ENHANCED SEGMENT PARTICLE SWARM OPTIMIZATION FOR LARGE-SCALE KINETIC PARAMETER ESTIMATION OF *ESCHERICHIA COLI* NETWORK MODEL

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SUPERVISOR'S DECLARATION

I hereby declare that I have checked this thesis and in my opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Doctor of Philosophy.

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I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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ABSTRAK

Yang pembangunan model metabolik berskala besar bagi *Escherichia Coli (E. Coli)* sangat diperlukan oleh industri untuk membantu mengenalpasti penyelesaian yang berpotensi yang boleh dilaksanakan bagi meningkatkan pengeluaran sesuatu produk. Namun begitu, anggaran parameter kinetik yang berskala besar masih tidak dilaksanakan di dalam model kinetik yang melibatkan laluan utama metabolik *E-coli* di samping kekurangan keputusan ketepatan anggaran dilaporkan di dalam kajian terdahulu. Oleh yang demikian, penyelidikan ini bertujuan untuk menganggar nilai kinetik berskala besar bagi laluan utama metabolik *E-coli*. Penyelidikan ini melibatkan adaptasi dan cadangan pelbagai teknik seperti Analisis Sensitiviti Setempat, Segmentasi Pengoptimuman Kumpulan Zarah (Se-PSO), Peningkatan Segmentasi Pengoptimuman Kumpulan Zarah (ESe-PSO) bagi menganggar nilai parameter kinetik tersebut. Di peringkat awal kajian, algoritma Pengoptimuman Kumpulan Zarah (Particle Swarm Optimization-PSO) di gunakan untuk pencarian hasil optimum secara global berdasarkan pergerakan zarah secara rawak (tidak teratur) di ruang carian tertentu. Seterusnya, Se-PSO dibangunkan dengan cara melaksanakan proses segmentasi kepada zarah bagi mendapatkan nilai optimum setempat sebelum proses PSO dilaksanakan. Selanjutnya, ESe-PSO di cadang untuk meningkatkan nilai linear pemberat insersia, ω, yang digunakan dalam Se-PSO. Satu proses redaman di tambah di dalam algoritma ini bagi membolehkan zarah meningkatkan proses penerokaan dan ekplorasi dalam ruangan carian dalam mencari penyelesaian global yang optimum. Pengubahsuaian terhadap algorithma SE-PSO ini, memberikan hasil dapatan nilai optimum yang lebih tepat. Keberkesanan algoritma yang dicadangkan ini diuji ke atas dua ekperimen data (Chassagnole dan Houque) dan bandingkan secara statistik dengan penggunaan algoritma PSO, Algoritma Genetik (*Genetic Algorithm*-GA), Pembezaan Evolusi (*Differential Evolution*- DE) berdasarkan nilai pengurangan jarak, Min, Sisihan Piawai dan Ujian-F. Hasil Se-PSO dan ESe-PSO menunjukkan kesan yang luar biasa dalam pengangaran parameter kinetik di mana dapat disimpulkan bahawa pengurangan jarak dicapai dalam kedua-dua algoritma. Algoritma ESe-PSO mencapai (28.94% dan 16.18%) pengurangan jarak bagi data Chassagnole dan Hoque berbanding dengan model asal kajian (45.56% dan 57.16%), manakala Se-PSO memberikan perbezaan (29.16%, 26.29%), PSO (29.36%, 37.09%), GA (35.58%, 33.9%), dan DE (35.55%, 35.34%). ESe-PSO juga mencapai nilai Min terbaik (7.04E-05 dan 7.41E-05) bagi fungsi objektif berbanding dengan algoritma Se-PSO, (0.000603 dan 0.00379), PSO (0.003893 dan 0.00549), GA (0.11476 dan 0.269007), dan DE (0.049185 dan 0.280478) masing-masing, untuk kedua-dua set data. ESe-PSO dilihat memberikan hasil yang lebih baik dalam pengurangan jarak (nilai ketepatan) dan nilai fungsi objektif yang lebih kecil berbanding Se-PSO, PSO, dan algortima lain, berdasarkan dua set data eksperimen yang digunakan. Secara keseluruhan, pengunaan algoritma ESe-PSO dan Se-PSO boleh digunakan untuk memberikan hasil yang lebih baik dalam menganggarkan parameter kinetik skala besar untuk dengan lebih tepat dan dapat diterima pakai.

ABSTRACT

The development of a large-scale metabolic model of *Escherichia coli* (*E. coli)* is very crucial to identify the potential solution of industrially viable productions. However, the large-scale kinetic parameters estimation using optimization algorithms is still not applied to the main metabolic pathway of the *E. coli* model, and they're a lack of accuracy result been reported for current parameters estimation using this approach. Thus, this research aimed to estimate large-scale kinetic parameters of the main metabolic pathway of the *E. coli* model. In this regard, a Local Sensitivity Analysis, Segment Particle Swarm Optimization (Se-PSO) algorithm, and the Enhanced Segment Particle Swarm Optimization (ESe-PSO) algorithm was adapted and proposed to estimate the parameters. Initially, PSO algorithm was adapted to find the globally optimal result based on unorganized particle movement in the search space toward the optimal solution. This development then introduces the Se-PSO algorithm in which the particles are segmented to find a local optimal solution at the beginning and later sought by the PSO algorithm. Additionally, the study proposed an Enhance Se-PSO algorithm to improve the linear value of inertia weight ω used in the Se-PSO. This algorithm added a damping process to increase the exploration and exploitation in the search space to support the particle to locate a global optimum solution. This modification facilitates an accurate determination of the optimal solution. The effectiveness of the adapted and proposed algorithms were evaluated using two experimental data (Chassagnole and Hoque) and statistically compared to the Particle Swarm Optimization algorithm (PSO), Genetic Algorithm (GA) and Differential Evolution (DE), based on the distance minimization, Mean, Standard Deviation (STD), and the F test ($Ftest$). The result of Se-PSO and ESe-PSO shows a tremendous impact on estimating the kinetic parameters where it can be inferred that distance minimization was achieved in all the algorithms. The ESe-PSO algorithm achieved (28.94% and 16.18%) distance minimization for Chassagnole and Hoque data as compared to the model under study (45.56% and 57.16%), Se-PSO (29.16%, 26.29%), PSO (29.36%, 37.09%), GA (35.58%, 33.9%), and DE (35.55%, 35.34%), respectively. Also, ESe-PSO achieved the best Mean (7.04E-05 and 7.41E-05) of the objective function compared to the Se-PSO algorithm best Mean (0.000603 and 0.00379), PSO (0.003893 and 0.00549), GA (0.11476 and 0.269007), and DE (0.049185 and 0.280478) respectively, for the 2 data set. Overall, the ESe-PSO and Se-PSO algorithms' can be adopted effectively to estimate large-scale kinetic parameters to obtain accurate and acceptable results. Notably, the ESe-PSO superior to the original Se-PSO, PSO, and other state-of-the-art approaches in terms of distance minimization ($accuracy$), and the smallest objective function's value produces appropriate fits to a two-set of experimental data.

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