MeSwarm: Memetic Particle Swarm Optimization

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ABSTRACT

In this paper, a novel variant of particle swarm optimization (PSO), named memetic particle swarm optimization algorithm (MeSwarm), is proposed for tackling the overshooting problem in the motion behavior of PSO. The overshooting problem is a phenomenon in PSO due to the velocity update mechanism of PSO. While the overshooting problem occurs, particles may be led to wrong or opposite directions against the direction to the global optimum. As a result, MeSwarm integrates the standard PSO with the Solis and Wets local search strategy to avoid the overshooting problem and that is based on the recent probability of success to efficiently generate a new candidate solution around the current particle. Thus, six test functions and a real-world optimization problem, the flexible protein-ligand docking problem are used to validate the performance of MeSwarm. The experimental results indicate that MeSwarm outperforms the standard PSO and several evolutionary algorithms in terms of solution quality.

Categories and Subject Descriptors

Ant Colony Optimization and Swarm Intelligence, Local Search

General Terms

Algorithms

Keywords

Evolutionary computation, Particle Swarm Optimization, Numerical Optimization, Solis and Wets Local Search strategy, Memetic algorithms

1. INTRODUCTION

Some important situations that often occur in PSO is *overshooting*, which is a key issue to premature convergence and essential to the performance of PSO. From the velocity update mechanism of PSO, it is observed that the *Pbest* and *Gbest* make the particles oscillated. The overshooting problem stands for that the velocity update mechanism may lead the particles to the wrong or opposite directions against the direction to the global optimum. As a consequence, the pace of convergence of the whole swarm to the global optimum slows down. One possible way to prevent the overshooting problem from happening is to appropriately adjust the algorithmic parameters of PSO. However, it is a difficult task because the parameter adjustment depends a lot on domain knowledge and the optimization problem.

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2. DISCUSSION

An *overshooting* problem may occur in the motion behavior. The particle may fails to reach suitable minima while the particle step-size is too large or too small. By analyzing the velocity update mechanism in Equation (1), it can be observed that the overshooting will occurred in the following two situations:

1. The *Gbest* and *Pbest* are on the same side of the particle's current position *X*, as shown in Figure 1. According to Equation (1), particle will be led to a local optimum region. In consequence, the particle will fail to reach the global optimum.

2. The *Gbest* and *Pbest* are on the opposite sides of the particle's current position *X*, and the *Gbest* provides the larger momentum, as $|Gbest-X|$ is greater than $|Pbest-X|$, as shown in Figure 2(a),. Thus, the particle will be dragged towards the *Gbest*. On the contrary, In the Figure 2(b), the *Pbest* provides the greater momentum, and the particle will be dragged towards the *Pbest*. Theoretically, the motion behavior of particle behavior refers to the momentum by computing the $|Gbest-X|$, $|Pbest-X|$, and V. If the large momentum was generated towards the opposite side, the particle may be led to an opposite direction against the direction to the global optimum.

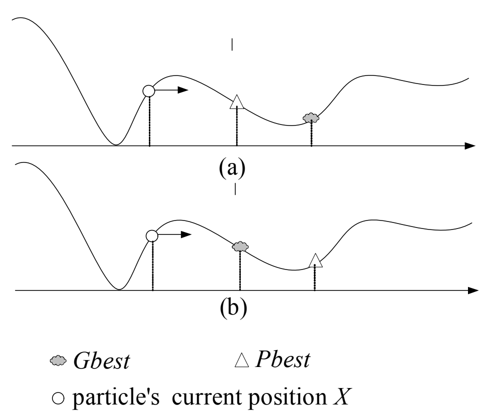

Figure 1: Gbest and Pbest are on the same side.

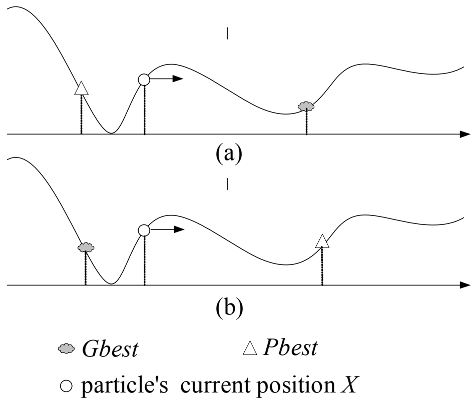

Figure 2: *Gbest* and *Pbest* are on the opposite sides.

In consequence of overshooting, the particle will move to the opposite direction against the direction to the global optimum. Two major approaches can be used to tackle the overshooting problem, described as follows.

1. Analysis of problems. By analyzing the structure of problems or identifying the fitness landscape of problems, a lethal movement could be prevented. It poses great challenge on automated problem structure analysis [1].
2. Generate and test strategies. There are many methods to generate a new solution for testing, such as heuristics of the specific problem, statistic sampling, and local search techniques. However, the computation costs in generating and testing new solutions may be high.

In order to develop a general-purpose algorithm and overcome the overshooting problem, an efficient local search strategy - the Solis and Wets local search strategy (SWs) [2] is adopted and combined with the standard PSO in this paper.

3. MESWARM

MeSwarm is a standard PSO combined with SWs. SWs is a randomized hill-climber with an adaptive step-size. The adaptive step-size is based on the recent probability of success. In the moving behavior of MeSwarm, when the traditional PSO moving mechanism of a particle is completed, SWs is applied to the particle with a probability Ps. The overall procedure of MeSwarm is shown in Figure 3.

Procedure SODOCK $t = 0$
Randomly initialize particles $X_i(t)$ and velocities $V_i(t)$
Evaluate $X_i(t)$
while not termination-condition
    Calculate $V_i(t+1)$
    Move $X_i(t)$ to $X_i(t+1)$ according to $V_i(t+1)$
    Evaluate $X_i(t+1)$
  Apply SWs to $X_i(t+1)$ with a probability $Prob_{ls}$ (Ps)
  Update P_i, and P_g
  $t = t+1$
result = $P_g(t)$

Figure 3: the Procedure of the MeSwarm.

4. EXPERIMENTS

In order to validate the feasibility of MeSwarm in improving PSO's search ability and preventing the overshooting problem, it is applied to solve a real-world optimization problem, flexible protein-ligand docking [3] and six parameter functions. The brief experimental results are shown in Table 1 and Table2, and the detail is in http://140.113.239.122/~meswarm/meswarm.pdf.

PDB	Dimensions	Best	Mean	Std. Dev.
2cpp	7	-22.73	-22.73	0
3ptb	7	-6.92	-6.782	0.13778
2mcp	11	-5.57	-5.51333	0.14761
1stp	12	-10.92	-10.92	0
1hvr	17	-21.41	-20.9097	1.55053
4hmg	18	-8.5	-8.371	0.41337

Table 1: Experimental results of MeSwarm in solving the protein-ligand docking problem.

	MeSwarm		PSO	
	Mean	S. D.	Mean	S. D.
f_1	0	0	6.496E-4	0.00142
f_2	0	0	5.43333E-6	1.01291E-5
f_3	1.966E-4	1.77729E-4	0.00243	0.00287
f_4	1.05867E-4	3.54298E-4	45.68483	118.20606
f_5	1.95629	0.76097	3.72502	1.03917
f_6	1	0	1.00004	6.29579E-5

Table 2: Experimental results of PSO and MeSwarm in solving the six test function

5. CONCLUSIONS

In this paper, a novel memetic particle swarm optimization MeSwarm is proposed to tackle the overshooting situations in the movement behavior of PSO. MeSwarm integrated the Solis and Wets local search strategy with the basic PSO in a well manner. A real-world application, flexible protein-ligand docking problems, and six test functions are used to validate the performance of MeSwarm. The experimental results indicate that MeSwarm outperforms the basic PSO and several EA-based algorithms in terms of the solution quality. From this study, it can be observed that adaptive local search is beneficial for PSO in identifying better solutions.

6. REFERENCES

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