



## IMPROVED SOCIAL SPIDER ALGORITHM FOR MINIMIZING MOLECULAR POTENTIAL ENERGY FUNCTION

<sup>1</sup>Emine BAŞ , <sup>2</sup>Erkan ÜLKER 

<sup>1</sup>Selcuk University, Kulu Vocational School, Computer Technologies Department, Konya, TURKEY

<sup>2</sup>Konya Technical University, Engineering and Natural Sciences Faculty, Computer Engineering Department, Konya, TURKEY

<sup>1</sup>emineozcan@selcuk.edu.tr, <sup>2</sup>eulker@ktun.edu.tr

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**ABSTRACT:** The social spider algorithm (SSA) is a new heuristic algorithm created on spider behaviors to solve continuous optimization problems. In this study, SSA is used in order to minimize a simplified model of the energy function of the molecule. The Molecular potential energy function problem is one of the most important real-life problems. The Molecular potential energy function problem attempts to predict the 3D structure of a protein. SSA is developed by various techniques (Crossover-mutation and  $G_{best}$  convergence-silent spider techniques) and SSA is called Improved SSA (ISSA). By these techniques, the exploration and exploitation capabilities of SSA in the continuous search space are improved. The general performances of SSA and ISSA are tested on low-scaled and large-scaled thirteen benchmark functions and obtained results are compared with each other. Wilcoxon signed-rank test is applied to SSA and ISSA results. Then, the general performance of the SSA and ISSA is tested on a simplified model of the molecule for different dimensions. Also, the performance of the ISSA is compared to various state-of-art algorithms in the literature. The results showed the superiority of the performance of ISSA.

**Key Words:** Constrained Optimization, Social spider algorithm, Molecular energy function

### Moleküler Potansiyel Enerji Fonksiyonu İçin Geliştirilmiş Sosyal Örümcek Algoritması

**ÖZ:** Sosyal örümcek algoritması (SÖA), sürekli optimizasyon problemlerini çözmek için örümcek davranışları üzerine oluşturulan yeni bir sezgisel algoritmadır. Bu çalışmada, SÖA molekülün enerji fonksiyonunun basitleştirilmiş bir modelini en aza indirmek için kullanılmıştır. Moleküler potansiyel enerji fonksiyonu problemi, en önemli gerçek hayat problemlerinden biridir. Moleküler potansiyel enerji fonksiyonu problemi, bir proteinin 3D yapısını tahmin etmeye çalışır. Sosyal örümcek algoritması çeşitli teknikler (Çaprazlama-mutasyon ve  $G_{best}$  yakınsaması-sessiz örümcek teknikleri) eklenerek geliştirilmiştir ve çeşitli tekniklerle geliştirilen SÖA 'ya Geliştirilmiş SSA (GSÖA) denilmiştir. Bu teknikler sayesinde, SÖA 'nın sürekli arama uzayında keşif ve sömürü yetenekleri geliştirilmiştir. SÖA ve GSÖA 'nın genel performansları, düşük ölçekli ve yüksek ölçekli on üç kıyaslama fonksiyonunda test edilmiştir ve elde edilen sonuçlar birbiriyle karşılaştırılmıştır. Wilcoxon işaretli testi, elde edilen SÖA ve GSÖA sonuçlarına uygulanmıştır. Daha sonra, SÖA ve GSÖA'nın genel performansı, farklı boyutlarda tanımlanan molekülün basitleştirilmiş bir modeli üzerinde test edilmiştir. Ayrıca, GSÖA'nın performansı, literatürdeki çeşitli sanatsal algoritmalarla da karşılaştırılmıştır. Sonuçlar, GSÖA 'nın performansının üstünlüğünü göstermiştir.

**Anahtar Kelimeler:** Sınırlı Optimizasyon, Sosyal örümcek algoritması, Moleküler enerji fonksiyonu

## 1. INTRODUCTION

Determining the global minimum potential energy conformation of proteins and peptides is known as the problem of energy minimization (Tawhid and Ali, 2017b). The minimization of the molecular potential energy function problem (MPEF) can be formulated as a global optimization problem. Finding the steady-state of the molecules in the protein can help to predict the 3D structure of the protein. The difficulty of the problem arises from the number of local minimizers of the energy function that grows exponentially with the size of the molecule (Wales and Scheraga, 1999). Many methods have been applied in the literature to solve this problem. Tawhid and Ali (2017a) proposed hybrid social spider optimization and genetic algorithm (HSSOGA) for MPEF. The social spider optimization (SSO) algorithm is a population-based algorithm proposed by Cuevas *et al.* (2013). SSO is another heuristic algorithm that is very similar to the SSA algorithm but different from it. Tawhid and Ali (2017b) proposed a hybrid Grey Wolf Optimizer and Genetic Algorithm (HGWOGA) for MPEF. The proposed HGWOGA algorithm is based on three procedures. In the first procedure, they apply the grey wolf optimizer algorithm with its powerful performance with the exploration and the exploitation processes and the second procedure is based on dimensionality reduction. The last procedure is to avoid premature convergence by applying the genetic algorithm mutation operator in the whole population. Tawhid and Ali (2017c) proposed hybrid flower pollination and genetic algorithm (HFPGA) and Tawhid and Ali (2016) improved a hybrid particle swarm optimization and genetic algorithm with population partitioning for large scale optimization problems for MPEF. Barbosa *et al.* (2005) proposed a steady-state real-coded genetic-simplex hybrid algorithm for MPEF. Pardalos *et al.* (1994) introduced some of the most commonly used potential energy functions and discuss different optimization methods used in the MPEF.

Yu and Li have offered Social Spider Algorithm (SSA) which is configured according to social spider behaviors (Yu and Li, 2015). Some spider species, which generally live solitary, can live as colonies. Spiders live in colonies can communicate with each other by web structure. The vibration they produce on the web enables this communication. They can make random walks to each other by the vibration information they share (Yu and Li, 2015). In this paper, we firstly propose an improved social spider algorithm (ISSA) and then ISSA is applied in order to solve the molecular potential energy function minimizations. Genetic algorithm operators are generally used in the literature to improve the exploration and exploratory ability of the algorithms. In this paper, we have added  $G_{best}$  convergence and silent spider techniques in addition to genetic algorithm operators. While crossover and  $G_{best}$  convergence techniques increase local search capacity of ISSA in continuous search space, mutation and silent spider techniques increase the global search capacity of ISSA in continuous search space. Crossover and  $G_{best}$  convergence techniques have been used to escape the local minima trap. Mutation and silent spider techniques ensure that global optimum points are found in the search space instead of local optimum points. The combination of these techniques accelerates the search and helps the algorithm to reach the optimal or near-optimal solution in a reasonable time. In this paper, the ISSA has been tested on various thirteen low-scaled and large-scaled benchmark functions. The molecular potential energy problem is solved by ISSA in various dimensions and the performances of ISSA are compared with well-known algorithms in the literature.

The general structure of the paper as follows. The related works and the definition of the molecular energy problem are details presented in section 1 and 2, respectively. In section 3, the original SSA and in section 4, ISSA is examined. In section 5, original SSA and ISSA are tested in various unimodal and multimodal benchmark functions in low-scale and large-scale dimensions. The performance of the SSA and ISSA is tested on a simplified model of the molecule with different dimensions. Obtained results are compared with each other and well-known heuristic and new methods in the literature. Finally, the results are interpreted and discussed. The paper is ended up with a conclusion and future works.

## 2. RELATED WORKS

Evolutionary computation has become an attractively efficient device of optimization for rapidly increasing complex modern optimization problems. For the last twenty years, swarm intelligence based algorithms, which are based on new evolutionary computation methods, attract attention. The term of a swarm expresses a community that consists of individuals who are in communication with each other. Swarm intelligence-based algorithms, study main social animal and insect behaviors for solving problems. These algorithms, imitate the behaviors of ant, fish, bird, bee, bacteria, butterfly, etc. Thus, the problems which seem hard are able to be solved (Talbi, 2009; Mallipeddi *et al.*, 2011; Parpinelli and Lopes, 2011; Kennedy and Eberhart, 1995).

One of the most popular heuristic algorithms in the literature is GA. GA has crossover and mutation operators (Holland, 1975). These operators have been used effectively in a variety of heuristic algorithms. Particle swarm optimization (PSO) is one of the most hybrid algorithms with GA. For example, GA-PSO and PSOGA (Robinson *et al.*, 2002) which are solved the particular electromagnetic application of profiled corrugated horned antenna, GSO (Grimaldi *et al.*, 2004) which is solved combinatorial optimization problems, GSO with several strategies (Grimaccia *et al.*, 2007) which is solved some multi-modal benchmark problems, and BS (Settles and Soule, 2005) which is resolved unconstrained optimization problems. In addition, there are many studies in the literature that have been hybridized with GA operators (Krink and Lvbjerg, 2002; Juang, 2004; Jian and Chen, 2006).

In this paper, one of the heuristic methods, the social spider algorithm has been selected. With the vibrations in SSA are shared some information in continuous spaces and the spiders are socialized at the evolutionary process. In the literature, SSA has been used in various papers. El-bages and Elsayed (2017) have solved a static transmission expansion planning problem by using SSA. In the proposed method; DC power flow sub-problem is solved by developing an original SSA based web and adding potential solutions to the result. Yu and Li (2016) have solved the Economic Load Dispatch (ELD) formulation by developing an original SSA based new approach. ELD is one of the essential components in power system control and operation. Mousa and Bentahar (2016) have adapted QoS-aware web service selection process to OSSA approach. Elsayed *et al.* (2016) have solved the non-convex economic load dispatch problem with an OSSA based approach.

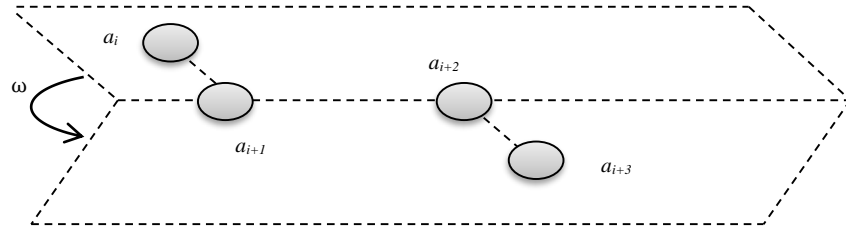
## 3. MOLECULAR POTENTIAL ENERGY PROBLEM

We test on a scalable simplified molecular potential energy function (MPEF) to examine the performance of ISSA. MPEF is first proposed in (Lavor and Maculan, 2004). The potential energy of a molecule is derived from molecular mechanics, which describes molecular interactions based on the principles of Newtonian physics (Tawhid and Ali, 2017).

The molecular model has formed consists of a chain of  $k$  atoms ( $a_1, a_2, \dots, a_k$ ) in a three-dimensional space. Similar models have been figured in the literature (Hedar *et al.*, 2011; Bansal *et al.*, 2010). In this paper, we define the potential energy as a function of the torsion angles as Equation 1.

$$E = \sum_i \left( 1 + \text{Cos}(3\omega_{i,i+3}) + \frac{(-1)^i}{\sqrt{10.60099896 - 4.141720682(\text{cos}(\omega_{i,i+3}))}} \right) \quad (1)$$

where  $i = 1, \dots, k-3$  and  $k$  is the number of atoms in the given model and  $\omega_{i,i+3}$  is the torsion angle by the atoms  $a_i, a_{i+1}, a_{i+2}$  and  $a_{i+1}, a_{i+2}, a_{i+3}$ . Figure 1 is shown in the torsion angle.



**Figure 1.** The torsion angle between the normal through the planes determined by the atoms  $a_i, a_{i+1}, a_{i+2}$  and  $a_{i+1}, a_{i+2}, a_{i+3}$ .

Our goal is to find  $\omega_{1,4}, \omega_{2,5}, \dots, \omega_{k-3,k}$  where  $\omega_{i,j} \in [0, 5]$ . Although the problem seems simple, it is a very difficult problem. A molecule with as few as 20 atoms has  $2^{17} = 131.072$  local minimizers.

In this paper,  $E$  is rewritten as  $f(x)$  for the large-scale unconstrained global optimization problem. Equations 2-4 show fitness function.

$$f(x) = \sum_{i=1}^n \left( 1 + \cos(3x_i) + \frac{(-1)^i}{\sqrt{10.60099896 - 4.141720682(\cos(x_i))}} \right) \tag{2}$$

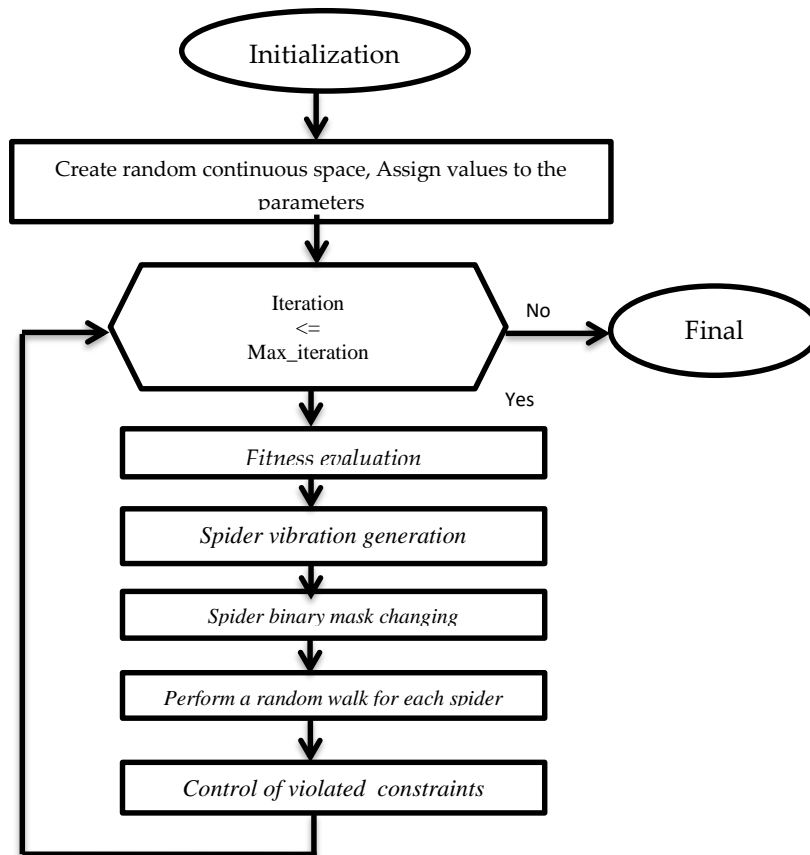
And  $0 \leq x_i \leq 5, \quad i = 1, \dots, n$  (3)

$\min f(x), \quad x \in R^n \quad l_b \leq x_i \leq u_b \quad i = 1, 2, \dots, n$  (4)

where  $f: R^n \rightarrow R$  is an objective function and  $x$  represents a decision variable vector.  $l_b$  and  $u_b$  are the lower and upper bounds of the decision variables  $x_i$ , respectively.

**4. ORIGINAL SOCIAL SPIDER ALGORITHM (SSA)**

Social spider algorithm (SSA) is a heuristic algorithm that is created by imitating spiders' behaviors in nature. SSA is created for organizing searching space of optimization problems as a high dimensional spider web. Each position on the web represents a convenient solution for the optimization problem and all convenient solutions to the problem correspond to positions on this web. This web also serves as a transmission medium of vibrations created by spiders. Each spider on the web is held in a position and the conformity value of the solution is calculated with the objective function. Spiders can move randomly on the web. But they can not move out of positions which represent convenient solutions for optimization problems. When a spider moves towards a new position, a vibration is produced and this vibration spreads on the web. Other spiders execute social information sharing via this vibration. Flowchart for the original SSA is shown in Figure 2.



**Figure 2.** Flowchart For SSA

There are two important terms in SSA: spider and vibration. Spider structure: Spiders are SSA agents that perform optimization. At the beginning of the algorithm, a predetermined number of spiders are placed on the web. The number of spiders cannot be changed afterward. “a” represents a spider and a memory is allocated for each spider a. Spider information is stored here. This information: the position of spider a on the web, the fitness value at the current position of spider a, the target vibration of spider a in the previous iteration, the iteration number where the target vibration last changed, the movement of spider a in the previous iteration and the dimension mask of spider a that guided the movement in the previous iteration. Spider locations are initially set at random. Each spider produces a vibration when it moves from a position to a different location. The severity of the vibration is related to the fitness value that the spider produces in that position. Vibration can spread over the web and other spiders on the web can feel it. Thus, other spiders on the web can obtain the personal information of the spider that produces the vibration, and information sharing takes place. Vibration structure: The vibration in the SSA is a very important term. It is one of the most important characteristics distinguishing SSA from other meta-heuristic algorithms. Two properties are used to define a vibration. a-) The source position b-) The source of vibration severity  $[0, +\infty)$  Equation 5 (Yu and Li, 2015) is used to calculate the vibration intensity.

$$I(P_a, P_a, t) = \log\left(\frac{1}{f(p_a) - C}\right) + 1 \quad (5)$$

Where a represents a spider and spider a generates vibration at its current position. It defines the position of spider a at time t as  $P_a(t)$ , or simply as  $P_a$  if the time argument is t. Where  $I(P_a, P_a, t)$  is the

vibration value produced by the spider in the source position at time  $t$ .  $f(P_a)$  represents the spider of fitness value in its current position. Where  $C$  is a confidently small constant such that all possible fitness values are larger than  $C$  for minimization problems.  $Dis(P_a, P_b)$  is showing the distance between spider  $a$  and spider  $b$ . This distance is calculated by Equation 6 (Yu and Li, 2015). Manhattan distance structure is used when calculating this distance. The vibration attenuation over distance is calculated by Equation 7 (Yu and Li, 2015).

$$Dis(P_a, P_b) = \|P_a - P_b\| \quad (6)$$

$$I(P_a, P_b, t) = I(P_a, P_a, t) \times \exp\left(-\frac{Dis(P_a, P_b)}{\bar{\sigma} \times r_a}\right) \quad (7)$$

Where  $\bar{\sigma}$  represents mean of the standard deviation of the positions of all spiders in each dimension.  $r_a$  is represented as a user-controlled parameter  $r_a \in (0, \infty)$ . This parameter controls the attenuation rate of the vibration intensity over the distance. Whenever a spider moves to a new position, it generates vibration at its current position.  $I(P_a, P_b, t)$  is the felt value of the spider's vibration in "a" point, by the spider in "b" point. The value of  $r_a$  is selected from the set  $\{1/10, 1/5, 1/4, 1/3, 1/2, 1, 2, 3, 4, 5, 10\}$  and the values of  $p_c$  and  $p_m$  are both selected from the set  $\{0.01, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.99\}$  (Yu and Li, 2015). After setting the values, the algorithm creates an initial population of spiders for optimization. Each spider is assigned a fixed size memory for storing spider information. The positions of spiders are randomly generated in the search space. Fitness values of the spiders calculated and stored. The initial target vibration of each spider in the population is set at its current position, and the vibration intensity is zero. All spiders produce vibration using their position. The algorithm uses vibrations to activate the propagation process.  $V$  represents spiders' vibrations. Each spider receives the vibrations generated by other spiders. A spider selects the strongest of these vibration values. This value shows as  $V_a^{best}$ ,  $a$  represents a spider. Spider  $a$  which is stored in the memory of the target vibration shows as  $V_a^{tar}$ .  $V_a^{best}$  compares vibration values and if the intensity of the  $V_a^{best}$  is not greater than the target vibration, the spider's memory is changed to  $V_a^{best}$ .  $cs$ , the number of iterations since spider  $a$  has last changed its target vibration, is reset to zero; otherwise, the original  $V_a^{tar}$  is retained and  $cs$  is incremented by one. The dimension mask  $m$  is determined so that a random walk can be performed towards the  $V_a^{tar}$ . The dimension mask is a  $\{0, 1\}$  binary vector of length  $n$  and  $n$  is the dimension of the optimization problem. Initially, all the values of this mask are zero. In each iteration, spiders have a probability of  $1 - p_c^{cs}$  to change its mask where  $p_c \in (0, 1)$  is a user-defined attribute that describes the probability of changing mask. If the mask is decided to be changed, each bit of the vector has a probability of  $p_m$  to be assigned with a one, and  $1 - p_m$  to be a zero.  $P_m$  is also a user-controlled parameter defined in  $(0, 1)$  (Yu and Li, 2015). Each bit of the mask is changed independently. The new mask does not have any correlation with the previous mask. In case all bits are zeros or ones, one random value of the mask is changed to one or zero. After the dimension mask is determined, a new following position  $P_a^{fo}$  is generated based on the mask for a spider.  $P_a^{fo}$  value is calculated by Equation 8 (Yu and Li, 2015).

$$P_{a,i}^{fo} = \begin{cases} P_{a,i}^{tar}, & m_{a,i} = 0 \\ P_{a,i}^r, & m_{a,i} = 1 \end{cases} \quad (8)$$

Where  $r$  is a random integer value generated in  $[1, \text{population\_size}]$  and  $m_{a,i}$  stands for the  $i$ th dimension of the dimension mask  $m$  of spiders. The random walk of each spider is calculated by Equation 9 (Yu and Li, 2015).

$$P_a(t+1) = P_a + (P_a - P_a(t-1)) \times r + (P_a^{fo} - P_a) \odot R \quad (9)$$

Where  $\odot$  denotes element-wise multiplication.  $R$  is a vector of random float-point numbers generated from zero to one uniformly. Before following  $P_a^{fo}$ , spider  $a$  first moves along its previous direction, which is the direction of movement in the previous iteration. The distance along this direction is a random portion of the previous movement. Then spider  $a$  approaches  $P_a^{fo}$  along each dimension with random factors generated in  $(0, 1)$ . After each spider performs a random walk, the spiders may move out of the web. It blocks the constraints of the optimization problem to be violated. The work steps of the original SSA is shown in Figure 3.

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- Step 1. Parameter setting:** Required constant parameter sets are adjusted. For example, lower and upper limits of variables, number of maximum iteration, etc.
- Step 2. Initialization:** Random starting position locations are determined for each spider in the swarm. Assign memory for them. The target vibration for each spider is started.
- Step 3. Evaluation:** Fitness value is calculated for each spider. The best in the swarm are detected and recorded.
- Step 4.** Vibration value for each spider calculated by using vibration Equations (5, 6, and 7). The best in the swarm are detected and recorded.
- Step 5. Vibration comparison:** The received the best vibration is compared to the target vibration values.
- Step 6.** Update the dimension mask.
- Step 7.**  $P_a^{fo}$  value is calculated by Equation 8
- Step 8. Movement:** Each spider moves to a new position by Equation 9 and a new population is obtained.
- Step 9. Repeat:** All criteria beginning from Step 3 are repeated until reaching stopping criteria.
- Step 10. Output:** Optimum outputs are obtained.
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**Figure 3.** The work steps of the original SSA

## 5. IMPROVED SOCIAL SPIDER ALGORITHM (ISSA)

The original SSA is an optimization algorithm that is developed for solving constant problems. In this paper, SSA is studied and it is improved by adding new four techniques enhancing its performance (ISSA). These techniques are crossover, mutation,  $G_{best}$  convergence, and silent spider techniques. In both techniques, ISSA develops the ability to search locally and globally in continuous search space. While crossover and  $G_{best}$  convergence techniques increase local search capacity of ISSA in continuous search space, mutation and silent spider techniques increase the global search capacity of ISSA in continuous search space. The working steps of ISSA are shown in Table 1 with general headings and details. In this Table, newly added to original SSA steps are indicated by bold letters. Fitness evaluation, vibration generation, mask changing, and spider random walk steps are taken from SSA and used similarly in ISSA.

**Table1.** General headings of the working steps of ISSA

Initialization
Iteration
<i>Fitness evaluation</i>
<i>Vibration generation</i>
<i>Mask changing</i>
<i>Spider random walk</i>
<b>Crossover-mutation techniques</b>
<b>G<sub>best</sub> convergence- silent spider techniques</b>
<i>Constraint handling</i>
Final

**Crossover-mutation Schema:** ISSA is avoided trapped around the local point with crossover and mutation operators. The value of crossover rate (cr) and the mutation rate (mr) is selected from the set {10%, %20, 30%, 40%, 50%, 60%, 70%, 80%, 90%}. The most appropriate cr value was found to be 90%. The most appropriate mr value was found to be 10%. Let N be the number of the population size, n show the dimension of the population; Figure 4 is shown in the crossover process. Figure 5 is shown in the mutation process.

Lets n=10, cr=90, Round(n\*90)/100= 9  
 N=1.spider

0	1	1	1	1	0	1	1	0	1
---	---	---	---	---	---	---	---	---	---

rand(N)=5.spider

1	0	0	1	0	0	1	0	0	0
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N<sub>new</sub> spider in crossover process

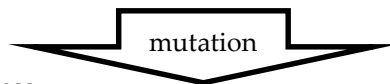
1	0	0	1	0	0	1	0	0	1
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**Figure 4.** Crossover process

Lets n=10, mr=10, Round(n\*10)/100= 1

N<sub>new</sub> spider in crossover process

1	0	0	1	0	0	1	0	0	1
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N<sub>new</sub> spider in mutation process

1	0	0	1	1	0	1	0	0	1
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**Figure 5.** Mutation process

**G<sub>best</sub> convergence Schema:** The G<sub>best</sub> convergence rate (gr) is selected from the set {10%, %20, 30%, 40%, 50%, 60%, 70%, 80%, 90%}. The most appropriate gr value was found to be 40%. The G<sub>best</sub> convergence improves the ability of ISSA to search locally in continuous space. Let N be the number of the population size, n show the dimension of the population; Figure 6 is shown G<sub>best</sub> convergence process.



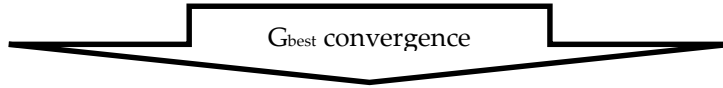
Lets  $n=10$ ,  $gr=40$ ,  $Round(n*40)/100= 4$

$N=$ Global best spider in population

1	1	1	0	0	0	0	1	1	1
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$N=1$ .spider

0	1	1	1	1	0	1	1	0	1
---	---	---	---	---	---	---	---	---	---



$N_{new}$  spider in  $G_{best}$  convergence process

0	1	1	1	0	0	0	1	1	1
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**Figure 6.**  $G_{best}$  convergence process

**Silent spider Schema:** The worst spider (silent spider) in the original SSA is hidden throughout each iteration. This spider has a small effect on the optimum result. ISSA has determined and omitted the worst spider (silent spider) and has added a new random spider ( $spider_{new}$ ) which can possibly have more effect on the optimum result. The fitness value of the new spider is controlled while adding it. If the fitness value of the new spider is worse than the fitness value of the worst spider (silent spider) of the population, it is never added to the population. The system preserves existing population members. If the fitness value of the new spider is better than the fitness value of the worst spider (silent spider) of the population, the silent spider is omitted from the population and a new spider is replaced ( $spider_{new}$ ). So, a predetermined fixed population amount is preserved. This process is repeated throughout each iteration. Figure 7 is shown a silent spider process.

Lets  $N=5, n=10$

Current Spider population( $N \times n$ )( $5 \times 10$ )

1	1	1	0	0	0	0	1	1	1
1	0	1	1	0	1	0	1	0	0
0	0	0	0	1	0	1	0	1	0
0	1	1	1	0	0	0	0	0	0
0	1	1	1	0	0	1	0	1	0

$N=3$  (the worst spider in population) (silent spider)

0	0	0	0	1	0	1	0	1	0
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*Spider<sub>new</sub>* (It is randomly generated)

1	0	1	0	0	1	0	1	1	1
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New Spider population( $N \times n$ )( $5 \times 10$ )

1	1	1	0	0	0	0	1	1	1
1	0	1	1	0	1	0	1	0	0
1	0	1	0	0	1	0	1	1	1
0	1	1	1	0	0	0	0	0	0
0	1	1	1	0	0	1	0	1	0

Figure 7. Silent spider process

Figure 8 shows a flowchart of ISSA and Figure 9 shows pseudocode of the ISSA.

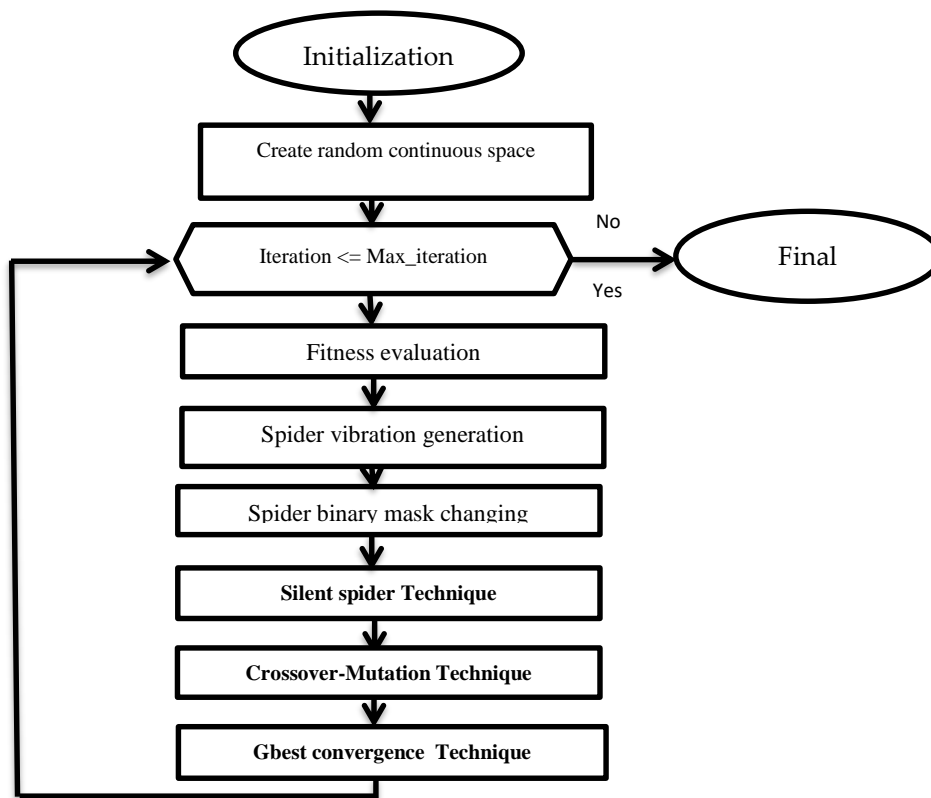
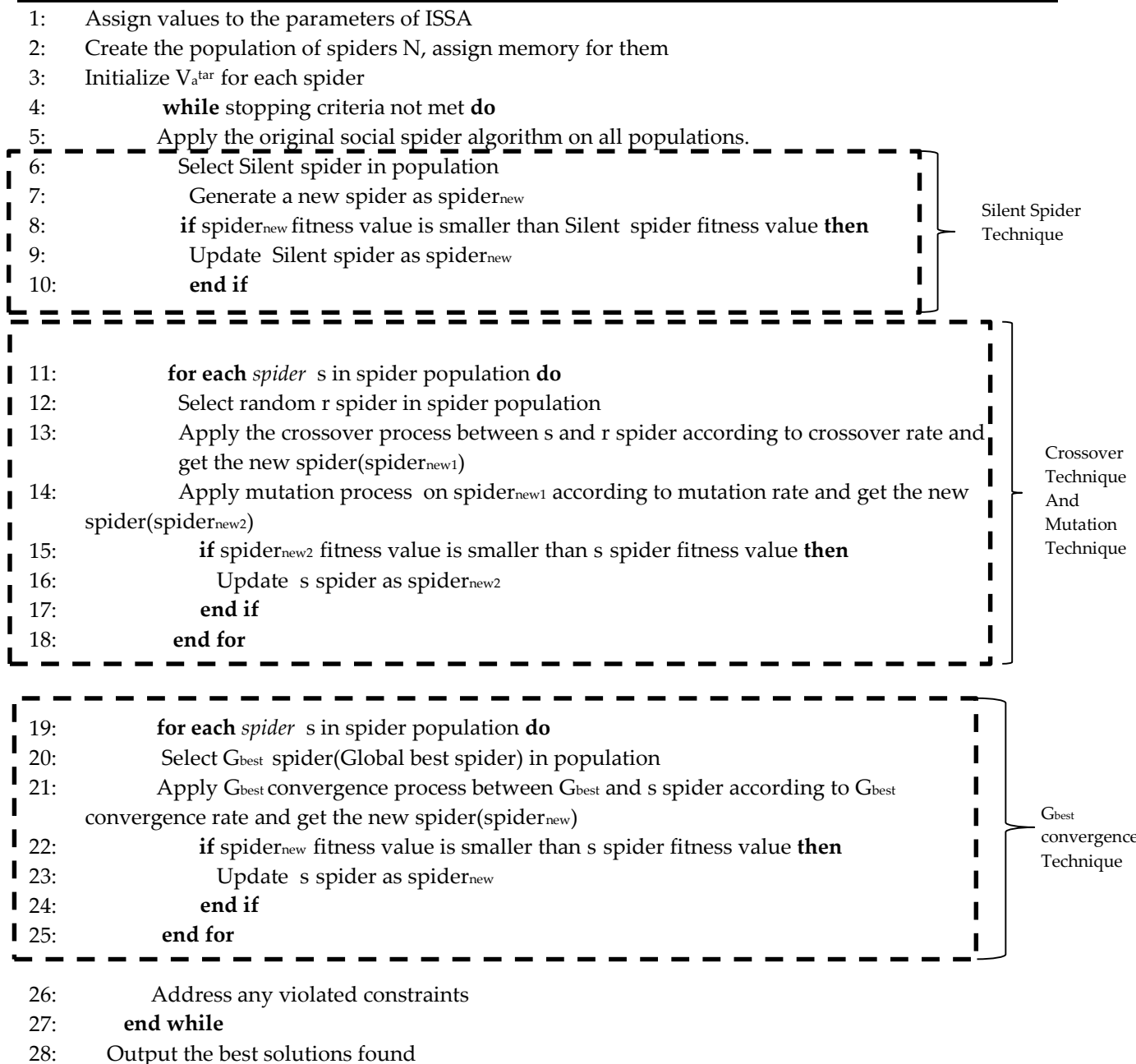


Figure 8. Flowchart For ISSA



**Figure 9.** Pseudocode of the ISSA

## 6. EXPERIMENTAL RESULTS AND ANALYSIS

ISSA and SSA are tested on Matlab R2014a that installed over windows 7, 64 bit, the system of 2.30 GHz processor with 4GB RAM. Common parameters used in ISSA and SSA comparison, which are population size (N), dimension (n), maximum iteration values,  $r_a$  value,  $p_c$  value,  $p_m$  value, crossover rate (cr), mutation rate (mr), and  $G_{best}$  convergence rate (gr) are shown in Table 2. The values of  $r_a$ ,  $p_c$ ,  $p_m$  are taken directly from SSA. The values of cr, mr, and gr are selected from the set {10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%}. In experimental studies, thirteen different unimodal and multimodal benchmark functions, which are shown in Table 3 with ISSA and SSA, are solved separately. The performance of ISSA is solved on both the global optimization problems and molecular potential energy problems, respectively.

**Table 2.** Parameters setup for ISSA and SSA

Parameters	Values
Population size (N)	25
Dimension (n)	{30, 100, 400, 1000}
Maximum iteration	1000
Crossover rate (cr)	90%
Mutation rate (mr)	10%
G <sub>best</sub> Convergence rate (gr)	40%
N <sub>run</sub>	20
Other parameters	r <sub>a</sub> =1; p <sub>c</sub> =0.7; p <sub>m</sub> =0.1 (Yu and Li, 2015)

**Table 3.** Classical Benchmark functions used in the experimental study.

Type	Name	Function	Range	f <sub>minimum</sub>
Unimodal	F1	$\sum_{i=1}^n x_i^2$	$[-100,100]^n$	$f(x^*)=0$
	F2	$\sum_{i=1}^n  x_i  + \prod_{i=1}^n  x_i $	$[-10,10]^n$	$f(x^*)=0$
	F3	$\sum_{i=1}^n \left( \sum_{j=1}^i x_j \right)^2$	$[-100,100]^n$	$f(x^*)=0$
	F4	$\max_i  x_i , 1 \leq i \leq n$	$[-100,100]^n$	$f(x^*)=0$
	F5	$\sum_{i=1}^{n-1} [100(x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$	$[-30,30]^n$	$f(x^*)=0$
	F6	$\sum_{i=1}^n [(x_i + 0.5)]^2$	$[-100,100]^n$	$f(x^*)=0$
	F7	$\sum_{i=1}^n ix_i^4 + \text{random}[0,1]$	$[-1.28,1.28]^n$	$f(x^*)=0$
Multimodal	F8	$\sum_{i=1}^n -x_i \sin(\sqrt{ x_i })$	$[-500,500]^n$	$f(x^*)=-418.9829 \times n$
	F9	$\sum_{i=1}^n [x_i^2 - 10\cos(2\pi x_i) + 10]$	$[-5.12,5.12]^n$	$f(x^*)=0$
	F10	$-20\exp\left(-0.2\sqrt{\frac{1}{n}\sum_{i=1}^n x_i^2}\right) - \exp\left(\frac{1}{n}\sum_{i=1}^n \cos(2\pi x_i)\right) + 20 + \exp(1)$	$[-32,32]^n$	$f(x^*)=0$
	F11	$\frac{1}{4000}\sum_{i=1}^n x_i^2 - \prod_{i=1}^n \cos\left(\frac{x_i}{\sqrt{i}}\right) + 1$	$[-600,600]^n$	$f(x^*)=0$
	F12	$1 - \cos\left(2\pi\sqrt{\sum_{i=1}^n x_i^2}\right) + 0.1\sqrt{\sum_{i=1}^n x_i^2}$	$[-100,100]^n$	$f(x^*)=0$
	F13	$-\sum_{i=1}^n \sin(x_i) \sin^{2m}\left(\frac{ix_i^2}{\pi}\right)$	$[0,\pi]^n$	n=30: $f(x^*)=-29,6309$ ; n=100: $f(x^*)=-99.6201940166$ ; n=400: $f(x^*)=-399,616795138572$ ; n=1000: $f(x^*)=-999.6161052093$

Benchmark functions divide into two groups according to their type as unimodal and multimodal benchmark functions. Functions F1-F7 (unimodal), which have only one global optimum

and can evaluate the exploitation capability of the investigated algorithms. Functions F8–F13 (multimodal), which include many local optima whose number increases exponentially with the problem size, become highly useful when the purpose is to evaluate the exploration capability of the investigated algorithms. These functions are obtained from various sources (Tawhid and Ali, 2017a; Yu and Li, 2015; Surjanovic and Bingham, 2017).

For each benchmark function, two measures are used to evaluate the performance of each algorithm to solve this function. These measures include (1) Average ( Mean ) and (2) Standard deviation ( S.D.). They defined as in Table 4. Where  $N_{run}$  represents the total number of runs.

**Table 4.** Performance measure

Mean	$\text{Mean} = \frac{1}{N_{run}} \times \sum_{i=1}^{N_{run}} \text{Fitness\_func}_i$
Standard Deviation	$\text{S. D.} = \sqrt{\frac{1}{N_{run}} \sum_{i=1}^{N_{run}} (\text{Gbest}_i - \text{Mean})^2}$

**6.1. Determine of crossover, mutation, and  $G_{best}$  convergence rates**

To determine the crossover rate (cr), population size = 25, dimension=30 and maximum iteration = 1000 parameter values are selected for ISSA. The crossover rate (cr) is tested in randomly selected five different unimodal benchmark functions (F1, F2, F4, F5, and F7) and randomly selected five different multimodal benchmark functions (F8, F9, F10, F11, and F13). Each benchmark function is run 20 times. Mean are done for obtained benchmark function results. Table 5 shows the results obtained. According to the results, the crossover rate (cr) is selected at 90%.

**Table 5.** Determine the crossover rate (cr) in 10 different unimodal and multimodal benchmark functions.

F	Crossover rate (cr)								
	10%	20%	30%	40%	50%	60%	70%	80%	90%
F1	27004,4900	26156,1900	17520,1100	18324,9400	10140,2200	8790,2180	7135,4120	3347,9670	<b>1175,5600</b>
F2	66,20135	69,99781	55,3307	53,31256	35,07983	37,10695	20,20037	22,91025	<b>11,5507</b>
F4	49,85766	45,78515	35,00857	28,66598	22,04498	21,00766	<b>19,00288</b>	20,91694	19,2189
F5	47536115	30431267	20364778	9716929	5907726	2776247	970753,500	1060099	<b>38362,99</b>
F7	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
F8	-3112,3900	-2690,1100	-2947,0400	-2547,1600	-3073,5100	-	<b>-3227,9500</b>	-	-
F9	244.9703	257,9103	188,5917	152.5475	112,2209	92,60459	64,57314	42,30282	<b>36,73263</b>
F10	18,92449	17,49768	17,00651	17,20581	15,78174	14,79526	13,53442	11,89024	<b>10,78819</b>
F11	283,2028	232,6389	188,1118	146,7355	84,3342	78,03849	54,26156	23,68114	<b>9,374057</b>
F13	-8,78887	-9,00019	-8,67862	-9,16455	-8,73005	<b>-9,33821</b>	-8,90599	-9,10591	-9,18917

To determine the mutation rate (mr), population size = 25, dimension=30 and maximum iteration = 1000 parameter values are selected for ISSA. The mutation rate (mr) is tested in randomly selected five different unimodal benchmark functions (F1, F2, F4, F5, and F7) and randomly selected five different multimodal benchmark functions (F8, F9, F10, F11, and F13). Each benchmark function is run 20 times. Mean are done for obtained benchmark function results. Table 6 shows the results obtained. According to the results, the mutation rate (mr) is selected at 10%.

**Table 6.** Determine the mutation rate (mr) in 10 different unimodal and multimodal benchmark functions.

F	Mutation rate (mr)								
	10%	20%	30%	40%	50%	60%	70%	80%	90%
F1	<b>0,394634</b>	0,702821	0,758151	0,617514	0,702059	0,671051	0,751396	0,905282	0,814592
F2	0,141074	<b>0,134244</b>	0,168751	0,210592	0,1827	0,199393	0,208086	0,208631	0,187357
F4	<b>18,04599</b>	21,89031	23,99734	24,45129	26,38615	25,51669	25,80048	24,79854	25,72667
F5	<b>282,6736</b>	313,285	327,3802	383,4963	331,8956	429,427	360,3212	383,9664	424,8467
F7	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
F8	-3325,990	-4201,030	-4000,200	-4730,400	-4522,850	<b>-5123,600</b>	-4961,060	-4514,820	-4711,540
F9	56,78534	53,34603	49,45195	46,10922	45,66494	47,71347	50,04745	<b>45,39075</b>	46,79847
F10	<b>0,267519</b>	0,316517	0,354352	0,340763	0,364685	0,317098	0,30045	0,390763	0,412149
F11	<b>0,679518</b>	0,745935	0,752064	0,819712	0,825792	0,84922	0,777499	0,923743	0,826685
F13	-8,9389	<b>-9,15235</b>	-9,13946	-8,75084	-9,03193	-9,09553	-9,04802	-9,04717	-8,79987

To determine the  $G_{best}$  convergence rate (gr), population size = 25 and maximum iteration = 1000 parameter values are selected for ISSA. The  $G_{best}$  convergence rate (gr) is tested in randomly selected five different unimodal benchmark functions (F1, F2, F4, F5, and F7) and randomly selected five different multimodal benchmark functions (F8, F9, F10, F11, and F13). Each benchmark function is run 20 times. Mean are done for obtained benchmark function results. Table 7 shows the results obtained. According to the results, the convergence rate (gr) is selected at 40%.

**Table 7.** Determine the  $G_{best}$  convergence rate (gr) in 10 different unimodal and multimodal benchmark functions.

F	$G_{best}$ convergence rate (gr)								
	10%	20%	30%	40%	50%	60%	70%	80%	90%
F1	0,2992	0,2075	0,1135	<b>0,1014</b>	0,3617	2,5722	1,4404	4,1672	6,6827
F2	0,0869	0,0541	0,0385	0,0363	<b>0,0250</b>	0,0482	0,1329	0,2004	0,3742
F4	15,3631	12,6156	10,9124	9,0924	8,6100	<b>7,9092</b>	8,8164	9,8505	8,7613
F5	252,0041	287,4710	230,5190	<b>141,4368</b>	317,3710	360,8188	708,5943	481,9163	643,2990
F7	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
F8	-	-	-	-	-	-	-	-	-
F9	6,3339e+03 50,7249	5,0872e+03 49,6798	7,6181e+03 38,4998	8,2660e+03 32,6286	1,0197e+04 25,8040	1,2587e+04 16,9285	1,0404e+04 9,2235	1,3402e+04 7,4238	<b>1,4866e+04</b> <b>5,7207</b>
F10	0,1855	<b>0,1092</b>	0,1908	0,3017	0,6169	0,8428	1,3251	1,3012	1,7077
F11	0,5491	0,4383	0,3003	<b>0,1847</b>	0,3639	0,5313	0,8443	1,0359	1,0551
F13	<b>-9,4599</b>	-8,8794	-9,1509	-8,6585	-9,2841	-8,9549	-8,5483	-8,9557	-8,5900

## 6.2. The contribution of crossover (cr), mutation (mr), $G_{best}$ convergence (gr), and silent spider techniques to the proposed algorithm

Each developed technique is applied individually with ISSA and its contribution to ISSA has been demonstrated. Each benchmark function is run 20 times. Mean and standard deviation (S.D.) are done for obtained benchmark function results. The results are shown in Tables 8 and 9. According to obtain results, all techniques have improved ISSA's local and global search capabilities.  $G_{best}$  convergence

and silent spider techniques are had good performance except for F5 and F6.  $G_{best}$  convergence and silent spider techniques have improved ISSA's local and global search capabilities. Crossover and mutation techniques are had sufficiently good performance except for F8, F12, and F13.

**Table 8.** The comparison of ISSA with cr, mr, gr, and silent spider techniques on dimension = {30}, the maximum number of iterations = 1000 in unimodal and multimodal benchmark functions.

F	ISSA							
	cr		mr		gr		silent spider	
	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
<i>F1</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F2</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F3</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F4</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F5</i>	178,9085	60,0856	177,8799	60,6647	183,7258	96,9333	231,9934	79,9607
<i>F6</i>	15,7213	6,7661	14,1819	4,1252	14,2264	4,1434	14,1882	4,1691
<i>F7</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F8</i>	-4,37e+03	8359,600	-3,29e+03	7960,018	-6,47e+03	4730,590	-6,60e+03	2650,303
<i>F9</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F10</i>	6,18e-10	0,00E+00	6,18e-10	0,00E+00	8,88e-16	0,00E+00	8,88e-16	0,00E+00
<i>F11</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F12</i>	0,6215	0,2514	11,7313	1,4812	0,1203	0,2302	0,3289	0,6639
<i>F13</i>	-8,4004	0,7053	-8,4930	0,7034	-8,7114	0,6902	-9,0613	0,6941

**Table 9.** The comparison of ISSA with cr-mr, and gr-silent spider techniques on dimension = {30}, the maximum number of iterations = 1000 in unimodal and multimodal benchmark functions.

F	ISSA			
	cr-mr		gr-silent spider	
	Mean	S.D.	Mean	S.D.
<i>F1</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F2</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F3</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F4</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F5</i>	177,8799	60,0856	180,71421	66,4571
<i>F6</i>	13,1852	3,8091	14,1852	4,7590
<i>F7</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F8</i>	-5,10e+03	3730,5997	-6,60e+03	2650,303
<i>F9</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F10</i>	8,18e-15	0,00E+00	8,88e-16	0,00E+00
<i>F11</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F12</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F13</i>	-8,5613	0,6802	-8,7613	0,6602



### 6.3. The general performance of the ISSA and SSA on low-scaled and large-scale optimization problems

ISSA is tested in seven unimodal benchmark functions. Each benchmark function is run 20 times. Mean and standard deviation (S.D.) are done for obtained benchmark function results. Mean and standard deviation (S.D.) comparison results, which are obtained for unimodal benchmark functions (F1-F7) by selecting population size (N) =25 and maximum iteration=1000 values for ISSA, are shown in Table 10. According to obtain results, ISSA is had super performance except for F5 and F6.

**Table 10.** The performance of ISSA with dimension = {30, 100, 400, 1000}, maximum number of iterations = 1000, population size = 25 in unimodal benchmark functions. S.D. is the standard deviation; Mean is the average of the unimodal benchmark function results.

		F1	F2	F3	F4	F5	F6	F7
30	Mean	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,78E+02	1,29E+01	0,00E+00
	S.D.	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,16E+01	3,59E+00	0,00E+00
100	Mean	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,15E+04	9,04E+01	0,00E+00
	S.D.	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,13E+04	1,29E+01	0,00E+00
400	Mean	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,57E+07	9,04E+01	0,00E+00
	S.D.	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,72E+06	1,29E+01	0,00E+00
1000	Mean	3,04E+05	inf	0,00E+00	0,00E+00	9,99E+02	6,97E+02	0,00E+00
	S.D.	2,60E+04	NaN	0,00E+00	0,00E+00	1,45E-02	1,39E+01	0,00E+00

ISSA is tested on six multimodal benchmark functions. Each benchmark function is run 20 times. Mean and standard deviation (S.D.) are done for obtained benchmark function results. Mean and standard deviation (S.D.) comparison results, which are obtained for multimodal benchmark functions (F8-F13) by selecting population size (N) =25 and maximum iteration=1000 values for ISSA, are shown in Table 11. According to obtain results, ISSA is had super performance except for F8, F10, and F13.

**Table 11.** The performance of ISSA with dimension = {30, 100, 400, 1000}, maximum number of iterations = 1000, population size = 25 in multimodal benchmark functions.

		F8	F9	F10	F11	F12	F13
30	Mean	-8,73E+03	0,00E+00	8,88E-16	0,00E+00	0,00E+00	-8,74E+00
	S.D.	2,67E+03	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,64E-01
100	Mean	-2,02E+04	0,00E+00	8,88E-16	0,00E+00	0,00E+00	-2,12E+01
	S.D.	4,82E+03	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,99E-01
400	Mean	-5,08E+04	0,00E+00	8,88E-16	0,00E+00	0,00E+00	-6,97E+01
	S.D.	2,57E+04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,95E+00
1000	Mean	-9,41E+04	0,00E+00	8,88E-16	0,00E+00	0,00E+00	-1,61E+02
	S.D.	3,42E+04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,97E+00

Original SSA and proposed ISSA are tested in low-scaled and large-scaled three different dimensions (dimension={30, 100, 1000}), thirteen different unimodal and multimodal benchmark functions. Each benchmark function is run 20 times. Mean and standard deviation are done for obtained benchmark function results. Mean and standard deviation comparison results, which are obtained for unimodal and multimodal benchmark functions by choosing dimension={30, 100}, and population size=25, maximum iteration=1000 values equally for original SSA and ISSA, are shown in Table 12. Mean and standard deviation comparison results, which are obtained for unimodal and multimodal benchmark functions by choosing dimension={1000}, and population size=25, maximum iteration=1000 values equally for original SSA and ISSA, are shown in Table 13. The results of the high performance of the ISSA are bold. According to the results, ISSA has shown better performance than SSA in unimodal

benchmark functions. According to the results, ISSA has shown better performance than SSA in multimodal benchmark functions.

Figure 10 is shown ISSA and SSA convergence graphs for unimodal *F1* and *F4*, and multimodal *F9* and *F10* benchmark functions. According to the convergence graphs results, the optimal solutions are obtained with ISSA.

**Table 12.** The comparison of SSA and ISSA with dimension = {30, 100}, maximum number of iterations = 1000 in unimodal and multimodal benchmark functions.

F	Dimension=30				Dimension=100			
	SSA		ISSA		SSA		ISSA	
	Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
<i>F1</i>	1,49E+00	7,48E-01	0,00E+00	0,00E+00	5,67E+02	1,18E+02	0,00E+00	0,00E+00
<i>F2</i>	5,23E-01	3,53E-01	0,00E+00	0,00E+00	8,51E+40	1,76E+41	0,00E+00	0,00E+00
<i>F3</i>	2,51E+02	7,02E+01	0,00E+00	0,00E+00	2,38E+03	6,38E+02	0,00E+00	0,00E+00
<i>F4</i>	3,42E+01	3,18E+00	0,00E+00	0,00E+00	6,35E+01	3,35E+00	0,00E+00	0,00E+00
<i>F5</i>	4,79E+02	1,04E+02	1,78E+02	6,16E+01	5,99E+04	1,85E+04	3,15E+04	1,13E+04
<i>F6</i>	4,27E+00	9,43E-01	1,23E+00	4,58E-01	6,79E+01	5,66E+00	6,56E+01	2,70E+00
<i>F7</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F8</i>	-2,80E+03	9,54E+02	-8,73E+03	2,67E+03	-4,82E+03	9,31E+02	-2,02E+04	4,82E+03
<i>F9</i>	4,45E+01	7,80E+00	0,00E+00	0,00E+00	5,36E+02	3,00E+01	0,00E+00	0,00E+00
<i>F10</i>	6,75E-01	2,14E-01	8,88E-16	0,00E+00	4,77E+00	2,45E-01	8,88E-16	0,00E+00
<i>F11</i>	9,96E-01	3,36E-02	0,00E+00	0,00E+00	6,42E+00	8,80E-01	0,00E+00	0,00E+00
<i>F12</i>	8,52E+01	5,76E+00	0,00E+00	0,00E+00	2,32E+02	1,51E+01	0,00E+00	0,00E+00
<i>F13</i>	-8,87E+00	7,17E-01	-9,03E+00	7,27E-01	-2,07E+01	9,87E-01	-2,22E+01	1,48E+00

**Table 13.** The comparison of SSA and ISSA with dimension = {1000}, population size=25, maximum number of iterations = 1000 in the unimodal and multimodal benchmark functions.

F	Dimension=1000			
	SSA		ISSA	
	Mean	S.D.	Mean	S.D.
<i>F1</i>	3,18E+05	1,20E+04	3,04E+05	2,60E+04
<i>F2</i>	Inf	NaN	Inf	NaN
<i>F3</i>	1,41E+03	1,93E+04	0,00E+00	0,00E+00
<i>F4</i>	9,94E+01	1,33E-01	0,00E+00	0,00E+00
<i>F5</i>	2,61E+08	2,09E+07	9,99E+02	1,45E-02
<i>F6</i>	2,52E+03	6,26E+01	6,97E+02	1,39E+01
<i>F7</i>	0,00E+00	0,00E+00	0,00E+00	0,00E+00
<i>F8</i>	-1,48E+04	3,79E+03	-9,41E+04	3,42E+04
<i>F9</i>	1,02E+04	1,46E+02	0,00E+00	0,00E+00
<i>F10</i>	1,54E+01	1,67E-01	8,88E-16	0,00E+00
<i>F11</i>	2,83E+03	1,35E+02	0,00E+00	0,00E+00
<i>F12</i>	8,73E+02	1,65E+01	0,00E+00	0,00E+00
<i>F13</i>	-1,41E+02	2,36E+00	-1,57E+02	2,18E+00

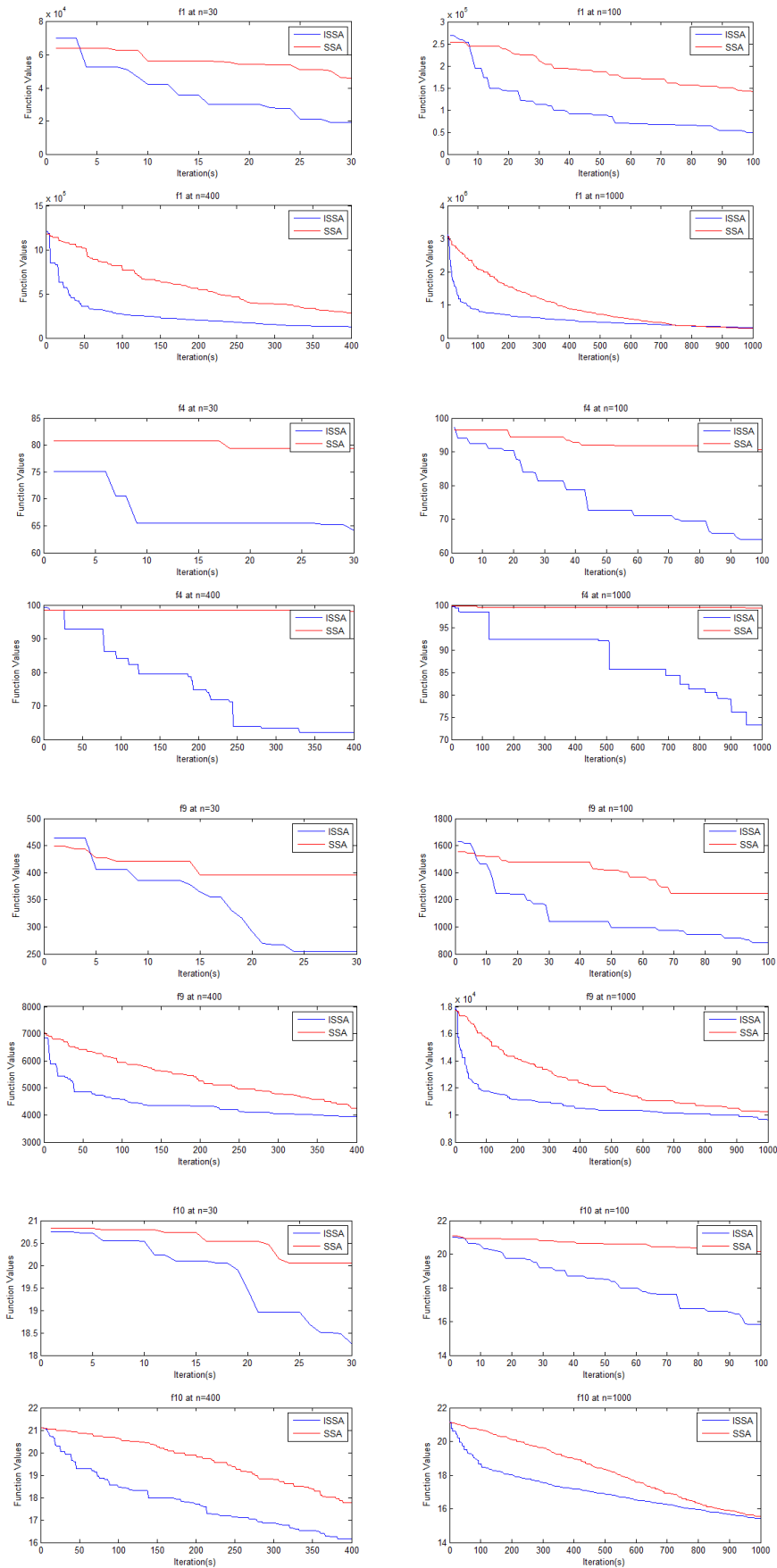


Figure 10. Convergence graphs for ISSA and Original SSA for benchmark functions (F1, F4, F9, and F10)

Wilcoxon signed-rank test is a pairwise test that aims to detect significant differences between the behavior of two algorithms (Acilar, 2013). In this paper, SSA-ISSA algorithms are operated with 20 times various unimodal and multimodal benchmark functions with the dimension  $(n)=\{30, 100, 1000\}$ , population size=25 and maximum iteration=1000 equal parameter and 20 trials are done in each dimension for each benchmark function and thirteen data sets are obtained. The results are shown in Table 14 for unimodal benchmark functions, Table 15 shows the multimodal benchmark In Wilcoxon signed-rank test, alpha is selected as 0.05 (Acilar, 2013).  $\rho$  is the probability of the null hypothesis is true.  $\rho$  values of the hypothesis are calculated by using Matlab R2014a software. According to the obtained results, there is a semantic difference between the results obtained from SSA and ISSA heuristic algorithms. The results showed that the ISSA has superior performance on thirteen unimodal and multimodal benchmark functions.

**Table 14.** Wilcoxon signed-rank test on SSA and ISSA in dimension= $\{30, 100, 1000\}$ , maximum number of iterations = 1000, population size=25 in unimodal benchmark functions.

<i>F</i>	<i>n=30</i>		<i>n=100</i>		<i>n=1000</i>	
	ISSA( $\rho$ )	<i>h</i>	ISSA( $\rho$ )	<i>h</i>	ISSA( $\rho$ )	<i>h</i>
<i>F1</i>	0,0419	1	0,9698	0	0,9097	0
<i>F2</i>	0,0211	1	0,0472	1	-	-
<i>F3</i>	1	0	0,0444	1	-	-
<i>F4</i>	0,5708	0	0,0757	0	0,2730	0
<i>F5</i>	0,0123	1	0,6756	0	0,9097	0
<i>F6</i>	0,9475	0	1	0	0,8172	0
<i>F7</i>	NaN	0	NaN	0	NaN	0

**Table 15.** Wilcoxon signed-rank test on SSA and ISSA in dimension= $\{30, 100, 1000\}$ , maximum number of iterations = 1000, population size=25 in multimodal benchmark functions.

<i>F</i>	<i>n=30</i>		<i>n=100</i>		<i>n=1000</i>	
	ISSA( $\rho$ )	<i>h</i>	ISSA( $\rho$ )	<i>h</i>	ISSA( $\rho$ )	<i>h</i>
<i>F8</i>	0,0247	1	0,0474	1	0,0408	1
<i>F9</i>	0,9698	0	0,7337	0	0,0103	1
<i>F10</i>	0,0452	1	0,7337	0	0,0474	1
<i>F11</i>	0,0123	1	0,0274	1	0,7337	0
<i>F12</i>	0,0447	1	0,0257	1	0,0001	1
<i>F13</i>	0,0347	1	0,0457	1	1	0

#### 6.4. The General Performance Of The ISSA For Minimizing The Potential Energy Function

We compare ISSA with SSA on dimension= $\{20, 40, 60, 80, 100, 120, 140, 160, 180, 200\}$ . According to the results, the performance of ISSA is better than the performance of SSA on the MPEF problem. The results are shown in Table 16.

**Table 16.** The comparison results of ISSA and SSA on dimension = {20, 40, 60, 80, 100, 120, 140, 160, 180, 200}.

n	SSA	ISSA
20	15,9100	<b>13,5926</b>
40	33,1715	<b>32,5559</b>
60	57,0631	<b>48,4384</b>
80	76,7605	<b>66,3655</b>
100	98,2967	<b>78,4906</b>
120	110,91	<b>105,76</b>
140	130,45	<b>124,16</b>
160	160,79	<b>148,94</b>
180	170,53	<b>156,09</b>
200	187,36	<b>186,60</b>

ISSA is compared in two different method series. In the first series, WX-PM, WX-LLM, LX-LLM and LX-PM which are variants of the GA, and ISSA are compared in molecular potential energy function in equal comparison parameters (Deep *et al.*, 2012; Deep and Thakur, 2007a; Deep and Thakur, 2007b). In the second series, VNS-123 which consists of a variable neighborhood search-based method, and ISSA are compared in molecular potential energy function in equal comparison parameters (Dražić *et al.*, 2008). rHYB method expresses a hybrid genetic algorithm (Barbosa *et al.*, 2005). The parameters settings used in all comparison algorithms are shown in Table 17.

**Table17.** The parameters settings of all algorithms

Key	Method Name
VNS-123	The combination of the VNS-1, VNS-2, and VNS-3 is made to diversify the search.
WX-PM	Crossover operator=WX and mutation operator=PM
WX-LLM	Crossover operator=WX and mutation operator=LLM
LX-LLM	Crossover operator=LX and mutation operator=LLM
LX-PM	Crossover operator=LX and mutation operator=PM
rHYB	
Common settings	Population size: N = 25; number of runs = 20; maximum iterations = [400-4000]; n=[20-200]

The function E in (1) is minimized in the specified search space  $[0, 5]^n$ . The function E grows linearly with n as  $E^*(n) = -0.0411183n$  (Lavor and Maculan, 2004) as shown in Table 18.

**Table 18.** Global minimum value E\* for different sizes

n	E*
20	-0,822366
40	-1,644732
60	-2,467098
80	-3,289464
100	-4,111830
120	-4,934196
140	-5,756562
160	-6,578928
180	-7,401294
200	-8,22366

The performance of ISSA is compared to SSA, VNS-123, WX-PM, WX-LLM, LX-LLM, LX-PM, and rHYB in dimension={20, 40, 60, 80, 100, 120, 140, 160, 180, 200} on MPEF problem. We take the results of comparison algorithms directly from (Barbosa *et al.*, 2005; Dražić *et al.*, 2008; Deep *et al.*, 2012; Deep and Thakur, 2007a; Deep and Thakur, 2007b ). The results are shown in Tables 19 and 20. Results of successful SSA are made in bold text.

**Table 19.** The comparison results of ISSA on dimension = {20, 40, 60, 80, 100}.

n	WX-PM	LX-PM	WX-LLM	LX-LLM	ISSA
20	15,574	23,257	28,969	14,586	<b>13,5926</b>
40	59,999	71,336	89,478	39,366	<b>32,5559</b>
60	175,865	280,131	225,008	105,892	<b>48,4384</b>
80	302,011	326,287	372,836	237,621	<b>66,3655</b>
100	369,376	379,998	443,786	320,146	<b>78,4906</b>

**Table 20.** The comparison results of ISSA on dimension = {20, 40, 60, 80, 100, 120, 140, 160, 180, 200}.

n	VNS-123	GA	rHYB	ISSA
20	23,381	36,626	35,836	<b>13,5926</b>
40	57,681	133,581	129,611	<b>32,5559</b>
60	142,882	263,266	249,963	<b>48,4384</b>
80	180,999	413,948	387,787	<b>66,3655</b>
100	254,899	-	-	<b>78,4906</b>
120	375,970	-	-	<b>105,76</b>
140	460,519	-	-	<b>124,16</b>
160	652,916	-	-	<b>148,94</b>
180	663,722	-	-	<b>156,09</b>
200	792,537	-	-	<b>186,60</b>

## 6.5. Discussion about ISSA

In this paper, the original SSA is improved by adding four techniques. Exploration and exploitation ability of SSA is increased with these techniques. Crossover (cr) and  $G_{best}$  convergence (gr) techniques allow ISSA to escape from the local traps in the search space and ISSA's local search capability is improved. Mutation (mr) and silent spider techniques allow ISSA to discover new points in search space. Thus, local optimum and global optimum points are guaranteed for ISSA. According to results, ISSA with  $G_{best}$  convergence and silent spider techniques shows performance at roughly 84,62% of benchmark functions for 11 out of 13 benchmark functions except for F5 and F6. ISSA with crossover (cr) and mutation (mr) techniques show performance at roughly 76,92% of benchmark functions for 10 out of 13 benchmark functions except for F8, F10, and F13. The results showed that none of the methods alone proved superior to all benchmark functions. All techniques develop a different ability of ISSA.  $G_{best}$  convergence and silent spider techniques developed ISSA's exploration and exploitation ability in multimodal functions, but not all unimodal functions. This is due to the low success of the silent spider technique in discovering new points, and the fact that the worst spiders are not thrown out of the system during each iteration. Furthermore, with the  $G_{best}$  convergence technique, some of the population members resemble the best spider of iteration. However, if the best spider of iteration is not the optimum point in the search space, it reduces the success of the algorithm. Therefore, while  $G_{best}$  convergence and silent spider techniques achieve 100% success in multimodal functions, they have not achieved in unimodal functions. Crossover and mutation techniques developed ISSA's exploration and exploitation ability in unimodal functions, but not all multimodal functions. This is because multimodal functions are more than one point of optimum and techniques can not discover these optimum points.

## 7. CONCLUSION

Social spider algorithm (SSA) is a heuristic algorithm that is created by imitating spider behaviors in nature. SSA regulates search space of optimization problems as a high dimensional spider web. SSA can be easily adapted to real-world problems and an easy to apply heuristic algorithm. In this paper, the original social spider optimization algorithm is studied details, an improved SSA (ISSA) based on SSA has been developed and applied on MPEF problem. MPEF problem is difficult to solve. Because the number of local minima increases exponentially with the molecular size. Four different techniques (Crossover, mutation,  $G_{best}$  convergence, and silent spider) are developed during the candidate solutions production schema in ISSA. With these four techniques, the ability of ISSA to search locally and globally in continuous space has been developed. The value of crossover rate (cr), mutation rate (mr), and  $G_{best}$  convergence rate (gr) are tested from the set {10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%} on ten different unimodal and multimodal benchmark functions. The most suitable values for these parameters are determined. The performances of SSA and ISSA are tested on thirteen unimodal and multimodal benchmark functions and the results obtained from SSA and ISSA are compared. Wilcoxon test was performed on the obtained results. The results showed that the ISSA has superior performance. The performance of the SSA and ISSA is evaluated on MPEF problem with different dimension={20, 40, 60, 80, 100, 120, 140, 160, 180, 200}. The results showed that the performance of ISSA is better than the performance of SSA. The performance of the ISSA is compared to various well-known seven algorithms in the literature. The results showed that the ISSA has superior performance and ISSA can be used as an alternative preference.

In future research, hybrid SSA will be created by using different heuristic methods. The random walk scene of SSA will be developed by inspiring from different heuristic methods. Weight value will be added to SSA's search space agents and the balance between the blasting and exploration will be provided.

## REFERENCES

- Acılar A.M., (2013), *Yapay Bağışıklık Algoritmaları Kullanılarak Bulanık Sistem Tasarımı*, Konya,Turkey, (Ph.D. thesis).
- Bansal J.C., Deep Shashi K., Katiyar V.K., (2010), Minimization of molecular potential energy function using particle swarm optimization. *Int J Appl Math Mech* 6(9):1–9.
- Barbosa H.J.C., Lavor C., Raupp F.M., (2005), A GA-simplex hybrid algorithm for global minimization of a molecular potential energy function. *Ann Oper Res* 138:189–202.
- Cuevas E., Cienfuegos M., Zaldívar D., Pérez-Cisneros M., (2013), A swarm optimization algorithm inspired in the behavior of the social-spider, *Expert Systems with Applications* 40, 6374–6384.
- Deep K., Barak S., Katiyar V.K., Nagar A.K., (2012), Minimization of molecular potential energy function using newly developed real coded genetic algorithms. *Int J Optim Control Theor Appl (IJOCTA)* 2(1):51–58.
- Deep K., Thakur M., (2007a), A new mutation operator for real coded genetic algorithms. *Appl Math Comput* 193(1):211–230.
- Deep K., Thakur M., (2007b), A new crossover operator for real coded genetic algorithms. *Appl Math Comput* 188(1):895–912.
- Dražić M., Lavor C., Maculan N., Mladenović N., (2008), A continuous variable neighborhood search heuristic for finding the three-dimensional structure of a molecule. *Eur J Oper Res* 185:1265–1273.
- El-bages M.S., Elsayed W.T., (2017), Social spider algorithm for solving the transmission expansion planning problem, *Electric Power Systems Research* 143, 235–243.

- Elsayed W.T., Hegazy Y.G., Bendary F.M., El-bages M.S., (2016), Modified social spider algorithm for solving the economic dispatch Problem, *Engineering Science and Technology, an International Journal* 19, 1672–1681.
- Grimaccia Gandelli F., Mussetta M., Pirinoli P., Zich R.E., (2007), Development and validation of different hybridization strategies between GA and PSO. In: *Proceedings of the IEEE Congress on Evolutionary Computation*, pp 2782–2787.
- Grimaldi E.A., Grimacia F., Mussetta M., Pirinoli P., Zich R.E., (2004), A new hybrid genetical swarm algorithm for electromagnetic optimization, In *Proceedings of the international conference on computational electromagnetics and its applications*, Beijing, China, pp 157–160.
- Hedar A., Ali A.F., Hassan T., (2011), Genetic algorithm and tabu search-based methods for molecular 3D-structure prediction. *Numer Algebra Control Optim* 1(1):191–209.
- Holland J.H., (1975), *Adaptation in natural and artificial systems*. University of Michigan Press, Ann Arbor.
- Jian M., Chen Y., (2006), Introducing recombination with dynamic linkage discovery to particle swarm optimization. In: *Proceedings of the genetic and evolutionary computation conference*, pp 85–86.
- Juang C.F., (2004), A hybrid of genetic algorithm and particle swarm optimization for recurrent network design. *IEEE Trans Syst Man Cybern Part B Cybern* 34:997–1006.
- Kennedy J., Eberhart R., (1995), Particle swarm optimization, in *Proc. IEEE Int. Conf. Neural Networks*, Perth, WA, pp. 1942–1948.
- Krink T., Lvbjerg M., (2002), The lifecycle model: combining particle swarm optimization, genetic algorithms, and hill climbers. In: *Proceedings of the parallel problem solving from nature*, pp 621–630.
- Lavor C., Maculan N., (2004), A function to test methods applied to global minimization of the potential energy of molecules. *Numer Algorithms* 35:287–300.
- Mallipeddi R., Mallipeddi S., Suganthan P.N., Tasgetiren M.F., (2011), Differential evolution algorithm with an ensemble of parameters and mutation strategies, *Appl. Soft Comput.* 11 1679–1696.
- Mousa A., Bentahar J., (2016), An Efficient QoS-aware Web Services Selection using Social Spider Algorithm, *The 13th International Conference on Mobile Systems and Pervasive Computing (MobiSPC 2016)*, *Procedia Computer Science* 94, 176 – 182.
- Pardalos P.M., Shalloway D., Xue G.L., (1994), Optimization methods for computing global minima of the nonconvex potential energy function. *J Glob Optim* 4:117–133.
- Parpinelli R.S., Lopes H.S., (2011), New inspirations in swarm intelligence: a survey, *Int.J. Bio-Inspired Comput.* 3 (1) 1–16.
- Robinson J., Sinton S., Samii Y.R., (2002), Particle swarm, genetic algorithm, and their hybrids: optimization of a profiled corrugated horn antenna. In: *Proceedings of the IEEE international symposium in Antennas and Propagation Society*, pp 314–317.
- Settles M., Soule T., (2005), Breeding swarms: a GA/PSO hybrid. In: *Proceedings of Genetic and Evolutionary Computation Conference*, pp 161–168.
- Surjanovic S., Bingham D., (2017), Virtual library of simulation experiments: test functions and datasets, <http://www.sfu.ca/~ssurjano>.
- Talbi E.G., (2009), *Metaheuristics: From Design to Implementation*, Wiley.
- Tawhid M.A., Ali A.F., (2016), A hybrid particle swarm optimization and genetic algorithm with population partitioning for large scale optimization problems, *Ain Shams Engineering Journal.*, xx, xxx-xxx.
- Tawhid M.A., Ali A.F., (2017a), A hybrid social spider optimization and genetic algorithm for minimizing molecular potential energy function, *Soft Computing*, 21:6499–6514 DOI 10.1007/s00500-016-2208-9.
- Tawhid M.A., Ali A.F., (2017b), A Hybrid grey wolf optimizer and genetic algorithm for minimizing potential energy function, *Memetic Comp.*, 9:347–359.



- Tawhid M.A., Ali A.F., (2017c), A Hybrid Flower Pollination and Genetic Algorithm for Minimizing the Non-Convex Potential Energy of Molecular Structure, *Trends Artif. Intell.*, 1(1):12-21.
- Wales D.J., Scheraga H.A., (1999), Global optimization of clusters, crystals, and biomolecules. *Science* 285:1368–1372.
- Yu J.Q.J., Li O.K.V., (2015), A social spider algorithm for global optimization, *Applied Soft Computing* 30 614–627.
- Yu J. J. Q., Li V. O. K., (2016), A social spider algorithm for solving the non-convex economic load dispatch problem, *Neurocomputing*, 171(C), 955–965.