

TRUST-REGION BASED METHODS FOR UNCONSTRAINED GLOBAL  
OPTIMIZATION

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## **DEDICATION**

**To My Beloved Family and Friends**

## ACKNOWLEDGEMENT

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## **ABSTRACT**

Convexity is an essential characteristic in optimization. In reality, many optimization problems are not unimodal which make their feasible regions to be non-convex. These conditions lead to hard global optimization issues even in low dimension. In this study, two trusted-region based methods are developed to deal with such problems. The developed methods utilize interval technique to find regions where minimizers reside. These identified regions are convex with at least one local minimizer. The developed methods have been proven to satisfy descent property, global convergence and low time complexities. Some benchmark functions with diverse properties have been used in the simulation of the developed methods. The simulation results show that the methods can successfully identify all the global minimizers of the unconstrained non-convex benchmark functions. This study can be extended to solve constrained optimization problems for future work.

## ABSTRAK

Kecembungan merupakan ciri yang penting dalam pengoptimuman. Sebenarnya, kebanyakan masalah pengoptimuman bukan bersifat unimod yang menyebabkan rantau tersaur masing-masing menjadi tak-cembung. Keadaan ini mengarah ke isu pengoptimuman sejagat susah walaupun dalam matra rendah. Dalam kajian ini, dua kaedah berdasarkan rantau-terpercaya telah dibangunkan untuk menyelesaikan masalah tersebut. Kaedah yang dibangunkan menggunakan teknik selang untuk mencari rantau tempat peminimum berada. Rantau yang dikenalpasti ini adalah cembung dengan sekurang-kurangnya satu peminimum. Kaedah yang dibangunkan telah terbukti memiliki sifat penurunan, penumpuan sejagat dan kekompleksan masa yang rendah. Beberapa fungsi bertanda aras yang mempunyai pelbagai sifat telah digunakan dalam simulasi kaedah yang dibangunkan. Keputusan simulasi menunjukkan kaedah ini berjaya mengesan semua peminimum sejagat fungsi-fungsi bertanda aras tak berkekangan tak-cembung. Kajian ini boleh dilanjutkan untuk menyelesaikan masalah pengoptimuman berkekangan untuk kerja masa hadapan.

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## LIST OF ABBREVIATIONS

DE	-	Differential Evolution
FR	-	Failure Rate
Freu	-	Freudenstein and Roth Function
GO	-	Global Optimization
GOM	-	Global Optimization Methods
HOM	-	Homotopy Optimization Method
HOPE	-	Homotopy Optimization with Perturbations and Ensembles
HSPM	-	Homotopy 2-Step Predictor-corrector Method
HSPM <sub>I</sub>	-	Improved HSPM
HSPM <sub>IE</sub>	-	Extended HSPM <sub>I</sub>
IP	-	Integer Programming
IVT	-	Intermediate Value Theorem
Jenn	-	Jennrich and Sampson Function
KRTI	-	Kerk and Rohanin's Trusted Interval
KRTR	-	Kerk and Rohanin's Trusted Region
LO	-	Local Optimization
LOM	-	Local Optimization Method
M8	-	Mathematica version 8.0
max	-	Maximize/ maximum
min	-	Minimize/ minimum
MILP	-	Mixed Integer Linear Programming
NA	-	Numerical Analysis
NM	-	Nelder Mead
NP	-	Nonlinear programming
N-S	-	N-modal Sine Function
PCH	-	Predictor-Corrector Halley's method
PMT	-	Poincaré-Miranda Theorem

QN	-	Quasi-Newton
RS	-	Random Search
ROA	-	Region of Attraction
SA	-	Simulated Annealing
SR	-	Success Rate
TF	-	Test Function
TI	-	Trusted Interval
TR	-	Trusted Region

## LIST OF SYMBOLS

$C_\alpha$	-	A collection of convex sets
$Z$	-	A continuous function
$K$	-	A corresponding value of $c$ over function $f$ , constant
$HOPE(x)$ ,	-	A function
$HSPM(x)$ ,		
$Z(x)$ , $Z(y)$		
$N$	-	A neighbourhood of an extremizer/ a point
$D$	-	A nonempty, closed set
$p, q, x_n, x_{n+1}$ ,	-	A point
$x_m, x_{m-1}$		
$l$	-	A solution set
$c$	-	A value/ element in between interval $[a, b]$
$A$	-	An algorithm
$g(x)$	-	Auxiliary function
$O$	-	Big oh notation, constant
$\theta$	-	Big theta notation
$[x_1, x_2]$ ,	-	Closed interval
$[y_1, y_2]$ ,		
$[a, b]$ , $[c, d]$ ,		
$I_x, I_y$		
$L, P$	-	Constant
$k$	-	Constant, number of iteration
$c_i(x)$	-	Constrained function
$m$	-	Controller of the sharpness of valley of Eq (5.7), parameter to adjust the step size $st$ ,

	-	Maximum number of iteration $k$
$h$	-	Convergence-control parameter
$C, S_1, S_2$	-	Convex set
$\bar{f}$	-	Currently smallest value of function $f$
$\nabla$	-	Derivative
$f_x$	-	Partial derivative of function $f$ with respect to $x$
$f_y$	-	Partial derivative of function $f$ with respect to $y$
■	-	End of proof
$x^*$	-	Extremizer
$f^*, y^*$	-	Extremum/ global minimum
$f(x)$	-	Function $f$ or target function
$x^{(1)}$	-	Global solution
$t(x)$	-	Generic homotopy function
$g_n$	-	Gradient or first derivative of function $f$
$F(x_n), H(x)$	-	Hessian function
$H(x, \lambda),$	-	Homotopy function
$H(x, y, \lambda)$		
$\lambda$	-	Homotopy parameter
$subinterval_i$	-	$i$ number of subintervals fulfilled the condition by HSPM/ KRTI within the. interval $[a, b]$
$\varepsilon$	-	Infinitesimal change of the dependent variable, error, stopping criterion
$\delta$	-	Infinitesimal increment of the independent variable
$x_0, x^0,$	-	Initial guess
$\{x_i, y_i\},$		
$(x_k, y_k)$		
$x_{i,0}$	-	Initial point, randomly select from $subinterval_i$
$l, \lambda_0$	-	Initial value for homotopy loop
$I_n, I^n$	-	Interval



$B$	-	Inverse matrix
$x_j^{(k-1)}$	-	$j^{th}$ point in the ensemble at the start of iteration $k$
$subinterval_k$	-	$k$ number of subintervals after the filtration
$\alpha$	-	Least upper bound for $A$
$I^-$	-	Left hand side of interval $I^n$
$a, f^R, \overline{f^R}$	-	Lower bound of an interval
$a_n$	-	Lower bound of interval $I_n$
$a_i$	-	Lower bound of $subinterval_i$
$c_{\max}$	-	Maximum number of points in an ensemble
$M$	-	Maximum number of $subinterval_i$ , constant
$subinterval_m$	-	$m$ number of subintervals fulfilled the condition by KRTR on $x$ -axis.
$n, j, i, k$	-	Number of iteration
$\hat{c}$	-	Number of perturbations generated of each point in the ensemble
$c^{(k-1)}$	-	Number of points in the ensemble at the beginning of iteration $k$
$subinterval_n$	-	$n$ number of subintervals fulfilled the condition by KRTR on $y$ -axis.
$F(x)$	-	Objective function
$\gamma$	-	Performing a single steepest descent step
$\xi$	-	Perturbation
$x_{j,0}^{(k)}$	-	Point found by minimization starting at $x_j^{(k-1)}$
$x_{j,i}^{(k)}$	-	Point found by minimization starting at the $i^{th}$ perturbation of $x_j^{(k-1)}$
$R$	-	Real number
$R^n$	-	Real coordinate space of $n$ dimensions,
$I^+$	-	Right hand side of interval $I^n$
$\nabla^2$	-	Second derivative
$X, Y, S$	-	Set

$O(g(n)),$	-	Set of complexity function
$O(h(n)),$		
$n$	-	Size input, number of iteration, constant
$\Delta\lambda, \Delta^{(k)}, \lambda, t,$	-	Step length/ step size
$s, st, sx, sy$		
$x^k$	-	Solution computed by local search
$[a_1, b_1] \times [a_n, b_n]$	-	Sub-region
$T_{HOPE}(n)$	-	Time complexity of HOPE
$T_{HSPM}(n)$	-	Time complexity of HSPM
$T_{KRTI}(n)$	-	Time complexity of KRTI
$T_{KRTR}(n)$	-	Time complexity of KRTR
$T(x)$	-	Tunnelling function
$c^2$	-	Twice-continuously differentiable
$b, f^L, \overline{f^L}$	-	Upper bound of an interval
$b_n$	-	Upper bound of interval $I_n$
$b_i$	-	Upper bound of <i>subinterval</i> <sub><math>i</math></sub>
$x, y, z, N$	-	Variable
$\lambda^{(k)}$	-	Value of parameter homotopy in iteration $k$

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# CHAPTER 1

## INTRODUCTION

### 1.0 Overview

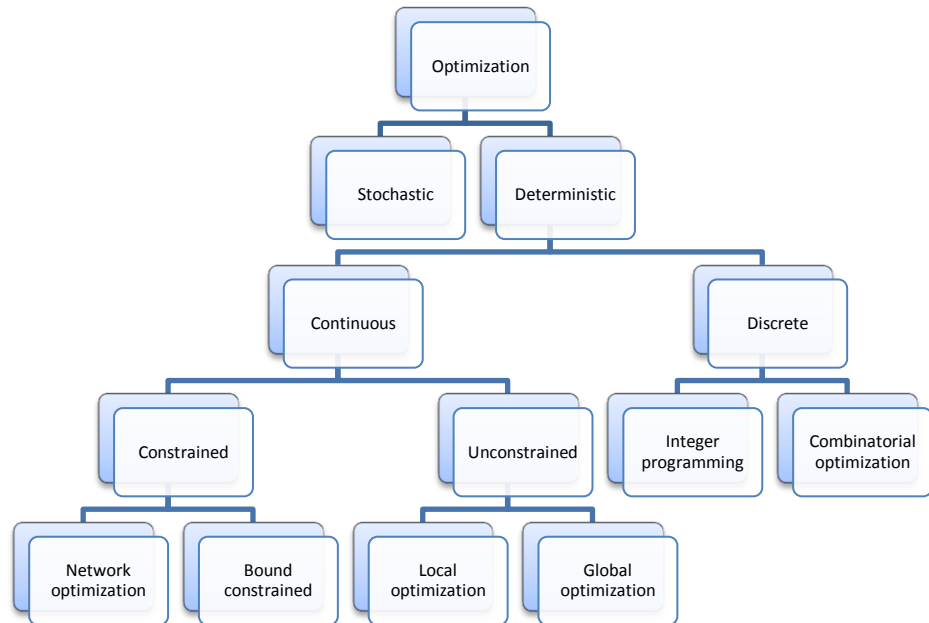
This chapter provides the definition and brief explanation to give a necessary and clearer understanding of this study. An introduction of optimization is described in Section 1.1. The background, statement, research questions, objectives, scope and significance of the study will be discussed in Section 1.2 to Section 1.7. A research outline is provided in Section 1.8.

### 1.1 Introduction

Optimization is used widely in our daily life. It is a powerful tool, especially in the engineering field. For instance, it helps engineers to design aircraft with minimum weight and maximum strength, maximize the power output of electrical networks and machinery while minimizing heat generation. Also, optimization has been applied in the economic field to minimize the total transportation cost of shipping  $x$  units of products from origin to destination to name a few.

Optimization problems can be classified into several categories as shown in Figure 1.1. Optimization problems can be divided into two main categories which are discrete and continuous optimization. Discrete optimization can be separated into

integer programming and combinatorial optimization. While continuous optimization problems involved nonlinear programming and these problems can be categorized into unconstrained and constrained problem. The optimization problems can be further classified. Details can be referred in Neos (2016).



**Figure 1.1:** Classes of optimization problem.

Each type of methods which used to solve these problems is a reliable tool in solving optimization problems. For example, the integer programming (IP), a well-known method in optimization that can help to solve an air-crew scheduling problem (Hoffman and Padberg, 1993). A mixed integer linear programming (MILP) is used to minimize the total control cost consisting of operating and investment cost (Rodrigues *et al.*, 2014). A nonlinear programming (NP) can be used to minimize the size of a tank, and its optimal result helps to explain why soft drink cans are long and thin while storage tanks are short and fat (Shaban *et al.*, 1997).

In general, optimization problems can be viewed as a decision problem that involves finding the "best" solution of the decision variables over all possible

candidates' solution in the feasible region. By the "best" solution, it can be defined as the smallest value of the objective function and such a solution is called a minimizer of the objective function over a feasible region. It also can be defined as the biggest value of the objective function and called as a maximizer.

An optimization problem consists of three important elements, which are objective function, constraints and variables. An objective function is needed to minimize or maximize the system. Constraints can comprise of a feasible region that defines limits of performance for the system. Variables used in the system are adjustable to satisfy the constraints (Biegler, 2010).

Today, optimization is a dominant and indispensable decision-making tool. Many industries apply optimization techniques in their daily operation. For example, it is applied in the area of chemistry to minimize the total cost of the heat exchange and used in biology field to predict new designs of movement and behaviours of animals that may yet evolved (Banga, 2008). Minimizing costs is a natural goal to use optimization (Antonioni and Lu, 2007). Besides that, wastage of materials, the way of arranging productions lines machinery, location of warehouses and products storage can also be optimized.

Based on Biegler (2010), optimization is encountered in all facets of chemical engineering from model and process development to process synthesis and design and finally to process operations, control, scheduling and planning. It becomes a major technique to keeps the chemical industry to remain competitive.

Optimization was used to solve the diet problem in 1940's (Banga, 2008). It helped to find the cheapest combination of foods that will satisfy all the daily nutritional requirements of a person. The main objective of the problem is minimizing the cost of foods, while the decision variables are the amounts of each

type of food which need to be purchased and the constraints are nutritional needs to be satisfied, like total calories, or amount of vitamins, and minerals in the diet.

In physics, a nonlinear multi-objectives technique is used to solve electromagnetic problem. The objective functions are highest efficiency, lowest cost, and minimum weight of active materials (Duan and Ionel, 2013).

In order to satisfy the requirement from various areas, many methods were established. From Figure 1.1, nonlinear unconstrained optimization can be categorized into local optimization (LO) and global optimization (GO). For example, unconstrained optimization can be used to calibrate a multi-surface-plasticity of a soil constitute model (Yang and Elgamel, 2003).

Existing methods for solving local optimization problem, called local search methods are Newton's method, Golden Section Search method, Steepest descent method to name a few. These methods are usually iterative methods. They will start by initial guesses and stop executing when they found one local solution (Chong and Zak, 2013). While global search methods like Hill Climbing Method, Tunneling Method, Multi-start method, etc are used to solve global optimization problems.

## **1.2 Background of Problems**

Optimization is central to any problem involving decision making, whether in engineering or economics. The area of optimization has received enormous attention in recent years, the realization of the global optimal solution of the problem is always preferred (Gould and Tolle, 1975).



Solving a general unconstrained nonlinear optimization can be very hard, even when the problem is small in size since the feasible region of the problem is not always convex (Guenin *et al.*, 2014). To illustrate the potential difficulty of general unconstrained nonlinear optimization, consider the following model instance taken from Pinter (2006).

$$\text{Minimize } f(x, y) = [\sin(xy) + \sin(3y - 5x) + \sin(x^2 - 4y)]^2 \quad (1.1)$$

$$\begin{aligned} \text{subject to } & -3 \leq x \leq 3 \\ & -2 \leq y \leq 5 \end{aligned}$$

Figure 1.2 shows the 3D plot of the model above, and its corresponding contour plot is displayed in Figure 1.3.

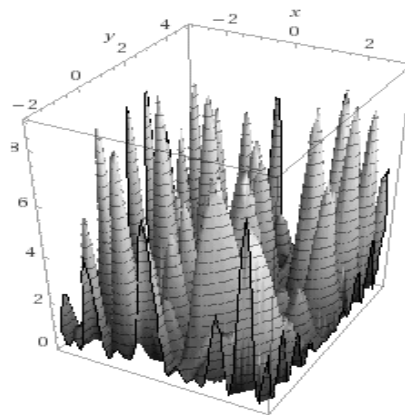


Figure 1.2: 3D plot of the Function (1.1).

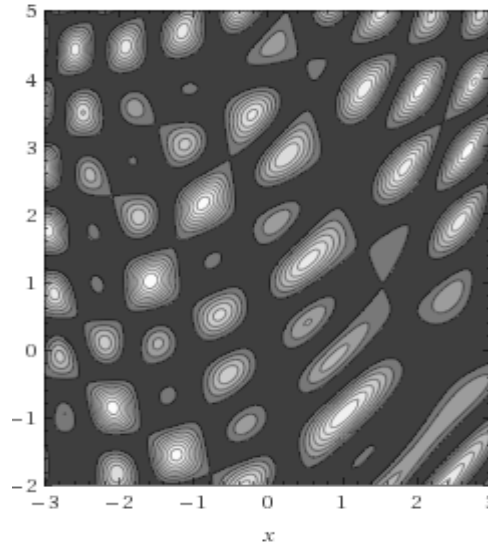


Figure 1.3: Contour plot of the Function (1.1),

The model provided above is a multi-extremal problem. It has a lot of local solutions. Generally, a function can have more than one local solution since they are not unimodal. Local optimization (LO) methods like Newton's method do not emphasize on exploration (Balaprakash *et al.*, 2012); hence it will be stuck in one local solution amongst many and the solution obtained might not be the most optimized one.

Many global optimization algorithms based on homotopy technique have been established such as Homotopy Optimization Method (HOM), and Homotopy Optimization with Perturbation and Ensembles method (HOPE). Homotopy is a fundamental concept in topology. In optimization, it acts like a medium to transfer solutions successively from one local minimum to another better one.

Generally, the global homotopy optimization methods require a significant amount of computation and only applicable to the problems with small number of local minimizers. To overcome this problem, Dunlavy and Leary (2005) introduced two optimization methods, which are Homotopy Optimization Method (HOM) and

Homotopy Optimization with Perturbation and Ensembles (HOPE). HOM is a local search method while HOPE is used as a global search.

HOPE applicability was shown on multi-extrema problems such as 60 modal Sine function which has 60 local minimizers. It can be concluded to be more efficient than quasi-Newton method and HOM based on the result by Dunlavy and Leary (2005).

Besides that, HOPE was proved to outperform Simulated Annealing (SA) on simple protein structure prediction problems (Dunlavy, 2005). SA method converges to a solution only when the probability is almost one, while HOPE was able to converge even when the probability is less than one (Dunlavy and Leary, 2005).

The basic concept of HOPE is to construct a simple auxiliary function with its minimizer known. Then it will use that minimizer as the initial point to locate the next minimizer on the homotopy function. A perturbation step will be applied to perturb the minimizers found so far in various directions. Those perturbed points are used as the next initial points to find the following minimizers. These two steps will be repeated as it deforms the auxiliary function continuously into the objective function. All the minimizers found will be stored in an ensemble.

HOPE seems like a promising algorithm in solving global optimization problems. However, we found two weaknesses from HOPE. In each iteration, the ensemble members carried forward the previous perturbed points and used as starting points to find other minimizers. Hence, it needs many function evaluations to complete its operation which makes it high in computational complexity.

Furthermore, the success rate in locating a solution is highly dependent on the step size and the number of perturbation. A small step size and a large number of perturbations will increase the chances of correctly predicting the global minimizer. In the meantime, it also increases the computational steps taken. However, increasing the amount of computational steps did not promise a significant success rate (Dunlavy and Leary, 2005).

There is an attempt to improve HOPE, which partially overcame the weaknesses of HOPE called Homotopy with 2 Step Predictor-corrector Method (HSPM). This method is introduced by Kerk (2014). There are three essential elements in HSPM, which are homotopy, Intermediate Value Theorem (IVT) and modified Predictor-Corrector Halley's method (PCH). The role of homotopy technique in HSPM is to find an approximate global solution when the trusted interval failed to be found on the target function due to poor choice of step-size parameter. A trusted interval is an interval which can be trusted to contain at least one minimizer. Such trusted interval can be identified by using IVT. Modified PCH method was used as the local search to find the minimizer from each trusted interval. The details of HSPM can be referred to Rohanin and Kerk (2017).

From the result obtained by Kerk (2014), HSPM was shown to have less time complexity than HOPE and able to obtain a 100% success rate in locating the global solution regardless the step size. The main difference between HSPM and HOPE is, HOPE is a stochastic GO method while HSPM is a deterministic GO method. Thus, the number of function evaluation of HOPE is uncountable while number of function evaluation of HSPM is countable. Besides that, the same minimizer can be located repeatedly by HOPE but not in HSPM. This characteristic makes the ensemble of HOPE contains a sequence of the same minimizer which contributes to its expensiveness.

However, the improvement of HOPE with HSPM is not complete since HSPM was designed for solving one variable unconstrained optimization problems. For versatility purpose, it needs to be extended. To extend HSPM, we need to find another possible technique to replace IVT such that a trusted region which contains at least one extremizer can be found.

### **1.3 Statement of Problems**

Global optimization can be hard even when the function involved has a low dimension. It is due to the non-convex feasible regions. Many optimization methods established are used to locate local minimizers. Such methods are called local optimization method (LOM). An LOM will stop executing when a minimizer is found, or the stopping criterion is met. Hence, there is no guarantee that no other solution is better than the current solution found. This issue occurs typically in a multi-extrema problem. The existence of multiple local minima of a general non-convex objective function makes global optimization a significant challenge (Horst *et al.*, 2000).

HOPE was shown as a reliable method to find the minimizer from non-convex optimization problems (Dunlavy and Leary, 2005). The result states that more computation efforts taken and the larger perturbation used, the performance of HOPE improves. In another word, to improve the chances of HOPE in locating a global minimizer, computational effort and cost of operation will need to increase as well.

Kerk (2014) introduced an unconstrained global optimization algorithm called HSPM. HSPM is a method modified from HOPE. HSPM was shown as an

excellent tool to solve one variable non-convex and unconstrained global optimization problems. However, it still has room for improvement such that it can be flexible to solve unconstrained multivariable optimization problems.

In this research, a global optimization algorithm which can be used to solve multi-variables optimization problems is developed. The proposed algorithm will use HSPM as the foundation. To avoid unnecessary computations, we will establish a promising area called the trusted region. At least one minimizer will lie in this region.

In HSPM, IVT technique enables HSPM to determine all intervals which contain at least one minimizer. The trusted interval was credited in reducing the unnecessary function evaluations since the local search step will be applied only on the trusted intervals found, and the same minimizer will not be located repeatedly. Besides that, since a trusted interval is expected to be convex, then we can say that HSPM is able to identify the convex parts from a non-convex feasible region.

To identify a trusted region for multivariable optimization problems, IVT is not compliant since it is only applicable for an interval. Therefore, in this study, we need to find another possible technique to replace IVT, such that a minimizer can be bounded successfully.

#### **1.4 Research Questions**

With regards to the problem statement, the results of this thesis will be answering the following questions:

- i. How to convert a non-convex optimization problems into piece-wise convex optimization problem?
- ii. How to reduce the time complexity of HSPM?
- iii. How to make HSPM deal with multivariable problems?
- iv. How to show the robustness of the proposed algorithm?
- v. How to establish the theoretical support for the proposed algorithm in solving unconstrained optimization problems?

## **1.5 Objectives of the Study**

The objectives of this method are

- i. to develop a technique to identify convex regions from a non-convex region.
- ii. to develop an algorithm to solve multi-variable optimization problems.
- iii. to measure the performance of the proposed algorithm on benchmark unconstrained optimization problems.
- iv. to establish a theoretical background for the proposed algorithm.

## **1.6 Scope of the Study**

This research is designed to solve nonlinear, and non-convex unconstrained global optimization problems. In this research, a GO method will be extended to deal with multivariable problems based on HSPM and functions which are at least twice continuously differentiable,  $C^2$  over a closed interval will be applied. The problems which only involved less than four variables are applied. There are many types of

methods to solve a GO problem such as deterministic, stochastic and heuristic. However, the deterministic will be the only approach utilized in this research. Furthermore, a trusted region will be determined by the method proposed. Software Wolfram Mathematica version 11.1.1 will be used.

## **1.7 Significance of the Study**

This study is expected to extend HSPM to solve multivariable unconstrained global optimization problems. The proposed algorithm is aimed to be able to convert a non-convex optimization problems into piece-wise convex optimization problems and achieve a hundred per cent success rate in locating the global solution such as HSPM. Besides that, this study also is anticipated to result in a reliable algorithm such that industries including the academia can benefit from it.

## **1.8 Research Outline**

This thesis consists of seven chapters, and the contents of each chapter are described as follows:

Chapter 1 is related to the introduction of the topic of research. The contents in this chapter includes background of the problem, statement of the problem, research question, objectives of the study, scope of the study and significance of the study.



Chapter 2 consists of the literature review for this research. Previous and recent studies are reviewed and discussed. Their strengths and weaknesses are analysed and concluded. The information from the materials such as journal will be stated.

Chapter 3 introduces the research methodology and plan for this research. It includes the overall research framework and methodology. The technique applied to complete research objectives is described.

In Chapter 4, the improved method from HSPM will be presented. Next, another extended method to solve multivariable optimization problems will be established in Chapter 5. The theoretical background will be provided for both proposed algorithms. The benchmark problems will also be solved to show their feasibility and robustness.

Then, the proposed algorithms will be compared to HOPE in Chapter 6. Chapter 7 shows the summary, the achievements accomplished and the suggestion for future works of this study.

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