

Integrated Evolutionary Algorithms for Michaelis-Menten Model Parameter Identification

Tuan, Ngo Anh、吳幸珍

E-mail: 360071@mail.dyu.edu.tw

ABSTRACT

The proposed research centers on the development a parameter identification method for Michaelis-Menten (M-M) model in Biological System by Evolution Algorithms. The inference of M-M model without knowledge of system parameters is a complicated task due to its nonlinearity and derivation. In this research, a parameter estimation algorithm is proposed for inferring M-M model parameters. This algorithm combines two parameter estimation methods: Genetic algorithm (GA) and Particle Swarm Optimization (PSO) in the strategy of parallel hybridization. The decoupling method is applied to predefine the parameter values in order to improve the accuracy estimation. The performance of the proposed algorithm is evaluated on two aspects: the parameter estimation error and structure identification accuracy. The proposed algorithm is applied to three different M-M models with simulated data. The results show that the proposed algorithm has lower estimation error and higher identification accuracy than the existing method although it processed in a wider search space (from 0 to 5,000).

Keywords : Parameter Identification, System Estimation, Evolutionary Algorithms

Table of Contents

中文摘要	iii Abstract
.....	iii Acknowledgements
.....	v Contents
.....	vi List of Figures
.....	viii List of Tables
.....	ix Acronyms
.....	x Chapter 1 - Introduction
.....	1 1.1. Motivation of research
.....	1 1.2. Thesis Outline
.....	2 Chapter 2 - Review of Evolutionary Algorithms (EAs)
.....	3 2.1. Introduction
Algorithm (GA).....	3 2.2. Genetic
.....	5 2.2.1. Initialization
.....	7 2.2.2. Selection
.....	7 2.2.3. Crossover
.....	10 2.2.4. Mutation
.....	11 2.2.5. Termination condition
.....	12 2.3. Particle Swarm Optimization (PSO)
Chapter 3 - Parameter Identification for M-M model by EAs	12
Systems	16 3.1. Michaelis-Menten-based Biological
Improvement for the proposed algorithm	16 3.2. Hybrid between GA and PSO for identification
.....	21 3.3.
.....	25 Chapter 4 - Simulations results
.....	27 4.1. System 1: 2 states M-M model with 18 parameters
.....	28 -vii- 4.2. System 2: 4 states M-M model with 8 parameters
states M-M model with 9 parameters	31 4.3. System 3: 4
Summary.....	33 4.4.
.....	35 Chapter 5 - Conclusion
.....	36 References
.....	37 -viii- List of Figures
procedure.....	Figure 2.1. Evolutionary Algorithm
.....	4 Figure 2.2. Diagram of Genetic Algorithm
.....	6 Figure 2.3. Selection probability for 10 individuals – population
Figure 2.4. Flowchart of the conventional PSO	8
pathway	15 Figure 3.1. M-M model 1: reversible
.....	17 Figure 3.2. M-M model 2: metabolic pathway with branch points
.....	19 Figure 3.3. M-M model 3: four-state kinetic model
.....	20 Figure 3.4. Process of

system identification	21	Figure 3.5. GA ' s individual data structure.....	24	
.....	24	Figure 3.6. PSO ' s particle data structure	24	
.....	24	Figure 3.7. Flowchart of parallel combination nGA – PSO algorithm	24	
26	Figure 4.1. Reversible pathway estimation in Case I	30	Figure 4.2. Reversible pathway estimation in Case II	31
.....	30	Figure 4.3. Metabolic pathway validation in the search space [0, 10]	31	
Figure 4.4. Metabolic pathway validation in the search space [0, 10.000]	32	Figure 4.5. Four-state kinetic estimation result in search space [0, 10]	33	
33	Figure 4.6. Four-state kinetic estimation result in search space [0, 50.000]	34	-ix- List of Tables Table 2.1. Fitness range for selection of a 10 individual-population	9
Table 3.1. Summary of parameters in reversible pathway	14	Table 2.2. Description of parameters meaning in PSO Algorithm	14	
.....	20	Table 3.2. Summary of parameters in metabolic pathway	20	
Summary of parameters in four-state kinetic model	20	Table 3.3. Table 4.1. Default parameter setting for GA and PSO	20	
.....	27	Table 4.2. The true and estimated kinetic parameter for reversible pathway	29	
Estimated parameter for metabolic pathway with branch points	32	Table 4.3. Table 4.4. The four-state kinetic model parameter validation	34	

REFERENCES

- [1]. P. K. Liu, F. S. Wang, Inverse problems of biological systems using multi-objective optimization, Journal of the Chinese Institute of Chemical Engineers 39; pp.339-406 (2008).
- [2]. D. Juki?, R. Scitovski, K. Sabo, A review of existence criteria for parameter estimation of the Michaelis – Menten regression model, Annali dell'Universita' di Ferrara. Vol.53, No.2, pp.281-291 (2007).
- [3]. C. Darwin, On the Origin of Species. London: John Murray, (1859), http://embryology.med.unsw.edu.au/pdf/Origin_of_Species.pdf
- [4]. J. T. Alander, On Optimal Population Size of Genetic Algorithms, IEEE, (1992).
- [5]. W. S. M. Elshamy, Using Artificial Intelligence Models in System Identification, (M.S thesis), (2007).
- [6]. A. H. Wright, Genetic algorithms for real parameter optimization, in: G. J. E. Rawlins (Ed.), Foundations of Genetic Algorithms I, Morgan Kaufmann, San Mateo, pp.205 – 218. (1991).
- [7]. K. Deep, M. Thakur, A new mutation operator for real coded genetic algorithms, Applied Mathematics and Computation N.193, pp.211-230 (2007).
- [8]. Z. Michalewicz, Genetic Algorithms + Data Structures = Evolution Programs, Springer-Verlag, New York (1992).
- [9]. J. Kennedy, R. C. Eberhart, and Y. Shi, Swarm Intelligence, ser. Evolutionary Computation Series. San Francisco: Morgan Kaufman (2001).
- [10]. J. Kennedy, The particle swarm: social adaptation of knowledge. Proceedings of IEEE International Conference on Evolutionary Computation. pp.303 – 308 (1997). -38- [11]. J. J. Liang, A. K. Qin, P. N. Suganthan and S. Baskar, Comprehensive Learning Particle Swarm Optimizer for Global Optimization of Multimodal Functions, IEEE Transaction on Evolutionary Computation, Vol.10, No.3, (Jun 2006).
- [12]. M. S. Voss and X. Feng, “ Emergent system identification using particle swarm optimization ” in Proceedings of SPIE: Complex Adaptive Structures, W. B. Spillman, Ed., vol. 4512, pp.193 – 202, (Oct. 2001), <http://citeseer.ist.psu.edu/voss01emergent.html>.
- [13]. M. Silva, Ferreira, E. N. Antonio, A. M. Tomas, C. Cordeiro, and A. P. Freire, Quantitative assessment of the Glyoxalase pathway in Leishmania infantum as a Therapeutic Target by Modeling and Computer and Simulation, The FEBS J., 270, 2388 (2005).
- [14]. B. Robertson and R. D. Astumian, Michaelis – Menten equation for an enzyme in an oscillating electric field, Biophysical Journal, V.58, pp.969-974 (1990).
- [15]. ode45 parameter solver for ordinary differential equations (ODEs) guideline: <http://www.weizmann.ac.il/matlab/techdoc/ref/ode45.html>
- [16]. N. M. Abbasi, Using Matlab ode45 to solve differential equations, (2012). http://12000.org/my_notes/matlab_ODE/document.pdf
- [17]. E. O. Voit, Computational Analysis of Biochemical Systems, p.91, Cambridge University Press, Cambridge, U.K. (2000).
- [18]. Rate equations for M-M model 2 (metabolic pathway with branch points) <http://jjj.biochem.sun.ac.za/database/silva/index.html>
- [19]. C. G. Moles, P. Mendes, and J. R. Banga, Parameter Estimation in Biochemical Pathways: A Comparison of Global Optimization Methods, Genome Research, 13(11), pp.2467-2474 (Nov 2003). <http://www.ncbi.nlm.nih.gov/pmc/articles/PMC403766/?tool=pubmed>
- [20]. T. P. Runarsson and X. Yao, Stochastic ranking for constrained evolutionary optimization, IEEE Trans Evol Comput, pp.284-294 (2000).