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An improved hybrid of particle swarm optimization and the gravitational search algorithm to produce a kinetic parameter estimation of aspartate biochemical pathways

Ahmad Muhaimin Ismail[a], Mohd Saberi Mohamad[c,g,h,*], Hairudin Abdul Majid[a], Khairul Hamimah Abas[b], Safaai Deris[c,g,h], Nazar Zaki[d], Siti Zaiton Mohd Hashim[e], Zuwairie Ibrahim[f], Muhammad Akmal Remli[a]

[a] Artificial Intelligence and Bioinformatics Research Group, Faculty of Computing, Universiti Teknologi Malaysia, Skudai, Johor, Malaysia
[b] Department of Control and Mechatronic Engineering, Faculty of Electrical Engineering, Universiti Teknologi Malaysia, Skudai, Johor, Malaysia,
[c] Faculty of Creative Technology and Heritage, Universiti Malaysia Kelantan, Bachok, Kelantan, Malaysia,
[d] College of Information Technology, United Arab Emirate University, Al Ain, United Arab Emirates
[e] Soft Computing Research Group, Faculty of Computing, Universiti Teknologi Malaysia, Skudai, Johor, Malaysia
[f] Faculty of Electrical and Electronic Engineering, Universiti Malaysia Pahang, Pekan, Pahang, Malaysia,
[g] Center For Computing and Informatics, Universiti Malaysia Kelantan, City Campus, Pengkalan Chepa, 16100 Kota Bharu, Kelantan, Malaysia
[h] Institute For Artificial Intelligence and Big Data, Universiti Malaysia Kelantan, City Campus, Pengkalan Chepa, 16100 Kota Bharu, Kelantan, Malaysia

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ABSTRACT

Mathematical modelling is fundamental to understand the dynamic behavior and regulation of the biochemical metabolisms and pathways that are found in biological systems. Pathways are used to describe complex processes that involve many parameters. It is important to have an accurate and complete set of parameters that describe the characteristics of a given model. However, measuring these parameters is typically difficult and even impossible in some cases. Furthermore, the experimental data are often incomplete and also suffer from experimental noise. These shortcomings make it challenging to identify the best-fit parameters that can represent the actual biological processes involved in biological systems. Computational approaches are required to estimate these parameters. The estimation is converted into multimodal optimization problems that require a global optimization algorithm that can avoid local solutions. These local solutions can lead to a bad fit when calibrating with a model. Although the model itself can potentially match a set of experimental data, a high-performance estimation algorithm is required to improve the quality of the solutions.

This paper describes an improved hybrid of particle swarm optimization and the gravitational search algorithm (IPSOGSA) to improve the efficiency of a global optimum (the best set of kinetic parameter values) search. The findings suggest that the proposed algorithm is capable of narrowing down the search space by exploiting the feasible solution areas. Hence, the proposed algorithm is able to achieve a near-optimal set of parameters at a fast convergence speed. The proposed algorithm was tested and evaluated based on two aspartate pathways that were obtained from the BioModels Database. The results show that the proposed algorithm outperformed other standard optimization algorithms in terms of accuracy and near-optimal kinetic parameter estimation. Nevertheless, the proposed algorithm is only expected to work well in small scale systems. In addition, the results of this study can be used to estimate kinetic parameter values in the stage of model selection for different experimental conditions.

* Corresponding author.
E-mail address: saberi@umk.edu.my (M.S. Mohamad).

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