UNIVERSITI PUTRA MALAYSIA

CROSSOVER AND MUTATION OPERATORS OF REAL CODED GENETIC ALGORITHMS FOR GLOBAL OPTIMIZATION PROBLEMS

LIM SIEW MOOI

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By

LIM SIEW MOOI

Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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DEDICATIONS

This thesis is dedicated to:
my beloved husband Wu Ta Hong,
my daughter Elvina Wu Jit Shern,
my son Enrico Wu Yew Ke,
my family and friends.

Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfillment of the requirement for the degree of Doctor of Philosophy

CROSSOVER AND MUTATION OPERATORS OF REAL CODED GENETIC ALGORITHMS FOR GLOBAL OPTIMIZATION PROBLEMS

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February 2016

Chairman: Associate Professor Md Nasir Sulaiman, PhD

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This study is primarily aimed at investigating two issues in genetic algorithm (GA) and one issue in conformational search (CS) problems. First and foremost, this study examines the proposed crossover and mutation operators on the problems of slow convergence and premature convergence to suboptimal solution. Second of all, this study operates within experimental design with Taguchi method to discover the optimal design factors for the two proposed genetic operators. On the other hand, the CS issue focuses on the effects of the combination of the two proposed genetic operators on two CS problems.

Past studies have revealed that GAs are one of the most prevalently used stochastic search techniques to date. The strength of the algorithm lies in the fact that it assists the evolution of a population of individuals who would thrive in the survival of the fittest towards the next generation. GA has been employed in resolving many complex combinatorial optimization problems such as CS problems.

However, the lack of diversity in a population and the difficulty to locally exploit the solutions within a population creates a setback for GA. Apart from that, its tuning variables are tricky, as it requires intricate setting properties. On another note, the drawback in CS is in locating the most stable conformation of a molecule with the minimum potential energy based on a mathematical function. The number of local minima grows exponentially with molecular size and this makes it that more difficult to arrive at a solution. As such, this research is aimed at resolving the issues mentioned.

The rationale behind developing algorithms using real encoding of chromosome representations is the limitations of binary encoding. In relation to this, Real Coded GA (RCGA) refers to GAs which incorporate real number vector representations of chromosomes. Because the representations of the solutions are similar to the natural formulation, RCGA gets better-customized to the optimization of problems in a continuous domain. Throughout the years, there has been a shift in focus on constructing new crossover and mutation operators to improve the performance of GA in function optimization.

GA operators employ two main strategies; that is, exploration and exploitation to locate the optimum solutions. This research employed a new generational GA based on a combination of the proposed Rayleigh Crossover (RX) and proposed Scale Truncated Pareto Mutation (STPM) called RX-STPM. It is applied in optimization problems like CS. While RX displays self-adaptive behavior and possesses exploration capabilities, STPM thrive in its exploitation features. Hence, RX-STPM becomes an optimal equilibrium between exploration and exploitation strategies in leading the system towards global optima. The explorative and exploitative features of the proposed GA are regulated by substantial crossover probability and mutation rate set up using the Taguchi method. Aside from that, tournament selections with proper tournament sizes, used in the design of the proposed operators, also led to strong exploration potentials.

As you will see in this study, the performance of all RCGAs is contrasted to the standard criteria used in GA literature, which involves accuracy (judged by average error, mean and standard deviation of the objective function values), efficiency and reliability (judged by success rate and average number of function evaluation). RX and STPM operators were separately tested on a dataset of ten benchmark global optimization problems according to the specified experimental procedure. The numerical findings gathered from performance evaluations for RX and STPM were promising and they have shown significantly better results in comparison to the other crossover and mutation operators found in the literature.

An accurate combination of GA operators is pivotal in securing effective resolution to the problem. In this study, the GA was analyzed on a few operators. The numerical results obtained from the performance evaluation indicated that the RX crossover is the most fitting pair to the STPM mutator in competently solving two CS problems i.e. minimizing a molecular potential energy function and finding the most stable conformation of pseudoethane through a molecular model, which involves a realistic energy function.

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Doktor Falsafah

PENGENDALI CROSSOVER DAN MUTASI ALGORITMA GENETIK KOD NYATA UNTUK MASALAH OPTIMUM SEJAGAT

Oleh

LIM SIEW MOOI

Februari 2016

Pengerusi: Profesor Madya Md Nasir Sulaiman, PhD

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Tujuan kajian ini adalah untuk meneliti dua isu dalam algoritma genetik (GA) serta satu isu penting melibatkan masalah carian konformasi (CS). Isu GA Pertama: Kajian ini meneliti pengendali crossover dan mutasi yang dicadangkan ke atas masalah penumpuan perlahan dan penumpuan pra-matang untuk penyelesaian suboptimal. Isu GA Kedua: Reka bentuk kajian ini adalah berasaskan kaedah Taguchi dalam mencari faktor-faktor reka bentuk optimum bagi kedua-dua pengendali genetik yang dicadangkan. Isu CS ditumpukan kepada kesan Algoritma Genetik Kod Nyata (RCGA) dengan menggabungkan dua pengendali genetik yang dicadangkan ke atas dua masalah CS.

GA merupakan salah satu teknik carian stokastik yang paling umum digunakan. Algoritma ini mengevolusi populasi individu yang bakal berkesinambungan dalam kehidupan dengan tujuan untuk menghala ke generasi akan datang. Berdasarkan kajian lepas, GA telah digunakan dalam menyelesaikan banyak masalah pengoptimuman kombinatorik yang sukar seperti masalah CS. Namun begitu, GA juga mempunyai kelemahan tersendiri disebabkan oleh kekurangan dalam kepelbagaian populasi dan kesulitan dalam mengeksploitasi penyelesaian dalam populasi.

Selain itu, sifat tetapan rumit dalam pembolehubah penalaan juga menambah cabaran. Kelemahan dalam CS adalah dalam pencarian pengesahan molekul yang paling stabil dengan menggunakan tenaga keupayaan yang minimum berdasarkan fungsi matematik. Bilangan tempatan minima berkembang sejajar dengan saiz molekul dan ini merupakan satu cabaran. Oleh yang demikian, kajian ini bertujuan untuk menyelesaikan isu-isu yang dinyatakan.

Faktor-faktor utama untuk membina algoritma menggunakan pengekodan sebenar kromosom representasi adalah bagi mengatasi batasan pengekodan perduaan. RCGA merupakan GA yang menggabungkan perwakilan vektor nombor nyata kromosom. Similariti antara representasi penyelesaian kepada formulasi semulajadi membolehkan RCGA diubahsuai untuk masalah pengoptimuman dalam domain yang berterusan. Baru-baru ini, kita dapat perhatikan bahawa tumpuan pada pembinaan pengendali crossover dan mutasi baru telah beralih untuk meningkatkan prestasi GA dalam fungsi pengoptimuman.

Pengendali GA menggunakan dua strategi utama; iaitu eksplorasi dan eksploitasi untuk mencari penyelesaian yang optimum. Oleh yang demikian, kajian ini telah melahirkan satu GA generasi baru dengan mengabungkan cadangan Rayleigh Crossover (RX) dan Scale Truncated Pareto Mutation (STPM) iaitu RX-STPM bagi menyelesaikan masalah pengoptimuman seperti CS. RX mempunyai sifat penyesuaian sendiri serta keupayaan eksplorasi, manakala STPM juga menonjolkan ciri-ciri eksploitasi. Oleh itu, RX-STPM dikatakan mampu mengekalkan keseimbangan yang baik antara strategi eksplorasi dan eksploitasi kearah sistem optima sejagat. Ciri-ciri penerokaan dan mengeksploitasi GA yang dicadangkan adalah dikawal oleh kebarangkalian crossover dan mutasi yang ditubuhkan dengan menggunakan kaedah Taguchi. Selain itu, pilihan berdasarkan pertandingan (dengan saiz pertandingan yang sesuai) bakal menaikkan potensi eksplorasi.

Berpandukan laporan dalam kajian ini, prestasi kesemua RCGA diukur-banding mengikut kriteria standard yang digunakan dalam kesusasteraan GA, iaitu ketepatan (dinilai dengan kesilapan skor, min dan sisihan piawai nilai fungsi objektif), kecekapan dan kebolehpercayaan (dinilai dengan kadar kejayaan dan nombor purata penilaian fungsi). Pengendali RX dan STPM yang dicadangkan telah diuji secara berasingan ke atas sepuluh dataset masalah pengoptimuman sejagat mengikut prosedur eksperimen yang dinyatakan. Hasil kajian yang dikumpul dari penilaian prestasi mengesyorkan bahawa RX dan STPM berpotensi dan ianya telah menghasilkan keputusan yang lebih baik berbanding dengan pengendali crossover dan mutasi lain yang ditemui dalam kesusasteraan .

Gabungan pengendali GA yang tepat adalah amat penting dalam mengecapi penyelesaian yang berkesan untuk kesemua masalah GA. Dalam kajian ini, GA telah dianalisis dengan mengunakan beberapa pengendali. Keputusan statistikal yang diperolehi daripada penilaian prestasi membuktikan bahawa pengendali RX dan STPM merupakan pasangan yang paling sesuai bagi menyelesaikan dua masalah CS. Ini dicapai dengan mengurangkan satu fungsi tenaga keupayaan molekul dan mencari pengesahan yang paling stabil untuk molekul pseudoethane melalui model molekul yang melibatkan fungsi tenaga realistik.

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This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Doctor of Philosophy. The members of the Supervisory Committee were as follows:

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DECLARATION

Declaration by graduate student

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LIST OF ABBREVIATIONS

ADM	Adaptive Directed Mutation
AE	Average Error
AFE	Average Number of Function Evaluation
BA	Bees Algorithms
BCGA	Binary Encoding Genetic Algorithms
BGAM	Breeder GA Mutation
CMA-ES	Covariance Matrix Adaptation Evolution Strategy
COP	Combinatorial Optimization Problem
CPU	Central Processing Unit
CS	Conformational Search
EA	Evolutionary Algorithms
F1	Test Function Number 1
F2	Test Function Number 2
F3	Test Function Number 3
F4	Test Function Number 4
F5	Test Function Number 5
F6	Test Function Number 6
F7	Test Function Number 7
F8	Test Function Number 8
F9	Test Function Number 9
F10	Test Function Number 10
GA	Genetic Algorithm

GAOT	Genetic Algorithm Optimization Toolbox
GSTM	Greedy Sub Tour Mutation
HYB	Stage Hybrid with Full Simplex
LLM	Log Logistic Mutation
LM	Logarithmic Mutation
LX	Laplace Crossover
MI-LXPM	Mixed Integer Laplace Crossover-Power Mutation
MM	Muhlenbein's Mutation
MNUM	Multi Non-Uniform Mutation
MPTM	Makinen, Periaux and Toivanen Mutation
NP	Non-Deterministic Polynomial
NUM	Non-Uniform Mutation
oHYB	Simplex as Operator Hybrid
OS	Operating System
P	Polynomial
PBIL	Population Based Incremental Learning Algorithms
PCA	Principal Component Analysis Mutation
PCX	Parent Centric Crossover
PLM	Polynomial Mutation
PM	Power Mutation
P_m	Mutation Rate
PoD	Pointed Directed Mutation
P_s	Population Size
P_c	Crossover Probability
QSAR	Quantitative Structure Activity Relationship

RCGA	Real Coded Genetic Algorithm
rHYB	Stage Hybrid with a Reduced Simplex
RX	Rayleigh Crossover
RX-STPM	Rayleigh Crossover-Scaled Truncated Pareto Mutation
S/N	Signal to Noise Ratio
SA	Simulated Annealing
SBX	Simulated Binary Crossover
SPX	Simplex Crossover
SR	Success Rate
SS	Systematic Search
STPM	Scaled Truncated Pareto Mutation
TS	Tabu Search
T_s	Tournament Size
UNDX	Unimodal Normal Distribution Crossover
WX	Weibull Crossover

CHAPTER 1

INTRODUCTION

1.1 Background of Studies

Global optimizations encompass issues, which arise in the financial, economic and engineering world. The solution to these problems involves countless variables, which are bound to a massive search parameter, dynamic environments and real-time performance restraints. Therefore, many studies have been aimed at looking for the optimum set of variables, which best fulfills the goals involved within said constraints.

This research is aimed at finding the global optimal solutions for conformational search (CS) which are mathematically represented as a continuous global optimization problem. CS is a term familiar to those in the field of applied mathematics and computational chemistry. In CS, the variables are the torsion angles or coordinates that are used to represent the conformation of the molecule (e.g. polypeptide chain). The objective function value is the potential energy function. By varying the values of the variables, the global minimum value of the objective function can be achieved; that is to locate the most stable conformation of a molecule with the minimum potential energy.

A global optimization problem can be formulated as:

given $f : \mathfrak{R}^n \rightarrow \mathfrak{R}$ a continuous function and $S \subset \mathfrak{R}^n$, find its global minimum $f^* = \min \{ f(x) : x \in S \}$ and the set X^* of all global minimizers $X^*(f) = \{x^* \in S : f(x^*) = f^*\}$ (Lavor et al. 2004).

Table 1.1 depicts the six categories of optimization algorithms. The table demonstrates that these six categories and their branches need not be mutually exclusive.

Table 1.1: Six Categories of Optimization Algorithms
(Haupt et al. 2004)

Category	Optimization Algorithms	
1	Function	Trial and error
2	Single variable	Multiple variables
3	Static	Dynamic
4	Discrete	Continuous
5	Constrained	Unconstrained
6	Random	Minimum seeking

Premature convergence, the no free lunch theorem, over fitting, and over simplification are among the underlying issues of optimization problems. That said, a major setback that is constantly present is that the algorithm is ambiguous in determining whether the proposed best solution is positioned on a local or global optimum. Therefore, for the last three decades, a lot of research has been fixed on finding the global optimal solution of nonlinear optimization problems. Weise (Weise et al. 2009) demonstrates the challenge in finding the optimal resolutions to overcome these problems.

Metaheuristic methods (nature or non-nature inspired) are the most sought after optimization algorithms. With one or more solutions in the beginning, this method follows with a more iterative approach to optimize the search in promising areas away from local solutions. This method is often employed in circumstances where the exact solution methods are unfeasible within a limited time frame.

One of the most popular metaheuristic algorithms advocated by Holland in the 1960s is the Genetic algorithm (GA) (Holland 1975). Being nature-inspired, it works mostly on different sophisticated computational glitches. Subsequently, in the early 90's, a new model, that is the real coded genetic algorithms (RCGA) was brought into light (Herrera et al. 1998). It incorporates real number vector representation of chromosomes and the RCGA can be easily tweaked to fit the optimization of problems in a continuous domain owing to the fact that the representations of the solutions are close to the natural formulation i.e. the genotype (coding) and the phenotype (search space) are very much alike.

However, the problems of slow and premature convergence to suboptimal solution remain an existing struggle that GA is facing. Due to lower diversity in a population, it becomes challenging to locally exploit the solutions. In order to resolve these issues, the focus is now on reaching equilibrium between the explorative and exploitative features of GA. Therefore, the search process can be prompted to produce suitable GA solutions (Yuan et al. 2010).

Although optimization algorithms with higher degree of exploitation may have higher convergence speed, the challenge lies in locating the optimal solution and chances are it may not get past a local optimum. On the other hand, algorithms that favor exploration over exploitation might consume more time in locating the global optimum, that is, coincidentally, due to its less sophisticated candidate solutions. Both features of GA are categorized based on the crossover and mutation operator, crossover probability (P_c), mutation rate (P_m), tournament size (T_s) and population size (P_s), all of which poses existing challenge to the current studies in GA. So the quality of GA solution and the computational time is governed by a fitting scheme of operators and parameter setting.

1.2 Problem Statement

The implementation of real chromosomes encoding stems from the limitations of binary encoding (Deep et al. 2007a). In RCGA, a chromosome length is a vector of floating point numbers to the problem; thus, each gene represents a variable of the problem. Through data gathered from the literature, the many pros of RCGAs have been made apparent over Binary Coding GA (BCGA) particularly in terms of optimizing numerical functions (Deb et al. 2014, Sawyerr et al. 2014). Therefore, the express purpose of this study is aimed at refining the growth in RCGAs instead of BCGAs.

The key focus of this study is narrowed down to the design of genetic operators. It is important to note that the success of exploration and exploitation in GA significantly depends on the efficient crossover and mutation search operators. It also depends on the appropriate coordination among the operators (Elsayed et al. 2014). These genetic operators will exchange information between the peaks and hinders the search from winding up at a local optimum. Over the years, there have been notable efforts in fine-tuning the existing operators by the evolutionary computation community.

The main search operator in GA is the crossover operator which equally as significant as mutation, selection and coding in GA. The crossover operator functions primarily in the survey of information that is accessible through the search space, which inadvertently improves the behavior of the GA. A lot of RCGA efforts are channeled toward designing new crossover operators to heighten the performance of function optimization (Chuang et al. 2015).

On another note, mutation is a secondary operator. It functions to alter the genes of the offspring. A mutator will diversify the existing population and this inadvertently allows GAs to exploit promising areas of the search space thus avoiding local solutions (Korejo et al. 2010). Some of the mutation operators are designed to explicitly overcome certain types of issues over others (Gong et al. 2015).

The performance among all the comparative of GA operators are easily validated and compared through unbiased test problems from the literature, which are diverse in properties in terms of complexity and modality.

Apart from that, the parameter settings of the GA is yet another key focus of this study. Significant attention has been shed in light of this to achieve exploration and exploitation in GA. The tuning methods involve increasing the algorithm performance or decreasing the effort. Since GA parameters can be divided into several levels, there are almost an infinite numbers of possibilities.

Therefore, this research proposes the ideal operators with appropriate parameters and mechanisms to overcome global optimization problems such as CS, which are extremely challenging due to the volume of the search space. In this case, CS occurs when the total number of possible conformations grows exponentially with the total number of degrees of freedom (usually the dihedral angles). It had been confirmed that CS belongs to the category of NP-hard (non-deterministic polynomial time) problem. Such complexity requires an equally long amount of time to achieve resolution. This phenomenon is thus known as the 'combinatorial explosion' (Leach 2007).

On the downside, the conventional experimental design is tedious due to the fact that the large number of experiments increases proportionally with the number of process parameters. These parameters are most likely to influence the performance of a studied system. To rectify that flaw, Genichi Taguchi (Taguchi 1962) presented an efficient and systematic approach called the Taguchi method to iron out the existing issues present in the conventional experimental design. Hence, this study incorporates the Taguchi method in the proposed operators.

1.3 Objectives

The main objective of this research is to propose new RCGA operators in the search for the optimum solution for continuous global optimization problems along with CS problems. The following details are identified to achieve the main objective of this study:

- To propose a mutation operator to exploit good solutions further in order to reach the optimum solution.
- To propose a crossover operator to perform a rapid and thorough discovery examination of the search space in order to speed up the exploration process.
- To propose a generic GA by combining the proposed crossover and mutator to achieve a good balance between exploration and exploitation.

- To apply the newly defined GA in the global minimization of a molecular potential energy function and finding stable conformations of small molecules.

1.4 Scope of the Study

This study focuses primarily on new genetic operators to achieve a balance between exploration and exploitation strategies in GA in order to solve global optimization problems. The two main tools used in the Taguchi method were incorporated in the proposed approach to study all the decision variables involved simultaneously and to measure the quality of solution.

The two proposed genetic operators were tested separately on a data set of ten standard global optimization test problems with varying properties and type of difficulty levels. The test set comprised five non-scalable problems and five scalable problems. The findings gathered from the proposed crossover and mutation operators were compared separately with other GA operators using different probability distributions namely the Laplace distribution, Log Logistic distribution and Power distribution. The effect of the two proposed operators were also tested on two CS application problems. For validity purposes, we adopted the method of analysis that is similar to previous related work to analyze the effect of the newly proposed genetic operators on the GA performance.

1.5 Research Contribution

This study substantially contributes in defining a new generational RCGA, which maintains a good balance between exploration and exploitation strategies while manufacturing the optimum GA solutions. The following highlights the strength of the proposed genetic operators:

The Pareto distribution employed in the new mutation operator has been altered to include a scale to the bounded Pareto. The scale limits the influence of the mutation on the offspring created by the crossover. To supplement that, the truncated Pareto distribution, which always has finite moments, is applied and a modulus is added into the distribution to eliminate the possible imaginary number. Therefore, the new mutator is named Scale Truncated Pareto Mutation (STPM). STPM facilitates the algorithm in generating new solutions from existing ones. It not only improves but also combines the traits of the currently known solution(s). This process can expedite the convergence giving a greater impact on the diversity of the populations.

In the new crossover operator, a Log is introduced to set the boundary of the Rayleigh distribution. A modulus is also included to select only the positive values of the Rayleigh distribution numbers. This operator produces two offspring solutions from two parents. Each offspring solution would inherit favorable elements from both parents. The new parent-centric approach crossover has a higher probability in generating the offspring solutions near each of the parents. This crossover operator exhibited self-adaptation features through the generation of additional diversity beginning from the current one. In other words, the operator seeks new solutions within an unexplored search space and this will inadvertently enhance the competence of GA performance.

1.6 Organization of Thesis

This thesis is structured in a way that it complies with the standard structure of thesis and dissertation of University Putra Malaysia. The thesis consists of seven chapters, which are organized as follow:

Chapter 1 is the introductory chapter, which includes the background, problems, objectives, scope and contributions of the study. This chapter outlines some fundamental information on the importance of this study and the outcomes of the research.

Chapter 2 reviews the theoretical foundation on the related topics about algorithms. The chapter begins with the introduction of combinatorial optimization and the role of algorithms starting from the big family of stochastic approaches followed by metaheuristic techniques, evolutionary methods and finally GA in solving these problems and related issues.

Chapter 3 explains the computational methods and computational steps for CS. This chapter also provides various algorithmic approaches that have been applied to various common CS problems over the last few decades. It covers an overview of five popularly used metaheuristic approaches and five other techniques with their respective mechanisms on solving all kind of CS problems.

Chapter 4 discusses the research methodology of this study. It covers the descriptions of ten benchmark datasets, two CS application problems, the relevant experimental procedures and detailed experimentation evaluations. It begins with the four major research phases, which cover the proposed algorithms, and the experimentation conducted to compare the performance among the algorithms.

Chapter 5 outlines the major contribution of the work. This chapter introduces an overview of a novel RCGA model called Rayleigh Crossover-Scale Truncated Pareto Mutator (RX-STPM) capable of solving two CS problems. Apart from that, the design and analysis of GA parameters using the Taguchi approach are also introduced in this chapter.

Chapter 6 discusses the computational results obtained from the proposed GA approach in Chapter 5 based on experiments performed on the ten benchmark test problems and two CS application problems. The discussions are presented in six different parts. The first four parts examine the results obtained from the final-parameter-tuning and performance analyses for the proposed RX crossover and STPM mutator operators over a set of ten benchmark global optimization test problems. Subsequently, the last two parts confers the results of the performance analysis in the minimization of a simplified molecular model and stable conformations of pseudoethane over the proposed RX-STPM algorithm.

Last but not least, **Chapter 7** concludes the core findings of the study and several recommendations are suggested for possible future research in various aspects of GA and CS problems.

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