A troop-search optimization for Lennard-Jones Potential Problem

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Abstract

In the defence security sector, a commander/captain attempts to prepare a bravery battalion with the help of efficient troops before/throughout each combat operation. In order to select the *best troop*, there could be a number of readjustments, shuffling and exchanging mechanisms applied over the combatants. The process of optimum troop selection has been computationally modelled in this paper to frame a robust optimization algorithm namely 'Troop Search Optimization (TSO) algorithm'. TSO takes utmost care to balance both exploration and exploitation in the population during simulation. In order to ensure the superiority of TSO, a typical real life problem namely 'Lennard-Jones Potential Problem' is being solved and result is compared with the state-of-the-art algorithms.

Keywords: Optimization Problem, Meta-heuristics, L-J potential problem

1. Introduction

Over the increasing complexity of the optimization problem, the classical optimization methods become handicapped. However, the bio-inspired optimization algorithms becomes an alternate paradigm. In each algorithmic design, the real challenge is to balance the exploration and exploitation. Hence continuous attempts are made by the researchers in order to establish a robust 'optimization algorithm' that can solve larger range of problems, if not to all of them.

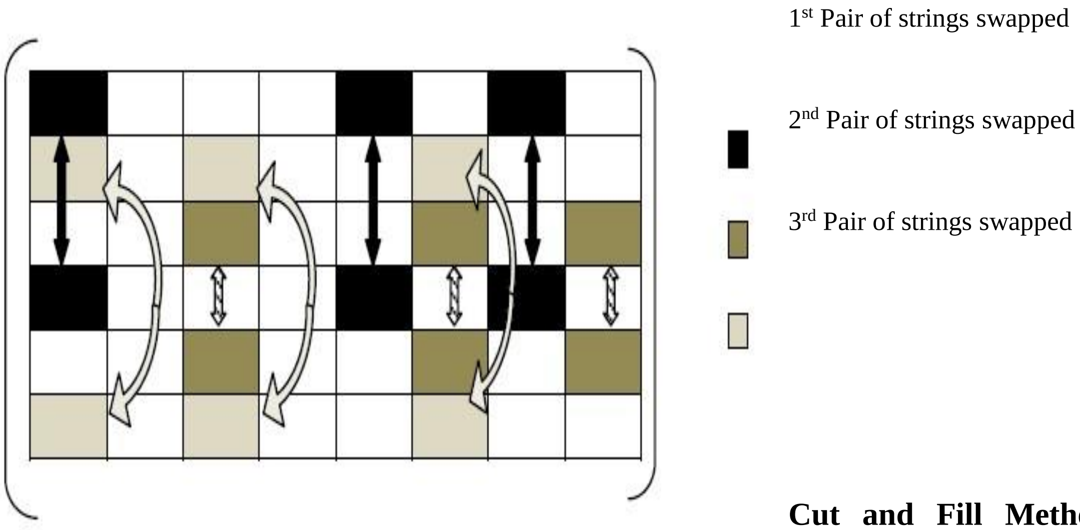
Rao et. al. [1] proposed an algorithm known as Teaching-Learning-Based Optimization (TLBO), which simulates the traditional teaching learning process of a classroom. Authors later improved the basic TLBO and named it as Improved TLBO (ITLBO) [2]. TLBO is also applied on combinatorial optimization problem [3], where the TLBO perfoms better over many algorithms. It is observed that proper balance of exploration and exploitation over the search space is still missing in the above cited methods. Therefore, an attempt is made in this paper to design a more robust and entirely new algorithm, namely 'Troop Search Optimization (TSO)' algorithm, whose concept is based on the mechanism of selecting best troop by the commander during a combat operation.

2. Major componets of the proposed algorithm

2.1 Swapping Crossover (SC) In 'Swapping Crossover' a D/2 number of stings (D: Dimension of the problem) are arbitrarily swapped under the following steps.

1. Select two arbitrary strings S1 and S2.
2. In S1, randomly select □□$D/2$□□ number of distinct variables x_i, □□1,2,...,D□. Store the 'i', chosen.
3. Select the corresponding variables y_i, □□1,2,...,D□ in S2.
4. Swap x_i and y_i chosen in step 2 and 3 respectively.
5. Repeat steps 1 to 4 for 2D number of times.

The concept of swapping crossover is diagrammatically represented in Fig.1, where 3 different pairs of strings are swapped.



2.2 Cut and Fill Method (CFM) A new concept of 'cut and fill' is employed in this paper, where 20% worse strings will be removed from the population and were refilled by generating new strings due to equation (1).

$$x_{i\,j} = x_{best\,j} + rand(0,1)\left(x_{r_1,j} - x_{r_2,j}\right) \qquad (1)$$

where $x_{i\,j}$ is the j^{th} variable of i^{th} string and x_{best} is the best fit string in the population. r_1 and r_2 are two random strings from the top 80% of population and 'j' represents the variable number. Rand (0, 1) is a random number between 0 and 1. If the value of any variable obtained by equation (1) lying outside the range, then that will be automatically replaced by the corresponding best value (x_{best}) of the best string.

3 Troop Search Algorithm (TSO)

3.1 Motivation and Methodology

The main idea behind this paper is based on the mechanism of selecting better troops before/during each combat operation. Especially in Naval sector (in defence), a battalion consists of many troops and a troop consists of many combatants. A troop is leaded by a commander and a battalion by a captain. Efficient supervision of combatants in a troop and troops in a battalion plays a significant role in optimizing the fortitude of battalion, leading them to vanquishing enemies and to achieve success triumphs over every contingent. In TSO, the mechanism is conceptualized as follows. A battalion is treated as a group of populations of individuals, a troop is treated as a population of strings, a combatant is treated as a string in the population and the strength of a particular combatant is being interpreted as the fitness of that string.

3.2 TSO algorithm

The Troop Search Optimization (TSO) Algorithm is the proposed algorithm in this paper, which consists of the following basic steps.

1. Initialization of population
2. Repeat steps 3 to 8 while stopping criteria is not satisfied
3. Apply swapping crossover

4. Apply greedy selection
5. Apply Cut & Fill Method
6. Apply Simplex Search Method
7. Apply Elitism
8. Apply NRS
9. Return the optimal solution and stop

4. The Lennard-Jones Potential Problem

The Lennard-Jones (LJ) potential energy is a simple mathematical model that approximates the interaction between the pair of atoms. This model is also known as LennardJones 6-12 potential. Lennard-Jones pair potential for the position of the molecular cluster of

N atoms by $x = (x_1, x_2, x_3, \ldots, x_N)$ where x_i is a three-dimensional vector denoting the position of the i^{th} atom, then the LJ potential energy function $E_{LJ}(r_{ij})$ of a pair of atoms (i, j) is given by equation (2).

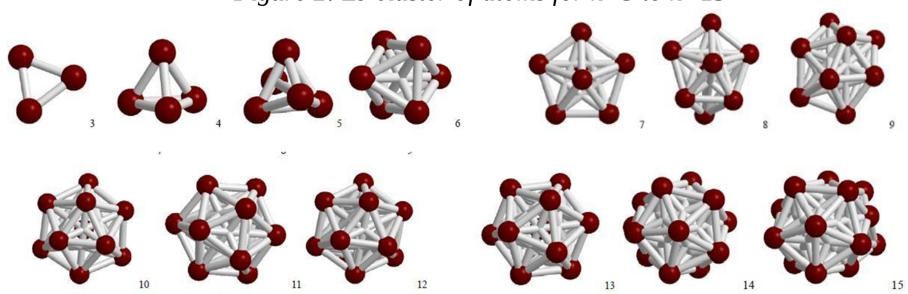
$$E_{LJ}(r_{ij}) = 4\varepsilon \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6} \right], \quad 1 \le i, j \le N \qquad (2)$$

where $r_{ij} = \| x_i - x_j \|$ the Euclidean distance between i^{th} and j^{th} atom. Here, ε is the depth of the potential well and σ is the finite distance at which the inter-particle potential is zero.

The main objective of LJ problem is to minimize the total potential energy $E_{LJ}(r_{ij})$ of the cluster. The LJ problem is very difficult to solve because it is multi-modal, non-convex and highly nonlinear, due to this it consists exponential number of local minima [4]. Hence the LJ problem a challenging standard test problem for the global optimization algorithms.

The concept of dimension of atoms are illustrated in [5]. In [6], the optimization structures of LJ cluster of atoms for n=3 to n=15 are given in Fig 2.

Figure 2: LJ cluster of atoms for n=3 to n=15



5. Experimental Setup, Results and Discussion

In order to verify the performance of TSO over the recent state-of-the-art algorithms, the Lennard-Jones Potential Problem has been solved by the proposed TSO. The TSO algorithm is coded in C++ and simulated in Linux platform. From Table 1 it is observed that out of 13 cases considered with different atomic structure, in 7 cases TSO performs better and in rest 6 cases TSO performs equally with PSO and MI-LXPM, in terms of minimizing the obtained energy.

Table 1: Comparison of obtained minimum potential energy of atoms

ATOM	PSO	MI-LXPM	TSO	ATOM	PSO	MI-LXPM	TSO
3	-3.0000	**-3.0000**	**-3.00000**	10	-24.294	**-28.4225**	**-28.4225**
4	-6.0000	**-6.0000**	**-6.00000**	11	-26.4812	-32.7659	**-32.766**
5	-9.1038	-9.1038	**-9.10385**	12	-32.1131	**-37.9676**	**-37.9676**
6	-12.2991	-12.7120	**-12.7121**	13	-33.2150	**-44.3268**	**-44.3268**
7	-15.0429	-16.5053	**-16.5054**	14	-34.4274	-47.8451	**-47.8452**
8	-19.1671	-19.8214	**-19.8215**	15	-37.3204	**-52.3226**	**-52.3226**
9	-21.8320	-24.1133	**-24.1134**				

From Table 2 it is clear that, except the case where number of atoms is 4, TSO outperforms others with much less effort as it takes very less number of function evaluations. Similarly, the success rate for PSO, MI-LXPM and TSO is reported in Table 3, from where it is observed that except atom 13 the TSO gives better success rate everywhere.

Table 2: Comparison of average function evaluation

ATOM	GA	DELP	PSO	MI-LXPM	TSO	ATOM	GA	DELP	PSO	MI-LXPM	TSO
3	1550	1973	13970	341	**312**	10	721370	4653805	623768	136846	**95153**
4	3673	10359	68400	**1144**	1480	11	*	*	687213	197514	**190797**
5	8032	31443	220800	5929	**4604**	12	*	*	740265	279910	**210928**
6	31395	67953	306854	9271	**8743**	13	*	*	789542	327712	**317042**
7	48900	103449	389641	24253	**20132**	14	*	*	847646	456716	**384416**
8	121247	207776	421032	31107	**28766**	15	*	*	996421	485462	**460484**
9	346397	1463183	516890	57208	**54336**						

*** No values reported in the literature [5, 7]**

Table 3: Comparison of success rate

ATOM	PSO	MI-LXPM	TSO	ATOM	PSO	MI-LXPM	TSO
3	**100**	**100**	**100**	10	0	**100**	**100**
4	**100**	**100**	**100**	11	0	70	**81**
5	**100**	**100**	**100**	12	0	**100**	**100**
6	74	**100**	**100**	13	0	**84**	80
7	60	**100**	**100**	14	0	**100**	**100**

8	0	**100**	**100**	15	0	64	**70**
9	0	**100**	**100**				

6. Conclusion

In this paper, a robust optimization technique with newly proposed swapping crossover and cut and fill method are introduced and simplex search method used. Lastly a Non Redundancy Search (NRS) with modified Quadratic Approximation are used to overcome repeated objective function values. It has been compared with the recent variants of ABC reported in the literature and other evolutionary optimization techniques. Firstly from the extensive numerical results and discussion it is seen that TSO outperforms many forms of ABC in maximum number of cases. Hence it has more reliability. Secondly the impact of TSO in less standard deviation implies its better stability. Therefore as a whole, TSO is more efficient, more reliable and more stable than the recent variants of ABC and other evolutionary optimization techniques.

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