., 200}	[0, 1]	$F1, F2, F6, F8, F10$ $F11, F12, F13$	$F3, F4, F5, F7$ 2 dimensions	$F3, F4, F5$, 10 dimensions $F14$, 20 dimensions	$F9$	{1, 2, ..., 15}

p_r and p_m represent the recombination and mutation probabilities, respectively.

these benchmark cases, $F3$ (De Jong), $F4$ (Shifted Rastrigin), $F5$ (Rotated Hybrid Composition function) and a shifted version of $F2$, which is presently referred to as $F6$, are further tested. In the end, a real-world problem of engineering design, as modeled by function $F14$, is included for a practical application of TSC2. The problems, together with the number of known peaks, are depicted in Table I.

Recent model-based investigations [24] have led to the conjecture that complex multimodal optimization algorithms may perform better than simple multistart methods only if the number of optima is relatively low. $F3$ is thus tested to show that starting from the simplest case of only one optimum, the considered methods indeed perform well. Moreover, any method that is due to optimize a difficult function should at least cope with a simple one.

Having equally distant optima would be an advantage for a radius-based EA, as a proper value for the radius would aid in detecting all peaks. But, as a real-world problem does not necessarily exhibit a regular fitness landscape, the original Six-Hump Camel Back function is rescaled in order to have the optima, two by two, more remote from each other ($F6$). The Waves test case is a function that is already asymmetric and has many peaks, some of which being even more difficult to find as they lie on the border or on flat hills.

The complete description of the Shifted Rastrigin function, as well as the one for the Rotated Hybrid Composition function, can be found in [25], as they are part of a set of 25 benchmark problems used in a contest during the Congress on Evolutionary Computation 2005 (Shifted Rastrigin is F_9 in the collection). The difficulty with $F4$ is that the global optimum is surrounded by a large number of very close local optima with only a small difference in their values as compared to the main peak. The $F5$ function represents a composition of five functions: Ackley, Rastrigin, Sphere, Weierstrass, and Griewank. According to [25], it has a huge number of optima, different functions properties are mixed together, the Sphere function adds some flat areas and a local optimum is set on the origin. Eleven algorithms were tested in the contest and none of them found the global optimum in any run when ten dimensions were considered. The reader is directed to [25] for a complete view of the function.

Branin RCOS contains three global optima, which are disposed within an irregular and asymmetric landscape. Shubert's function possesses eighteen global, equally far disposed optima, and many other local peaks are in between. Ackley's function has one global optimum and a large number of local optima, as it has the appearance of a "spiny" landscape. Michalewicz' function has one global optimum and a local one. Ursem's $F1$ function contains one global optimum, a local peak and has a smooth landscape that should not yield difficulties for a typical multimodal EA. Ursem's $F3$ and $F4$ have each one global optimum and four local peaks. The former, called by Ursem "5 hills–4 valleys," has five very close hills with lines of valleys between them, while the latter, named "1 center peak and 4 neighbors," has the four local optima on the edge of the intervals and a global one in the middle.

In order to test the applicative side of the proposed methodology, Keane's Bump problem [26] from engineering design is finally taken into consideration in the suite. The $F14$ function has a highly bumpy surface and the global optimum is given by the product constraint.

TABLE III
CONSIDERED PARAMETER INTERVALS FOR THE NCMA-ES

Niche Number	q_{eff} (New Niches)	κ (Niche Lifetime)	Radius/Mutation Strength
$\{2, \ldots, 20\}$	$[1, 2]$	$\{2, \ldots, 20\}$	$[0.001, 0.3 \cdot d_{\max}]$

$q_{\text{eff}} \cdot (q - 1)$new niches are regularly introduced and live for at least k generations.

In summary, the test problems include:

1) one function with one global optimum ($F3$) considered for 2 and 10 variables;
2) three functions with one global optimum and a very large number of local optima, with spiny surfaces ($F4$, $F5$, and $F9$). $F4$ and $F5$ are considered for 2 and 10 dimensions;
3) one function with 2 optima and large plateaus ($F10$);
4) five functions with several optima disposed on a smooth landscape ($F2$, $F6$, $F11$, $F12$, and $F13$);
5) two functions with multiple optima that are irregularly disposed, with unexpected valleys situated very close to high optima ($F1$, $F7$);
6) one function with a large number of global optima and many local ones ($F8$);
7) one function to model a real-world application and chosen as a practical test ($F14$).

For $F1$, $F2$, $F6$, $F7$, $F10$–$F13$ the task is to find all optima they exhibit, global, and local, while for the rest the job is to concentrate the search on the global optimum/optima and to escape the local, unimportant, peaks.

All functions are considered for maximization, therefore, when the definitions were given for minimization, the functions were reversed. The constraints in Keane's real-world problem were chosen to be treated by penalizing the infeasible individuals. The employed penalty function reduces their fitness according to the distance to the feasible region [1].

A. Direct Performance Comparison

1) *Pre-Experimental Planning:* In the previous TSC version [14], a maximum limit for the number of seeds was not set. This parameter was revealed to be vital when it was dealt with the $F5$ function: the results were very poor, even when the test function was considered for two variables. The number of seeds was exponentially increasing as generations were passing. Having a population of 200 individuals, about 180 seeds were chosen in less than 30 generations, meaning that 90% of the population was blocked from the start of the algorithm. However, after setting the MAX_{Seeds} value within TSC2, this situation was successfully handled. In all the undertaken experiments, an amount of 20% of the population size for the value of MAX_{Seeds} seemed to achieve a good control.

2) *Task:* The first aim is to put TSC2 in contrast to the original TSC version [14] and examine whether the pertained

TABLE IV

BEST/AVERAGE RESULTS OBTAINED IN 30 LHS POINTS, EACH REPLICATED 30 TIMES, FOR FUNCTIONS $F1$–$F5$

Method	Peak Ratio		Basin Ratio		Peak Accuracy		Distance Accuracy	
	Best	Avg.	Best	Avg.	Best	Avg.	Best	Avg.
$F1$, 1 global optimum, 9 local ones								
TSC2	**0.99**	**0.84**	1	0.88	**0.13**	1.84	**0.04**	0.79
CDE	0.88	0.79	0.98	**0.93**	0.52	**1.59**	0.11	**0.41**
TSC [14]	0.85	0.64	0.83	0.66	4.52	7.7	1.29	3.26
NCMA-ES	0.8	0.49	0.9	0.59	1.85	8.89	0.88	3.87
SCGA	0.66	0.18	0.99	0.264	8.74	18.59	0.98	11.56
DFS	0.37	0.16	0.37	0.16	14.46	20.93	5.24	11.52
$F2$, 2 global, 4 local optima								
TSC2	1	**0.77**	1	**0.77**	**6.93e−04**	**2.91**	0.02	2.09
NCMA-ES	1	0.59	1	0.61	1.72e−03	3.9	0.02	3.19
CDE	1	0.75	1	0.76	0.02	3.3	0.1	**1.99**
SCGA	0.96	0.32	1	0.35	0.39	6.37	0.44	7.02
DFS	0.67	0.26	0.67	0.26	4.64	7.27	2.73	6.22
TSC [14]	0.63	0.46	0.66	0.44	3.93	6.18	3.44	6.18
$F3$, 2 dimensions, 1 optimum								
NCMA-ES	1	1	1	1	**4.6e−68**	3.92e−06	**6.48e−35**	5.84e−04
CDE	1	1	1	1	9.47e−40	4.48e−04	1.96e−20	5.25e−03
TSC2	1	1	1	1	5.85e−12	1.81e−07	1.61e−06	9.32e−05
SCGA	1	1	1	1	1.53e−11	2.86e−07	2.41e−06	1.65e−04
TSC [14]	1	1	1	1	2.48e−10	**1.75e−07**	4.9e−06	**9.08e−05**
DFS	1	1	1	1	2.55e−09	4.17e−06	4.23e−05	8.12e−04
$F3$, 10 dimensions, 1 optimum								
CDE	1	**0.83**	1	1	**2.66e−25**	0.11	**4.07e−13**	**0.15**
NCMA-ES	1	0.73	1	1	1.28e−17	**0.08**	2.51e−09	0.19
TSC2	1	0.73	1	1	2.36e−06	0.15	0.001	0.23
TSC [14]	1	0.74	1	1	2.79e−06	0.12	0.003	0.51
SCGA	1	0.72	1	1	1.03e−05	1.43	0.003	0.45
DFS	1	0.72	1	1	3.12e−05	0.14	0.005	0.22
$F4$, 2 dimensions, 1 global optimum/many local ones								
NCMA-ES	1	0.86	1	0.88	**0**	0.19	**9.05e−9**	0.14
DFS	1	0.98	1	0.98	9.13e−08	0.02	7.24e−06	0.02
SCGA	1	**0.99**	1	**0.99**	1.4e−07	**0.01**	1.46e−05	**0.01**
CDE	1	0.88	1	0.98	4.29e−07	0.11	3.93e−05	0.03
TSC2	1	0.8	1	0.94	2.23e−06	1.63	8.23e−05	0.05
TSC [14]	1	0.74	1	0.93	5.04e−05	1.73	5.1e−04	0.07
$F4$, 10 dimensions, 1 global optimum/many local ones								
SCGA	1	**0.35**	1	**0.66**	0.002	18.42	0.003	1.71
TSC2	1	0.04	1	0.27	0.002	39.78	0.003	2.57
DFS	1	0.31	1	0.44	0.003	**8.93**	0.003	**1.44**
TSC [14]	0.97	0.03	1	0.28	0.03	51.46	0.03	6.08
CDE	0.9	0.12	0.97	0.19	0.09	18.68	0.04	1.68
NCMA-ES	0	0	0	0	26.9	23.6	2.46	3.32
$F5$, 2 dimensions, 1 global optimum/many local ones								
TSC2	**0.77**	**0.26**	**0.97**	**0.67**	14.74	369.93	**9.4e−04**	0.49
DFS	0.7	0.21	0.73	0.24	58.09	164.85	1.34	3.05
TSC [14]	0.63	0.19	0.73	0.29	273.64	934.45	0.96	1.07
SCGA	0.47	0.21	0.6	0.31	81.47	317.24	0.11	2.51
CDE	0	0.003	1	0.96	**20.65**	**134.64**	0.01	**0.07**
NCMA-ES	0	0	0	0	1700	1840	1.62	0.71
$F5$, 10 dimensions, 1 global optimum/many local ones								
NCMA-ES	0	0	0	0.01	1810	1900	**9.44**	**8.82**
TSC2	0	0	0	0	770.48	1234.14	9.64	11.24
DFS	0	0	0	0	**569.6**	**870.64**	11.08	12.85
CDE	0	0	0	0	1076.2	1301.02	11.99	9.32
SCGA	0	0	0	**0.3**	762.8	1311.85	12.95	11.49
TSC [14]	0	0	0	0	961.59	1151.36	33.33	32.37

For each function, the methods are presented in decreasing order based on the quality of results in the best configuration, first by *peak ratio* and then by *distance accuracy.*

TABLE V

BEST/AVERAGE RESULTS OBTAINED IN 30 LHS POINTS, EACH REPLICATED 30 TIMES, FOR FUNCTIONS $F6$–$F14$

Method	Peak Ratio		Basin Ratio		Peak Accuracy		Distance Accuracy	
	Best	Avg.	Best	Avg.	Best	Avg.	Best	Avg.
*F*6, 2 global, 4 local optima								
TSC2	**0.99**	0.79	**0.99**	0.79	**0.15**	2.77	**0.01**	0.54
CDE	0.98	**0.85**	0.98	**0.85**	0.23	**1.78**	0.02	**0.22**
SCGA	0.72	0.23	0.94	0.27	3.89	7.06	0.34	5.31
NCMA-ES	0.67	0.49	0.67	0.50	4.64	5.12	0.34	1.48
TSC [14]	0.59	0.46	0.64	0.45	4.15	5.99	1.82	3.94
DFS	0.5	0.24	0.5	0.25	4.64	6.89	0.34	4.55
*F*7, 3 global optima								
TSC2	1	**0.98**	1	**0.98**	**2.74e−07**	0.02	**5.54e−04**	0.45
DFS	1	0.72	1	0.72	6.17e−06	**3.42e−04**	0.003	3.63
CDE	1	0.97	1	1	1.41e−05	0.1	0.004	**0.21**
SCGA	0.99	0.62	1	0.77	0.02	0.73	0.15	6.04
TSC [14]	0.96	0.75	0.94	0.85	0.8	1.79	2.43	5.48
NCMA-ES	0.67	0.66	0.67	0.92	0.04	1.96	1.16	4.56
*F*8, 18 global, many local optima								
CDE	**0.99**	0.27	**1**	**0.92**	0.26	115.4	**0.04**	**3.12**
NCMA-ES	0.89	**0.41**	0.94	0.43	4.24	52.6	1.63	31.0
TSC2	0.7	0.3	0.81	0.3	99.07	727.9	4.23	33.2
DFS	0.44	0.21	0.44	0.21	**0.04**	**0.11**	44.55	88.2
TSC [14]	0.36	0.13	0.26	0.21	750.8	1628.46	78.8	59.2
SCGA	0.27	0.08	0.3	0.32	589.7	1381.05	42.75	22.1
*F*9, 1 global, many local								
NCMA-ES	1	0.97	1	1	**0**	0.01	**2.56e−16**	2.96e−03
DFS	1	1	1	1	4.14e−05	0.003	1.46e−05	**8.18e−04**
SCGA	1	1	1	1	4.61e−05	0.003	1.63e−05	9.78e−04
TSC2	1	0.72	1	1	2.25e−04	0.85	7.95e−05	0.21
TSC [14]	1	0.91	1	1	0.001	0.23	4.18e−04	0.06
CDE	1	0.69	1	0.98	0.001	0.24	4.61e−04	0.05
*F*10, 1 global, 1 local								
TSC2	1	0.99	1	0.99	1.01e−07	0.009	**7.83e−05**	0.02
NCMA-ES	1	0.93	1	0.93	**6.87e−08**	0.07	9.41e−05	0.15
CDE	1	**1**	1	**1**	1.71e−07	**0.006**	1.18e−04	**0.01**
TSC [14]	1	0.99	1	0.99	1.08e−06	0.01	2.4e−04	0.03
DFS	1	0.6	1	0.62	8.0e−04	0.37	0.005	0.72
SCGA	1	0.58	1	0.63	0.002	0.48	0.007	0.92
*F*11, 1 global, 1 local								
CDE	1	1	1	1	**2.87e−07**	**0.002**	**2.83e−04**	**0.009**
TSC2	1	0.97	1	0.97	3.82e−07	0.1	6.04e−04	0.21
NCMA-ES	1	0.75	1	0.75	4.23e−07	0.64	6.49e−04	1.42
TSC [14]	1	1	1	1	3.87e−07	0.005	7.67e−04	0.01
DFS	1	0.65	1	1.66	6.31e−07	0.92	8.12e−04	1.87
SCGA	0.98	0.75	1	0.76	0.006	0.76	0.03	1.55
*F*12, 1 global optimum, 4 local ones								
CDE	1	**0.97**	1	0.98	**0.003**	**0.1**	**0.01**	**0.12**
TSC2	1	0.94	1	0.94	0.008	0.32	0.03	0.34
NCMA-ES	1	0.55	1	0.69	0.01	1.89	0.04	1.99
SCGA	0.99	0.33	1	0.38	0.07	4.28	0.15	4.32
TSC [14]	0.96	0.68	0.94	0.67	0.2	1.68	0.28	1.77
DFS	0.81	0.28	0.79	0.3	0.17	4.3	0.2	4.29
*F*13, 1 global optimum, 4 local ones								
CDE	1	**0.97**	1	**0.98**	**5.89e−04**	**0.12**	0.001	**0.36**
TSC2	1	0.94	1	0.93	8.33e−04	0.28	0.001	0.95
NCMA-ES	1	0.56	1	0.56	1.02e−03	1.02	0.002	5.42
DFS	0.99	0.38	1	0.38	0.07	2.11	0.15	7.36
TSC [14]	0.99	0.84	0.89	0.64	0.15	0.89	1.22	7
SCGA	0.89	0.32	1	0.49	0.37	2.53	0.54	7.68
*F*14, 20 dimensions, 1 global, many local								
TSC2	1	0.03	0.13	0.42	0.05	0.46	3.2	8.73
NCMA-ES	1	**1**	**1**	**1**	**0**	**0**	6.6	10.4
SCGA	0.97	0.25	0.17	0.48	0.04	0.29	3.22	7.49
CDE	0.9	0.6	0.93	0.53	0.05	0.23	**1.15**	**4.16**
DFS	0.87	0.04	0	0.09	0.07	0.35	3.98	7.63
TSC [14]	0.5	0.02	0.2	0.66	0.11	0.51	10.18	34.8

For each function, the methods are presented in decreasing order based on the quality of results in the best configuration, first by *peak ratio* and then by *distance accuracy*.

TABLE VI

p-VALUES CALCULATED BY MEANS OF t-TEST AND WILCOXON RANK-SUM TEST FOR TSC2 VERSUS THE OTHERS FOR $F1$–$F5$

TSC2	Peak Ratio		Distance Accuracy	
Versus	t-Test	Wilcoxon	t-Test	Wilcoxon
$F1$, 1 global optimum, 9 local ones				
+CDE	2e−08	1.8e−08	–	–
+TSC [14]	2.7e−10	2.7e−09	–	–
+NCMA-ES	<2.2e−16	6.1e−14	–	–
+SCGA	<2.2e−16	1.9e−12	–	–
+DFS	<2.2e−16	1.9e−12	–	–
$F2$, 2 global, 4 local optima				
+NCMA-ES	–	–	0.71	0.01
+CDE	–	–	<2.2e−16	<2.2e−16
+SCGA	0.02	0.01	<2.2e−16	<2.2e−16
+DFS	–	1.69e−14	–	–
+TSC [14]	3.1e−12	9.1e−13	–	–
$F3$, 2 dimensions, 1 optimum				
−NCMA-ES	–	–	4.2e−05	<2.2e−16
−CDE	–	–	4.2e−05	<2.2e−16
+SCGA	–	–	4.8e−07	0.28
+TSC [14]	–	–	0.24	2.6e−07
+DFS	–	–	3.5e−04	1.2e−14
$F3$, 10 dimensions, 1 optimum				
−CDE	–	–	1.5e−12	<2.2e−16
−NCMA-ES	–	–	1.5e−12	3.1e−11
+TSC [14]	–	–	3.7e−04	7.7e−05
+SCGA	–	–	2.1e−04	2.3e−04
+DFS	–	–	5.8e−15	8.6e−15
$F4$, 2 dimensions, 1 global optimum/many local ones				
−NCMA-ES	–	1.69e−14	0.34	6.4e−08
-DFS	–	–	0.34	6.9e−11
-SCGA	–	–	0.34	2.3e−11
−CDE	–	–	0.34	4.1e−05
+TSC [14]	–	–	0.34	9.8e−04
$F4$, 10 dimensions, 1 global optimum/many local ones				
-SCGA	–	–	0.35	0.53
+DFS	–	–	0.008	0.02
+TSC [14]	0.33	0.33	2.1e−12	<2.2e−16
+CDE	0.08	0.08	0.23	3.6e−10
+NCMA-ES	–	–	<2.2e−16	3.1e−11
$F5$, 2 dimensions, 1 global optimum/many local ones				
+DFS	0.57	0.57	6.8e−04	0.62
+TSC [14]	0.27	0.27	1.5e−04	0.22
+SCGA	0.02	0.02	0.04	0.84
+CDE	1.1e−10	1.5e−09	–	–
+NCMA-ES	1.1e−10	1.5e−09	–	–
$F5$, 10 dimensions, 1 global optimum/many local ones				
−NCMA-ES	–	–	0.19	0.18
+DFS	–	–	0.008	0.19
+CDE	–	–	3.9e−07	2.1e−07
+SCGA	–	–	<2.2e−16	6.3e−15
+TSC [14]	–	–	<2.2e−16	<2.2e−16

When the *peak ratio* difference is not significant, *distance accuracy* is also considered. +/− stands for TSC2 being better/worse.

TABLE VII

p-VALUES CALCULATED THROUGH A t-TEST AND A WILCOXON RANK-SUM TEST FOR TSC2 VERSUS THE OTHERS FOR $F6$–$F14$

TSC2	Peak Ratio		Distance Accuracy	
Versus	t-Test	Wilcoxon	t-Test	Wilcoxon
$F6$, 2 global, 4 local optima				
+CDE	0.65	0.65	0.08	3.5e−07
+SCGA	3.2e−10	3.1e−10	–	–
+NCMA-ES	<2.2e−16	4.1e−14	–	–
+TSC [14]	1.9e−14	3.3e−12	–	–
+DFS	<2.2e−16	4.1e−14	–	–
$F7$, 3 global optima				
+DFS	–	–	6.1e−04	3.0e−05
+CDE	–	–	7.8e−04	9.7e−14
+SCGA	0.33	0.33	8.9e−08	<2.2e−16
+TSC [14]	0.04	0.04	0.004	<2.2e−16
+NCMA-ES	–	–	<2.2e−16	7.6e−12
$F8$, 18 global, many local optima				
−CDE	<2.2e−16	6.4e−12	–	–
−NCMA-ES	2.1e−13	1.5e−10	–	–
+DFS	<2.2e−16	2.1e−11	–	–
+TSC [14]	<2.2e−16	2.2e−11	–	–
+SCGA	<2.2e−16	1.8e−11	–	–
$F9$, 1 global, many local				
−NCMA-ES	–	–	0.005	3.0e−11
−DFS	–	–	0.009	8.9e−05
−SCGA	–	–	0.009	2.6e−04
+TSC [14]	–	–	0.02	0.005
+CDE	–	–	0.1	0.002
$F10$, 1 global, 1 local				
+NCMA-ES	–	–	0.13	0.008
+CDE	–	–	6.7e−09	4.1e−10
+TSC [14]	–	–	0.32	3.1e−13
+DFS	–	–	1.2e−08	<2.2e−16
+SCGA	–	–	4.5e−07	<2.2e−16
$F11$, 1 global, 1 local				
−CDE	–	–	1.8e−06	6.8e−06
+NCMA-ES	–	–	0.53	0.02
+TSC [14]	–	–	0.92	0.18
+DFS	–	–	0.04	7.3e−04
+SCGA	–	–	1.4e−09	<2.2e−16
$F12$, 1 global optimum, 4 local ones				
−CDE	–	–	6.4e−09	3.6e−09
+NCMA-ES	–	–	2.4e−06	1.5e−05
+SCGA	0.32	0.32	1.1e−11	<2.2e−16
+TSC [14]	0.03	0.02	3.2e−04	4.9e−11
+DFS	1.99e−09	1.32e−09	–	–
$F13$, 1 global optimum, 4 local ones				
−CDE	–	–	3.1e−15	3.5e−14
+NCMA-ES	–	–	0.03	2.6e−06
+DFS	–	–	0.16	4.9e−11
+TSC [14]	0.33	0.33	0.003	<2.2e−16
+SCGA	9.1e−05	2.7e−05	–	–
$F14$, 20 dimensions, 1 global, many local				
+NCMA-ES	–	–	<2.2e−16	1.2e−12
+SCGA	0.33	0.33	0.06	0.1
+CDE	0.08	0.08	2.8e−10	1.6e−09
+DFS	0.04	0.04	0.17	0.2
+TSC [14]	8.7e−06	9.6e−06	–	–

When the *peak ratio* difference is not significant, *distance accuracy* is also considered. +/− stands for TSC2 better/worse.

modifications indeed yield the expected significant difference in results. Secondly, it is targeted to perform a direct comparison between the radius-dependent species conservation technique of inspiration, the SCGA, and the novel radius-free TSC2 approach. The MGA was not used in the comparison here because previous work [14] had shown that it was less efficient than both SCGA and the earlier TSC formulation in terms of acquired performance relative to the number of spent fitness evaluations. Additionally, two other radius-propelled evolutionary techniques were taken for a contrast: DFS, which was very competitive in the experiments described in [7] and is fundamentally related to TSC2, and the NCMA-ES, which achieved very good results within validation [15]. In order to also have a completely different method to weigh against, the crowding differential evolution (CDE) presented in [11] is also included in the comparison. The method does not possess a radius, but it has a different parameter, the *scaling* *factor*, that is used for creating new offspring. Consequently, the hypotheses to be tested are as follows.

1) The enhanced TSC2 is more efficient than the initial TSC combination in [14], in terms of the balance between the achieved performance and the number of invested fitness evaluations.
2) TSC2, having an additional parameter that must be a positive integer and represents a several-choice number of individuals, is at least as good as SCGA, DFS, and NCMA-ES, all three with a radius parameter that is real, free-valued.
3) TSC2 has significantly better performance on several types of test problems than the methods of comparison. Accordingly, the conditions under which TSC2 is able to outperform the others are identified.

3) *Experimental Setup:* In order to achieve an objective comparison, the only user interaction in setting the parameters for the examined techniques appears in defining the ranges for their values. The statistical method of Latin hypercube sampling (LHS) (e.g., [27]) is employed to generate a space-filling (fair) sample of the algorithm parameters. For small sample sizes, it is well known to generate more even distributions than random sampling. For this reason, it is also the first step in the tuning algorithm sequential parameter optimization (SPO) [28]. Here, we use it to generate a disposition of plausible parameter sets from a multidimensional distribution, which is conducted on all test functions for automatically setting the values for every involved parameter within all compared methods. It is clear that there is further room for improvement of algorithm parameters by applying a full tuning method, but the LHS already gives a good estimation of the performance values under parameter variation. Thereby, we can avoid comparing algorithms under bad parameter settings.

For all considered test functions and all techniques, we employ the same budget of 3×10^4 fitness evaluations. For all methods, except NCMA-ES, the evolutionary variables are set as follows. The upper bound of the population size is restricted to 200. The mutation and crossover probabilities are selected by the LHS in the interval [0, 1] in all experiments. The upper limit for the mutation strength parameter is similarly set for all compared techniques, but differently for each benchmark function. The interval from which the LHS takes the values for the mutation strength is actually identical to the one of the radius parameter within the SCGA and DFS, which depends on the problem to be solved. The radius value is computed for each function using the Deb and Goldberg formula (1) and then the upper bound of the interval is appointed as approximately the double of that value, in order to make sure a proper configuration is included in the ones generated by the LHS. For all benchmark problems, the number of gradations in TSC2 is considered from the set $\{1, 2, \ldots, 15\}$. Table II illustrates the sets and intervals used for each tuned parameter.

For the NCMA-ES, parameter intervals (Table III) have to be chosen in a different fashion as it knows no base population but only niches holding one individual each. Furthermore, the probabilities for mutation and crossover cannot be easily changed. Mutation is usually always done in CMA-ES variants, and recombination is implicitly performed in one step with selection. However, the NCMA-ES possesses other parameters, namely q_{eff} and κ. The first one resembles the number of total niches, that is the number of "stable" niches plus a number of "test" niches. In contrast to the additive fashion that would lead to unwanted dependencies on the original niche number, a multiplier in the interval [1, 2] is used to compute q_{eff} as the product of this parameter and the number of "stable" niches. The second one, κ, is set as the discrete minimum lifespan of the "test" niches between 2 and 20. The initial stepsize and the niche radius are varied in the interval of $[0.001, 0.3] \cdot d_{\max}$, the latter meaning the maximum search space expansion in one dimension. These values have been chosen according to the recommendation of the authors of [10].

There are 30 LHS points taken into account for each test function and every configuration is replicated 30 times for all techniques in turn. The average over the 30 repeated runs of the best configuration and the mean over all 30 different configurations are recorded. The latter is reported to indicate how sensitive each technique is to changes in the parameter values. It does not necessarily demonstrate the superiority of a method upon another, but shows that tuning the methods can require different amounts of effort, where one that gives good results for a large variety of configurations shall be preferred. Naturally, if the number of parameters is smaller, the available space is explored better when the number of tested configurations is held constant.

A peak is considered as found if at least one individual of the population of the last generation is situated in the basin of attraction of that optimum, with an accuracy of at least 10^{-1}. Several measures are used for evaluating success of the different algorithms.

1) The *peak ratio* computes the fraction between the number of detected peaks and the amount of peaks to be found.
2) *Basin ratio* is meant to be broader than the previous measure, as it counts a basin as found if an individual entered the basin, even if not closer than 10^{-1} in fitness. When an individual is in the right basin, it will most likely find the desired peak with a few more evaluations. We detect an individual inside a basin via the *detect-multimodal* method with ten interior points. The actual measurement is given as ratio between the number of detected basins and the number of desired optima (and basins, accordingly).
3) The *peak accuracy* measure is calculated as follows. For each optimum to be found, the nearest individual x in the population is taken and the absolute difference in fitness values is computed. Then, all these differences are summed as in (3), where the fitness of an individual x is denoted by $f(x)$

$$\text{peak acc.} = \sum_{i=1}^{\#\text{peaks}} \mid f(\text{peak}_i) - f(x) \mid . \tag{3}$$

4) When there are more peaks that have very close or identical peak height, the previous metric may produce good results even if all the population is situated in

the basin of the attraction of the same peak. As a precaution, the *distance accuracy* that refers to the dissimilarity in the genotypic space between each peak and its closest individual is also computed and stands for a ranking field of compared methods. It is derived in the same manner as in (3), with the only change that the difference between fitness values is substituted by the Euclidean distance between the two individuals. Current and previous measure should stay poised, or otherwise, a peak accuracy error caused by coincidental close evaluations may appear.

The first two measures were also considered in [5], the third appears in [11] and the last is proposed herein.

Besides the newly proposed TSC2 approach, the other techniques considered for comparison have also been implemented by the current authors. The only exception is the NCMA-ES whose code, made available by its authors, was interfaced. Additionally, the same type of (common) operators [1] are employed for all algorithms (except NCMA-ES).

1) Binary tournament selection.
2) Intermediate recombination with probability p_r, so that the genes of an offspring O are obtained from two parents P and Q according to (4), where R is a uniformly distributed random number over [0, 1]

$$O = P + R \cdot (Q - P). \tag{4}$$

3) Mutation with normal perturbation with probability p_m. A gene of an individual X selected to be modified through mutation is changed according to (5). MS and $N(0, 1)$ represent the mutation strength and a normally distributed random variable with expected mean 0 and variance 1, respectively

$$X' = X + MS * N(0, 1). \tag{5}$$

4) *Results:* The results derived from the LHS parameterization are depicted in Tables IV and V. While for peak ratio and basin ratio, higher values signify better results (1 being the best), for the other two measures, better results correspond to smaller values, meaning that the individuals came closer to the actual solutions in accuracy (see peak accuracy), as well as in genotype (distance accuracy). The best configuration of a method refers first to the peak ratio results, then, in case of equality, it is chosen with respect to the distance accuracy. The corresponding values from the *best* basin ratio and *best* peak accuracy are the ones obtained in the configuration that is chosen to be the best with respect to the peak ratio or distance accuracy. Besides the average results of the best configuration repeated 30 times, the mean over all generated design points, each replicated 30 times, is presented. For each function, the techniques involved in the comparison are ranked upon the quality of the best configuration results, these too ordered first by peak ratio and then by distance accuracy. The best result with respect to each of the four applied measures is highlighted.

Fig. 2 enables a quick visual comparison for the best configuration of relative distance and peak accuracies of every function over all algorithms.

In order to verify the significance of the results and to validate the hypotheses formulated in the task subsection, two statistical tests are conducted for the results obtained in the 30 repeats of the best configurations. A *t*-test for independent samples is used to compare the difference in means between TSC2 and every other algorithm. As the normality assumption may not hold, the Wilcoxon rank-sum test is employed as a nonparametric alternative. The tests are performed on the peak ratio (best LHS configuration repeated 30 times). If two algorithms are not significantly different concerning this measure, their distance accuracies are also tested. The statistical results for all the functions are presented in Tables VI and VII. In these two tables, the methods are ordered according to the quality of their results as reported in Tables IV and V. The labels + or − assigned to each referenced technique signify the fact that TSC2 obtained better or worse results in comparison to it.

5) *Observations:* A brief look over Tables IV and V confirms that the compendium of benchmark functions is well chosen. Note that the method rankings change, depending on the problem properties, i.e., dimensionality, multimodality, and deceptive character.

We now analyze result Tables IV and V and the significance Tables VI and VII with the purpose of identifying for what problem types TSC2 performs significantly better than the other algorithms. TSC2 is placed first, or *ex aequo* with results similar (according to the statistical tests) to the method ranking first, for $F1$, $F2$, $F4$ with 10 variables, $F5$ with two variables, $F6$, $F7$, $F10$, and $F14$. The only other cases that have multiple peaks, all to be found, are $F11$, $F12$, and $F13$ and for these TSC2 is second best, with only minor (but statistically significant) differences in distance accuracy below CDE. Most of these functions have an irregular landscape, with optima often situated on the margins of the intervals, facts that disadvantage the other, radius-based methods. $F8$ is a different case because, although it has 18 global optima to be detected, it also possesses many local optima that are to be omitted. Nevertheless, the result for this case places TSC2 third out of the six techniques as regards the number of discovered peaks. The proposed technique does not disappoint for the remaining functions either, as it gives competitive results in most of the cases. Nevertheless, TSC2 seems best suited for the test cases with irregular landscapes that have up to 10 optima, all of which have to be located.

For the above mentioned test cases with optima haphazardly disposed, like $F1$, $F6$, $F7$, $F11$, $F12$, and $F13$, TSC2 is more accurate in finding the peaks than the radius-based techniques. CDE is outperformed by TSC2 when there is one optimum to be detected that has many local peaks in its vicinity and the discrepancy becomes higher when the number of dimensions raises to 10 or 20. To continue with the clarifications regarding the formulated hypotheses, TSC2 is superior to TSC [14] in all considered test cases. Checking the significance of the difference in results from Tables VI and VII, the only cases where TSC2 is not statistically better are $F9$ and $F11$; however, the resulting values still place the new technique above its previous version in the standings.

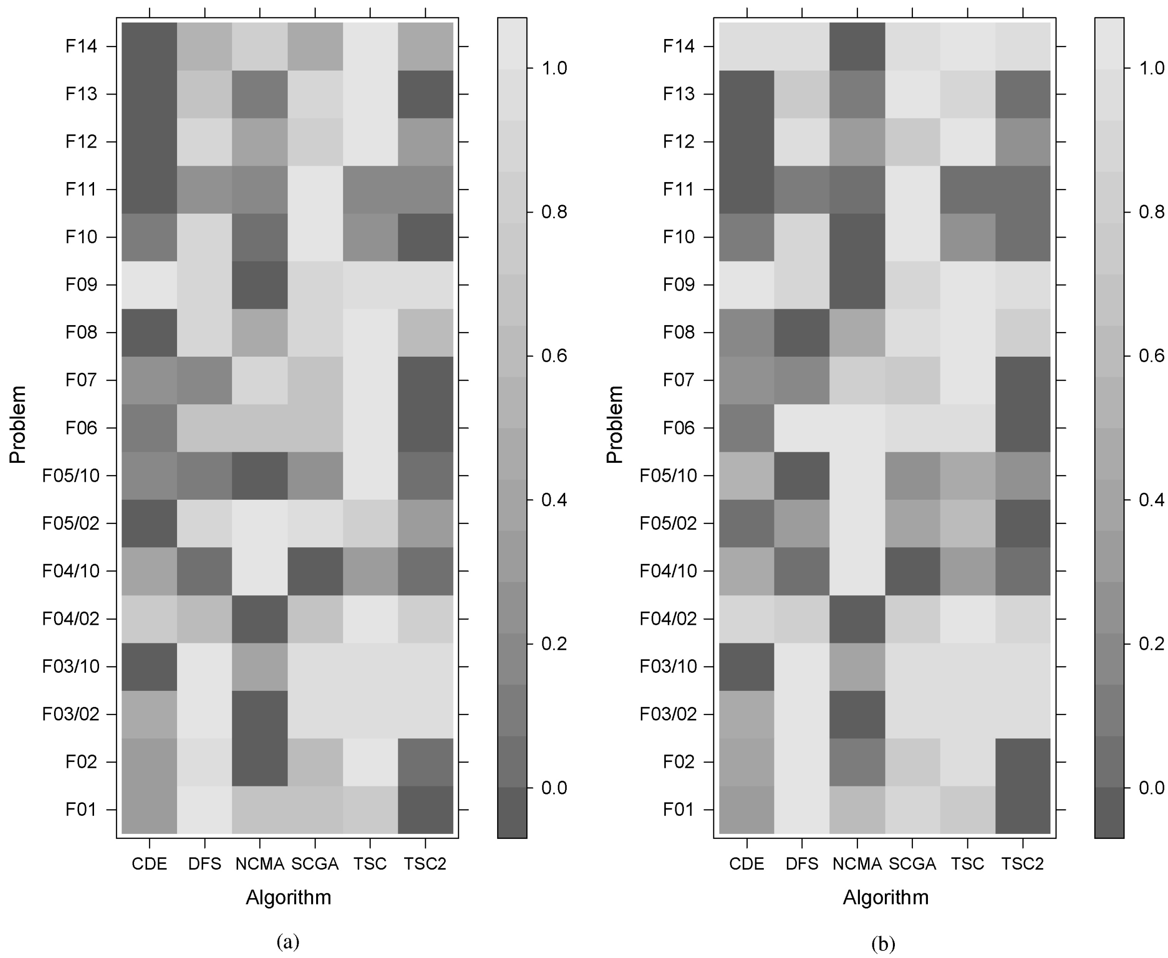


Fig. 2. Overview of relative (a) distance and (b) peak accuracies for the best LHS configurations of each algorithm. Results are log 10-transformed and then separately normalized for each problem, so that 0.0 refers to the best and 1.0 to the worst algorithm. Both measures lead to similar impressions, with three predominant algorithms: CDE, NCMA-ES, and TSC2.

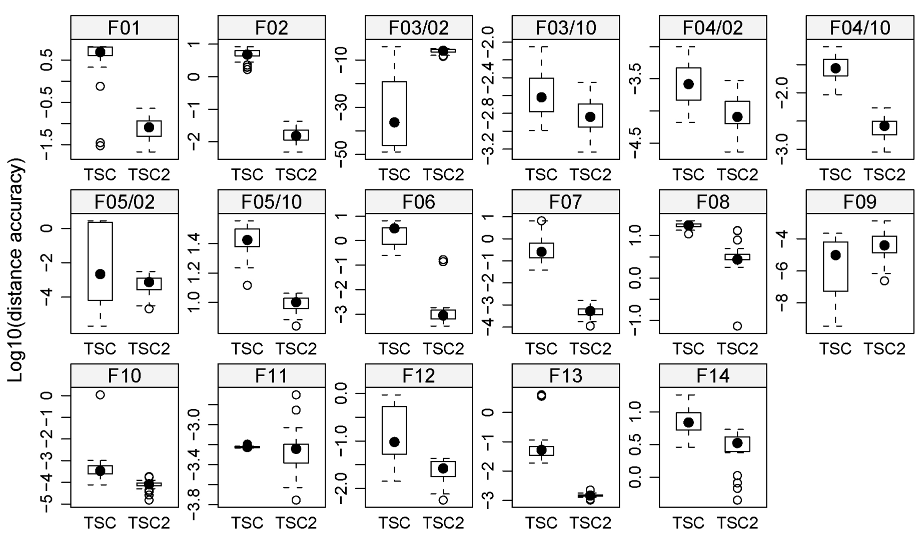


Fig. 3. Log 10-transformed distance accuracies of 30 runs of TSC2 against 30 runs of TSC. Best LHS configurations are compared over all test problems. TSC2 is better except for two cases.

TABLE VIII
OVERALL BEST/AVERAGE RESULTS OBTAINED FOR CLASSES OF TEST FUNCTIONS

Method	Peak Ratio		Basin Ratio		Peak Accuracy		Distance Accuracy	
	Best	Avg.	Best	Avg.	Best	Avg.	Best	Avg.
One optimum, $F4$ 2 and 10 dimensions, $F5$ 2 and 10 dimensions, $F9$, $F14$								
TSC2	**4.77**	1.85	4.1	3.3	785.27	1646.8	**12.97**	23.29
DFS	4.57	2.54	3.73	2.75	**627.76**	**1044.8**	16.13	24.99
SCGA	4.44	2.8	3.77	**3.74**	844.31	1647.8	17.8	23.21
TSC [14]	4.1	1.89	3.93	3.16	1235.4	2139.7	44.26	74.45
CDE	3.8	2.29	**4.9**	3.64	1097	1454.9	13.19	**15.31**
NCMA-ES	3	**2.83**	3	2.89	3516.8	3742.6	20.12	23.39
Multiple optima, $F1$, $F2$, $F6$, $F7$, $F10$–$F13$								
TSC2	**7.98**	7.22	**7.99**	7.25	**0.29**	8.25	**0.12**	5.39
CDE	7.86	**7.3**	7.96	**7.5**	0.77	**7**	0.25	**3.33**
SCGA	7.19	3.33	7.93	3.91	13.49	40.8	2.64	44.4
NCMA-ES	7.14	5.02	7.24	5.55	6.55	23.49	2.44	22.08
TSC [14]	6.98	5.82	6.9	5.7	13.75	24.25	10.48	27.67
DFS	6.34	3.29	6.33	4.35	23.98	42.79	8.67	40.16
More than 2 dimensions, $F3$, $F4$, $F5$, $F14$								
TSC2	**3**	0.8	2.13	1.69	770.5	1274.5	**12.9**	22.8
SCGA	2.97	1.32	2.17	**2.44**	762.8	1332	16.2	21.1
DFS	2.87	1.07	2	1.53	**569.7**	**880.1**	15.1	22.1
CDE	2.8	1.55	**2.9**	1.72	1076.4	1320	13.2	**15.3**
TSC [14]	2.47	0.79	2.2	1.94	961.7	1203.5	43.5	73.8
NCMA-ES	2	**1.73**	2	2.01	1816.8	1902.4	18.5	22.7
Peak ratio 1, $F3$ 2 and 10 dimentions, $F4$ 2 dimensions, $F9$, $F10$								
NCMA-ES	5	**4.49**	5	4.81	**6.8e−08**	**0.35**	**1e−04**	0.48
CDE	5	4.4	5	**4.96**	0.001	0.47	6e−04	**0.25**
TSC2	5	4.24	5	4.93	2e−04	2.64	0.001	0.51
TSC [14]	5	4.38	5	4.92	0.001	2.09	0.004	0.67
DFS	5	4.3	5	4.60	9e−04	0.53	0.01	0.96
SCGA	5	4.29	5	4.62	0.002	1.92	0.01	1.38
Overall								
TSC2	**15.45**	11.1	14.9	12.85	884.6	2383.1	17.3	62.1
CDE	14.65	**11.69**	**15.86**	**14.06**	1098	1577.4	**13.5**	**21.9**
SCGA	13.9	7.93	14	9.97	1447.5	3071.1	63.2	90.2
TSC [14]	13.44	9.58	13.1	11.1	1999.9	3792.6	133.5	161.8
DFS	13.35	7.76	12.5	9.31	**651.8**	**1087.8**	69.4	153.6
NCMA-ES	13.03	9.99	13.18	10.9	3527.6	3818.7	24.2	76.7

Methods are presented in decreasing order based on the quality of results in the best configuration, first by *peak ratio* and then by *distance accuracy*. The best result with respect to each of the four applied measures is highlighted.

A conclusive illustration of the considerable difference between TSC2 and the initial TSC is given in Fig. 3. For each test case, the distance accuracy is compared for the two for all 30 repeats of the best configuration. The black circle represents the median value; the rectangles plot the range for the middle half of the values (the two inner quartiles), while the grey circles represent the outliers. Note that except F3 in 2 dimensions and F9, TSC2 is always better. However, even in these two cases, TSC2 has the distance accuracy mean values (Tables IV and V) better than TSC, while the median pushes the latter in front only because it has a high-standard deviation.

In order to verify the above affirmations, Table VIII gathers the results from Tables IV and V in only one place, as it sums the values from all corresponding attributes according to groups of test functions.

For only one global optimum in a landscape perturbed by many local ones, we take $F4$ and $F5$ with 2 and 10 dimensions, $F9$ and $F14$. According to the peak ratio of the best configurations, TSC2 ranks first and is followed by DFS and SCGA. The proposed method also dominates the ranking when judging on the distance accuracy measure. However, the average over all LHS configurations positions TSC2 on the last place because, for these test cases and with the limit of fitness evaluations calls, good results are obtained only when the number of gradations is small, while for the rest it performs poorly. Regarding the peak accuracy, wherever $F5$ with 10 variables is included, DFS will definitely dominate the rest because for this test case it has a difference of about 200 to the second best and, even if summed over all the other cases, the amount is enough to put it on the first position.

The functions that possess many optima and all of them are to be found (there are 8 of them and they are enumerated in the table) are included in the second group. TSC2 is again first with respect to the peak ratio in the best configuration and is closely followed by CDE. For this type of problems, TSC2 performs well for all 30 LHS configurations, as it can be noticed from the 7.22 in average peak ratio. TSC2 also dominates the other four attributes that are measured for this group of functions, so the previous assumption remains valid.

The test problems considered for more than 2 dimensions are further on gathered. TSC2 is the only method that has the peak ratio equal to 3, meaning that except for $F5$, it found the desired optimum in the best configuration. However, the average peak ratio indicates the same behavior as for the first

TABLE IX
p-VALUES OF t-TEST AND WILCOXON RANK-SUM TEST FOR RESULTS OF $F2$ VERSUS $F6$ OBTAINED BY ALL METHODS

Method	p-Values for $F2$ Versus $F6$			
	Peak Ratio		Peak Accuracy	
	t-Test	Wilcoxon	t-Test	Wilcoxon
TSC2	0.16	0.16	0.16	2.67e−10
CDE	0.08	0.08	0.10	6.63e−09
SCGA	1.35e−08	6.55e−08	–	–
TSC	0.45	0.45	0.64	0.55
DFS	–	1.69e−14	–	–
NCMA-ES	–	1.69e−14	–	–

group (as many functions coincide): TSC2 performs well only for some configurations, while for others it gives poor results. It is the same number of gradations that has to be set small in order not to lose too many fitness evaluation calls and reach the limit.

The five functions for which all methods have the peak ratio equal to 1 are then collected and the techniques are ordered in this case according to the best configuration of the distance accuracy. NCMA-ES and CDE give the most accurate results and are then followed by the proposed TSC2.

Finally, the last case contains the summed results over all considered test functions. TSC2 ranks first, CDE is second and SCGA is third when it comes to the number of found peaks in the best configuration. For the distance accuracy attribute, CDE changes the place with TSC2 and is then followed by NCMA-ES. Eventually, according to peak accuracy, DFS is best (due to $F5$ with 10 variables).

The runtime differences are insignificant from one method to another. Except for $F5$ and $F14$ functions, the average runtime for one run is around the 10th of a second. For $F5$ with two variables, one run finishes in about 4.5 s and for 10 variables it takes about 16 s, while for $F14$ a run lasts around 1 s. The reason for the similar runtime of all techniques can be attributed to the common amount of fitness function calls. It must be remarked that the discussed enhancement regarding the economy in fitness calls within TSC2 as opposed to the previous TSC cannot offer a superiority in runtime in the current experimental setup. Since a maximum number of fitness evaluations is set as a stop condition, it is the saving in fitness evaluations that accelerates TSC2 in comparison to TSC.

6) *Discussion:* The main advantage of TSC2 over NCMA-ES, SCGA, and DFS is that the first does not make use of a radius for separating the individuals into subpopulations. Instead, it solely uses the fitness evaluations of some interior solutions to recognize the geometrical form of the landscape, and therefore, creates subpopulations that include only individuals which track the same peak. On the other hand, TSC2 has the disadvantage that it uses a higher number of fitness evaluations just for separating the subpopulations, while the NCMA-ES, SCGA, and DFS do not spend any in their budget for this purpose. However, in the undertaken experiments, the same budget of 3×10^4 fitness evaluations was set for all compared techniques and the results clearly indicate that TSC2 performs better than SCGA, NCMA-ES, and DFS in the cases when several optima are searched for, as it can be seen in Table VIII, second group of functions. The difference is important when analyzing the peak ratio for the best configuration and it increases when the average values are compared for the same measure, meaning that for this type of functions the radius-based methods are very dependant on the chosen parameters. Notable differences can be also perceived for the peak and distance accuracy attributes again, not only for the best configuration, but also in average over all LHS parameter settings. When the task was to find only the global optimum and avoid the local ones, TSC2 ranks at the top again, but this time closely followed by DFS and SCGA. It is the time for TSC2 to be more dependent on parameter values than the others, as the average results for peak ratio now advantage the radius-based methods.

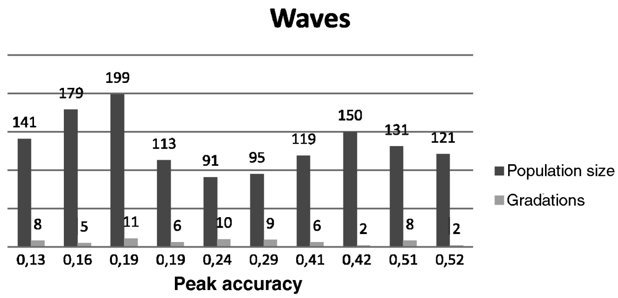
In the conducted experiment, DFS was able to escape local optima in favor of the global one, also meaning that suboptimal regions with sought local optima were abandoned. This weakness comes from the restriction which requires that a species has to contain at least two individuals. Despite the employed fitness sharing, the species that track solutions which are not very fit tend to decrease in constitution to one individual. As a species with only one individual does not conserve from one generation to another, it disappears rapidly.

SCGA performs better than DFS when the aim is to find various optima, because the minimum size of a species is not restricted and seeds are copied along the generations.

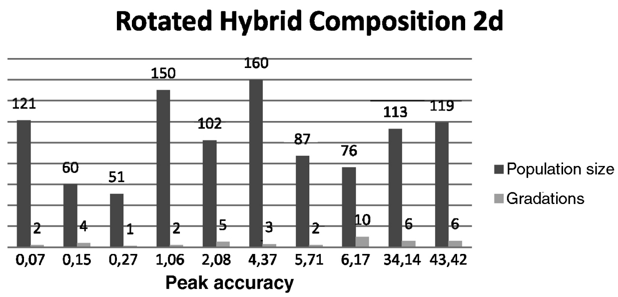
CDE is also very powerful when dealing with test cases that have many optima to be found, as it is placed second in Table VIII for that group of functions, while it performs best for Shubert function, the only one where several global optima are intertwined with local peaks. Moreover, when looking at the overall results, CDE is second, close to TSC2. However, when the task is to find only one global optimum with many local ones around it and when the number of dimensions is raised, CDE drops many positions in the rankings. The main advantage of CDE over the other methods is given by the ease to parameterize it, not only because it has only three parameters, but also because its average values over all LHS configurations are very good in most of the cases and they also place it first in the overall rankings for mean results in Table VIII.

NCMA-ES is by far the most accurate when checking the peak accuracy of the found optima. However, it demonstrated inconsistency, as for $F4$ with ten dimensions or for $F5$ with two dimensions it performed unbelievably weak. That is the reason why in the overall standings in Table VIII it occupies only the last position.

TSC2 does not make use of a radius, but it employs another parameter, i.e., the number of gradations. It is obvious that this parameter is easier to set than the radius within the NCMA-ES, SCGA or DFS cases, as the former is a positive integer value, while the latter is a positive real number. The main task of the current experiment was to perform an objective comparison between the chosen techniques for the same test cases and in similar circumstances. One of the imposed restrictions referred to the stop condition, i.e., the total number of fitness evaluation calls of 3×10^4. So, it was not in the aim of the current experiment to find all the desired optima for the test cases by any price, but merely to see how the techniques can



(a)



(b)

Fig. 4. Population size and number of gradations of TSC2 in best ten configurations for functions (a) $F1$ and (b) $F5$ with two variables. Average peak accuracy over 30 repeats is included on the horizontal axis.

handle the problems with all the requisite constraints. When several peaks are to be achieved, TSC2 performs better for the parameter setting configurations that have a large population and a high number of interior points so that all, or most of the attraction basins are detected by means of the *detect-multimodal* procedure. The population size and the number of gradations of the best ten LHS configurations with respect to the peak accuracy value are illustrated for $F1$ function in Fig. 4(a). When the function has an immense number of local optima and one global that has to be detected, the best choices for the two parameters seem to be a small number of gradations and various values for the population size, but the two kept in an equilibrium. When the population size is high, the number of gradations has to be very small or when the population size is small, the number of interior points can increase [Fig. 4(b)] in order to spend the evaluations wisely. The dependency of TSC2 upon these variables for some configurations can also be observed in the first group of test functions in Table VIII, where for the best configuration TSC2 ranks first, while for the average over all LHSs, it is positioned at the bottom of the ranking. However, as it can be seen in Fig. 4(b), in order to get the best results, the solution for this kind of problem is to use a small number of gradations. Nevertheless, if the stop condition had been changed to a higher allowed number of fitness evaluation calls, the best configuration would possibly be different.

Further on, the dependency of the models on changes in the function landscape and on their specific parameter for subpopulation differentiation are attentively investigated.

B. Model Dependency on Changes in the Function Landscape

1) *Pre-Experimental Planning:* The formation of subpopulations by only taking the topology of the fitness landscape into consideration and not relating to a radius can be an advantage because it shall react less sensitively to landscape modifications via simple mathematical transformations. In order to demonstrate that, two of the previous test functions are considered for all compared techniques, i.e., $F2$ and its shifted version, $F6$. While TSC2, TSC, and CDE should behave in a similar manner for the two functions, it is expected that the radius-dependent algorithms are sensitive to the fact that the optima in $F6$ are not equidistant any more.

2) *Task:* The following hypothesis is tested: the accuracy remains invariable in nonradius-based techniques for both $F2$ function and its shifted version ($F6$), while it changes when radius-powered methods are employed for the reallocation of the existing peaks.

3) *Experimental Setup:* The same LHS points as for the first experiment are considered for comparing the results for $F2$ and $F6$. However, because the locations of the optima are changed for the two functions, instead of using the distance as the second measure for comparing the difference, the peak accuracy is employed as the optima have the same height.

4) *Results and Visualization:* The results are visualized in Tables IV and V. While TSC2, CDE, and TSC have approximately no change in results when moving from $F2$ to $F6$, all the other methods show a performance decrease when the optima are not equally distant, i.e., in the case of the $F6$ function. Table IX presents the p-values obtained through the application of a t-test for independent samples and a Wilcoxon rank-sum test for measuring whether the difference in the results of the same method for $F2$ and its shifted version $F6$ is significant. Tests are employed for peak ratio and, if the difference is not considerable, the same tests are performed for the peak accuracy measure. As the results show, there is a significant difference for peak ratio for SCGA, DFS, and NCMA-ES for the t-test and/or Wilcoxon rank-sum test. For DFS and NCMA-ES the t-test could not be computed because the standard deviation in the case of $F6$ was null. The p-values obtained for TSC2, CDE, and TSC for peak ratio indicate that this difference is not important. Moving the attention to the tests for peak accuracy, it can be noticed that the Wilcoxon rank-sum test shows significant differences for both TSC2 and CDE, while according to the t-test this is not true. TSC, however, is even more steady as both statistical tests point out, but it is constant in providing modest results for these functions. To conclude, TSC2, CDE, and TSC are not sensitive to optima reallocation as regards the number of found peaks. This sustains the formulated hypothesis, although the values in peak accuracy are disrupted by the rescaling between the two functions for TSC2 and for CDE.

5) *Discussion:* The assumptions within the current experiment were verified. When counting the detected optima, TSC2, CDE, and TSC are independent of the fact of whether the optima are equally remote or not, while NCMA-ES, SCGA, and DFS are very sensitive to such changes in the peaks location. This is an important drawback of the radius-based techniques involved in this comparison as it cannot be assumed that a real-world problem has equally distant optima.

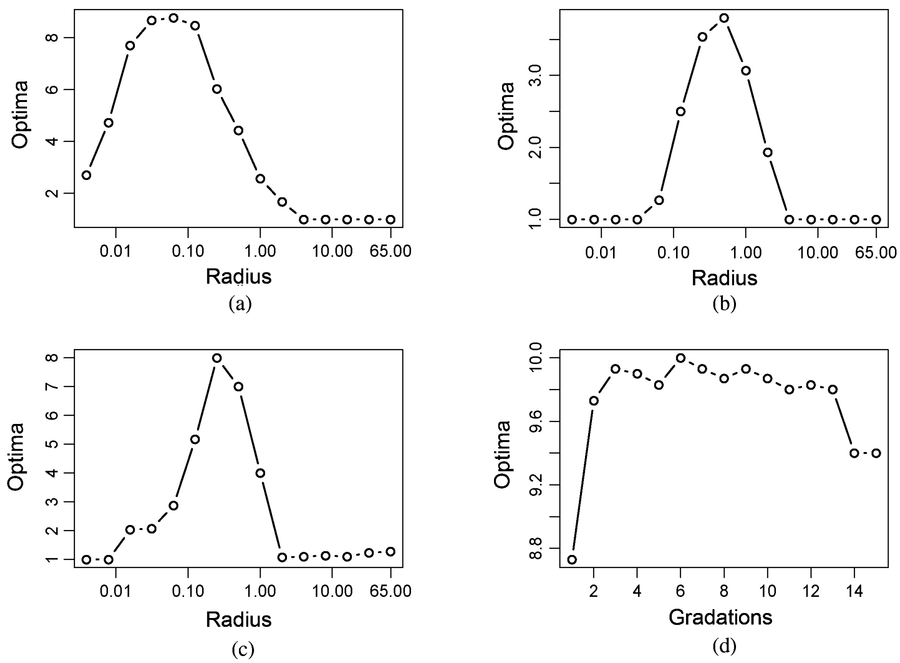


Fig. 5. Average number of optima in 30 repeats that are detected for the Waves function ($F1$) for different radius values within (a) SCGA, (b) DFS, and (c) NCMA-ES. The distinct values for the number of gradations in TSC2 and the amount of detected optima are represented in (d).

C. Model Dependency on Niche Radius or Number of Gradations Parameters

1) *Pre-Experimental Planning:* As radius-based techniques ranked below the other methods for the asymmetric function $F1$ in the first experiment, finding a proper value for the radius and subsequently investigating how dependent these methods are on the values of this parameter is of great interest. Plus, the reliance of TSC2 to the number of gradations parameter is also of major concern.

2) *Task:* Investigate how sensitive TSC2, on the one hand, and the radius-based methods, on the other hand, are on the specific parameters for determining multimodality, i.e., number of gradations and radius, respectively. Different values are tried for the radius/number of gradations on the $F1$ test function. The hypothesis to be tested is the following: TSC2 is not as sensitive to the changes in the values of the number of gradations parameter as SCGA, DFS, and NCMA-ES are to the variations in their corresponding radius parameter when optimizing a function with many peaks.

3) *Experimental Setup:* In order to find the best values for the radius/number of gradations when tackling the $F1$ function, the best LHS configuration found in the first experiment is used for all the parameters, except the two examined ones. For each configuration, 30 repeats are performed. While for TSC2, the number of gradations is tried for all possible values considered in the direct comparison experiment (1–15), for the others, the radius is exponentially scaled. The starting value is computed using the Deb and Goldberg formula (1) and then the value is multiplied with integer powers of 2 taken from the interval $\{-7, -6, \ldots, 6, 7\}$.

4) *Results and Visualization:* Results obtained for $F1$ by SCGA, DFS, and NCMA-ES with different values for the radius parameter are shown in Fig. 5(a)–(c). The actual value found using Deb and Goldberg formula is approximately 0.5. It can be noticed, however, from the SCGA and NCMA-ES graphics that the best average result is not obtained for this value, but for smaller ones, to be more specific, for 0.126 and 0.25, respectively. Nevertheless, for DFS, the best configuration was precisely the one that had the radius computed by Deb and Goldberg formula, but the method could only reach a modest result, that is 3.8 peaks in average. None of the values generated for the radius was proper for detecting all 10 optima of the function through the three methods. Moreover, when the value for the radius is higher than 1, the number of detected optima decreases to only approximately one solution.

Fig. 5(d) outlines the average number of detected optima when trying different values for the number of gradations parameter within TSC2. As it can be seen, by increasing the value of the number of gradations from 2 up to 13, more than 9.6 optima are detected in average for 30 runs of the same configuration. The results shown in the four figures indicate that the tested hypothesis is correct.

Finally, as a distinct reinforcement of the validity of the given hypothesis, Fig. 6 illustrates the parameters influence on performance (in terms of found peaks) of the same SCGA, DFS, NCMA-ES, and TSC2 methods on problem $F1$. The visualization method divides the measured 30 LHS configurations into three equally sized groups, i.e., a good, middle, and a badly performing set. Instead of a usual box plot bar, an approximated percentile depiction is chosen as it emphasizes more where the single points are located. The dot in the middle of each bar represents the average (in parameter values of this group), the largest vertical line stands for the median, while the others represent the hinges. As it can be seen in the Fig. 6(a) and (b), the only parameter that has a great influence over the results for SCGA and DFS is the radius, which is set in average around 1 for the best 10 configurations,

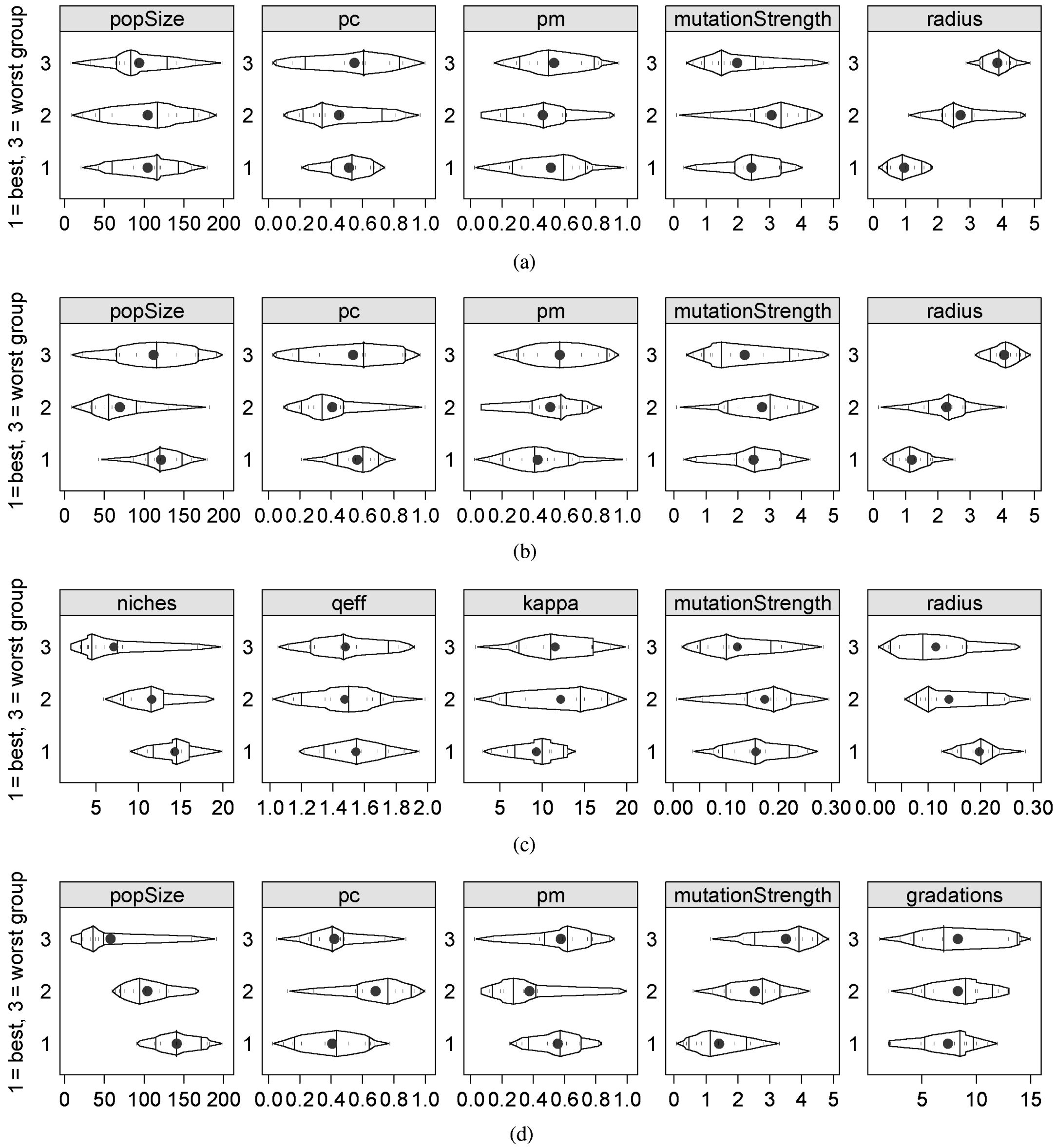


Fig. 6. Box percentile plots of LHS (30) parameters for (a) SCGA, (b) DFS, (c) NCMA-ES, and (d) TSC2 on the Waves function ($F1$). Note that the three quality groups reflect relative and not absolute quality (in terms of best and worst).

while for the second 10 configurations it is moved to 3 and the worst 10 configurations had it with the greatest value, that is approximately 4. For NCMA-ES, the radius parameter still remains important, however, its significance is not of the same magnitude, as it allows other parameters to matter. The niche parameter is also taken around 15 for the best 10 configurations and the results get worse when its value decreases. The important parameters for TSC2 are the size of the population and the mutation strength and the best results are achieved when the former is high and the latter is low. The number of gradations is not relevant for this test case, fact that also sustains the conclusions derived from Fig. 5. To conclude, in Fig. 6, apart from a visualization of the other parameters weight on the peak accuracy, the variability of the radius value as opposed to the consistency of the number of gradations once more supports the formulated hypothesis.

5) *Discussion:* It can be noticed that TSC2 does not very much depend on the value that is chosen for the number of gradations parameter, while the picking of the right value for the radius parameter within SCGA, DFS, and NCMA-ES is vital in obtaining good results. Figs. 5 and 6 also show this, the former taking into account the best configuration averaged over several repeats, while the latter considering only relative performance values and not the absolute ones for one tested algorithm. It may be argued that adjusting the radius by the use of a metaheuristic would be the trivial solution to the problem of setting its value. However, if the various attraction basins have unequal sizes, a unique value for the radius to differentiate between species connected to each peak cannot be appointed. Plus, this would add complexity to the respective technique, while the proposed TCS2 approach is not sensitive to an otherwise easy to calibrate corresponding value for the number of gradations.

V. Conclusion

In this paper, a multimodal evolutionary technique deriving from an earlier integration of concepts of two modern methods was further augmented by imposing several control variables, supporting diversity and aiming for a prolonged search time by inherently saving fitness evaluations. The novel TSC2 was tested for the optimization of several benchmark functions and a real-world instance. To justify its development, results were directly compared to the original TSC version [14] and the better one of the parent techniques, the SCGA [6]. To be even more critical, experiments were further performed in contrast to one related, recent evolutionary multimodal approach, the DFS [7], to another competitive radius-based methodology, the NCMA-ES [15] and, finally, to a complementary method of crowding differential evolution (CDE) [11].

TSC2 aimed to inherit the strengths from SCGA and the manner of detecting multimodality within the MGA [5], while avoiding their shortcomings and going beyond the initial TSC combination in the construction of a more robust algorithm, able to deal with real-valued multimodal optimization problems. In the first respect:

1) the fitness landscape-triggered methodology obsoletes the use of the radius threshold for species differentiation;
2) the sizes of the species are thus directly correlated with those of the basins to which they are connected, as they flexibly adapt to the shape of the landscape. Therefore, the species are not forced to be formed within equally spaced hyperspheres that depend on the value of a threshold, as it is the case in radius-based evolutionary approaches;
3) the preservation of the most prolific individuals within each subpopulation takes place in order to maintain the spread of the potential solutions over the search space;
4) a manner of keeping track of all individuals species is proposed in order to reduce the expenses regarding the amount of consumed fitness evaluations.

In the second regard, the extensions of TSC2 above the previous TSC targeted the following.

1) For the purpose of further carefully saving fitness calls and thus of an extension of evolutionary time, a notion of similarity is employed when possible, instead of repeatedly referring the $detect - multimodal$ procedure.
2) Exploration is increased by broadening the opportunities for new diverse species as a result of reproduction.
3) The species seeds are not directly copied into the population of the next generation, but their possible redundancy is checked and prevented beforehand.
4) A fixed upper bound for the number of seeds to record is set, in order to avoid the whole population of individuals turning into prototypes for an overestimated number of species.

Experiments show that the new TSC2 technique achieves both liberation from a crucial parameter and significantly better performance than the algorithms it is compared to, especially for the test functions that have an irregular landscape representation. Additionally, the results of the expansions on top of the preliminary TSC argued in favor of the new TSC2 approach.

From a practical perspective, the results on the traditional benchmark problems bring evidence of the type of real-world problems that can reach solution by means of TSC2. Although many 2-D functions are employed for testing purposes, the experiments specifically answered 10 to 20-D tasks as a reasonable model substitute for real instances. Moreover, cases of higher multimodality (as usual in practice), ranging from 10 to 20 important optima to be found, were additionally successfully solved. Very importantly, all these specific assignments are resolved with a relatively small budget of fitness evaluations (30 000), which is a primary concern in real applications. Finally, TSC2 has been shown to deal well with asymmetric landscapes that can be expected for many real-world applications.

A first step to extend the current work would be to add mutation step size adaptation mechanisms, as this will surely open a path leading to substantially increased performance.

Secondly, for a complete and general multimodal instrument, it would be interesting to study and further tailor the proposed approach in application to problems of dynamic nature. Since the landscape changes over time, the topologically-triggered TSC2 flexibility in subpopulation formation should deal with this situation in a useful manner.

Another task that is currently under development is the enhancement of a tool for estimating the number of local/global optima within the landscape of a function [29], this time by taking advantage of the novel features within TSC2. Knowing this information in advance can be very valuable for a technique dealing with a specific problem. It can help in setting the proper values for parameters or even in deciding the method that should be employed for solving the task. TSC2 represents a good inspiration for this purpose as it keeps track of all the different detected peaks through direct landscape inspection and it would help to estimate how many niches exist in the search space from the very early stages of the evolutionary process.

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Catalin Stoean (M'08) was born in Craiova, Romania, on August 31, 1979. He received the M.S. AQ:6 degree from the University of Craiova, Craiova, Romania, and the Ph.D. degree from the Babes-Bolyai University, Cluj-Napoca, Romania, both in computer science, in 2003 and 2008, respectively.

Since 2003, he has been an Assistant Professor at the Department of Computer Science, Faculty of Mathematics and Computer Science, University of Craiova. For the last couple of years, he has been lecturing on the topic of artificial intelligence. He has been active in the fields of evolutionary computation and machine learning. He AQ:7 has been a Visiting Scholar of the University of Dortmund and the University of Cologne, Germany, courtesy of two grants from the German Academic Exchange Service.

Dr. Stoean is a Member of the IEEE Computer Society. In 2008, he was part of a group of four people who won the 2008 Romanian Academy Grigore Moisil Award for computer science research conducted in 2006.

Mike Preuss (M'08) was born in Ahlen/Westfalen, Germany, on March 23, 1969. He received the Diploma degree from the Department of Com- AQ:8 puter Science, Dortmund University of Technology, Dortmund, Germany, in 1998.

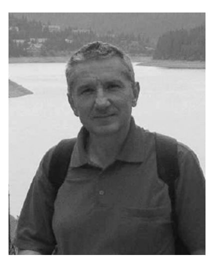
Since 2000, he has been a Research Associate with the Department of Computer Science, Dortmund University of Technology. His mission is to further develop the experimental methodology for nondeterministic optimization algorithms by means of tuning, adaptability measures, and other experimental analysis techniques. These are essential for the design of specific evolutionary algorithms (EA)-based algorithms for industrial optimization in various engineering domains, e.g., thermodynamics and ship propulsion technology. His research interests include the field of EA for real-valued problems, namely for multimodal and multiobjective niching.

Prof. Preuss is active in designing authentic artificial intelligence compo- AQ:9 nents for believable opponents and increased player satisfaction as a member of the IEEE Computational Intelligence Society (CIS) Games Technical Committee and the Chair of the CIS task force on realtime strategy games.

Ruxandra Stoean (M'08) was born in Craiova, Romania, on August 2, 1979. She received the M.S. degree from the University of Craiova, Craiova, Romania, and the Ph.D. degree from the Babes-Bolyai University, Cluj-Napoca, Romania, both in computer science, in 2003 and 2008, respectively.

She is currently an Assistant Professor with the Department of Computer Science, Faculty of Mathematics and Computer Science, University of Craiova, where she lectures on nonprocedural programming and laboratories of artificial intelligence and logic AQ:10 programming. Her current research interests include support vector machines, evolutionary computation, and data mining. She has been the guest of the Universities of Cologne and Dortmund, Germany, with the support of a German Academic Exchange Service grant.

Dr. Stoean was awarded a 2008 Computer Science Prize from the Romanian Academy for a collection of papers in evolutionary computation as part of a four-person group. She is a member of the IEEE Computer Society.



D. Dumitrescu received the M.S. and Ph.D. AQ:11 degrees from Babes-Bolyai University, Cluj-Napoca, Romania. AQ:12

He is currently a Professor with the Department of Computer Science, Babes-Bolyai University. His AQ:13 current research interests include natural computing, complexity, and computational game theory.