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HYBRID MULTI-OBJECTIVE OPTIMIZATION METHODS FOR *IN SILICO*
BIOCHEMICAL SYSTEM PRODUCTION

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**HYBRID MULTI-OBJECTIVE OPTIMIZATION METHODS FOR *IN SILICO*
BIOCHEMICAL SYSTEM PRODUCTION**

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A thesis submitted in fulfilment of the
requirements for the award of the degree of
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LIST OF ABBREVIATIONS

ABC	-	Artificial Bee Colony
BST	-	Biochemical Systems Theory
CA	-	Co-evolutionary Algorithm
ComCA	-	Competitive Co-evolutionary Algorithm
CooCA	-	Cooperative Co-evolutionary Algorithm
DE	-	Differential Evolution
EA	-	Evolutionary Algorithm
GA	-	Genetic Algorithm
GP	-	Genetic Programming
GMA	-	Generalized Mass Action
IP	-	Integer Programming
LP	-	Linear Programming
MCA	-	Metabolic Control Analysis
NSPABC	-	Newton Strength Pareto Artificial Bee Colony
NSPComGA	-	Newton Strength Pareto Competitive Genetic Algorithm
NSPCooGA	-	Newton Strength Pareto Cooperative Genetic Algorithm
NSPDE	-	Newton Strength Pareto Differential Evolution
NSPGA	-	Newton Strength Pareto Genetic Algorithm
NSPPSO	-	Newton Strength Pareto Particle Swarm Optimization
ODE	-	Ordinary Differential Equation
PSO	-	Particle Swarm Optimization
SI	-	Swarm Intelligence

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ABSTRACT

In silico approach for multi-objective constraint optimization of biochemical system production is a computational process that aims to improve the biochemical system production. Besides the biochemical system production, the component concentrations involved also need to be considered. The optimization process involves the process of altering and ne-tuning of components in the biochemical system. The optimization process becomes complicated and difficult when a large biochemical system with many components is involved. In addition, the optimization process involves multi-objective problem which maximizes the biochemical system production and at the same time minimizing the total of component concentrations involved. Beside that, several constraints of biochemical system which are the steady state condition and component concentration constraint also contribute to the complication and difficulty in optimization process. This study aims to design and develop an optimization method that efficiently and effectively maximizes the biochemical system production and minimizes the total component concentrations involved simultaneously. To achieve this goal, an improved method was proposed known as Advance Newton Strength Pareto Cooperative Genetic Algorithm. The proposed method combined Newton method, Strength Pareto approach, Cooperative Coevolutionary Algorithm (CooCA) and Genetic Algorithm (GA). The use of Newton method is for dealing with biochemical system, Strength Pareto approach is for the multi-objective problem, GA is to maximize the production, and CooCA is to minimize the total component concentrations involved. The effectiveness of the proposed method was evaluated using two benchmark case studies. The experimental results showed that the proposed method was able to generate the highest results compared to other studies. Statistical validation confirmed that the proposed method is competent in producing good results in terms of maximizing the biochemical system production and minimizing the total of component concentrations involved. In conclusion, this study has presented an improved optimization method, capable to simultaneously maximize the biochemical system production and minimize the total of component concentrations involved.

ABSTRAK

Pendekatan *in silico* untuk pengoptimuman kekangan pelbagai-objektif dalam pengeluaran sistem biokimia ialah proses komputeran yang bermatlamat untuk meningkatkan pengeluaran sistem biokimia. Selain daripada pengeluaran sistem biokimia, jumlah kepekatan biokimia yang terlibat juga perlu diambil kira. Proses pengoptimuman melibatkan proses mengubah dan menukar komponen di dalam sistem biokimia. Proses pengoptimuman menjadi lebih rumit dan sukar apabila melibatkan sistem biokimia yang besar dan mengandungi banyak komponen. Tambahan pula, proses pengoptimuman melibatkan masalah pelbagai-objektif seperti memaksimumkan pengeluaran sistem biokimia dan pada masa yang sama meminimumkan jumlah kepekatan komponen yang terlibat. Selain itu, beberapa kekangan sistem biokimia seperti keadaan bentuk tetap dan kekangan kepekatan komponen juga menyebabkan proses pengoptimuman menjadi semakin rumit dan sukar. Kajian ini bertujuan untuk mereka bentuk dan membangunkan satu kaedah pengoptimuman yang cekap dan berkesan di mana ia mampu memaksimumkan pengeluaran sistem biokimia dan pada masa yang sama mampu meminimumkan jumlah kepekatan komponen yang terlibat. Bagi mencapai tujuan ini, satu kaedah lanjutan telah dicadangkan dan dikenali sebagai Algoritma Lanjutan Newton Kekuatan Pareto Kerjasama Genetik. Kaedah yang dicadangkan menggabungkan kaedah Newton, pendekatan Kekuatan Pareto, Algoritma Evolusi Bekerjasama (CooCA) dan Algoritma Genetik (GA). Kegunaan kaedah Newton adalah untuk berurusan dengan sistem biokimia, pendekatan Kekuatan Pareto adalah untuk masalah pelbagai-objektif, GA adalah untuk memaksimumkan pengeluaran sistem biokimia dan CooCA adalah untuk meminimumkan jumlah kepekatan komponen yang terlibat. Keberkesanannya yang dicadangkan telah dinilai dengan menggunakan dua piawaian kajian kes. Hasil eksperimen menunjukkan kaedah yang dicadangkan mampu menjana keputusan yang lebih tinggi berbanding kajian yang lain. Pengesahan statistik mengesahkan bahawa kaedah yang dicadangkan adalah memuaskan dan menghasilkan keputusan yang baik daripada segi memaksimumkan pengeluaran sistem biokimia dan meminimumkan jumlah kepekatan komponen yang terlibat. Kesimpulannya, kajian ini telah menunjukkan satu kaedah pengoptimuman lanjutan yang mampu memaksimumkan pengeluaran sistem biokimia dan pada masa yang sama mampu meminimumkan jumlah kepekatan komponen yang terlibat.

REFERENCES

- Ab Wahab, M. N., Nefti-Meziani, S. and Atyabi, A. (2015). A comprehensive review of swarm optimization algorithms. *PloS one*. 10(5), e0122827. doi:10.1371/journal.pone.0122827.
- Abbass, H. A. and Sarker, R. (2011). The Pareto Differential Evolution Algorithm. *International Journal on Artificial Intelligence Tools*. 11(4), 531–552.
- Adiwijaya, B. S., Barton, P. I. and Tidor, B. (2006). Biological network design strategies: discovery through dynamic optimization. *Molecular BioSystems*. 2(12), 650–659.
- Akay, B. (2012). Synchronous and asynchronous Pareto-based multi-objective Artificial Bee Colony algorithms. *Journal of Global Optimization*. 57(2), 415–445.
- Alba, E. and Luque, G. (2007). Designing a Parallel GA for Large Instances of the Workforce Planning Problem. In *Seventh International Conference on Intelligent Systems Design and Applications (ISDA 2007)*. oct. IEEE, 823–830.
- AlRashidi, M. and El-Hawary, M. (2009). A Survey of Particle Swarm Optimization Applications in Electric Power Systems. *IEEE Transactions on Evolutionary Computation*. 13(4), 913–918.
- Amat, S. and Busquier, S. (2003). On a higher order Secant method. *Applied Mathematics and Computation*. 141(2-3), 321–329.
- Argyros, I. K. (2005). New sufficient convergence conditions for the secant method. *Czechoslovak Mathematical Journal*. 55(1), 175–187.
- Axelrod, R. (2006). *The Evolution of Cooperation (Revised ed.)*. New York, USA: Basic Books.
- Babaei, M. (2013). A general approach to approximate solutions of nonlinear differential equations using particle swarm optimization. *Applied Soft Computing*. 13(7), 3354–3365.
- Bachrathy, D. and Stepan, G. (2012). Bisection method in higher dimensions and the efficiency number. *Periodica Polytechnica Mechanical Engineering*. 56(2), 81–86.

- Back, T. (1996). *Evolutionary Algorithms in Theory and Practice*. United Kingdom: Oxford University Press.
- Bailey, J. E. (1998). Mathematical modeling and analysis in biochemical engineering: past accomplishments and future opportunities. *Biotechnology Progress*. 14(1), 8–20.
- Balsa-Canto, E., Banga, J. R., Egea, J. A., Fernandez-Villaverde, A. and de Hijas-Liste, G. M. (2012). Global optimization in systems biology: stochastic methods and their applications. *Advances in experimental medicine and biology*. 736, 409–24.
- Banga, J. R. (2008). Optimization in computational systems biology. *BMC Systems Biology*. 47(2).
- Barr, R. S., Golden, B. L., Kelly, J. P., Resende, M. G. C. and Stewart, W. R. (2001). Designing and Reporting on Computational Experiments with Heuristic Methods. In *Proceedings of International Conference on Metaheuristics for Optimization*. 1–17.
- Bartz-Beielstein, T., Limbourg, P., Melmen, J., Schmitt, K., Parsopoulos, K. and Vrahatis, M. (2003). Particle swarm optimizers for Pareto optimization with enhanced archiving techniques. In *The 2003 Congress on Evolutionary Computation, 2003. CEC '03.*, vol. 3. IEEE, 1780–1787.
- Benfenati, E., Gini, G., Hoffmann, S. and Luttik, R. (2010). Comparing In Vivo, In Vitro and In Silico Methods and Integrated Strategies for Chemical Assessment: Problems and Prospects. *Alternatives to laboratory animals*. 38(2), 153–166.
- Beni, G. and Wang, J. (1993). Swarm Intelligence in Cellular Robotic Systems. In Dario, P., Sandini, G. and Aebischer, P. (Eds.) *Robots and Biological Systems: Towards a New Bionics?* SE - 38. (pp. 703–712). *NATO ASI Series*, vol. 102. Springer Berlin Heidelberg.
- Berrocal-Plaza, V., Vega-Rodriguez, M. A., Sanchez-Perez, J. M. and Gomez-Pulido, J. A. (2012). Solving the Location Areas problem with Strength Pareto Evolutionary Algorithm. In *2012 IEEE 13th International Symposium on Computational Intelligence and Informatics (CINTI)*. nov. IEEE, 49–54.
- Birgin, E. G., Krejić, N. and Martínez, J. M. (2003). Globally Convergent Inexact Quasi-Newton Methods for Solving Nonlinear Systems. *Numerical Algorithms*. 32(2-4), 249–260.
- Boussaïd, I., Lepagnot, J. and Siarry, P. (2013). A survey on optimization metaheuristics. *Information Sciences*. 237, 82–117.

- Boyd, S., Kim, S.-J., Vandenberghe, L. and Hassibi, A. (2007). A tutorial on geometric programming. *Optimization and engineering*. 8(1), 67–127.
- Bradley, S. P., Hax, A. C. and Magnanti, T. L. (1977). *Applied Mathematical Programming*. Reading, MA: Addison-Wesley.
- Chellapandi, P., Sivaramakrishnan, S. and Viswanathan, M. B. (2010). Systems biotechnology: An emerging trend in metabolic engineering of industrial microorganisms. *Journal of Computer Science & Systems Biology*. 3(2), 43–49.
- Chong, C. K., Mohamad, M. S., Deris, S., Shamsir, M. S., Chai, L. E. and Choon, Y. W. (2014). Parameter Estimation by Using an Improved Bee Memory Differential Evolution Algorithm (IBMDE) to Simulate Biochemical Pathways. *Current Bioinformatics*. 9(1), 65 – 75.
- Cruz-Ramírez, M., Hervás-Martínez, C., Jurado-Expósito, M. and López-Granados, F. (2012). A multi-objective neural network based method for cover crop identification from remote sensed data. *Expert Systems with Applications*. 39(11), 10038–10048.
- Darwin, C. (2007a). *Fertilisation of Orchids. (reprint)*. New York, USA: Cosimo, Inc.
- Darwin, C. (2007b). *On the Origin of Species: By Means of Natural Selection Or the Preservation of Favored Races in the Struggle for Life. (reprint)*. New York, USA: Cosimo, Inc.
- Das, S., Abraham, A. and Konar, A. (2008). Particle Swarm Optimization and Differential Evolution Algorithms: Technical Analysis, Applications and Hybridization Perspectives. *Studies in Computational Intelligence Volume*. 116, 1–38.
- de Souza, L., Haida, H., Thévenin, D., Seidel-Morgenstern, A. and Janiga, G. (2013). Model selection and parameter estimation for chemical reactions using global model structure. *Computers & Chemical Engineering*. 58, 269–277.
- Dehghan, M. and Hajarian, M. (2012). Fourthorder variants of Newton's method without second derivatives for solving nonlinear equations. *Engineering Computations*. 29(4), 356–365.
- Díez, P. (2003). A note on the convergence of the secant method for simple and multiple roots. *Applied Mathematics Letters*. 16(8), 1211–1215.
- Dorigo, M., Birattari, M. and Stutzle, T. (2006). Ant colony optimization. *IEEE Computational Intelligence Magazine*. 1(4), 28–39.
- Durillo, J. J. and Nebro, A. J. (2011). jMetal: A Java framework for multi-objective optimization. *Advances in Engineering Software*. 42(10), 760–771.
- El-Emary, I. M. M. and El-Kareem, M. M. A. (2008). Towards Using Genetic

- Algorithm for Solving Nonlinear Equation Systems. *World Applied Sciences Journal*. 5(3), 282–289.
- Elbeltagi, E., Hegazy, T. and Grierson, D. (2005). Comparison among five evolutionary-based optimization algorithms. *Advanced Engineering Informatics*. 19(1), 43–53.
- Elhossini, A., Areibi, S. and Dony, R. (2010). Strength Pareto particle swarm optimization and hybrid EA-PSO for multi-objective optimization. *Evolutionary computation*. 18(1), 127–56.
- Fell, D. (2005). Metabolic Control Analysis. In Alberghina, L. and Westerhoff, H. V. (Eds.) *Systems Biology SE - 80*. (pp. 69–80). *Topics in Current Genetics*, vol. 13. Springer Berlin Heidelberg.
- Fernández, M. Á. and Moubarac, M. (2005). A Newton method using exact jacobians for solving fluidstructure coupling. *Computers & Structures*. 83(2-3), 127–142.
- Floreano, D. and Nolfi, S. (1997). Adaptive Behavior in Competing Co-Evolving Species. In Husband, P. and Harvey, I. (Eds.) *In Proceedings of the Fourth European Conference on Artificial Life*. (pp. 378–387). Cambridge, MA: MIT Press.
- Fogel, L. J. (1962). Autonomous Automata. *Industrial Research*. 4(2), 14–19.
- Fourer, R., Gay, D. M. and Kernighan, B. W. (1990). A Modeling Language for Mathematical Programming. *Management Science*. 36(519-554).
- Galazzo, J. L. and Bailey, J. E. (1990). Fermentation pathway kinetics and metabolic flux control in suspended and immobilized *Saccharomyces cerevisiae*. *Enzyme and Microbial Technology*. 12(3), 162–172.
- Gong, W. and Cai, Z. (2008). A multiobjective differential evolution algorithm for constrained optimization. In *2008 IEEE Congress on Evolutionary Computation (IEEE World Congress on Computational Intelligence)*. jun. IEEE, 181–188.
- Grimaccia, F., Mussetta, M., Pirinoli, P. and Zich, R. E. (2006). Genetical Swarm Optimization (GSO): a class of Population-based Algorithms for Antenna Design. In *2006 First International Conference on Communications and Electronics*. oct. IEEE, 467–471.
- Grosan, C. and Abraham, A. (2008). A New Approach for Solving Nonlinear Equations Systems. *Systems, Man and Cybernetics, Part A: Systems and Humans, IEEE Transactions on*. 38(3), 698–714.
- Gutierrez, C., Gutierrez, F. and Rivara, M.-C. (2007). Complexity of the bisection method. *Theoretical Computer Science*. 382(2), 131–138.

- Hernández, M. and Rubio, M. (2002). The Secant method for nondifferentiable operators. *Applied Mathematics Letters*. 15(4), 395–399.
- Holland, J. H. (1975). *Adaptation in natural and artificial systems*. University of Michigan Press.
- Hood, L. and Perlmutter, R. M. (2004). The impact of systems approaches on biological problems in drug discovery. *Nature Biotechnology*. 22(10), 1215–1217.
- Ismail, M. A., Deris, S., Mohamad, M. S. and Abdullah, A. (2014). A Hybrid of Newton Method and Genetic Algorithm for Constrained Optimization method of the Production of Metabolic Pathway. *Life Science Journal*. 11(9s), 409–414.
- Ismail, M. A., Deris, S., Mohamad, M. S. and Abdullah, A. (2015). A newton cooperative genetic algorithm method for in silico optimization of metabolic pathway production. *PloS one*. 10(5), e0126199. doi:10.1371/journal.pone.0126199.
- Jalilzadeh, S., Darabian, M. and Azari, M. (2013). Power System Stability Improvement via TCSC Controller Employing a Multi-objective Strength Pareto Evolutionary Algorithm Approach. *Journal of Operation and Automation in Power Engineering*. 1(1), 33–42.
- Jeniefer Kavetha M. (2013). Coevolution Evolutionary Algorithm: A Survey. *International Journal of Advanced Research in Computer Science*. 4(4), 324–328.
- Jiang, L. L., Maskell, D. L. and Patra, J. C. (2013). Parameter estimation of solar cells and modules using an improved adaptive differential evolution algorithm. *Applied Energy*. 112, 185–193. ISSN 03062619. doi:10.1016/j.apenergy.2013.06.004. Retrievable at <http://www.sciencedirect.com/science/article/pii/S0306261913005114>.
- Jiang, S. and Yang, S. (2015). A Fast Strength Pareto Evolutionary Algorithm Incorporating Predefined Preference Information. In *Proceedings of the 15th UK Workshop on Computational Intelligence*.
- Jin, J. H. and Lee, J. (2005). In silico analysis of lactic acid secretion metabolism through the top-down approach: Effect of grouping in enzyme kinetics. *Biotechnology and Bioprocess Engineering*. 10(5), 462–469.
- Kacser, H. and Burns, J. A. (1973). The control of flux. *Symposia of the Society for Experimental Biology*. 27, 65–104.
- Karaboga, D. and Basturk, B. (2007). A powerful and efficient algorithm for numerical function optimization: artificial bee colony (ABC) algorithm. *Journal of Global Optimization*. 39(3), 459–471.

- Kennedy, J. and Eberhart, R. (1995). Particle Swarm Optimization. In *Proceedings of IEEE International Conference on Neural Networks*, vol. 4. 1942–1948.
- Kolias, C., Kambourakis, G. and Maragoudakis, M. (2011). Swarm intelligence in intrusion detection: A survey. *Computers & Security*. 30(8), 625–642.
- Konak, A., Coit, D. W. and Smith, A. E. (2006). Multi-objective optimization using genetic algorithms: A tutorial. *Reliability Engineering & System Safety*. 91(9), 992–1007.
- Koza, J. R., Andre, D., Bennett, F. H. and Keane, M. A. (1999). *Genetic Programming III: Darwinian Invention & Problem Solving*. San Francisco, CA, USA: Morgan Kaufmann Publishers Inc.
- Ku, C.-Y., Yeih, W. and Liu, C.-S. (2010). Solving Non-Linear Algebraic Equations by a Scalar Newton-homotopy Continuation Method. *International Journal of Nonlinear Sciences and Numerical Simulation*. 11(6), 435–450.
- Kulturel-Konak, S., Konak, A. and Coit, D. W. (2007). Multiobjective Metaheuristic Approaches to Reliability Optimization. In Levitin, G. (Ed.) *Computational Intelligence in Reliability Engineering*. (pp. 37–62). Berlin Heidelberg: Springer Berlin Heidelberg.
- Lages, N. F., Cordeiro, C., Sousa Silva, M., Ponces Freire, A. and Ferreira, A. E. N. (2012). Optimization of time-course experiments for kinetic model discrimination. *PloS one*. 7(3), e32749.
- Liiving, T., Baker, S. M. and Junker, B. H. (2011). Modeling in Systems Biology. In Koch, I. and Schreiber, F. (Eds.) *Computational Biology*. (pp. 19–36). vol. 16. London: Springer-Verlag.
- Link, H., Vera, J., Weuster-Botz, D., Darias, N. T. and Franco-Lara, E. (2008). Multi-objective steady state optimization of biochemical reaction networks using a constrained genetic algorithm. *Computers and Chemical Engineering*. 32(8), 1707–1713.
- Liu, C.-S. (2009). A modified Newton method for solving non-linear algebraic equations. *Journal of Marine Science and Technology*. 17(3), 238–247.
- Liu, C.-S. and Atluri, S. N. (2008). A novel time integration method for solving a large system of non-linear algebraic equations. *Computer Modeling in Engineering and Sciences*. 31(2), 71–83.
- Liu, H., Zhou, Y. and Li, Y. (2011). A Quasi-Newton Population Migration Algorithm for Solving Systems of Nonlinear Equations. *Journal of Computers*. 6(1), 36–42.
- Luo, Y.-Z., Tang, G.-J. and Zhou, L.-N. (2008). Hybrid approach for solving systems

- of nonlinear equations using chaos optimization and quasi-Newton method. *Applied Soft Computing*. 8(2), 1068–1073.
- Mahant, M., Choudhary, B., Kesharwani, A. and Rathore, K. S. (2012). A Profound Survey on Swarm Intelligence. *International Journal of Advanced Computer Research*. 2, 31–36.
- Mariano, A. P., Costa, C. B. B., de Angelis, D. d. F., Filho, F. M., Atala, D. I. P., Maciel, M. R. W. and Filho, R. M. (2009). Optimization strategies based on sequential quadratic programming applied for a fermentation process for butanol production. *Applied Biochemistry and Biotechnology*. 159(2), 366–381.
- Mariano, A. P., Costa, C. B. B., de Angelis, D. d. F., Filho, F. M., Atala, D. I. P., Maciel, M. R. W. and Filho, R. M. (2010). Optimisation of a fermentation process for butanol production by particle swarm optimisation (PSO). *Journal of Chemical Technology and Biotechnology*. 85(7), 934–949.
- Marin-Sanguino, A. and Torres, N. V. (2000). Optimization of tryptophan production in bacteria. Design of a strategy for genetic manipulation of the tryptophan operon for tryptophan flux maximization. *Biotechnology Progress*. 16(2), 133–145.
- Marin-Sanguino, A. and Torres, N. V. (2003). Optimization of biochemical systems by linear programming and general mass action model representations. *Mathematical Biosciences*. 184(2), 187–200.
- Marin-Sanguino, A., Voit, E. O., Gonzalez-Alcon, C. and Torres, N. V. (2007). Optimization of biotechnological systems through geometric programming. *Theoretical Biology and Medical Modelling*. 4, 38–54.
- Maynard-Smith, J. (1982). *Evolution and the Theory of Games*. Cambridge, UK: Univ. Press.
- Metivier, L., Brossier, R., Virieux, J. and Operto, S. (2013). Full Waveform Inversion and the Truncated Newton Method. *SIAM Journal on Scientific Computing*. 35(2), B401–B437.
- Mezura-Montes, E., Reyes-Sierra, M. and Coello, C. A. C. (2008). Multi-objective optimization using differential evolution: a survey of the state-of-the-art. In Chakraborty, U. K. (Ed.) *Advances in differential evolution*. (pp. 173–196). Springer Berlin Heidelberg.
- Michalewicz, Z. (1996). *Genetic Algorithms + Data Structures = Evolution Programs*. Berlin, Heidelberg: Springer-Verlag.
- Mo, Y., Liu, H. and Wang, Q. (2009). Conjugate direction particle swarm optimization solving systems of nonlinear equations. *Computers & Mathematics*

with Applications. 57(11-12), 1877–1882.

- Nam, J. W., Hana, K. H., Yoon, E. S., Shin, D. I., Jin, J. H., Lee, D. H., Lee, S. Y. and Lee, J. (2004). In silico analysis of lactate producing metabolic network in *Lactococcus lactis*. *Enzyme and Microbial Technology*. 35, 654–662.
- Ngatchou, P., Zarei, A. and El-Sharkawi, A. (2005). Pareto Multi Objective Optimization. In *Proceedings of the 13th International Conference on, Intelligent Systems Application to Power Systems*. IEEE, 84–91. doi:10.1109/ISAP.2005.1599245.
- Omkar, S., Senthilnath, J., Khandelwal, R., Narayana Naik, G. and Gopalakrishnan, S. (2011). Artificial Bee Colony (ABC) for multi-objective design optimization of composite structures. *Applied Soft Computing*. 11(1), 489–499.
- Palsson, B. (2000). The challenges of in silico biology. *Nature Biotechnology*. 18(11).
- Passino, K. (2002). Biomimicry of bacterial foraging for distributed optimization and control. *IEEE Control Systems Magazine*. 22(3), 52–67.
- Patil, M., Irani, J. and Jagtap, V. (2014). Survey Of Different Swarm Intelligence Algorithms. *International Journal of Advance Engineering and Research Development*. 1(12), 2348 – 4470.
- Pendharkar, P. C. (2008). A threshold varying bisection method for cost sensitive learning in neural networks. *Expert Systems with Applications*. 34(2), 1456–1464.
- Planes, F. J. and Beasley, J. E. (2008). A critical examination of stoichiometric and path-finding approaches to metabolic pathways. *Briefings in Bioinformatics*. 9(5), 422–436.
- Polisetty, P. K., Gatzke, E. P. and Voit, E. O. (2008).. Yield optimization of regulated metabolic systems using deterministic branch-and-reduce methods. *Biotechnology and Bioengineering*. 99(5), 1154–1169.
- Potter, M. A. and De Jong, K. A. (2000). Cooperative Coevolution: An Architecture for Evolving Coadapted Subcomponents. *Evolutionary Computation*. 8(1), 1–29.
- Prajapati, B. S. and Srivastava, L. (2012). Multi-Objective Reactive Power Optimization Using Artificial Bee Colony Algorithm. *International Journal of Engineering and Innovative Technology*. 2(1), 126–131.
- Price, N. D., Reed, J. L., Papin, J. A., Famili, I. and Palsson, B. O. (2003). Analysis of Metabolic Capabilities Using Singular Value Decomposition of Extreme Pathway Matrices. *Biophysical Journal*. 84(2), 794–804.
- Qin, H., Zhou, J., Li, Y., Liu, L. and Lu, Y. (2008). Enhanced Strength Pareto Differential Evolution (ESPDE): An Extension of Differential Evolution for Multi-

- objective Optimization. In *2008 Fourth International Conference on Natural Computation*, vol. 1. IEEE, 191–196.
- Raul Curto, Albert Sorribas and Cascante, M. (1995). Comparative Characterization of the Fermentation Pathway of *Saccharomyces cerevisiae* Using Biochemical Systems Theory and Metabolic Control Analysis: Model Definition and Nomenclature. *Mathematical Biosciences*. 130(1), 25–50.
- Rechenberg, I. (1973). *Evolutionsstrategie: Optimierung technischer Systeme nach Prinzipien der biologischen Evolution*. Stuttgart, Germany: Frommann-Holzboog Verlag.
- Reyes-sierra, M. and Coello, C. A. C. (2006). Multi-Objective particle swarm optimizers: A survey of the state-of-the-art. *International Journal Of Computational Intelligence Research*. 2(3), 287–308.
- Rivara, M.-C. (2009). Lepp-bisection algorithms, applications and mathematical properties. *Applied Numerical Mathematics*. 59(9), 2218–2235.
- Rodriguez-Acosta, F., Regalado, C. M. and Torres, N. V. (1999). Non-linear optimization of biotechnological processes by stochastic algorithms: Application to the maximization of the production rate of ethanol, glycerol and carbohydrates by *Saccharomyces cerevisiae*. *Journal of Biotechnology*. 65(1), 15–28.
- Sahoo, N., Ganguly, S. and Das, D. (2012). Multi-objective planning of electrical distribution systems incorporating sectionalizing switches and tie-lines using particle swarm optimization. *Swarm and Evolutionary Computation*. 3, 15–32.
- Sakamoto, N. (2003). Characterization of the transit and transition times for a pathway unit of MichaelisMenten mechanism. *Biochimica et Biophysica Acta (BBA) - General Subjects*. 1623(1), 6–12.
- Salleh, A., Mohamad, M., Deris, S. and Illias, R. (2013). Identifying Minimal Genomes and Essential Genes in Metabolic Model Using Flux Balance Analysis. In Selamat, A., Nguyen, N. and Haron, H. (Eds.) *Intelligent Information and Database Systems SE - 43*. (pp. 414–423). *Lecture Notes in Computer Science*, vol. 7802. Springer Berlin Heidelberg.
- Sánchez, L. N. G. (2015). Parallel Genetic Algorithms on a GPU to Solve the Travelling Salesman Problem. *Revista en Ingeniería y Tecnología, UAZ*. 8(2), 79–85.
- Savageau, M. A. (1976). *Biochemical systems analysis: a study of function and design in molecular biology*. Reading, Massachusetts: AddisonWesley.
- Schwacke, J. H. and Voit, E. O. (2005). Computation and analysis of time-dependent

- sensitivities in Generalized Mass Action systems. *Journal of theoretical biology*. 236(1), 21–38.
- Sendín, O. H., Vera, J., Torres, N. V. and Banga, J. R. (2007). Model based optimization of biochemical systems using multiple objectives: a comparison of several solution strategies. *Mathematical and Computer Modelling of Dynamical Systems*. 12(5), 469–487.
- Sharma, J. R., Guha, R. K. and Sharma, R. (2012). An efficient fourth order weighted-Newton method for systems of nonlinear equations. *Numerical Algorithms*. 62(2), 307–323.
- Sheng, W., Liu, Y., Meng, X. and Zhang, T. (2012). An Improved Strength Pareto Evolutionary Algorithm 2 with application to the optimization of distributed generations. *Computers & Mathematics with Applications*. 64(5), 944–955.
- Singh, S. and Gupta, D. K. (2014). A New Sixth Order Method for Nonlinear Equations in R. *The Scientific World Journal*. 2014.
- Sorribasa, A., Pozo, C., Vilaprinyo, E., Guillén-Gosálbez, G., Jiménez, L. and Alves, R. (2010). Optimization and evolution in metabolic pathways: Global optimization techniques in Generalized Mass Action models. *Journal of Biotechnology*. 149(3), 141–153.
- Srinath, S. and Gunawan, R. (2010). Parameter identifiability of power-law biochemical system models. *Journal of Biotechnology*. 149(3), 132–140.
- Steuer, R. and Junker, B. H. (2009). *Computational Models of Metabolism: Stability and Regulation in Metabolic Networks*. New Jersey: John Wiley & Sons.
- Storm, R. and Price, K. (1997). Differential Evolution A Simple and Efficient Heuristic for global Optimization over Continuous Spaces. *Journal of Global Optimization*. 11(4), 341–359.
- Sun, J., Garibaldi, J. M. and Hodgman, C. (2012). Parameter estimation using meta-heuristics in systems biology: a comprehensive review. *IEEE/ACM transactions on computational biology and bioinformatics / IEEE, ACM*. 9(1), 185–202.
- Tashkova, K., Korošec, P., Silc, J., Todorovski, L. and Džeroski, S. (2011). Parameter estimation with bio-inspired meta-heuristic optimization: modeling the dynamics of endocytosis. *BMC systems biology*. 5(1), 159.
- Uchibe, E. and Asada, M. (2006). Incremental Coevolution With Competitive and Cooperative Tasks in a Multirobot Environment. *Proceedings of the IEEE*. 94(7), 1412–1424.

- Ujevic, N. (2006). A method for solving nonlinear equations. *Applied Mathematics and Computation*. 174(2), 1416–1426.
- Vanitha, S. and Padma, T. (2014). A Survey on Swarm Intelligence Algorithms. *International Journal of Computer Science and Mobile Computing*. 3(5), 994–998.
- Vera, J., Gonzalez-Alcon, C., Marin-Sanguino, A. and Torres, N. (2010). Optimization of biochemical systems through mathematical programming: Methods and applications. *Computers & Operations Research*. 37(8), 1427–1438.
- Vesterstrom, J. and Thomsen, R. (2004). A comparative study of differential evolution, particle swarm optimization, and evolutionary algorithms on numerical benchmark problems. In *Proceedings of the 2004 Congress on Evolutionary Computation (IEEE Cat. No.04TH8753)*, vol. 2. IEEE. ISBN 0-7803-8515-2, 1980–1987. doi:10.1109/CEC.2004.1331139. Retrievable at <http://ieeexplore.ieee.org/articleDetails.jsp?arnumber=1331139>.
- Voit, E. O. (2013). Biochemical Systems Theory: A Review. *ISRN Biomathematics*. 2013.
- Wahid, A., Gao, X. and Andreae, P. (2015). Multi-Objective Clustering Ensemble for High-Dimensional Data based on Strength Pareto Evolutionary Algorithm (SPEA-II). In *IEEE International Conference on Datasience and Advance Analytics (DSAA)*.
- Xie, Q., Li, S. and Yang, G. (2008). Studies on Fast Pareto Genetic Algorithm Based on Fast Fitness Identification and External Population Updating Scheme. In Yan, X.-T., Ion, W. J. and Eynard, B. (Eds.) *Global Design to Gain a Competitive Edge*. (pp. 539–548). Springer London.
- Xiu, Z.-L., Zeng, A.-P. and Deckwer, W.-D. (1997). Model analysis concerning the effects of growth rate and intracellular tryptophan level on the stability and dynamics of tryptophan biosynthesis in bacteria. *Journal of Biotechnology*. 58(2), 125–140.
- Xu, G. (2012). Bi-objective optimization of biochemical systems by linear programming. *Applied Mathematics and Computation*. 218(14), 7562–7572.
- Xu, G. (2013). Steady-state optimization of biochemical systems through geometric programming. *European Journal of Operational Reseach*. 225(1), 12–20.
- Xu, G., Shao, C. and Xiu, Z. (2008). A Modified Iterative IOM Approach for Optimization of Biochemical Systems. *Computers and Chemical Engineering*. 32(7), 1546–1568.
- Yang, X.-S. (2009). Firefly algorithms for multimodal optimization. In Watanabe, O. and Zeugmann, T. (Eds.) *Stochastic Algorithms: Foundations And Applications*.

- Sapporo, Japan: Springer, 178–178.
- Zhang, J., Xiea, L. and Wang, S. (2006). Particle swarm for the dynamic optimization of biochemical processes. *Computer Aided Chemical Engineering*. 21, 497–502.
- Zhang, Y. H. P., Ye, X. and Wang, Y. (2008). Biofuels Production by Cell-Free Synthetic Enzymatic Technology. In Richter, F. W. (Ed.) *Biotechnology: Research, Technology and Applications*. (pp. 143–157). Nova Science Publisher.
- Zhao, M., Liu, R., Li, W. and Liu, H. (2010). Multi-objective Optimization Based Differential Evolution Constrained Optimization Algorithm. In *2010 Second WRI Global Congress on Intelligent Systems*, vol. 1. dec. IEEE. ISBN 978-1-4244-9247-3, 320–326. doi:10.1109/GCIS.2010.50.
- Zhou, A., Qu, B.-Y., Li, H., Zhao, S.-Z., Suganthan, P. N. and Zhang, Q. (2011). Multiobjective evolutionary algorithms: A survey of the state of the art. *Swarm and Evolutionary Computation*. 1(1), 32–49.