Nelder-Mead based Marriage in Honey Bees Optimization C-means (NM-MBOC) algorithm for Clustering and it's Convergence Analysis

Chenguang Yang^{1, a}, Qiaoge Liu Li^{2, b}

¹ Chinese Electronic Equipment System Corporation Institute, Beijing, P. R. China

² Agricultural Bank of China, Beijing, P.R .China

^aemail: yangcgemail@126.com, ^bemail: liuqgmail@126.com

Keywords: Marriage in honey bees optimization (MBO); C-means, Nelder-Mead method; Markov chain

Abstract. Clustering is the method to partition unlabeled data, whitch is very important in bioinformatics. To overcome the difficult of balancing between different cluster criteria, we use multi-objective optimization to solve the problem. In this paper, we propose an Nelder-Mead based Marriage in Honey Bees Optimization C-means (NM-MBOC) algorithm for clustering. The pareto-optimal front that gives the optimal number of clusters as a solution set is obtained by NM-MBOC. The convergence is proven by Markov Chain Theory. In the end, tested with the UCI datasets, the effectiveness of the proposed approach is shown.

1. Introduction

Clustering is an unsupervised classification method to partition data into subgroups in bioinformatics. One popularly known problem of clustering is that there isn't clustering criteria can satisfy all the aspects. Some papers compliance with local density distributions [1], others integrate the results of a variety of different clustering methods [2][3].

To solve the problem of improper clustering criterion, one solution is to combine the results of several clustering methods; the other is to integrate several clustering criteria. The later one is an optimization problem of multi-objective and it has been shown to be superior to the former[7]. Many papers aim at providing choice for a decision maker[4][5] and a few paper work on the situation of the clusters number determining the clustering criterion[6].

Optimization is a basic problem for many areas, such as bioinformatics, computational biology. Not only traditional optimization but also multiple objectives optimization is arousing a great interest[8].

Multi-objective optimization focuses on the optimization problem with multiple goals. A general format is to minimize y that defined in (1).

$$y = f(x) = (f_1(x), f_2(x), ..., f_m(x)),$$

$$x = (x_1, x_2, ..., x_n) \in X$$
(1)

where x is the decision vector and X is the solution space. y is the objective function.

In this paper, we will propose a new algorithm of Nelder-Mead based Marriage in Honey Bees Optimization C-means (NM-MBOC), utilizing the algorithm named Nelder-Mead based Marriage in Honey Bees Optimization (NM-MBO) as the multi-objective optimization tool. The pareto-optimal will be obtained after running the multi-objective algorithm.

Marriage in Honey Bees Optimization (MBO) is a swarm intelligence method was proposed by Jason Teo and Hussein A. Abbass[9][10] and has been updated by Jason Teo, Hussein A. Abbass [11] and Omid Bozorg Haddad et al [12][13]. Combing with Nelder-Mead method and C-means method, NM-MBOC is used for clustering. And its convergence is analyzed based on the theory of Markov Chain.

The paper is organized as follows. As the basis of the study, Marriage in Honey Bees Optimization (MBO) algorithm and Nelder-Mead method are shown first in Section 2. The

proposed algorithm of Nelder-Mead based Marriage in Honey Bees Optimization C-means (NM-MBOC) is given in Section 3. Section 4 uses Markov Chain theory to analyze the proposed algorithm's convergence. Finally, some simulations, use UCI datasets, are done and conclusion is given.

2. Nelder-Mead method and marriage in honey bees optimization (NM-MBO)

2.1. Algorithm of marriage in honey bees optimization

The behavior of honey-bees shows many features like cooperation and communication, so honey-bees have aroused great interests in modeling intelligent behavior these years.

Marriage in Honey Bees Optimization (MBO) is a kind of swarm-intelligence method. And such swarm-intelligence has some successful applications. Ant colony is an example and the search algorithm is inspired by its behavior. Mating behavior of honey-bees is also considered as a typical swarm-based optimization approach. The behavior of Honey-bees is related to the product of their genetic potentiality, ecological and physiological environments, the social conditions of the colony, and various prior and ongoing interactions among these three [9][10].

The five main processes of MBO are: (a) the mating-flight of the queen bees with drones encounter at some probabilistically. (b) creating new broods by the queen bees, (c) improving the broods' fitness by workers, (d) updating the workers' fitness, and (e) replacing the least fittest queen(s) with the fittest brood(s).

2.2. Nelder-Mead method

The Nelder-Mead method is a commonly used nonlinear optimization algorithm, proposed by Nelder & Mead [15]. It is a direct search method and does not use numerical or analytic gradients. The method uses the concept of simplex and finds a local minimum of a function with several variables. Nelder-Mead method can generate a new point by extrapolating the objective function measured at each point arranged as a simplex, and will replace one of them with the new one to keep the algorithm run.

The basic process in a iteration is the following.

- Order. Order the n+1 vertices to satisfy $f(x_1) \le f(x_2) \le \dots \le f(x_{n+1})$, using the tie-breaking rules given below.
- Reflect. Compute the reflection point x_r from $x_r = \overline{x} + \rho(\overline{x} x_{n+1})$, $\overline{x} = \sum_{i=1}^n \frac{x_i}{n}$ is the centroid of the *n* best points (all vertices except for x_{n+1}). Evaluate $f_r = f(x_r)$. If $f_1 \le f_r < f_n$, accept x_r

and terminate the iteration.

- Expand. If $f_r < f_1$, calculate the expansion point x_e . $x_e = \overline{x} + \lambda(x_r \overline{x})$ and evaluate $f_e = f(x_e)$. If $f_e < f_r$, accept x_e ; otherwise accept x_r . Terminate the iteration.
- Contract. If $f_r > f_n$, perform a contraction between \overline{x} and the better of x_{n+1} and x_r .
- Perform a shrink step. Evaluate *f* at the *n* points $v_i = x_1 + \sigma(x_i x_1)$, i = 2,...n+1. The vertices of the simplex at the next iteration consist of $x_1, v_2, ..., v_{n+1}$.

The merit of Nelder-Mead method is that it is not sensitive to starting values and neither does it rely on derivatives nor on continuity of the objective function.

3. Nelder-Mead based Marriage in Honey Bees Optimization C-means (NM-MBOC) algorithm

3.1. Algorithm of NM-MBO

One of the most important advantages of MBO over Genetic Algorithm is MBO does a local search in each iteration. So MBO can avoid solely using crossover operator and mutation operator who is of worse local search ability.

But MBO algorithm chooses some simple and random local searching methods, such as random walk and random flip 0, which will reduce the probability of obtaining optimal solution. So such low efficiency of Worker in MBO badly influences the whole performance of MBO.

So we utilize the local search ability and replace the Worker of MBO algorithm by the Nelder-Mead method.

Some studies related to MBO have been carried out in our research. One of them is to increase the convergence speed. Here we make some introduce about it, because the main work in this paper will based on such improved MBO algorithm.

In MBO algorithm, the probability of a drone makes with a queen is defined by the annealing function 0. Not only the calculation of probability is complex, but also its calculation participants are complicated. So the whole process has a large computation burden.

On the other hand, we have found that MBO with low speed need enough iteration times to approach optimization result. But several variables in MBO, such as energy, speed, can't make sure about this. As the process going, the mating probability becomes smaller, which neither help the calculation process put up, nor help converge globally. So based on the original MBO algorithm, we have done some improvement on the original MBO algorithm. That is, by random initializing drones and restricting the condition of iteration, the computation process will become easier. The detail about this improvement has been discussed in other papers before.

Here we further our research to improve the performance of MBO and propose an algorithm of Nelder-Mead -Marriage in Honey Bees Optimization (NMMBO) by taking the Nelder-Mead method and C-means method as the Workers.

3.2. C-means clustering based on NM-MBOC

In Fig.1, we can define four operators: Crossover, Mutation, Heuristic(NM) and C-means. Crossover and Mutate are same as that in GA. But the Heuristic and C-means operator is a new one proposed in NM-MBOC.

Crossover: Crossover operator exchanges the pieces of genes between chromosomes. Through crossover, it introduces new chromosomes to the population, and hence the possibility of having fitter chromosomes. In this algorithm one-point crossover can produced better results compared to multi-point after some initial experiments.

Mutation: Mutation operation alters individual alleles at random locations of random chromosomes at a very probability. It might create a better or worse chromosome, which will either thrive or diminish through next selection.

Heuristic: Heuristic operator improves a set of broods. It help conduct local search on broods. For the good local convergence performance, we use Nelder-Mead method as the heuristic operator.

C-means: C-means is used to reanalyze cluster value; it calculates the cluster centre for each cluster; and then it re-assigns each gene to the cluster that is the closest one to the instance in the gene. Hence, C-means operator is used to speed up the convergence process.

By the way, in Fig1, every Nelder Mead method is followed by a fix box. The reason is: it is possible for Nelder Mead method to create illegal results.

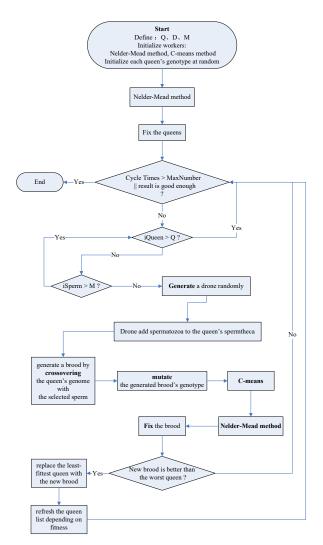


Fig.1. Nelder-Mead-Marriage in Honey Bees Optimization C-means algorithm (NM-MBOC)

4. Convergence analysis of NM-MBOC algorithm

4.1. Markov chain

Markov chain has been widely applied to GA. Markov chains (MCs) have been used extensively to study convergence characteristic. Such as many GA methods' performance were analyzed by modeling the GA process as a Markov process.

A Markov chain is a sequence of random values whose probability at a time interval depends upon the value of the number at the previous time. The probabilities of a Markov chain are usually entered into a transition matrix indicating which state or symbol follows which other state or symbol.

Definition 1[14]: A square matrix is $A = [a_{ij}]_{n \times n}$

(a) if
$$\forall i, j \in \{1, ..., n\}$$
 : $a_{ij} > 0$, A is positive $(A > 0)$;
(b) if $\forall i, j \in \{1, ..., n\}$: $a_{ij} \ge 0$, A is nonnegative $(A \ge 0)$;
(c) if $A \ge 0$ and $\exists m \in \mathbb{N} : A^m > 0$, A is primitive;
(d) if $A \ge 0$ and $\forall i \in \{1, ..., n\}$: $\sum_{i=1}^{n} a_{ij} = 1$, A is stochastic.
(2)

Definition 2[14]: If the state space *s* is finite (|s|=n), and the transition probability $p_{ij}(t)$ are independent from *t*,

$$\exists i, j \in S, \exists u, v \in \mathbb{N}, p_{ij}(u) = p_{ij}(v)$$
(3)

the Markov chain is said to be finite and homogeneous. $p_{ij}(t)$ is the probability of transitioning from state $i \in S$ to state $j \in S$ at step t.

Theorem 1[14]: For a homogeneous finite Markov chain, with the transition matrix $P=(p_{ij})$, If

$$\exists m \in \mathbf{N} : P^m > 0 \tag{4}$$

then this Markov chain is ergodic and with finite distribution. $\lim_{t\to\infty} p_{ij}(t) = \overline{p_j}, i, j \in S$ is the steady distribution of the homogeneous finite Markov Chain.

Theorem 2[14] (The basic limit theorem of Markov chain): If P is a primitive homogeneous Markov chain's transition matrix, then

it is a $n \times n$ matrix and it's all rows are same to ω^T .

Theorem 3[14]: Let *P* be a reducible stochastic matrix, where $C:m \times m$ is a primitive stochastic matrix and $R \neq 0, T \neq 0$. Then

$$P^{\infty} = \lim_{k \to \infty} P^{k} = \lim_{k \to \infty} \begin{pmatrix} C^{k} & 0\\ \sum_{i=0}^{k-1} T^{i} R C^{k-i} & T^{k} \end{pmatrix} = \begin{pmatrix} C^{\infty} & 0\\ R^{\infty} & 0 \end{pmatrix}$$
(6)

is a stable stochastic matrix.

4.2 Convergence analysis

The proposed algorithm is against solving Multi-Objective Optimization problem. And two objective functions are given: minimizing the number of clusters and minimizing the partitioning error.

A common difficulty with the multi-objective optimization is the conflict between the objective functions. None of the feasible solutions allows optimal solutions for all the objectives. Pareto-optimal is the solution, which offers the least objective conflict.

When output(s1) of one objective function is fixed, turn to optimize the other objective function's output(s2). If s2 can reach the optimal value, we can get the optimal solution under the condition of s1 is fixed. Then the problem is converted to a one objective optimization problem.

If the following two can be proved, the proposed algorithm is convergent.

For any fixed s1, the corresponding optimal solution of s2 can be gotten.

On the other side, for any fixed s2, the corresponding optimal solution of s1 can be gotten. Then the problem is to prove the convergence of the above two one-objective optimization problem.

Then we use Markov Chain to analysis the convergence of the Nelder-Mead-Marriage in Honey Bees Optimization C-means algorithm.

There are only four ways to change from one generation to another, Crossover, Mutate, C-means and Heuristic. These operators depend only on the inputs and not restricted with time. Then we can get the following theorem.

Definition 3: The state space of NM-MBOC is

$$X = \left\{ x = [t_1, t_2, \dots, t_N] \middle| t_i \in \{0, 1\}, i = 1, \dots, N \right\}$$
(7)

where $[t_1, t_2, ..., t_N]$ is the binary bit cluster listed in turn.

Define f(x) as the fitness function based on X and y is the fitness. So the fitness aggregate Y is

$$Y = \left\{ y \middle| y = f(x), x \in X \right\}$$
(8)

It is easy to see

$$\forall x \in X, y > 0 \tag{9}$$

Define g = |Y|, we can get a ordered aggregate

$$\{y_1, y_2, \dots, y_g\}, y_1 > y_2 > \dots > y_g$$
 (10)

Crossover, Mutate, C-means and Heuristic operators lead to probable transition in the state space. And we use four transition matrix C, M, Cm and H to describe their infections respectively. Finally, we can get

$$Tr = C \cdot M \cdot Cm \cdot H \tag{11}$$

where Tr is the transition matrix of the Markov chain of the NM-MBOC algorithm. Theorem 4: The Markov Chain of NM-MBOC is finite and homogeneous.

Proof:

The aggregate $\{x_1, x_2, ..., x_M\}$ is finite. So the Markov chain composed of $\{x_1, x_2, ..., x_M\}$ is finite. This finite space can also be said as a state space *x*.

With $\rho_i, \rho_j \in X$, the probability of transformation from the state ρ_i to the state ρ_j at step *t* only depends on ρ_i and is independent of time. So the Markov chain of the NM-MBOC algorithm is homogeneous.

End.

Theorem 5: The transition matrixes of the crossover probability (C), Heuristic probability (H) and C-means probability (Cm) in the NM-MBOC algorithm are all stochastic.

Proof:

The square matrix *C* is $C = \left[c_{ij}\right]_{n \times n}$. Then

$$\forall i, j \in \{1, ..., n\} : c_{ij} \ge 0 \text{ and } \forall i \in \{1, ..., n\} : \sum_{j=1}^{n} c_{ij} = 1$$
(12)

So C is stochastic.

The square matrix *H* is $H = [h_{ij}]_{n \times n}$. Then,

$$\forall i, j \in \{1, \dots, n\} : h_{ij} \ge 0 \text{ and } \forall i \in \{1, \dots, n\} : \sum_{j=1}^{n} h_{ij} = 1$$
(13)

So *H* is stochastic.

C-means operator is used to speed up the convergence process. So it's operation is similar to Heuristic.

The square matrix Cm is $Cm = [cm_{ij}]_{n\times n}$. Then

$$\forall i, j \in \{1, \dots, n\} : c_{ij} \ge 0 \text{ and } \forall i \in \{1, \dots, n\} : \sum_{j=1}^{n} cm_{ij} = 1$$
(14)

So *Cm* is stochastic.

End

Theorem 6: The transition matrix of the NM-MBOC with mutation probability (M) is stochastic and positive.

Proof:

 $M = [m_{ij}]_{n \times n}$ is a square matrix. Then

$$\forall i, j \in \{1, \dots, n\} : m_{ij} \ge 0 \text{ and } \forall i \in \{1, \dots, n\} : \sum_{j=1}^{n} m_{ij} = 1$$
 (15)

So *M* is stochastic.

And the mutation has an influence on every position of a state vector. We can easily know $\forall x_i, x_j \in X$. Each position of x_i can mutate to the value of x_j . So the probability of x_i mutate to x_j is positive. So *M* is positive.

End

Theorem 7: The Markov Chain of the NM-MBOC (*Tr*) is ergodic and with finite distribution $\lim_{t \to T} tr_{ij}(t) = \overline{tr_j} > 0, i, j \in X$.

Proof:

According to Theorem 5, Theorem 6 and(11), Tr is positive. And according to Theorem 1, this proposition is proved.

End

Definition 4: The fitness of one generation is the largest one of the individuals in this generation.

$$f(\{x_{1}, x_{2} \dots x_{K}\}) = \max_{i=1,2,\dots,K} \{f(x_{i})\}$$
(16)

Define $X_i = \{x_i, x_2, ..., x_k | f(\{x_i, x_2, ..., x_k\}) = y_i, x_i, x_2, ..., x_k \in X\}$, y_i are defined at(10), that is, the fitness of all the individuals in X_i is equal to y_i .

Definition 5: For an arbitrary initial generation X(0), y_1 is of the largest fitness,

$$\lim_{t \to \infty} \Pr(f(X(t)) = y_1) = 1 \tag{17}$$

Then the algorithm is global convergence. Theorem 8: The NM-MBOC converges to the global optimum. Proof: We can define

$$TX = \left\{ X_i \middle| i \in N \right\} \tag{18}$$

For Definition 4 and Theorem 4, TX is a Markov Chain. In the same time, we define

$$P(X_i) = P\left\{iX \in X_i\right\} \tag{19}$$

iX is defined in (12).

We can see that $P(X_i) > 0$ and $\sum_{i=1}^{n} P(X_i) = 1$

Define $P(X_i, X_j)$ is the probability state X_i go to X_j , we can get

$$P(X_i, X_j) = \sum_{ni=1}^{N_i} \sum_{nj=1}^{N_j} P(x_{ni}, x_{nj}), x_{ni} \in X_i, x_{nj} \in X_j$$
(20)

Because NM-MBOC saves the best individual at every generation, $P(X_i, X_j) = 0, i < j$. And the transition matrix of *TX* 's Markov Chain can be write as follows:

$$P = \begin{bmatrix} P(X_{1}, X_{1}) & \cdots & P(X_{1}, X_{n}) \\ \vdots & \cdots & \vdots \\ P(X_{n}, X_{1}) & \cdots & P(X_{n}, X_{n}) \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & \cdots & 0 \\ P(X_{2}, X_{1}) & P(X_{2}, X_{2}) & \ddots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ P(X_{n}, X_{1}) & \cdots & \cdots & P(X_{n}, X_{n}) \end{bmatrix}$$
(21)

For Theorem 3,

$$C = 1, T = \begin{bmatrix} P(X_2, X_2) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ P(X_n, X_2) & \cdots & P(X_n, X_n) \end{bmatrix}, R = \begin{bmatrix} P(X_2, X_1) \\ \vdots \\ P(X_n, X_1) \end{bmatrix}$$
(22)

$$P^{\infty} = \lim_{k \to \infty} P^{k} = \lim_{k \to \infty} \left(\sum_{i=0}^{k-1} T^{i} R C^{k-i} \quad T^{k} \right) = \begin{pmatrix} C^{\infty} & 0 \\ R^{\infty} & 0 \end{pmatrix}$$
(23)

For Theorem 7 and Theorem 1, P^{∞} is a stable random matrix, So $R^{\infty} = 1$. That is

$$R^{\infty} = \lim_{k \to \infty} R^{k} = \begin{bmatrix} \lim_{k \to \infty} \left(P(X_{2}, X_{1}) \right)^{k} \\ \vdots \\ \lim_{k \to \infty} \left(P(X_{n}, X_{1}) \right)^{k} \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$
(24)

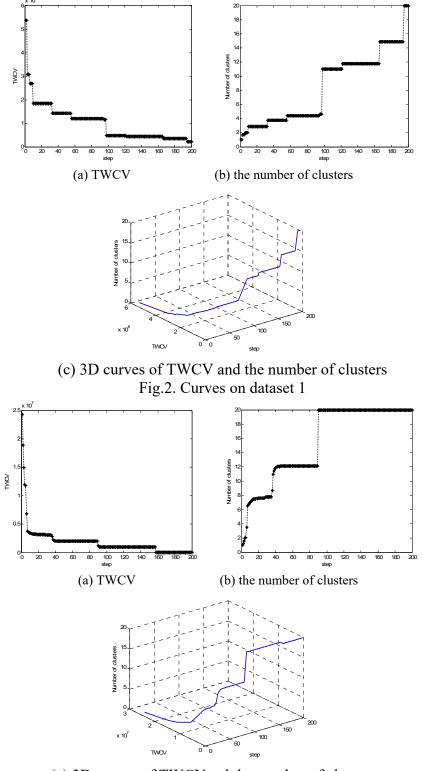
So every state in TX will go to X_1 , if the iteration number is big enough, this proposition is proved.

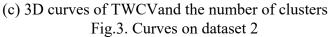
End

It is applicable to the two conditions, so the algorithm can converge to the Pareto surface.

5. Simulation

To test the performance of proposed algorithm, we will do some simulations. We choose three datasets in UCI database and draw the dynamic curves of TWCV[6] and the number of clusters respectively. Fig.2 to Fig.3 are the test results





From the above, we can see that the proposed algorithm can converged according to the objective functions.

6. Conclusions

Using multi-objective optimization methods to solve clustering problem is useful, which can avoid weighting different results obtained from different clustering criteria. In this paper we proposed a new algorithm to solve clustering problem, naming as. Nelder-Mead Method based Honey Bees Optimization C-means (NM-MBOC) algorithm. NM-MBOC can not only avoid the local optimum, but also converge to the Pareto surface. Also NM-MBOC is easy to implement and has few parameters to adjust. And the global convergence is proved. Simulating on three UCI datasets show that the NM-MBOC is effective for clustering.

References

[1] J. Handl, J. Knowles, and D.B. Kell, "Computational Cluster Validation in Post-Genomic Data Analysis" Bioinformatics, vol. 21, no. 15, pp. 3201-3212, 2005.

[2] A. Strehl and J. Ghosh, "Cluster Ensembles—A Knowledge Reuse Framework for Combining Multiple Partitions," J. Machine Learning Research, vol. 3, pp. 583-617, 2002.

[3] A. Topchy, A.K. Jain, and W. Punch, "Clustering Ensembles: Models of Consensus and Weak Partitions," IEEE Trans. Pattern Analysis and Machine Intelligence, vol. 27, no. 12, pp. 1866-1881, Dec. 2005.

[4] M.B. Dale and P.T. Dale, "Classification with Multiple Dissimilarity Matrices," Coenoses, vol. 9, no. 1, pp. 1-13, 1994.

[5] A. Ferligoj and V. Batagelj, "Direct Multicriterion Clustering," J. Classification, vol. 9, pp. 43-61, 1992.

[6] Y. Liu, T. Oezyer, R. Alhajj, and K. Barker, "Integrating Multi-Objective Genetic Algorithm and Validity Analysis for Locating and Ranking Alternative Clustering," Informatica, vol. 29, pp. 33-40, 2005.

[7] J. Handl and J. Knowles, "An Evolutionary Approach to Multiobjective Clustering," IEEE Trans. Evolutionary Computation, vol. 11, no. 1, pp. 56-76, 2007.

[8] D.F. Jones, S.K. Mirrazavi, and M. Tamiz, "Multi-Objective Meta-Heuristics: An Overview of the Current State-of-the-Art," EuropeanJ. Operational Research, vol. 137, no. 1, pp. 1-9, 2002.

[9] H.A. Abbass, "Marriage in Honey Bees Optimization (MBO): A Haplometrosis Polygynous Swarming Approach", Congress on Evolutionary Computation, CEC2001, Seoul, Korea, 2001, pp. 207-214.

[10]H.A. Abbass, "A Single Queen Single Worker Honey-Bees Approach to 3-SAT", Proceedings of the Genetic and Evolutionary Computation Conference, GECCO2001, San Francisco, USA, 2001, pp. 807-814.

[11]Jason Teo, Hussein A. Abbass, "An Annealing Approach to the Mating-Flight Trajectories in the Marriage in Honey Bees Optimization Algorithm", Technical Report CS04/01, School of Computer Science, University of New South Wales at ADFA, 2001.

[12]Omid Bozorg Haddad, Abbas Afshar, Miguel A. Marin O., "Honey-Bees Mating Optimization (HBMO) Algorithm: A New Heuristic Approach for Water Resources Optimization", Water Resources Management, 20, 2006, pp. 661-680.

[13]Hyeong Soo Chang, "Converging Marriage in Honey-Bees Optimization and Application to Stochastic Dynamic Programming", Journal of Global Optimization, 35, 2006, pp. 423-441.

[14]Rudolph G., "Convergence analysis of canonical genetic algorithms", IEEE Transaction Neural Networks. 5(1), 1994, pp. 96-101.

[15]Lagarias, J C, J A Reeds, M H Wright, P E Wright, "Convergence Properties of the Nelder-Mead Simplex Method in Low Dimensions", SIAM Journal of Optimization, 9(1), 1998, pp. 112-147.