INTERNATIONAL RESEARCH JOURNAL OF PHARMACY

www.irjponline.com

ISSN 2230 – 8407

Review Article

APPLICATIONS OF SWARM BASED INTELLIGENCE ALGORITHM IN PHARMACEUTICAL INDUSTRY: A REVIEW

Rajeshkumar J *[1], Kousalya K [2]

[1]Assistant Professor, SNS College of Technology, Coimbatore, Tamil Nadu, India

[2]Professor, Kongu Engineering College, Erode, Tamil Nadu, India

*Corresponding Author Email: rajeshresearch88@gmail.com

Article Received on: 31/10/17 Approved for publication: 29/11/17

DOI: 10.7897/2230-8407.0811212

ABSTRACT

A swarm is a large number of homogeneous, uncomplicated agents collaborating locally among themselves, and their circumstances, with no central control to allow a global interesting behaviour to emerge. Swarm based algorithms are nature inspired, population based algorithms that are clever in producing optimal solution for several complex and combinatorial problems. In the pharmaceutical industry, the product and other process development problems usually involve a numerous of independent variables and it incorporated with multiple constraints. To solve problems related to pharmaceutical industry requires accurate result and it's very hard to solve using traditional method. Swarm based intelligence technique is a collection of knowledge based algorithms which having capable of solving complex problems and can obtain optimal or accurate solution. This paper discusses swarm based intelligent algorithms to solve different pharmaceutical field related complex problems such as drug design, pharmacovigilance, alignment of sequence etc.

Keywords: Swarm Intelligence, Pharmaceutical Industry, Optimization Algorithms, Combinatorial Problems, Pharmacovigilance

INTRODUCTION

Swarm intelligence is a sub area of artificial intelligence which concentrates on designing an intelligent multi-agent system by using the collective behaviour of natural agents such as ants, birds, fish, ant lion etc.., Self organization and decentralized control based working environment are the main features of social insects or other natural swarms in their collective activities. Optimization techniques are the mathematical domain which finds the best or optimum solutions from the initial feasible solutions for a given problem. There are various types of optimization techniques available to solve single, multi variable functions. Functions may or may not hold constraints. Swarm intelligence optimizes the functions and produce optimal results which satisfy the constraints related to the problem.

Pharmaceutical industry is one of the most critical level areas which rely on decision oriented and has a noticeable impact on every society's hygiene and treatment part of human being. Pharmaceutical industries have large size of data sets that have not been used to make any meaningful decision directly for further process. So it requires efficient system to infer meaningful decision in no time. Swarm based optimization algorithm provides such an environment to pharmaceutical industry and it can adopt for any problems. For example, drug discovery problem requires enormous data and factors to be processed to receive meaningful information[1]. If we use traditional methods, it requires more time to attain solution which may be a non optimal solution. But in that situation if we apply heuristic based algorithms, we can attain optimal solutions using multiple knowledge based swarms within fraction of time. This is the main feature which enforces the researchers to concentrate on swarm based procedures for solving combinatorial optimization problems.

Ant colony optimization (ACO), Particle swarm optimization, Gases Brownian motion optimization (GBMO), Chemical reaction optimization (CRO), Intelligent water drop optimization (IWO) are some of the swarm based algorithms available to solve different optimization problems. Each algorithm has its own individual characteristics while solving the problems but which follows same framework. Swarm based algorithms will not change its population from generation to generation which happens in evolutionary algorithms. Choosing proper algorithm based on problems characteristics and parameter settings are the other important major research issues.

In this paper, the authors discussed some of the swarm intelligence based optimization algorithms, which are more efficient for solving different problems related to pharmaceutical industry. Section 2 deals with application of swarm algorithms in drug discovery and design. Section 3 discusses concept of pharmacovigilance and applications of swarm algorithm in the same. Section 4 deals with sequencing and alignment concepts. Section 5 deals with data mining and swarm algorithms in pharmaceutical industry problems.

SWARM INTELLIGENCE AND ITS APPLICATIONS IN PHARMACEUTICAL PROBLEMS

Drugs are obligatory for human survival. Designing a drug is a system of detecting or creating a molecule which has a specific activity on a specific biological living thing. Inventing a new drug is an expensive and time consuming process[2]. An average of 10 to 15 years and up to 800 million US dollars is consumed

by new drug development[3]. One of the main problems of drug design is exploring the chemical space of many possible molecules to obtain the new scarcely any suitable molecule. Drug discovery process is a collection three major process namely Lead Discovery, Lead Optimization and Clinical Candidate. Many swarm based intelligence algorithms were developed by different authors to simplify and enhance the process of drug discovery.

Quantum based binary version of particle swarm optimization algorithm (QBPSO)[4] was developed in which active site of the target protein is known. In this method fitness evaluation considers interaction energy of the residue, chemical properties of the pair and closest functional group. This binary version of PSO on drug design problem provides optimal solution by producing minimum interaction energy.

Pharmacovigilance is a major area in pharmaceutical industry in which safety of the drug monitored. This field discusses with detecting, monitoring the adverse affects of drugs and other possible medication errors[5]. Pharmacovigilance field requires high level knowledge to retrieve meaningful decision from the available data. Knowledge discovery process in this area is an important and PSO/ACO approach[6] applied successfully and received meaningful data from the large set of available data. This method supports high accuracy in spotting presence of previously undetected causal relationships between therapeutics, patient characteristics and inauspicious events.

Data mining has acquired a vital role during all phases of drug development from drug discovery to surveillance of post marketing. Post marketing is the main theme in pharmacovigilance field in which large number of data collected and processed using data mining or other data processing algorithms. Two broad areas of pharmacovigilance in which data mining concepts required are: 1) Pinpointing new effects of drugs 2) Fittingness in usage of drug. Mining infrequent causal associations[7] was performed using exponential particle swarm optimization algorithm. It also used the working methodology of fuzzy model to identify the best causal relationship and their reactions of drug in potent manner. Proposed system also uses fuzzy recognition primed decision principle to extract causal relationship among drug and pairs of symptoms among different patient. Data and rule are extracted from health care report of the patients. This system takes minimum amount of time and cost to extract decision from available reports.

Some of the data mining methods have introduced by many researchers to identify disease and other factors from available medical data. This system adopted by different swarm intelligence based techniques in many of its phases while processing input data set. Disease risk evaluation and earlier detection is the recent research in which many swarm intelligence based algorithms employed. Firefly algorithm for breast cancer risk evaluation[8], Hybrid finite difference frequency domain and particle swarm optimization techniques[9] and hybrid intelligent bees algorithm for breast cancer detection[10], Myocardial Infarction detection using Hybrid Firefly Algorithm[11], Dynamic protein complexes detection using fruit fly optimization algorithm[12], PSO based detection of dengue disease[13], Diabetic disease detection using bat optimization and fuzzy rule miner[14], Lymph diseases prediction using particle swarm optimization algorithm and random forest[15] are some research findings for disease detection using different combinations of swarm algorithms.

Another important problem is sequence alignment of genes. Sequence alignment is defined as a comparison procedure which involves two or more biological sequences. This sequence alignment helps in many areas such as classifying proteins and genes; biological function prediction etc., Pair wise alignment and multiple sequence alignment are the two important classification of sequence alignment. The overall objective of the sequence alignment is focusing on understanding predicting the structures of molecules. Multiple sequence alignment problems are considered as NP-Hard[16] and it requires swarm intelligence to get optimal solution.

Hybrid method for multiple sequence alignment was proposed[17] in which tabu search and simulated annealing algorithms combined to get optimal solution. In this method proper guidance was initiated to maintain the balancing between intensification and diversification. Simulated annealing method was considered as exploitation tool for search space. Local minima trapping was avoided by tabu search as well as simulated annealing characteristics. Ant colony optimization based sequencing method on deoxyribonucleic acid (DNA) was proposed[18] with multi level framework feature. This algorithm was compared with many optimization algorithms and it outperforms other algorithm. Multi level ant colony algorithm for DNA sequencing was introduced[19] with additional information utilization factor. This methodology has the capability of reconstructing the sequence using available partial information also.

Bacterial foraging optimization algorithm based multiple sequence alignment[20] was proposed and it considered multiple objectives such as non-gap percentage, maximization of similarity, conserved blocks and minimization of gap penalty. In this paper authors proposed two swarm intelligence based algorithm namely hybrid genetic algorithm with artificial bee colony and bacterial foraging optimization algorithm. BaliBase 3.0 database was consumed by proposed algorithm to show its performance. In the experimental analysis, the hybrid genetic algorithm failed to produce conserved block. But bacterial algorithm worked efficiently and produced conserved block. Proposed algorithm was compared with particle swarm optimization, ant colony optimization, artificial bee colony and genetic algorithm. Proposed multi objective bacterial algorithm outperforms other algorithms.

Ribonucleic Acid (RNA) sequence structure alignment[21] using two level particle swarm optimization algorithm was developed for pair wise analysis of RNA structure. Proposed approach optimizes the length of sequences and evaluates the conflicting constraints. Ant colony based hybrid algorithm for multiple sequence alignment considers genetic algorithm[22] additional component to provide efficiency in aligning multiple sequence.

Combination of ant colony optimization and genetic algorithm has been proposed for sequence alignment[23]. In this algorithm ACO algorithm is used to receive set of alignments and genetic algorithm (GA) is used to improve the quality of alignments which obtained in ACO. But this algorithm was only applied for single sequence alignment. Particle swarm optimization algorithm was combined with hidden markov model[24] for multiple sequence alignment. This method guaranteed optimal training using hidden markov model. Baum–Welch algorithm is also involved in this system and to avoid local optima.

Many new swarm based algorithms have been developed recently by many researchers which derives many living things characteristics in their working methodology. In the following table the recent swarm based algorithms are given with their basic working characteristics:

Algorithm Name	Characteristics
Whale Optimization Algorithm[25]	• Mimics the social behaviour of Humpback whales
Moth Flame Optimization Algorithm[26]	• Inspires the navigating method of moths in nature
Magnetic Optimization Algorithm[27]	• Inspires the principle of magnetic field theory
Thermal Exchange Optimization Algorithm[28]	• Working principle is based on the Newton's law of cooling
Grasshopper Optimisation Algorithm[29]	• Working principle inspires the behaviour of grasshopper in nature
Competitive Optimization Algorithm[30]	• This algorithm mimics the competitive behaviour of various living creatures such as birds, cats, ants and bees etc.,
Chaotic Grey Wolf Optimization Algorithm[31]	• Algorithm inherits the hunting behaviour of grey wolves

Many other algorithms are also available in the area of optimization algorithm. Similarly more than one algorithm can be combined to increase the overall optimality of the output. This concept is also called as hybrid metaheuristic algorithm. In hybrid metaheuristic algorithm, the disadvantages of one algorithm can be tolerated by other in order to increase the efficiency. Finding good combinations of algorithm is the other research issue in the same field. By using any of the above swarm based algorithm and hybrid versions of that swarm algorithm, many pharmaceutical industry problems can be solved in efficient manner.

CONCLUSION

In this paper, we discussed many pharmaceutical problems and their solving methodology using swarm based intelligence algorithms. Pharmaceutical problems are very complex in nature which requires more accurate results because it directly affects the life of living creature. So most of the traditional problem fails due to its time and cost complexity. But swarm based intelligence algorithm can solve the problem efficiently by using their iterative process. Based on the characteristics of the problems, user can choose appropriate one or more algorithm to solve. Data mining also plays major role in pharmaceutical data handling processes which come up with meaningful decision from available raw data. In medical data mining also, it is possible to use swarm intelligence in order to improve the decision quality. Swarm intelligence based algorithm can provide good quality of solution in any sort of the problems in pharmaceutical industry and their sub areas.

REFERENCES

1. Ruud EH, Smits M and Wouter PCB. The Role of Users in Innovation in the Pharmaceutical Industry. Drug Discovery Today 2008; 13.
2. Muller G. Medicinal Chemistry of Target Family-Directed Masterkeys. Drug Discovery Today 2003; 681-691.
3. DiMasi JA, Hansen RW and Grabowski HG. The Price of Innovation: New Estimates of Drug Development Costs. Journal of Health Economics 2003; 22:151-185.
4. Ghosh A, Chowdhury and Hazra J. An Evolutionary Approach to Drug-Design Using Quantum Binary Particle Swarm Optimization Algorithm. Electrical, Electronics and Computer Science (SCEECS) 2012;1-4.
5. Naik P. The Future of Pharmacovigilance. J Pharmacovigilance. 2015; 3: 159
6. Margarita Sordo, Shawn N, Murphy. APSO/ACOApproach to Knowledge Discovery in a Pharmacovigilance Context. Harvard MedicalSchool, Charlestown, MA. USA.
7. Poorani M, Nithya P and Umamaheshwari B. A Method for Mining Infrequent Causal Associations with Swarm Intelligence Optimization for Finding Adverse Drug Reaction. International Journal of Computing, Communications and Networking. 2014; 3: 25-32.
8. Saravana Kumar K and Arthanariee AM. Breast Cancer Risk Evaluation By Firefly Optimization Algorithm. International Journal of Engineering Technology Science and Research. 2017; 4: 214 – 219.
9. Zainud-Deen SH, Hassen WM, Ali EM, Awadalla KH and Sharshar HA. Breast Cancer Detection Using a Hybrid Finite Difference Frequency Domain and Particle Swarm Optimization Techniques. 2008; 3: 35 - 46.
10. Jaliladdeh, Ata Ebrahimzadeh. Breast Cancer Recognition Using a Novel Hybrid Intelligent Method. Journal of Medical Signals & Sensors 2012; 2:95 – 102.
11. Padmavathi Kora. ECG based Myocardial Infarction detection using Hybrid Firefly Algorithm. Computer Methods and Programs in Biomedicine. 2017; 152: 141 – 148.
12. Lei Xiujuana, Ding Yuliana, Hamido Fujitab and Zhang Aidongc. Identification of Dynamic Protein Complexes Based on Fruit Fly Optimization Algorithm. Knowledge-Based Systems 2016; 105:270 – 277.
13. Shalini Gambhir, Sanjay Kumar Malik and Yugal Kumar. PSO-ANN based Diagnostic Model for the Early Detection of Dengue Disease. New Horizons in Translational Medicine 2017;
14. Ramalingaswamy Cheruku, Damodar Reddy Edla, Venkatanareshbabu Kuppili and Ramesh Dharavath:RST-BatMiner. A Fuzzy Rule Miner Integrating Rough Set Feature Selection and Bat Optimization for Detection of Diabetes Disease. Applied Soft Computing 2017;
15. Waheeda Almayyan:Lymph Diseases Prediction Using Random Forest and Particle Swarm Optimization. Journal of Intelligent Learning Systems and Applications. Journal of Intelligent Learning Systems and Applications. 2016; 8:51 – 62.
16. Wang L and Jiang T. On the Complexity of Multiple Sequence Alignment. Journal of Computational Biology 1994; 1:337 – 348.
17. Lamiche Chaabane and Moussaoui Abdelouahab. A Hybrid Method Applied to Multiple Sequence Alignment Problem. Wseas Transactions on Computers2015; 14:465 – 473.
18. Christian Blum, Mateu Yábar Vallès and Maria J.Blesa. An Ant Colony Optimization Algorithm for DNA Sequencing by Hybridization. Computers & Operations Research 2008; 35:3620 – 3635.
19. Kamil Kwarciak, Marcin Radom, Piotr Formanowicz. A Multilevel Ant Colony Optimization Algorithm for Classical and Isothermic DNA Sequencing by Hybridization with Multiplicity Information Available. Computational Biology and Chemistry 2016; 61:109 – 120.
20. Ranjani Rani R and Ramyachitra. Multiple Sequence Alignment Using Multi-Objective Based Bacterial Foraging Optimization Algorithm. Biosystems. 2016; 150:177 – 189.
21. SoniyaLalwani, RajeshKumar and KusumDeep. Multi-Objective Two-Level Swarm Intelligence Approach for Multiple RNA Sequence-Structure Alignment. Swarm and Evolutionary Computation. 2017; 34:130 – 144.

22. Zne-Jung Lee, Shun-Feng Su, Chen-Chia Chuang and Kuan-Hung Liu. Genetic Algorithm with Ant Colony Optimization (GA-ACO) for Multiple Sequence Alignment. Applied Soft Computing. 2008; 8:55 – 78.
23. Jangam SR, Chakraborti N. A Novel Method for Alignment of Two Nucleic Acid Sequences using Ant Colony Optimization and Genetic Algorithms. Applied Soft Computing 2007; 7:1121 – 1130.
24. Thomas Kiel Rasmussen, Thiemo Krink. Improved Hidden Markov Model Training for Multiple Sequence Alignment by a Particle Swarm Optimization—Evolutionary Algorithm Hybrid. Biosystems. 2003; 72: 5 – 17.
25. Seyedali Mirjalili and AndrewLewis. The Whale Optimization Algorithm. Advances in Engineering Software. 2016; 95:51 – 67.
26. Seyedali Mirjalili:Moth-Flame Optimization Algorithm. A Novel Nature-Inspired Heuristic Paradigm. Knowledge-Based Systems. 2015; 89:228 – 249.
27. Tayarani NMH, Akbarzadeh MRT. Magnetic-Inspired Optimization Algorithms: Operators and Structures. Swarm and Evolutionary Computation. 2014; 19:82 – 101.
28. Kaveh A and Dadras A. A Novel Meta-Heuristic Optimization Algorithm: Thermal Exchange Optimization. Advances in Engineering Software 2017; 110:69 – 84.
29. Shahrzad Saremi, Seyedali Mirjalili and Andrew Lewis. Grasshopper Optimisation Algorithm: Theory and Application. Advances in Engineering Software 2017; 105:30 – 47.
30. Yousef Sharafi Mojtab Ahmadieh Khanesar and Mohammad Teshnehlab. COOA: Competitive Optimization Algorithm. Swarm and Evolutionary Computation 2016; 30:39 – 63.
31. Mehak Kohli and Sankalap Arora. Chaotic Grey Wolf Optimization Algorithm for Constrained Optimization Problems. Journal of Computational Design and Engineering 2017

Cite this article as:

Rajeshkumar J and Kousalya K. Applications of swarm based intelligence algorithm in pharmaceutical industry: A review. Int. Res. J. Pharm. 2017;8(11):24-27 http://dx.doi.org/10.7897/2230-8407.0811212

Source of support: Nil, Conflict of interest: None Declared