



Improved Exploration and Exploitation in Particle Swarm Optimization

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Abstract. Exploration and exploitation are analyzed in Particle Swarm Optimization (PSO) through a set of experiments that make new measurements of these key features. Compared to analyses on diversity and particle trajectories, which focus on particle motions and their potential to achieve exploration and exploitation, our analysis also focuses on the *pbest* positions that reflect the actual levels of exploration and exploitation that have been achieved by PSO. A key contribution of this paper is a clear criterion for when restarting particles can be expected to be a useful strategy in PSO.

Keywords: Exploration · Exploitation
Particle Swarm Optimization · Multi-modal search spaces

1 Introduction

To improve “exploration” and “exploitation”, we must first have clear measurements on existing levels of these features, and these measurements require precise definitions. We begin by dividing a multi-modal search space into attraction basins which each have a single local optimum. Each point in an attraction basin has a monotonic path of increasing (for maxima) or decreasing (for minima) fitness to its local optima. A search point (e.g. the current position of a particle) is then defined to be performing “exploration” if it is in a different attraction basin than its reference solution (e.g. the particle’s *pbest* position), and it is defined to be performing “exploitation” if it is in the same attraction basin as its reference solution.

Optimization in a multi-modal search space involves exploration to find the best attraction basin and exploitation to find the local optimum within this attraction basin. The performance of a search technique in multi-modal search spaces thus depends on its ability to perform both exploration and exploitation, and it is noted that Particle Swarm Optimization (PSO) [1] has several weaknesses in its ability to perform each of these two critical tasks. A large number of modifications have been proposed to address these weaknesses [2], but most of these modifications do not have consensus acceptance (e.g. by becoming part of a standard implementation such as [3]).

We believe the lack of precise definitions for the concepts of “exploration” and “exploitation” [4] have interfered with the ability to specifically identify PSOs weaknesses in these critical tasks, and thus to subsequently measure if any of the proposed modifications have had the intended effect. The improved precision of the above definitions for exploration and exploitation allow us to conduct quantitative experiments in which the effects of modifications can be measured at both the operational level (e.g. more exploitation has been observed) and at the performance level (e.g. average results on benchmark functions has improved).

Our research begins with an analysis on the operational characteristics of a standard implementation of PSO [3]. The first key observation we make is that many *pbest* positions in the final swarm do not represent local optima. This result exposes a weakness in the ability of PSO to perform exploitation. If PSO was able to fully exploit all of the attraction basins represented by its *pbest* positions, its performance could improve. Additional measurements also indicate that a very small number of attraction basins are fully exploited/have their local optimum reached, and this observation raises concerns about the effectiveness of exploration in PSO.

Based on the above analysis, we make several modifications to PSO. The effects of these modifications are measured using an experimental procedure that is presented as part of the Background Section. Baseline measurements of exploration and exploitation in standard PSO are then presented in Sect. 3. In Sect. 4, we introduce a modification to improve exploitation in PSO, and we present both operational and performance data to support the usefulness of this modification. We then add another modification to improve exploration in Sect. 5, and we again present both operational and performance data to verify its benefits. We then provide a Discussion of our experiments and results before some brief Conclusions close the paper.

2 Background

“Exploration” and “exploitation” are highly discussed topics in metaheuristics and evolutionary computation. However, these concepts often lack precise definitions. A broad survey of over 100 papers led Crepinšek, Liu, and Mernik to the unexpected conclusion that “The fact that until now exploration and exploitation have only been implicitly defined in EAs comes as a big surprise” [4]. We

believe the lack of precise definitions hinders the ability to specify and collect quantitative data for in-depth analysis. A subsequent complaint of contemporary research is that a large amount of it has “only presented experimental results [on benchmark problem sets] and did not provide adequate discussion (neither from theoretical perspective, nor general discussions) on merits of the proposed approach” [2].

The theoretical perspective that we will provide in this paper is based on quantitative data collected on the Rastrigin function. The basic experimental procedure was first presented as part of the development of Leaders and Followers? [5], and it leverages the known structure of the search space for the Rastrigin function. Specifically, every point in the search space with an integer value in each dimension is a local optimum, and the nearest local optimum for every other point can be found by rounding that point’s coordinate values to their nearest integer. These features allow us to divide the search space into non-overlapping attraction basins, know the fitness of (the local optimum of) an attraction basin, and calculate the difference in fitness between an existing solution and its nearest local optimum. We believe that an analysis based on these types of quantitative data can provide a more “adequate discussion” as requested in [2].

Our analysis will also focus specifically on the achievement of exploration and exploitation as opposed to “inputs” such as diversity and particle trajectories. For example, it has been said that “Diversity is related to the notions of exploration and exploitation: the more diverse a swarm is, the more its particles are dispersed over the search space, and the more the swarm is exploring” [6]. However, it should be noted that even though a diverse swarm has the potential for more exploration, there is nothing that prevents a diverse swarm from performing exploitation instead (according to our definitions). In fact, studies which analyze the oscillatory nature of particle trajectories [7] clearly demonstrate that even particles which travel far away from their reference solutions (e.g. a *pbest* attractor) often spend significant time near these reference solutions as well. By focusing on the effects to *pbest* positions, our experiments measure what has happened in terms of exploration and exploitation as opposed to what was hoped to happen.

3 An Analysis of Standard PSO

We base our experiments on a version of standard particle swarm optimization [3] with a ring topology and the key parameter values of $\chi = 0.72984$ and $c_1 = c_2 = 2.05$. Additional implementation details are the use of $p = 50$ particles [3], zero initial velocities [8], and Reflect-Z for particles that exceed the boundaries of the search space (i.e. reflecting the position back into the search space and setting the velocity to zero) [9]. The source code for this implementation is available online [10].

All of our experiments with Rastrigin are based on averages for 30 independent trials in $n = 30$ dimensions using a termination condition of $10,000 \cdot n$

total function evaluations (FEs). As shown in (1), Rastrigin develops a globally convex, multi-modal search space by superimposing a sinusoid over a parabolic base function. The standard parameters are $A = 10$ and $x_i \in [-5.12; 5.12]$. Rastrigin is an n -dimensional minimization problem with a single global optimum of zero when all $x_i = 0$, and it contains a high number of local optima evenly distributed across the entire search space. These optima are located at the integer coordinates of a regular grid of size one, which means that the function has 11^n optima within the search boundaries defined above. Given a solution in this well-structured search space, the nearest (local) optimum for any solution x can be easily determined by rounding each component x_i to its nearest integer.

$$f(x) = An + \sum_{i=1}^n [x_i^2 - A \cos(2\pi x_i)] \quad (1)$$

Knowing the location of every local optima and the boundaries of their attraction basins allows us to easily and directly measure aspects of exploration and exploitation according to our previous definitions. We can also measure what we call the “fitness of an attraction basin” – i.e. the fitness of the local optimum of an attraction basin. For our implementation of standard PSO, we have recorded the fittest solution (i.e. the solution that would be *gbest* when using a star topology), the fittest attraction basin represented by the *pbest* positions, and the fittest attraction basin visited by any particle (see Fig. 1). It should be noted that the three curves plateau after about 50% of the allocated function evaluations. This premature convergence happens despite PSO’s inability to fully exploit all of the attraction basins represented by *pbest* positions, and in particular the fittest of these attraction basins. It should be noted that the fittest attraction basin is not necessarily associated with the fittest overall solution, and this situation is the likely cause of the gap between the curves for the fittest solution and the fittest attraction basin represented by a *pbest* position.

It is also worthwhile to note the large gap between the fittest attraction basin visited by a particle and the fittest attraction basin retained by a *pbest* position. This gap indicates a large divergence between what is happening at the particle level (e.g. their diversity and trajectories) and with their *pbest* positions (i.e. what updates are actually being stored). We thus focus our attention on *pbest* positions by recording the fitness of each *pbest* and its associated attraction basin. The difference between these two values is a measure of the amount of exploitation that has occurred in that attraction basin. For the Rastrigin function in 30 dimensions, we define a difference of less than 10 between these two values to indicate that the represented attraction basin has been “fully exploited”. The total height of each attraction basin is at least 600, so a gap of less than 10 represents significant exploitation.

Table 1 shows the average number of *pbest* positions that represent fully exploited attraction basins at the end of the 30 independent trials. We also report the total number of distinct attraction basins that have been fully exploited, the number of times a *pbest* which is within 10 of the local optimum of its current attraction basin moves into another attraction basin (i.e. that its particle has

Table 1. Analysis of standard PSO

Algorithm	Fully exploited final <i>pbests</i>	Fully exploited attraction basins	Fully exploited <i>pbests</i> moved	Function fitness
PSO	38.2	13.1	0.0	66.8

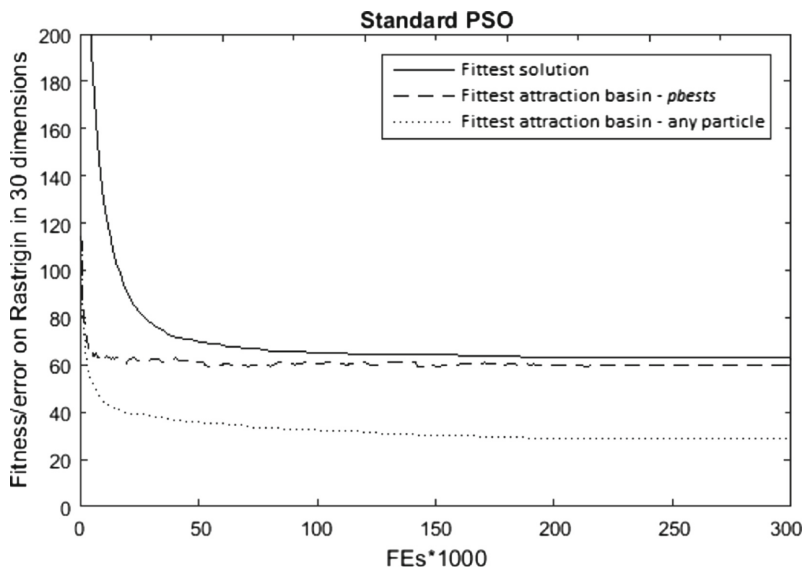


Fig. 1. Analysis of Standard PSO. The gap between the fittest solution and the fittest attraction basin represented by a *pbest* position shows a weakness in the ability of PSO to perform exploitation.

performed successful exploration after full exploitation), and the fitness of the best overall solution at the end of the allocated 300,000 FEs.

Two key observations can be made from the collected data. First, a large number of *pbest* positions (i.e. 11.8/50 or 23.6%) are still a large distance away from their nearest local optimum (i.e. they have a fitness difference of at least 10). This indicates a weakness in the ability of PSO to perform exploitation in the vicinity of these *pbest* positions. Second, no particles (i.e. 0.0) that achieve “full exploitation” of an attraction basin ever move their *pbest* position into a different attraction basin (i.e. perform exploration according to our definitions). At the end of the allocated FEs, the *pbest* positions represent an average of 13.1 distinct attraction basins that have been fully exploited.

These observations contradict a common narrative on the operation of PSO. The goal of a ring topology (compared to a star topology) is to slow down, not stop, communication amongst the particles. However, our results indicate that all of the particles and their *pbest* positions have not converged to a single optimum, and that at least 13 distinct attraction basins remain on average. The

communication chain in PSO is broken by the inability of a particle which has achieved full exploitation of one attraction basin to ever successfully explore (i.e. move its *pbest* to) another attraction basin – this includes known attraction basins such as the (fitter) attraction basins represented by the *pbest* positions for other particles in the swarm. In combination with the observation of (11.8) particles which never achieve the full exploitation of any attraction basin, we believe these experiments demonstrate that the particle trajectories achieved by standard PSO have weaknesses in both their ability to perform exploration and their ability to perform exploitation.

4 A Modification for Improved Exploitation

The preceding observations lead us to make the following hypothesis about the operation of PSO. Exploitation to find improving solutions in the attraction basins for the Rastrigin function in 30 dimensions requires sufficiently slow moving particles to ensure a fine-grained sampling of the search space around each *pbest* attractor/reference solution. This might only happen if both of the attractors for a particle (i.e. *pbest* and *lbest*) are in the same attraction basin (e.g. by being the same position). In PSO with a ring topology, the *lbest* positions represent the fittest *pbest* from the current particle and its two neighbours. This strategy makes it possible for some *pbest* positions to never be *lbest*, and we believe this could be necessary to allow exploitation in the attraction basin that the given *pbest* position represents. We propose a modification to ensure that every *pbest* position has the opportunity to also be an *lbest* position at some time so as to increase the probability of fully exploiting its represented attraction basin.

Our modification will select the *lbest* position for a given particle by rotating through the usual *pbest* positions from which it normally selects its *lbest* position. This rotation involves four steps in each cycle which repeat until allocated function evaluations are exhausted. In the first step, *lbest* is selected as usual, i.e. the *lbest* of particle i is the fittest of $\{pbest_{i-1}, pbest_i, pbest_{i+1}\}$. In the next three steps, the *lbest* of particle i is selected as $pbest_{i-1}$ first, then $pbest_i$, and finally $pbest_{i+1}$. A simple parameter tuning revealed that, for Rastrigin, a suitable frequency for the rotation cycle is to move to the next step every 40 iterations (i.e. 2000 function evaluations if the population size is 50).

The goal of this modification is to promote the exploitation of more attraction basins. As it is shown in Table 2, this goal has been achieved as the number of particles which can fully exploit an attraction basin as evidenced by the location of its final *pbest* position increases to an average of 44.6 per trial. As these particles perform exploitation, they are less likely to abandon their attraction basins, and this leads in an increase in the number of distinct attraction basins that are fully exploited – which now averages 42.9 per trial. Another positive outcome, as Fig. 2 shows, is that premature convergence of the fittest solution no longer occurs, and this helps the swarm achieve a better overall performance on Rastrigin. However, the number of *pbest* positions that are in fully exploited attraction

basins which move to another attraction basin remains at 0.0, and this limits the ability of this modification to reduce the gap between the fittest attraction basin visited by any particle and the fittest attraction basin represented by a *pbest* position.

Table 2. Analysis of rotate PSO

Algorithm	Fully exploited final <i>pbests</i>	Fully exploited attraction basins	Fully exploited <i>pbests</i> Moved	Function fitness
Rotation PSO	44.6	42.9	0.0	46.5

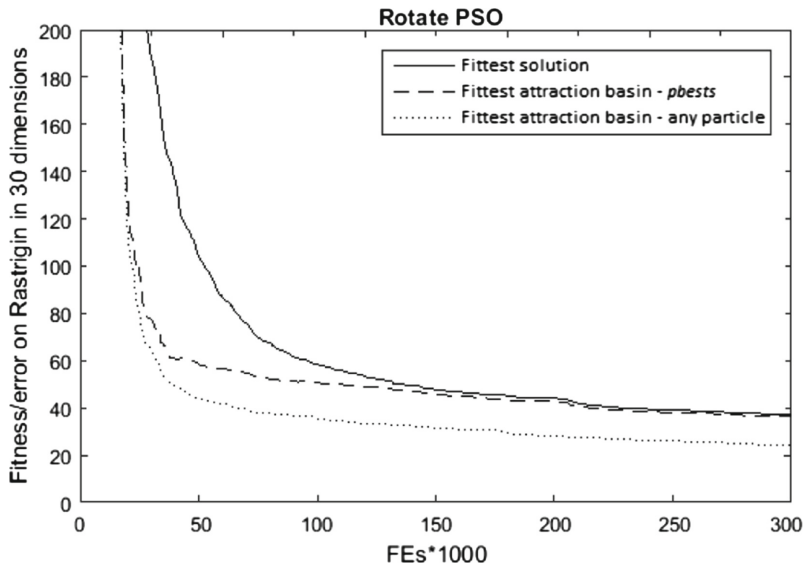


Fig. 2. Analysis of Rotate PSO. The gap between the fittest solution and the fittest attraction basin represented by a *pbest* position has been reduced.

5 A Modification for Improved Exploration

The previous modification was able to improve the number of fully exploited attraction basins, but it is still a very small number. A key weakness in PSO appears to be the inability of a particle which has performed exploitation in one attraction basin to ever achieve successful exploration in another attraction basin. Based on our hypothesis that exploitation to find a better solution around a *pbest* position requires sufficiently slow particle speeds, the ability of a particle

to find a highly fit solution (e.g. one that has experienced a large amount of exploitation) in another attraction basin will be extremely unlikely due to the relatively high speeds caused by the large attraction vectors that result from having attractors at least as far apart as the size of an attraction basin. If particle speeds which allow the visiting of different attraction basins (i.e. our definition of exploration) make finding highly fit solutions in these attraction basins next to impossible, then modifications that alter more than particle trajectories (e.g. increasing diversity) will be necessary to achieve “successful” exploration (i.e. exploration which leads to a moved/updated *pbest* position).

Our next modification aims to restart particles that have fully exploited their current attraction basin without improving the best overall fitness of the swarm. During the normal operation of PSO, we cannot measure the fitness of an attraction basin, so we instead predict that a particle has fully exploited its attraction basin if the fitness of its *pbest* position has not improved during a rotation cycle by at least 1% of the difference between the fittest and least fit *pbest* positions in the swarm. A secondary benefit of this threshold is that it adapts the restart criteria to the search space (e.g. the height of the attraction basins which will of course vary across different problem domains). If exploitation is continuing for a given particle, then we will allow it to continue. Otherwise, if insufficient improvement has been recorded, we will assume that the stalled particle has already fully exploited its attraction basin and restart it. A restart involves relocating the particle to a uniform random position in the search space, setting its velocity to zero, and setting the *pbest* fitness to infinity. A simple parameter tuning revealed that good results can be achieved if rotation steps occur every 40 iterations and restarts are performed every cycle or 160 iterations.

Table 3. Analysis of Rotate + Restart PSO

Algorithm	Fully exploited final <i>pbests</i>	Fully exploited attraction basins	Fully exploited <i>pbests</i> moved	Function fitness
Rotation + Restart PSO	38.0	218.2	209.9	21.5

Table 3 shows that the most distinctive feature of adding restarts to PSO is the large number of *pbests* from fully exploited attraction basins that are now moved/updated (through being restarted). This measurement is based on the actual fitness difference between the *pbest* position and its attraction basin being less than 10 as opposed to the predictive estimate used to restart the particle. The ability to restart particles once they have fully exploited their attraction basins improves exploration as indicated by the increase in the number of attraction basins that are fully exploited. As Fig. 3 shows, this improved exploration greatly reduces the gap between the curves for the fittest attraction basin represented by a *pbest* position and the fittest attraction basin visited by any particle. The effect on performance is also observed with a large improvement for PSO on the Rastrigin function.

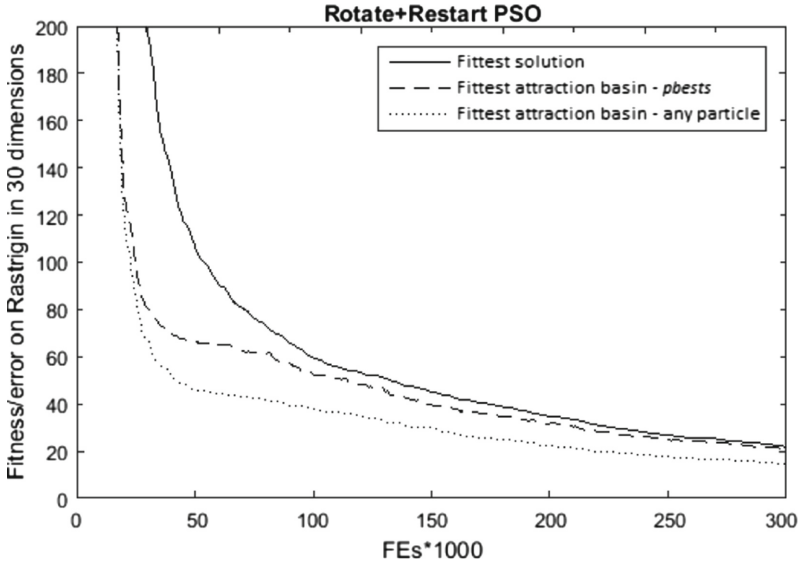


Fig. 3. Analysis of Rotate + Restart PSO. The gap between the fittest attraction basin represented by a *pbest* position and the fittest attraction basin visited by any particle has been reduced.

To further study the proposed modifications, we tested them on the CEC 2013 benchmark [11] (see Table 3). This benchmark consists of 28 unimodal and multi-modal functions divided into three sets: unimodal functions (1 to 5), basic multi-modal functions (6 to 20), and composite multi-modal functions (21 to 28). The experimental setup follows the directions given in [11]: a total of 51 randomized trials with a maximum allocation of 300,000 function evaluations were performed on each function.

We report the mean and standard deviation of the fitness errors and the relative differences of the mean errors (%-diff). The %-diff of the mean error m_1 of standard PSO with respect to the mean m_2 of the modified PSO is given by $100 \cdot (m_1 - m_2) / \max(m_1, m_2)$. Hence, positive %-diff values indicate that the modified PSO outperforms standard PSO. A *t*-test between the two results is also reported in order to make a comparison on the basis of statistically significant differences at the 5% level. However, we are unable to report additional insights for *pbest* positions since these previous experiments leveraged a unique feature from Rastrigin which allowed precise measurements of exploration and exploitation.

6 Discussion

An unexpected observation in the operation of standard PSO is that we never detected a *pbest* position from a “fully exploited” attraction basin being replaced

Table 4. Comparison PSO and Rotate + Restart PSO.

No.	PSO		Rotate + Restart PSO			<i>t</i> -test
	Mean	Stdev	Mean	Stdev	%-diff	
1	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00%	-
2	2.12E+06	1.06E+06	3.21E+06	1.72E+06	-34.07%	0.00
3	7.09E+07	6.03E+07	2.09E+07	2.22E+07	70.59%	0.00
4	1.73E+04	3.83E+03	2.13E+04	6.61E+03	-18.69%	0.01
5	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00%	-
1-5					3.57%	
6	1.62E+01	8.98E+00	1.72E+01	8.94E+00	-5.88%	0.07
7	6.46E+01	1.81E+01	1.50E+01	5.58E+00	76.72%	0.00
8	2.09E+01	5.74E-02	2.09E+01	4.75E-02	-0.05%	0.22
9	2.89E+01	2.26E+00	1.54E+01	1.89E+00	46.56%	0.04
10	1.19E-01	5.31E-02	1.39E-01	1.80E-01	-14.56%	0.05
11	6.08E+01	1.20E+01	2.06E+01	5.66E+00	66.08%	0.00
12	8.34E+01	1.78E+01	4.09E+01	8.32E+00	50.95%	0.01
13	1.36E+02	2.34E+01	9.01E+01	1.56E+01	33.63%	0.03
14	2.59E+03	4.09E+02	1.11E+03	2.74E+02	57.33%	0.00
15	3.98E+03	6.36E+02	3.42E+03	6.19E+02	14.02%	0.04
16	1.65E+00	3.73E-01	2.11E+00	2.83E-01	-21.78%	0.04
17	1.04E+02	1.63E+01	8.02E+01	7.86E+00	22.81%	0.00
18	1.68E+02	2.84E+01	2.11E+02	1.89E+01	-20.42%	0.00
19	5.89E+00	1.60E+00	3.32E+00	6.02E-01	43.70%	0.00
20	1.17E+01	4.93E-01	1.10E+01	4.15E-01	5.61%	0.15
6-20					23.65%	
21	2.24E+02	5.81E+01	2.16E+02	4.12E+01	3.85%	0.05
22	3.09E+03	4.80E+02	1.05E+03	2.68E+02	66.04%	0.00
23	4.57E+03	6.42E+02	3.48E+03	5.13E+02	24.01%	0.00
24	2.76E+02	6.26E+00	2.48E+02	8.31E+00	10.06%	0.00
25	2.92E+02	7.16E+00	2.65E+02	6.27E+00	9.20%	0.13
26	2.30E+02	6.57E+01	2.03E+02	2.16E-01	11.80%	0.03
27	1.04E+03	4.86E+01	7.53E+02	5.64E+01	27.68%	0.00
28	3.00E+02	2.80E+01	2.94E+02	6.50E+01	2.00%	0.74
21-28					19.33%	
1-28					18.83%	

by a new *pbest* position in a different attraction basin. This implies that once exploitation of an attraction basin occurs, no further exploration for new attraction basins is ever successful. This statement only applies directly to the Rastrigin function and the current experiments (and specifically the current implementation of PSO), so it is useful to study this function more closely to see how the current results might extend to other functions and other modified versions of PSO.

The study on Rastrigin presented in [5] shows how the potential for successful exploration drops from over 50% to near zero as the reference solution experiences more and more exploitation. In PSO, the reference solutions are *pbest* positions, and for *pbest* positions that have a fitness within 10 of their nearest local optimum, the experiments in [5] suggest that a vanishingly small proportion of the (fitter) attraction basins in Rastrigin will have solutions that are fitter than this (fully exploited) reference solution. Essentially, the operational characteristics of PSO turn any multi-modal search space (like Rastrigin) with a large number of relatively steep attraction basins into a “needle in the haystack” type search space. High speed particles which are necessary to travel between attraction basins cannot perform the fine-grained search in these newly explored attraction basins to find a solution in them that is fitter than their current *pbest*. Across the CEC benchmark (see Table 4), the modified version of PSO tends to perform significantly better than standard PSO on the functions that (like Rastrigin) have many steep attraction basins. Conversely, in accordance with “No Free Lunch” [12], the current modifications can perform significantly worse on fitness landscapes such as *f18* that appear to have larger and shallower attraction basins.

Many other modified versions of PSO have also led to significant improvements on benchmark functions. However, a large amount of them have “only presented experimental results [on benchmark problem sets] and did not provide adequate discussion (neither from theoretical perspective, nor general discussions) on merits of the proposed approach” [2]. The modifications in this paper are supported by measurements of actually achieved exploration and exploitation. In particular, an analysis of particle positions (e.g. diversity [6] or particle trajectories [7]) can still miss the limited effect that their associated modifications can have on the movement of *pbest* positions. We believe that any (modified) form of PSO that has 0.0 *pbest* positions which move from a fully exploited attraction basin to a different attraction basin can benefit from the restarting of these stalled particles.

A large amount of research on restart methods for PSO has been conducted (e.g. [13, 14]), and the restart methods used in the current modifications are highly rudimentary in comparison. Nonetheless, we believe the presented experimental methods which can accurately measure the number of distinct attraction basins that achieve full exploitation can be useful for on-going research in this area. One consideration for future research is to ensure that stalled particles which are to be restarted do not represent fitter attraction basins than those that have been more fully exploited by the swarm. Our *lbest* rotation strategy

which attempts to support the full exploitation of all attraction basins represented by a *pbest* position seems to work well in combination with our simple restart strategy to achieve good initial results.

7 Conclusions

The presented analysis of exploration and exploitation in Particle Swarm Optimization has benefited from the ability to make direct measurements on aspects of these important concepts. Unexpected weaknesses in the ability of PSO to perform exploration and to perform exploitation have been observed through specific measurements on *pbest* positions. The presented modifications represent only the first step in a line of research that will focus on increasing the number of attraction basins that PSO can fully exploit in a multi-modal search space. Targeted restarts are expected to be a key component of this future research.

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