OPTIMAL COMPUTING BUDGET ALLOCATION FOR SIMULATION BASED OPTIMIZATION AND COMPLEX DECISION MAKING

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Declaration

I hereby declare that the thesis is my original work and it has been written by me in its entirety. I have duly acknowledged all the sources of information which have been used in the thesis.

This thesis has also not been submitted for any degree in any university previously.

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2 Apr 2013

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Table of Contents

Summary

Optimal Computing Budget Allocation (OCBA) considers the problem how to get a best result based on the simulation output under a computing budget constraint. It is not only an efficient ranking and selection procedure for simulation problems with finite candidate solutions but also an attractive concept of resource allocation under stochastic environment. In this thesis, the framework of optimal computing budget allocation is studied in detail and improved from both theoretical aspect and practical aspect. From the perspective of problem setting, we extend OCBA to optimal subset selection problem and optimization problem with correlation between designs. From the perspective of OCBA application, we firstly explore the efficient way to use OCBA framework to help random search algorithms solving the simulation optimization problems with large solution space. The computing budget allocation models are built for a popular search algorithm Particle Swarm Optimization (PSO). Two asymptotic allocation rules PSOs_OCBA and PSOe_OCBA are specifically developed for two versions of PSO to improve their efficiency on tackling simulation optimization problems. The application of OCBA framework into complex decision making problems beyond simulation is also studied. We use the decision making technique Analytic Hierarchy Process (AHP) as an example. The resource allocation problem for AHP is modelled from the perspective of OCBA framework. One specific approximated optimal allocation rule AHP_OCBA is derived for it to demonstrate the efficiency improvement on decision making techniques by applying OCBA. The research work of this thesis may provide a more general and more efficient computing allocation scheme for optimization problems.

List of Tables

List of Figures

List of Symbols

The following are some selected notations.

k : The total number of designs.

m : The number of designs contained in the optimal subset.

T : Computing budget of simulation.

N_i : Number of replications allocated to design i, decision variables of the problem.

α_i : The proportion of the total computing budget allocated to design i, i.e. $\alpha_i = N_i / T$.

X_{ij} : A random variable denoting the performance of design i in the *j-th* replication.

$\bar{X}_i$: A statistic denoting the sample mean of the performance of design *i*, that is $\bar{X}_i = \frac{1}{N_i}\sum_{j=1}^{N_i} X_{ij}$.

σ_i^2 : The variance of the performance of design *i*.

μ_i : The mean of the performance of design *i*.

ρ_{ij} : the correlation coefficient between any two random variables *i* and *j*,

$P\{\text{CS}\}$: The probability of correct selection.

$P\{\text{IS}\}$: The probability of incorrect selection.

n_0 : The initial number of replications for sequential algorithm.

Δ : The number of replication increment.

List of Abbreviations

AHP	= Analytic Hierarchy Process,
CS	= Correct Selection,
EA	= Equal Allocation,
IS	= Incorrect Selection,
IZ	= Indifference Zone,
OCBA	= Optimal Computing Budget Allocation,
$P\{CS\}$	= Probability of Correct Selection,
$P\{IS\}$	= Probability of Incorrect Selection,
PSO	= Particle Swarm Optimization,
R&S	= Ranking and Selection.

Chapter 1 Introduction

In real industry, there exist various optimization problems in these complex systems with many decision variables and certain level of uncertainty such as the electronic circuit design problem in manufacturing industry, the portfolio selection problem in financial investment, and the spare parts inventory planning for airlines in service industry. Two main difficulties to solve these optimization problems are the evaluation of the performance of these complex systems (e.g. the logistics system of spare parts for airlines) and the searching of optimal solutions (e.g. the best inventory configuration of spare parts for airlines) for these optimization problems. Most of these complex systems cannot be modeled analytically, Even if analytical models can be built, analytical solutions are often unavailable due to the complexities of the real-world problems and the uncertainties involved. Therefore, simulation has been applied as a useful tool for evaluating the performance of such complex systems. Because of the black-box character of simulation, some traditional optimization methods such as linear programming cannot be applied to. So some new optimization approaches need to be developed for finding the best solution in simulation environment. Simulation optimization is the process of finding the best values of some decision variables for a system where the performance is evaluated based on the output of a simulation model of this system (Ólafsson and Kim, 2002).

Various techniques for simulation optimization have been developed. Most of these methods pay their main attention to the searching mechanism of finding a better solution for the system based on the system performance under current solutions and finally finding the optimal solution. However, using simulation to evaluate system performance under each solution needs time and the run time will be quite consuming when the system evaluated is very complicated. Therefore, we need to consider not only the quality of the final solutions we obtain but also the cost we take to get these final solutions. Compared with the study on searching mechanisms, very few studies have included the computing efficiency (cost) as one more concern of simulation optimization methods. This chapter will provide a brief overview of the current techniques for simulation optimization and more attention will be given to the introduction of computing efficiency in simulation optimization.

1.1 Overview of simulation optimization methods

Different problem settings own different simulation optimization techniques. Taking the nature of the feasible region, the set containing all candidate solutions represented by decision variables, to be the primary distinguishing factor, simulation optimization methods can be classified into two main categories: method with continuous decision variables and method with discrete decision variables.

Most methods for simulation optimization with continuous decision variables use the gradient information as a guidance to determine the direction to move. A most popular one among them is stochastic approximation (SA) (Robbins and Monro, 1951), which have the similar methodology of the steepest descent gradient search in nonlinear optimization. Besides the gradient based search methods, there are also several alternatives such as sample path method (Gurkan et al., 1994) that fix one sample path and change the problem to deterministic, and Response surface methodology (RSM) (Box and Wilson, 1951) aiming to study the functional relationship between input variables and output variables.

For the simulation optimization problems with discrete decision variables, ranking and selection (R&S) and multiple comparison procedures (MCP) are developed for the case that the feasible region contains just a few of alternatives. These procedures evaluate the performance of every alternative and select the best from them. When the number of candidate solutions is very large or uncountable, it is impossible to simulate each alternative. In this situation, random search approach or metaheuristics (e.g. genetic algorithms (GA), simulated annealing, tabu search) are usually employed to intelligently decide the moving path going to local optimal or global optimal solutions. Because of the capability to tackle problems with large solution spaces, random search and metaheuristics sometimes can also be applied to the continuous problems.

1.2 Computing cost for simulation optimization

The computing cost of simulation optimization methods is made up by two parts. One is the total number of solutions visited before the method finds the optimal solution. For most simulation optimization methods mentioned above except the approaches belonging to R&S or MCP, the total number of visited solutions is determined by search mechanism which decides where the candidate solution(s) should move so that the optimal solution can be gradually found. The literatures related to simulation optimization also mainly focus on search mechanism. Although it does help simulation optimization approaches reduce, intentionally or unintentionally, the total number of visited solutions, the main objective for search mechanism is still to find the local optimal or global solutions. Computing cost is not the concern for most literature.

The other part for computing cost is the time spent on simulating all visited solutions. Due to the stochastic environment, each selected solution in simulation optimization methods should be repeatedly evaluated and the performance of each solution is determined based on simulation output. The accuracy of the estimation depends on the number of simulation runs. The more we run simulation for one solution, the more accurate the estimation of that solution's performance will be. Since it is impossible to run simulation infinite times to get the 100% correct estimation, the determination of the number of simulation replications for each solution is the other question that each simulation optimization approaches need to tackle with. The simplest way is giving each visited solution the same number of simulation replications, which is also most approaches currently do. However, considering from the perspective of computing cost saving, this simplest way may be not the most efficient way. Intuitively, if we are already confident that one solution is very bad after a few times of simulation, it is no need to continue running it and more computing effort should be given to the more important solutions. The study on this part is still very limited.

Although they cannot reduce the number of visited solutions and need to simulate all candidate solutions, some methods belonging to R&S or MCP do consider the computing cost about simulation time for simulation optimization problems. The key idea for R&S or MCP approaches is the determination of number of simulation times for each solution such that the good solution(s) can be found with high probability. One of effective R&S approaches is the optimal computing budget allocation (OCBA) procedure developed in Chen et al. (2000) which aims at obtaining an effective allocation rule such that the probability of correctly selecting the best alternative from a finite number of solutions can be maximized under a limited computing budget constraint. Since computing cost is an important criterion for simulation optimization problems because of the increasing complexity of systems in real industry and OCBA is an efficient R&S approach, it is worthwhile to do more extension work on OCBA to further study the computing efficiency for simulation optimization problems. A detailed literature review about R&S approaches and OCBA will be provided in Part 2.

1.3 Objectives and Significance of the Study

The main aim of this study is to extend the OCBA to more general problems and improve the theoretical framework of OCBA. The specific objectives of this research are as follows:

- Extend the OCBA to the optimal subset selection problem and derive an allocation rule for this more general problem by using OCBA framework and KKT conditions.

- Model the computing budget allocation problem for the optimal subset selection problem with correlated sampling among designs by maximizing the convergence rate of incorrect selection probability based on the large deviation theory.

- Develop an OCBA framework for improving the efficiency of the random search algorithms when they are used to tackle simulation optimization problem. In particularly, we use Particle Swarm Optimization (PSO) to demonstrate how this framework works, and also the improvement by employing this framework.

- Apply OCBA framework beyond the simulation problem. We aim to show OCBA can be used to improve the efficiency of decision making techniques such as Analytic Hierarchy Process (AHP) by exploring the best resource allocation scheme for AHP from the perspective of OCBA framework.

The results of this study may have a significant impact on the further study of OCBA. In theoretical aspect, it may provide a more general allocation rule and more rational modeling framework. In practical aspect, this study may provide clearer guidelines for the application of OCBA in simulation optimization problems by integrating searching algorithms and the application into decision making problems which is beyond the area of simulation optimization.

It is understood that OCBA framework is built based on some assumptions. Like previous research work on OCBA, some common assumptions are made in this study to make the problem tractable. Firstly, the allocation rule was derived under the assumption of asymptotic environment. We also assumed that the performance of each design is the normally distributed.

1.4 Organization

This thesis contains 7 chapters. The rest of this thesis is organized as follows. In chapter 2, literatures related to this research are reviewed. Chapter 3 studies the problem of maximizing the probability of correctly selecting the top-m designs out of k designs under a computing budget constraint. The problem is modeled from the perspective of large deviation theory and extended for the situation with correlated sampling in chapter 4. In chapter 5, we explore the OCBA framework to improve the efficiency of random search algorithms in solving simulation optimization problems by taking PSO as an example. Chapter 6 considers the extension of OCBA concept to the decision making technique AHP to efficiently tackle complex decision making problems which is beyond the area of simulation optimization. Chapter 7 concludes the whole thesis.

Chapter 2. Literature Review

In this section, we review the literatures relevant to Ranking and Selection (R&S), especially the work about the optimal computing budget allocation (OCBA). Section 2.1 provides a brief literature review on R&S procedures which focus on simulation optimization problems containing just a few alternate solutions. In section 2.2, we specifically review OCBA, a popular R&S approach, and its following development. This is followed by the review addressing the application of OCBA into real industry and searching algorithms in section 2.3. Section 2.4 summarizes the specific research gaps which motivates our study in the following chapters.

2.1 Ranking and Selection (R&S)

When the number of alternative solutions is fixed, the simulation optimization problem reduces to a statistical selection problem called as Ranking and Selection. There are a vast number of literatures in this area (Bechhofer et al., 1995; Goldsman and Nelson 1998; Kim and Nelson, 2003; Kim and Nelson, 2006; Kim and Nelson, 2007; Chick and Inoue, 2001ab; Branke et al., 2007).

Ranking and Selection is originally developed for statistics. Conway (1963) compared it with analysis of variance (ANOVA) and suggested that R&S was a more proper approach used in the analysis of experimental data. It goes one step further than ANOVA because it can always provide decision makers the information of the best alternatives no matter the null hypothesis is rejected or not.

The aim of R&S procedures is to determine the number of simulation replications in selecting the best design or the optimal subset from a discrete number of alternative solutions. It can be usually classified into two types based on different fulfilled criteria. The first type is to guarantee a desired probability of correct selection, in which a correct selection means the best alternative is selected in the experiments. A traditional work in this group is a conservative two-stage procedure, also called Dudewicz-Dalal procedure proposed in Dudewicz and Dalal (1975). Rinott (1978) then built some inequalities as the lower bound of the probability of correct selection to improve the two-stage procedure. This updated procedure runs equal replications on each alternative at the first stage, and then allocates additional replications to each alternative in the second stage based on the variance of each design's performance obtained at the first stage. Kim and Nelson (2001) and Nelson et al. (2001) proposed the fully-sequential procedures in which one simulation replication was sampled for each alternative until it was eliminated by the screening criteria. In their procedures, the difference of two alternatives' performances is assumed to be indifferent if it is smaller than a specified parameter. Therefore, they are called as Indifference-zone (IZ) procedures. Another popular type for R&S procedures is to maximize the probability of correct selection (PCS) given a computing budget named as Optimal Computing Budget Allocation (OCBA). A detailed review for OCBA is in section 2.2.

In the above literatures of this section, most of them are developed from the frequentist perspective. There are also some other R&S procedures developed from the Bayesian perspective, such as Chick and Inoue (2001a) and Chick et al. (2010) which chose the expected value of information instead of the probability of correct selection (PCS) as the measure of selection quality.

2.2 Optimal computing budget allocation (OCBA)

The optimal computing budget allocation (OCBA) framework proposed by Chen et al. (2000) is a popular R&S procedure which aims to find an efficient way to determine the number of replications allocated to each alternative solution, such that the correctness of selection can be maximized under limited computing budget. The correctness of selection is usual measured by the probability of correct selection which is the probability that the alternative(s) we select are the true best alternative(s).

Traditional R&S procedures allocate the replications based on the variance only such as Dudewicz and Dalal (1975) and Rinott (1978). The larger the variance the more replications are allocated. However, for some alternatives with high variances but far away from the mean of the best alternative's performance, it is unnecessary to give them many replications because it is a waste of computing resources. Intuitively, to ensure a high probability of correctly selecting the desired optimal alternatives, a larger portion of the computing budget should be allocated to those alternatives that are critical in identifying the ordinal relationship with the best alternative. For example, for the alternatives whose performances are very close to the performance of the best alternative, we may need to give them more computing budget to guarantee the estimation accuracy of their performances because it has a high chance to wrongly them as the best. Based on this original idea, Chen et al. (1996) proposed a gradient approach using the information from both the sample mean and variance of designs' performance. Further, Chen et al. (1997) simplified the gradient approach into a greedy heuristics by developing another simple way of estimating the complicated gradient information. However, these budget allocation rules are still not necessarily optimal. Hence, Chen et al. (2000) introduced the concept of mathematical optimization into computing budget allocation problem and finished the fundamental development work for the asymptotic OCBA framework which shows better performance than many other R&S procedures.

OCBA formulates the R&S problem as an optimization model, whose objective is maximizing PCS, constraint is the computing budget and decision variables are the number of replications given to each alternative. Therefore, the two key issues for OCBA are 1) the formulation of PCS, and 2) the way to solve the non-linear optimization problem. For evaluation of probability of correct selection, there is usually no mathematically closed form expression and a proper lower bound of it is used instead as the objective. The Karush-Kuhn-Tucker (KKT) conditions can then be applied to the formulation and the optimality conditions can be derived under the asymptotic environment assumption.

The fundamental OCBA framework is proposed for selecting the best alternative for R&S problems with just one objective and without any constraints. Because of its property of high computing efficiency, OCBA are extended to more complicated problems. For the problem also considering feasibility of the designs, the OCBA model is formulated and an efficient allocation rule, OCBA-CO, is derived (Pujowidianto et al. 2009). For the problem with designs evaluated with multiple objectives, the concept of Pareto optimality is employed to obtain good allocation rules (Lee et al., 2004; Chen and Lee, 2009; Lee et al., 2010). For the problem selecting the optimal subset instead of one best alternative solution, Chen et al. (2008) applied a boundary c separating the optimal subset from the remaining designs and developed a procedure named OCBAm. Besides, the extension considering the correlation between alternatives is discussed in Fu et al. (2004, 2007). Glynn and Juneja (2004) addressed the problem whose performance measure is not normally distributed. Morrice et al. (2008, 2009) extended OCBA concept into regression to deal with transient mean which was a function of other variable such as time. These OCBA procedures perform better than other compared R&S procedures in the related numerical testing. Branke et al. (2007) also show that OCBA and EVI approach are the two top performers among the selection procedures.

2.3 The application of OCBA

Because of their good performance to obtain a high confidence level under certain computing budget constraint, OCBA procedures show great potential in improving simulation efficiency for tackling real industry problems and simulation optimization problems. Therefore, the application of OCBA procedures is studied by many researchers.

For the simulation optimization problems given a fixed set of alternatives, OCBA can be directly applied to select the optimal one among all these solutions. As many problems in real industry are large scaled, without an analytical structure of the problem, and with high uncertainties, OCBA provides an effective way to solve these difficult operation problems, such as the combinatorial optimization problems which include machine clustering problems (Chen et al., 1999), electronic circuit design problems (Chen et al., 2003), and semiconductor wafer fab scheduling problems (Hsieh et al., 2001; Hsieh et al. 2007). In Chen and He (2005), the authors applied OCBA to a design problem in US air traffic management due to the high complexity of this system. For multi-objective problems, Lee et al. (2005) employed MOCBA to optimally select the non-dominated set of inventory policies for the differentiated service inventory problem and an aircraft spare parts inventory problem. In these papers, although certain changes to OCBA are made according to different problems, its main idea is still retained. All numerical results in these papers show that OCBA can save a lot of computing cost compared with the traditional ordinal optimization methods.

For the simulation optimization problems with enormous size or continuous solution space, the application of OCBA is indirect by integrating it with search algorithms. Some frameworks about how to integrate OCBA with search algorithms have been developed. We can classify these papers based on the different search algorithms integrated with OCBA. For the integration with Nested Partition (NP), Shi et al. (1999) showed its application in discrete resource allocation. Shi and Chen (2000) then gave a more detailed hybrid NP algorithm and prove its global optimal convergence. For the integration with evolutionary algorithms, Lee et al. (2008) discussed the integration of MOCBA with MOEA. In Lee et al. (2009), GA is integrated with MOCBA to deal with the computing budget allocations for Data Envelopment Analysis. The integration of OCBA with Coordinate Pattern Search for simulation optimization problems with continuous solution space is considered in Romero et al. (2006). Chen et al. (2008) showed numerical examples on the performance of the algorithm combining OCBA-m with Cross-Entropy (CE). The theoretical part about the integration of OCBA with CE is then further analyzed in He et al. (2010). The numerical result in these papers demonstrates the significant improvements gained by integrating OCBA with search algorithms.

2.4 Summary of research gaps

The OCBA procedures derived or applied in the above reviewed papers show high superiority over other ranking and selection procedures. Therefore, OCBA framework is a valuable research area worthy to be studied. Although Chen et al. (2000) already provided a solid fundamental framework of OCBA, the current research on OCBA still has much room to improve.

- From the aspect of problem setting, most of the studies on OCBA still focus on selecting the best solution. In real industry problems and searching algorithms, the selection of more than one solution is also a popular problem, but the research on this aspect is very little except Chen et al. (2008).

- From the aspect of problem assumption, it is observed that most allocation rules for computing budget allocation are developed under the assumption that each simulation replication for any solutions is independent to each other. However, the technique common random number is usually used in simulation for real industry problem to reduce the variance. Although Fu et al. (2004, 2007) considered correlation between alternative solutions, the discussion is still for selecting one best solution. The optimal subset selection problem under correlation has not been studied.

- From the application perspective, OCBA framework is mainly for finding the best solution(s) given a finite set of design alternatives. Therefore, one obvious limitation for OCBA is that it is only useful for optimization problems with small number of candidate solutions. The large scale problem or problems with continuous feasible region are out of its capacity. There are already some researches on combing OCBA with search algorithms to circumvent this limitation. Most related work directly apply OCBA procedures into search algorithms but ignore the fact that different search algorithms requires different information. Therefore, this kind of combination between OCBA and search algorithms will have limitation and might not be able to produce the best possible efficiency improvement.

Based on the literature review and research gaps, this study aims to extend OCBA to more general problems, even problems beyond the domain of simulation optimization, and improve the theoretical framework of OCBA.

Chapter 3 Asymptotic Simulation Budget Allocation for Optimal Subset Selection

In this chapter, we consider the problem of selecting the optimal subset of top-*m* (*m* can be one) solutions out of *k* alternatives, where the performance of each alternative is estimated using stochastic simulation. The goal is to determine the best allocation of simulation replications among the various alternatives in order to maximize the probability of correctly selecting all top-*m* solutions. Section 3.1 introduces the optimal subset selection problem and specifies the significance of this chapter's study. In section 3.2, we introduce the general computing budget allocation model for the optimal subset selection problem and we propose a new approximated probability of correctly selecting the top-*m* alternatives in section 3.3. Section 3.4 derives an asymptotically optimal simulation allocation rule, OCBAm+, to maximize this approximated probability. Section 3.5 proposes a sequential algorithm to implement OCBAm+. A framework for the asymptotic convergence rate analysis of the probability of correct selection for the optimal subset selection problem is developed in section 3.6, in which the efficiencies of several allocation procedures including OCBAm+ are also compared according to their convergence rates. In section 3.7, we show a series of numerical experiments to support our theoretical claims. Section 3.6 concludes the whole chapter.

3.1 Introduction

Most procedures in ranking and selection are developed for identifying the best alternative. Typically these are two-stage or sequential procedures that ultimately return a single choice as the estimated optimum, e.g., Branke, Chick and Schmidt (2007), Chen et al. (1997, 2000), Chick and Inoue (2001ab), Fu et al. (2007), and Kim and Nelson (2006).

However, sometimes, the return of one best alternative by computer model seems insufficient for decision makers. “All models are wrong” because they are the abstraction of real systems. Therefore, instead of unconditionally trusting the result provided by computer models, decision makers sometimes may prefer to have several good alternatives provided by computer instead of one and make the final selection by considering some conditions neglected by computer model, such as some qualitative criteria and political feasibility. This guarantees that the final decision can be not only best in the criteria considered within the model but also applicable and still quite good in real system. Hence, the optimal subset selection provides decision makers a more flexible and people oriented way to support decision making by computer information.

In addition, the optimization problems in practice are usually with large solution space, such as the product design problems, operation scheduling problems and vehicle routing problems. For these large scaled combinatorial optimization problems, it is a useful way to reduce computing cost by screening the solution space with a rough model and evaluating the remaining alternatives in the subset with an accurate model. This also falls under the optimal subset selection problem.

The development of ranking and selection procedures for selecting the *m* best alternatives is not only applicable to the multiple alternatives selection problems in real industry but also beneficial to some recent developments in simulation optimization that require the selection of an “elite” subset of good candidate solutions in each iteration of the algorithm. Examples of these include the cross entropy method (CE, see Rubinstein and Kroese 2004), the model reference adaptive search method (Hu, Fu and Marcus 2007ab), genetic algorithms (Holland 1975), and more generally, evolutionary population-based algorithms that require the selection of an “elite” population in the evolutionary process (see Fu, Hu and Marcus 2006). The reason for this requirement is that this entire subset is used to update the subsequent population or sampling distribution that drives the search for additional candidates. A subset with poor performing solutions will result in an update that leads the search onto a possibly misleading direction. The overall efficiency of these types of simulation optimization algorithms highly depends on how efficiently we simulate the candidates and correctly select the top-*m* alternatives.

Although the optimal subset selection problem is a meaningful problem worthy of study, not much work had been done to address the optimal subset selection problem until Koenig and Law (1985) developed a two-stage procedure for selecting all the *m* best alternatives (see also Section 10.4 of Law 2007 for an extensive presentation of the problem and procedure). This procedure was developed based on a least favorable configuration and only the information of variances is used to determine the simulation replications' allocation, resulting in very conservative results. It also has a higher computational cost than necessary, since the computing budget is allocated mostly to alternatives with large variances.

Intuitively, to ensure a high probability of correct selection, a large portion of the computing budget should be allocated to those alternatives that are critical to the process of identifying the top-*m* solutions, rather than to alternatives with large variances, as Koenig and Law (1985) does. A key consequence is the use of both the means and variances in the allocation procedure. Following the notion of the Optimal Computing Budget Allocation (OCBA) approach (Chen and Yücesan, 2005), Schmidt, Branke and Chick (2006) proposed a procedure $OCBA_{\delta^*}^{EA}\left(\alpha^*\right)$ specifically for evolutionary algorithms to help them efficiently solve simulation optimization problems. However, this procedure is only applicable to optimization problems using evolutionary algorithms. More importantly, this procedure is still a feasible procedure to guarantee certain level of the probability of correct selection instead of maximizing the probability. Subsequently, Chen et al. (2008) maximized a simple heuristic approximation of the correct selection probability and developed a procedure called OCBAm for general optimal subset selection problems. It has been shown empirically that OCBAm is more efficient than traditional approaches such as Koenig and Law (1985). It should be noted, however, that the probability of correct selection in OCBAm is approximated by employing a constant which separates the optimal subset from the remaining alternatives. The performance of the procedure highly depends on the determination of this constant. One proposed way is to obtain the value of this constant by using a heuristic in each iteration of the sequential OCBAm algorithm, which increases the complexity of implementing the procedure.

In this chapter, we take a different approach to develop a better procedure, called OCBAm+, in which the determination of the constant required in OCBAm is no longer necessary, resulting in a more efficient and robust performance. More importantly, we improve the process of deriving OCBAm and propose a more rigorous theoretical derivation process for computing budget allocation problems. Furthermore, a framework to analyze the asymptotic convergence rate of the probability of correctly selecting the top-*m* alternatives is developed in this chapter. Generally speaking, most research work uses a numerical result as an empirical measure to evaluate different algorithms. The framework of convergence rate proposed in this chapter provides a theoretical measure to comparing these algorithms. Based on this framework, we show that OCBAm+ has a higher convergence rate than OCBAm and other procedures under some conditions. Numerical testing supports this convergence rate analysis and shows the superiority of OCBAm+ over other procedures even in various general cases.

3.2 Formulation for optimal subset selection problem

In this section, we make a problem statement. We consider a finite number of alternatives, i=1, 2, …,k, each with an unknown objective value $\mu_i \in \mathbb{R}$, and we want to select top-m alternatives with the lowest objective values, that is finding the set

$$S = \left\{ i \left| \left(\max_{i \in S} \mu_i \right) < \left(\min_{j \notin S} \mu_j \right),\ i, j \in \{1, ..., k\},\ \text{and } |S| = m \right. \right\}.$$

In stochastic environment, the simulation result for each alternative's performance is a random variable. We assume μ_i is its expectation, which is estimated by sample mean, $\bar{X}_i$, through simulation and a finite value $\sigma_i^2 \in \mathbb{R}_{++}$ as its variance, which is estimated by sample variance. Let $\alpha = (\alpha_1, \alpha_2, ..., \alpha_k)$, in which $\sum_{i=1}^{k} \alpha_i = 1$ and $\alpha_i \geq 0$ for all i=1,…,k, denote the proportion of the total computing budget T given to each alternative. In general, the alternatives whose estimated objective values are smaller than the m^{th} smallest are selected as the estimated solution of the set S. Then, the problem we study is what value of $\alpha = (\alpha_1, \alpha_2, ..., \alpha_k)$ maximizes the probability that the selection based on estimators are the true optimal subset S.

For research convenience, let i denote the index of i^{th} smallest objective value, that is $\mu_1 < \mu_2 < \cdots < \mu_k$. Let $\bar{x}_{(1)} < \bar{x}_{(2)} < \cdots < \bar{x}_{(k)}$ be the ordering of sample mean values of all alternatives. So the selected subset S_m will be $\{(1), (2), \ldots, (m)\}$, while the true optimal subset is $\{1, 2, \ldots, m\}$. Thus, the event of correct selection is $\{\{(1), (2), \ldots, (m)\} = \{1, 2, \ldots, m\}\}$ and the probability of correct selection can be formulated as

$$P\{CS\} \equiv P\{S_m = \{1, 2, \ldots, m\}\}. \tag{3.1}$$

We assume the performance of each alternative is mutually independent, and the performance of each alternative in each replication is also independent of each other. In addition, the alternatives' performances are assumed to be normally distributed. For the non-normal distribution case, we can use a batch-means method so that the original subset selection problem with non-normal distribution can be approximated by the one with normal distribution. Following the concept of the Optimal Computing Budget Allocation, the optimal subset selection problem can be modeled as follows.

$$\begin{aligned} &\max_{N_1, N_2, \ldots, N_k} P\{CS\} \\ &s.t. \quad \sum_{i=1}^{k} N_i = T \\ &\qquad\quad N_i \geq 0, \quad for \ i = 1, 2, \ldots, k. \end{aligned} \tag{3.2}$$

in which $N_i = \alpha_i T$.

3.3 The approximated probability of correct selection

In the model (3.2), we face the modeling challenge of how to formulate the probability of correct selection ($P\{CS\}$). For general parameter settings, there is no closed-form formula for $P\{CS\}$. Although $P\{CS\}$ can be estimated via Monte Carlo simulation by using the sample mean to approximate each alternative's true mean, the computing cost will be very high. Thus, to simplify the calculation of $P\{CS\}$ and eliminate the need for extra Monte Carlo simulation, researchers often use lower bounds of $P\{CS\}$ to approximate its true value, which are called the *Approximated Probability of Correct Selection* (*APCS*).

In Koening and Law (1985), the authors employ the least favorable configuration concept to formulate *APCS*, which results in the very conservative performance of the two-stage allocation rule. In Chen et al. (2008), a better *APCS*, denoted by *APCSm* shown below, is established by using a constant, *c*, to separate the optimal subset from other alternatives.

$$APCSm \equiv \prod_{i \in S_m} \Phi\left(\frac{c - \bar{x}_i}{\sigma_i / \sqrt{N_i}}\right) \prod_{j \notin S_m} \Phi\left(\frac{\bar{x}_j - c}{\sigma_j / \sqrt{N_j}}\right).$$

The value of *c* is determined based on some simple heuristic. The quality of $APCSm$ is highly sensitive to the value of *c*. If we choose a different *c*, $APCSm$ and the allocation rule developed based on it will also be different. Moreover, it is required that the value of *c* lies between $\bar{x}_{(m)}$ and $\bar{x}_{(m+1)}$. If the performances of these two alternatives are very close to each other, it will be difficult to choose *c*. To avoid these limitations, we develop a more robust *APCS* that does not require the determination of a constant value.

Our idea is to utilize the performances of alternatives as the subset boundaries. The correct selection event $\{S_m = \{1, 2, \ldots, m\}\}$ means the sample means from alternative 1 to alternative *m* are not greater than the sample means of other alternatives, i.e. $\max\{\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_m\} \le \min\{\bar{x}_{m+1}, \bar{x}_{m+2}, \ldots, \bar{x}_k\}$. So the probability in (3.1) is equivalent to

$$P\{CS\} = P\left\{\bigcap_i \bigcap_j \left(\bar{X}_i \le \bar{X}_j\right), \text{ for } i = 1, 2, \ldots, m \text{ and } j = m+1, m+2, \ldots, k\right\}. \quad (3.3)$$

Alternatives whose means are less than the mean of alternative *m* (or *m+1*) should be contained in the optimal subset while alternatives whose means are greater than the mean of alternative *m* (or *m+1*) should be out of the optimal subset. Hence, among all random variables in the formula of $P\{CS\}$ in (3.3), we choose the sample mean of alternative *m* and the sample mean of alternative *m+1*, i.e., $\bar{X}_m$ and $\bar{X}_{m+1}$, as thresholds to establish our new lower bound of $P\{CS\}$, *APCSm+*, which is given by Lemma 3.1.

Lemma 3.1. *The probability of correct subset selection can be bounded as follows.*

$$\begin{aligned} P\{CS\} &\geq \max(1-\sum_{i=1}^{m-1} P\left\{\bar{X}_i \geq \bar{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\bar{X}_m \geq \bar{X}_j\right\}, 1-\sum_{i=1}^{m} P\left\{\bar{X}_i \geq \bar{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\bar{X}_{m+1} \geq \bar{X}_j\right\}) \\ &\equiv \max\left(APCSm_1, APCSm_2\right) \equiv APCSm+. \end{aligned} \tag{3.4}$$

Proof. See Appendix A.

The interpretation for the bounds in Lemma 3.1 is as follows. If $APCSm_1$ goes to one, both $\sum_{i=1}^{m-1} P\left\{\bar{X}_i \geq \bar{X}_m\right\}$ and $\sum_{j=m+1}^{k} P\left\{\bar{X}_m \geq \bar{X}_j\right\}$ go to zero. In this case, the selected subset S_m is exactly the optimal subset and $P\{CS\}$ also goes to one. For the case of $APCSm_2$, we have a similar conclusion. Therefore, $APCSm_1$ and $APCSm_2$ are two lower bounds of $P\{CS\}$. To make our lower bound tighter, we choose the higher one between $APCSm_1$ and $APCSm_2$ as our new approximated probability of correct selection *APCSm+*. As *APCSm+* goes to one, the true probability of correct selection also goes to one.

3.4 Derivation of the allocation rule OCBAm+

Using $APCSm+$ given by Lemma 3.1, we approximate the original optimal subset selection model (3.2) by the following model and derive a new computing budget allocation rule, OCBAm+.

$$
\begin{aligned}
\max_{N_1,N_2,\ldots,N_k} APCSm+ = \max(&1-\sum_{i=1}^{m-1} P\left\{\overline{X}_i \ge \overline{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\overline{X}_m \ge \overline{X}_j\right\}, \\
&1-\sum_{i=1}^{m} P\left\{\overline{X}_i \ge \overline{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\overline{X}_{m+1} \ge \overline{X}_j\right\}) \\
s.t. \quad & \sum_{i=1}^{k} N_i = T \\
& N_i \ge 0, \quad for\ i = 1,2,\ldots,k.
\end{aligned}
\tag{3.5}
$$

Similar to several other researches in the literature (e.g., Chen et al. 2000, Glynn and Juneja 2004), we consider an asymptotic condition, i.e., $T \to \infty$, when deriving the optimal allocation rule, and solve the above problem (3.5) by solving the following two sub-problems separately.

1. Sub-problem 1

$$
\begin{aligned}
\max_{\alpha_1,\alpha_2,\ldots,\alpha_k} APCSm_1 &= 1-\sum_{i=1}^{m-1} P\left\{\overline{X}_i \ge \overline{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\overline{X}_m \ge \overline{X}_j\right\} \\
s.t. \quad & \sum_{i=1}^{k} \alpha_i = 1 \\
& \alpha_i \ge 0, \quad \text{for } i = 1,2,\ldots,k.
\end{aligned}
\tag{3.6}
$$

2. Sub-problem 2

$$
\begin{aligned}
\max_{\alpha_1,\alpha_2,\ldots,\alpha_k} APCSm_2 &= 1-\sum_{i=1}^{m} P\left\{\overline{X}_i \ge \overline{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\overline{X}_{m+1} \ge \overline{X}_j\right\} \\
s.t. \quad & \sum_{i=1}^{k} \alpha_i = 1 \\
& \alpha_i \ge 0, \quad \text{for } i = 1,2,\ldots,k.
\end{aligned}
\tag{3.7}
$$

Lemma 3.2. *There exist T_1^* and T_2^* such that sub-problem 1 is convex with respect to the vector $\alpha = \left\{(\alpha_1,\alpha_2,\ldots,\alpha_k)\right\}$ (>0) when $T > T_1^*$ and, sub-problem 2 is convex with respect to the vector α >0 when $T > T_2^*$.*

Proof. See Appendix B in which the values of T_1^* and T_2^* are also defined.

Because of the convexity of these two sub-problems, the solutions obtained from the Lagrangian method under the asymptotic framework are asymptotically global optimal allocation rules for these two sub-problems. Let F_1 and F_2 be the Lagrangian functions of sub-problem 1 and sub-problem 2 respectively. Then, we have

$$F_1 = 1 - \sum_{i=1}^{m-1} P\left\{\bar{X}_i \geq \bar{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\bar{X}_m \geq \bar{X}_j\right\} - \lambda\left(\sum_{i=1}^{k}\alpha_i - 1\right) - \sum_{i=1}^{k}\nu_i\alpha_i \text{ , and} \tag{3.8}$$

$$F_2 = 1 - \sum_{i=1}^{m} P\left\{\bar{X}_i \geq \bar{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\bar{X}_{m+1} \geq \bar{X}_j\right\} - \lambda\left(\sum_{i=1}^{k}\alpha_i - 1\right) - \sum_{i=1}^{k}\nu_i\alpha_i \text{ .} \tag{3.9}$$

By Karush-Kuhn-Tucker (KKT) conditions, the allocation rules satisfy the equations in the following lemma will be optimal for sub-problem 1 and sub-problem 2.

Lemma 3.3. (a) *The allocation rule* $\alpha^{*1} = \left(\alpha_1^{*1}, \alpha_2^{*1}, \ldots, \alpha_k^{*1}\right)$ *is asymptotically optimal for sub-problem 1 if it satisfies the following conditions:*

(i) $\alpha_m = \sigma_m \sqrt{\sum_{i \neq m}^{k} \frac{\alpha_i^2}{\sigma_i^2}}$ *;*

(ii) $\frac{\left(\mu_x - \mu_m\right)^2}{\sigma_x^2/\alpha_x + \sigma_m^2/\alpha_m} = \frac{\left(\mu_y - \mu_m\right)^2}{\sigma_y^2/\alpha_y + \sigma_m^2/\alpha_m}$, $x, y \neq m$

(iii) $\sum_{i=1}^{k}\alpha_i = 1$*;*

(iiii) $\alpha_i > 0$.

(b) *The allocation rule* $\alpha^{*2} = \left(\alpha_1^{*2}, \alpha_2^{*2}, \ldots, \alpha_k^{*2}\right)$ *is asymptotically optimal for sub-problem 2 if it satisfies the following conditions:*

(i) $\alpha_{m+1} = \sigma_{m+1}\sqrt{\sum_{i\neq m+1}^{k} \frac{\alpha_i^2}{\sigma_i^2}}$ *;*

(ii) $\frac{\left(\mu_x - \mu_{m+1}\right)^2}{\sigma_x^2/\alpha_x + \sigma_{m+1}^2/\alpha_{m+1}} = \frac{\left(\mu_y - \mu_{m+1}\right)^2}{\sigma_y^2/\alpha_y + \sigma_{m+1}^2/\alpha_{m+1}}$, $x, y \neq m+1$

(iii) $\sum_{i=1}^{k} \alpha_i = 1$*;*

(iiii) $\alpha_i > 0$.

Proof. See Appendix C.

Based on lemma 3.3, the values of optimal solutions for problem 3.6 and 3.7 can be solved by nonlinear programming (NLP) solvers. We can give the values of parameters to NLP as input and obtain the values of optimal solution, but we cannot find the explicit formula that link the solution with parameter. In addition, once we have a new value setting of parameters, we need to run NLP again. It is a little bit time-consuming. Therefore, we can make some reasonable assumptions such that some closed-form allocation rule can be derived and implemented as a good allocation rule (no guarantee of optimality) into some algorithms. We assume $\alpha_m^{*1} >> \alpha_i^{*1}, \forall\ i \neq m$ for sub-problem 1 and $\alpha_{m+1}^{*2} >> \alpha_i^{*2}, \forall\ i \neq m+1$ for sub-problem 2. This assumption can be justified by the following Proposition 3.1.

Proposition 3.1. *Under the asymptotic environment,* $T \to \infty$ *, if the means of alternatives satisfy that* $\mu_1 < \mu_2 < \cdots < \mu_k$ *and the variances are all strictly positive and bounded, we have*

$\lim_{k\to\infty}\left(\alpha_i^{*1}/\alpha_m^{*1}\right) = 0,\ \left(\alpha_i^{*1}/\alpha_m^{*1}\right) = O\left(1/\sqrt{k}\right),\ \forall\ i \neq m$ *and*

$$\lim_{k\to\infty}\left(\alpha_j^{*2}/\alpha_{m+1}^{*2}\right)=0,\ \left(\alpha_j^{*2}/\alpha_{m+1}^{*2}\right)=\mathrm{O}\left(1/\sqrt{k}\right),\ \forall\ j\neq m+1.$$

Proof. See Appendix D.

Based on the above assumption, we can simplify the conditions in lemma 3.3 and get approximated optimal solutions for these two sub-problems in closed-form as follows.

Lemma 3.4. (a) *As* $T\to\infty$, $APCSm_1$ *in sub-problem 1 can be asymptotically maximized when*

$$\alpha_i^{*1}=\frac{\beta_i^{*1}}{\sum_{i=1}^{k}\beta_i^{*1}}\text{, in which }\beta_i^{*1}=\frac{\sigma_i^2}{\left(\mu_i-\mu_m\right)^2},\forall\ i\neq m\text{ and }\beta_m^{*1}=\sigma_m\sqrt{\sum_{i\neq m}^{k}\frac{\left(\beta_i^{*1}\right)^2}{\sigma_i^2}}. \quad (3.10)$$

(b) *As* $T\to\infty$, $APCSm_2$ *in sub-problem 2 can be asymptotically maximized when*

$$\alpha_i^{*2}=\frac{\beta_i^{*2}}{\sum_{i=1}^{k}\beta_i^{*2}}\text{, in which }\beta_i^{*2}=\frac{\sigma_i^2}{\left(\mu_i-\mu_{m+1}\right)^2},\forall\ i\neq m+1\text{ and }\beta_{m+1}^{*2}=\sigma_{m+1}\sqrt{\sum_{i\neq m+1}^{k}\frac{\left(\beta_i^{*2}\right)^2}{\sigma_i^2}}. \quad (3.11)$$

Theorem 3.1. *Let* $\alpha^{*1}\equiv\left(\alpha_1^{*1},\alpha_2^{*1},\cdots,\alpha_k^{*1}\right)$ *and* $\alpha^{*2}\equiv\left(\alpha_1^{*2},\alpha_2^{*2},\cdots,\alpha_k^{*2}\right)$ *be the rule given by Lemma 3.4. As* $T\to\infty$, *the asymptotically optimal solution rule for problem (3.5), named as OCBAm+, is*

$$\alpha^*\equiv\left(\alpha_1^*,\alpha_2^*,\cdots,\alpha_k^*\right)=\begin{cases}\alpha^{*1} & \text{if } APCSm_1\left(\alpha^{*1}\right)\geq APCSm_2\left(\alpha^{*2}\right)\\ \alpha^{*2} & \text{if } APCSm_1\left(\alpha^{*1}\right)<APCSm_2\left(\alpha^{*2}\right)\end{cases}.$$

Proof. For the objective in problem (3.5), we have

$$\max_{N_1,N_2,\ldots,N_k} APCSm+=\max\left(\max_{N_1,N_2,\ldots,N_k} APCSm_1,\ \max_{N_1,N_2,\ldots,N_k} APCSm_2\right).$$

Lemma 3.3 shows that $\max_{N_1, N_2, \ldots, N_k} APCSm_1$ and $\max_{N_1, N_2, \ldots, N_k} APCSm_2$ are equal to $APCSm_1(\alpha^{*1})$ and $APCSm_2(\alpha^{*2})$ respectively when $T \to \infty$. Therefore, under the asymptotic limit, $APCSm+$ is maximized when the allocation rule is OCBAm+ shown in Theorem 3.1. □

Remark 3.1. To directly apply Theorem 3.1, we need to calculate the values of $APCSm_1(\alpha^{*1})$ and $APCSm_2(\alpha^{*2})$ to determine whether α^{*1} or α^{*2} should be applied. When the means and the variances of alternative *m* and alternative *(m+1)* do not have very huge difference, by making some mild approximations, we can simplify the conditions, $APCSm_1(\alpha^{*1}) \geq APCSm_2(\alpha^{*2})$ and $APCSm_1(\alpha^{*1}) < APCSm_2(\alpha^{*2})$ to $(\mu_{m+2} - \mu_{m+1}) \leq (\mu_m - \mu_{m-1})$ and $(\mu_{m+2} - \mu_{m+1}) > (\mu_m - \mu_{m-1})$ respectively (see Appendix E for illustration). Obviously, these simplified conditions are much easier to calculate than the original conditions.

Based on Theorem 3.1, we have the following corollary when *m* equals one.

Corollary 3.1. *When m equals one and the variances of all alternatives are equal, the allocation rule OCBAm+ will be as follows.*

$$\frac{\alpha_x}{\alpha_y} = \left(\frac{\sigma_x / \delta_x}{\sigma_y / \delta_y} \right)^2, \quad x, y \neq 1 \tag{3.12}$$

$$\alpha_1 = \sigma_1 \sqrt{\sum_{i \neq 1}^{k} \frac{\alpha_i^2}{\sigma_i^2}} , \tag{3.13}$$

in which $\delta_x = \mu_x - \mu_{i_1}$ *for all* $x \neq 1$.

Proof. See Appendix F.

Corollary 3.1 shows that OCBAm+ can reduce to OCBA1 in Chen et al. (2000) when *m* equals one in equal variance case. The corollary also shows us that OCBAm+ is more general than OCBAm, because, on the other hand, OCBAm does not directly reduce to OCBA1 as OCBAm+ does. This can be a potential advantage for OCBAm+ because it is has been shown that OCBA1 is superior to OCBAm in numerical testing when *m* equals one.

3.5 Sequential allocation procedure for OCBAm+

The allocation rule in Theorem 3.1 depends on the function of distributions. A sequential heuristic procedure is provided here to apply the allocation rules. In the procedure, each solution is initially simulated with n_0 replications in the first stage. The allocation proportion vector $\alpha \equiv (\alpha_1, \alpha_2, \cdots, \alpha_k)$ can be estimated by the sample mean and sample variance of each solution. Based on the updated $\alpha \equiv (\alpha_1, \alpha_2, \cdots, \alpha_k)$, the algorithm will decide which alternative can get one more replication in this iteration following the rule that alternative *i* (*i*=1,2,…,*k*) can get this replication with probability α_i. At each iteration, the algorithm just allocates one replication and each alternative *i* have the probability α_i to obtain this replication. Based on the rule, additional replications are allocated to individual solution one by one based on the value of $\alpha \equiv (\alpha_1, \alpha_2, \cdots, \alpha_k)$ which is updated by sample means and sample variances at each iteration.

Algorithm OCBAm+ Procedure

INTIALIZE Let n equal to $n_0 k$; Set $N_1^n = N_2^n = \cdots = N_k^n = n_0$ and $T^n = \sum_{i=1}^{k} N_i^n$; Perform n_0 replications for all alternatives. Calculate sample mean and sample variance of each alternative.

LOOP **WHILE** $T^n < T$ **DO**

ALLOCATE Calculate the value of $\alpha^n \equiv \left(\alpha_1^n, \alpha_2^n, \cdots, \alpha_k^n\right)$ according to (3.10) and (3.11) based on different situations; Generate a replicate s_n from the p.m.f $\alpha^n \equiv \left(\alpha_1^n, \alpha_2^n, \cdots, \alpha_k^n\right)$.

SIMULATE Set $N_s^{n+1} = N_s^n + 1$, $N_i^{n+1} = N_i^n, i \neq s_n$ and $T^{n+1} = \sum_{i=1}^{k} N_i^{n+1}$; Perform additional one replication of alternative s_n; Set n=n+1;

UPDATE Calculate sample mean of each alternative to estimate its true mean.

END OF LOOP

OUTPUT Select the alternatives whose performances' means are less than the *(m+1)*th smallest sample mean into the optimal subset and end the procedure.

In the sequential algorithm, although we use sample mean and sample variance to estimate the true mean and variance, the impact of these approximations will decay asymptotically.

Theorem 3.2. As $T \to \infty$, $\frac{N_i^n}{T} \to \alpha^*$ *almost surely.*

Proof. See Appendix G.

3.6 Asymptotic convergence rate analysis on allocation rules

In this section, we present a theoretical framework to analyze the asymptotic convergence rate of the correct selection probability for the optimal subset selection problem. We also utilize this framework to estimate and compare the efficiency of different simulation allocation rules.

3.6.1 The framework for asymptotic convergence rate analysis on allocation rules

Denote $P\{IS\}$ as the probability of incorrect selection, i.e., $P\{IS\}=1-P\{CS\}$. As T increases, $P\{CS\}$ increases and $P\{IS\}$ decreases. Let S_1 denote the set $\{1,2,\ldots,m\}$ and S_2 denote the set $\{m+1,m+2,\ldots,k\}$. Then the probability of incorrect selection can be expressed as

$$P\{IS\}=P\left\{\max_{i\in S_1}\bar{X}_i(\alpha_i T)\geq \min_{j\in S_2}\bar{X}_j(\alpha_j T)\right\}. \tag{3.14}$$

If $\alpha_i > 0$ for all i, $P\{IS\}$ goes to zero as $T\rightarrow\infty$. Based on large deviation theory (cf. Dembo and Zeitouni 1992, Szechtman and Yücesan 2008), $P\{IS\}$ in (3.14) can be bounded by

$$\max_{i\in S_1,\, j\in S_2} P\left\{\bar{X}_i(\alpha_i T)\geq \bar{X}_j(\alpha_j T)\right\}\leq P\{IS\}\leq |S_1|\times|S_2|\max_{i\in S_1,\, j\in S_2} P\left\{\bar{X}_i(\alpha_i T)\geq \bar{X}_j(\alpha_j T)\right\}.$$

As T increases, the convergence rate of $P\{IS\}$ approaches the convergence rate of $\max_{i\in S_1,\, j\in S_2} P\left\{\bar{X}_i\geq \bar{X}_j\right\}$.

For any given $i\in S_1$ and $j\in S_2$, there exists a rate function G_{ij} such that

$$\lim_{T\rightarrow\infty}\frac{1}{T}\log P\left\{\bar{X}_i(\alpha_i T)\geq \bar{X}_j(\alpha_j T)\right\}=-G_{ij}\left(\alpha_i,\alpha_j\right), \tag{3.15}$$

so we have

$$\lim_{T\rightarrow\infty}\frac{1}{T}\log\left(\max_{i\in S_1,\, j\in S_2} P\left\{\bar{X}_i(\alpha_i T)\geq \bar{X}_j(\alpha_j T)\right\}\right)=-\min_{i\in S_1,\, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right).$$

Thus,

$$\lim_{T\rightarrow\infty}\frac{1}{T}\log P\{IS\}=-\min_{i\in S_1,\, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right).$$

This means that $P\{IS\}$ will decay exponentially with increasing T at a rate given by $-\min_{i\in S_1, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right)$, and $\min_{i\in S_1, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right)$ can be considered as the convergence rate of $P\{CS\}$.

According to Glynn and Juneja (2004), we have

$$G_{ij}\left(\alpha_i,\alpha_j\right)=\inf_x\left(\alpha_i I_i\left(x\right)+\alpha_j I_j\left(x\right)\right),$$

in which $I_i\left(x\right)$ and $I_j\left(x\right)$ are the Fenchel-Legendre transform of the log-moment function of random variables X_i and X_j. For a normal distributed random variable $X_i \sim N\left(\mu_i,\sigma_i^2\right)$,

$$I_i\left(x\right)=\frac{\left(x-\mu_i\right)^2}{2\sigma_i^2}.$$

Calculating the derivative of the function $\left(\alpha_i I_i\left(x\right)+\alpha_j I_j\left(x\right)\right)$ with respect to x and letting the derivative equal to zero, we can get the expression of the optimal x to minimize this function. Substituting this optimal x into $\left(\alpha_i I_i\left(x\right)+\alpha_j I_j\left(x\right)\right)$, we obtain

$$G_{ij}\left(\alpha_i,\alpha_j\right)=\inf_x\left(\alpha_i I_i\left(x\right)+\alpha_j I_j\left(x\right)\right)=\frac{\left(\mu_i-\mu_j\right)^2}{2\left(\sigma_i^2/\alpha_i+\sigma_j^2/\alpha_j\right)}.$$

The convergence rate for an allocation rule is

$$\min_{i\in S_1, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right)=\min_{i\in S_1, j\in S_2}\frac{\left(\mu_i-\mu_j\right)^2}{2\left(\sigma_i^2/\alpha_i+\sigma_j^2/\alpha_j\right)}.$$

3.6.2 Asymptotic convergence rates for different allocation rules

Note that the convergence rate depends on not only the budget allocation α but also the problem itself (i.e., μ and σ under the normality assumption). Therefore, it will be generally difficult to get a closed-form expression for the convergence rate obtained by allocation rules. In this situation, we can estimate it numerically by repeatedly running experiment under large computing budget and estimating the convergence rate by the original formula (3.15). However, in some conditions, it is possible to know the expression and compare allocation rules based on their convergence rates. In this sub-section, we compare the convergence rate for OCBAm+ with the rates for OCBAm and the equal allocation rule (EA) under some conditions to theoretically show the superiority of OCBAm+ over OCBAm and EA.

Consider a simple case where the variances of all alternatives are equal ($\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$). Given the equal allocation rule, i.e., $\left(\alpha_1{}^E, \alpha_2{}^E, \cdots, \alpha_k{}^E\right)$, where $\alpha_i^E = 1/k$ for $i = 1, 2, \ldots, k$, we have

$$G_{ij}\left(\alpha_i^E, \alpha_j^E\right) = \frac{\left(\mu_i - \mu_j\right)^2}{4k\sigma^2} \text{ for } i \in S_1 \text{ and } j \in S_2 .$$

Among these $G_{ij}\left(\alpha_i^E, \alpha_j^E\right)$, the $G_{m(m+1)}\left(\alpha_m^E, \alpha_{m+1}^E\right)$ is always the minimum, because $\left|\mu_m - \mu_{m+1}\right|$ is the smallest one among $\left|\mu_i - \mu_j\right|$ for all $i \in S_1$ and $j \in S_2$. Therefore, the convergence rate for EA is

$$\min_{i \in S_1, j \in S_2} G_{ij}\left(\alpha_i, \alpha_j\right) = G_{m(m+1)}\left(\alpha_m^E, \alpha_{m+1}^E\right) = \frac{\left(\mu_m - \mu_{m+1}\right)^2}{4k\sigma^2} .$$

Similarly we can also obtain the asymptotic convergence rates for OCBAm and OCBAm+, also in the equal variance case.

Lemma 3.5. *Suppose* $\left(\alpha_1, \alpha_2, \cdots, \alpha_k\right)$ *and* $\left(\alpha_1{}^L, \alpha_2{}^L, \cdots, \alpha_k{}^L\right)$ *are the computing proportions allocated to all alternatives by OCBAm and OCBAm+ respectively. Then, if all alternatives have the same variance, i.e.,* $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$ *, we have the following result.*

(a) *The asymptotic convergence rate for OCBAm is*

$$\min_{i\in S_1, j\in S_2} G_{ij}\left(\alpha_i, \alpha_j\right) = \min\left\{G_{mk}\left(\alpha_m, \alpha_k\right), G_{1(m+1)}\left(\alpha_1, \alpha_{(m+1)}\right)\right\}$$
$$= \min\left\{\frac{\left(\mu_m - \mu_k\right)^2}{2\sigma^2\left(1/\alpha_m + 1/\alpha_k\right)}, \frac{\left(\mu_1 - \mu_{m+1}\right)^2}{2\sigma^2\left(1/\alpha_1 + 1/\alpha_{m+1}\right)}\right\};$$

(b) *The asymptotic convergence rate for OCBAm+ is*

$$\min_{i\in S_1, j\in S_2} G_{ij}\left(\alpha_i, \alpha_j\right) = G_{m(m+1)}\left(\alpha_m^L, \alpha_{m+1}^L\right) = \frac{\left(\mu_m - \mu_{m+1}\right)^2}{2\sigma^2\left(1/\alpha_m^L + 1/\alpha_{m+1}^L\right)}.$$

Proof. See Appendix H.

Lemma 3.5 enables us to perform further convergence rate analysis and comparison, and leads to the following two theorems.

Theorem 3.3. *The asymptotic convergence rate for OCBAm+ is greater than the asymptotic convergence rate for the equal allocation rule (EA), when the variances of all alternatives are equal (* $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$ *) and* $\left(\mu_{m+1} - \mu_m\right) \le \min\left(\mu_{m+2} - \mu_{m+1}, \mu_m - \mu_{m-1}\right)$.

Proof. See Appendix I.

Theorem 3.4. *If the means of all alternatives form an arithmetical progression, and the variances of all alternatives are equal, i.e.* $\mu_{i+1} - \mu_i = d$, for $i = 1, 2, \ldots, k-1$ *and* $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$*, the asymptotic convergence rate for OCBAm+ is no less than OCBAm when m=1, or* $m \ge 2$ and $k \ge m+5$.

Proof. See Appendix J.

It can also be proved the asymptotic convergence rate of OCBAm is greater than EA's under the same condition in Theorem 3.3. Therefore, OCBAm+ has the highest convergence rate and

OCBAm has the second highest convergence rate among EA, OCBAm and OCBAm+, if all alternatives have similar variances and their ranked means are similar to an arithmetical progression.

3.7 Numerical experiments

In this section, we conduct some numerical experiments to test the performance of OCBAm+ compared with OCBAm and EA. We use $P\{CS\}$ as the empirical performance measure and the asymptotic convergence rate as the theoretical performance measure. $P\{CS\}$ is estimated by the fraction of times the procedure successfully finds all the true top-*m* alternatives out of 10,000 independent experiments. Following the guidelines in Chen et al. (2008), we set n_0 equals to 20 in all numerical experiments.

3.7.1 The Base Experiment

We want to select top-5 solutions from 50 alternatives, with distribution $N(i\ , 10^2)$ for alternative i = 1, 2, …, 50. The performances of EA, OCBAm and OCBAm+ with an increasing computing budget *T* is shown in figure 3.1. Table 3.1.a displays the speed-up factors of OCBAm over EA and OCBAm+ over EA. The speed-up factor of OCBAm(OCBAm+) over EA equals to the average computing replications needed for EA to attain 90% $P\{CS\}$ divided by the average computing replications needed for OCBAm(OCBAm+) to attain 90% $P\{CS\}$. Table 3.1.b shows the theoretical convergence rates of $P\{CS\}$ for these three allocation rules.

Figure 3. 1 Performance comparison of P{CS} in the Base Experiment.

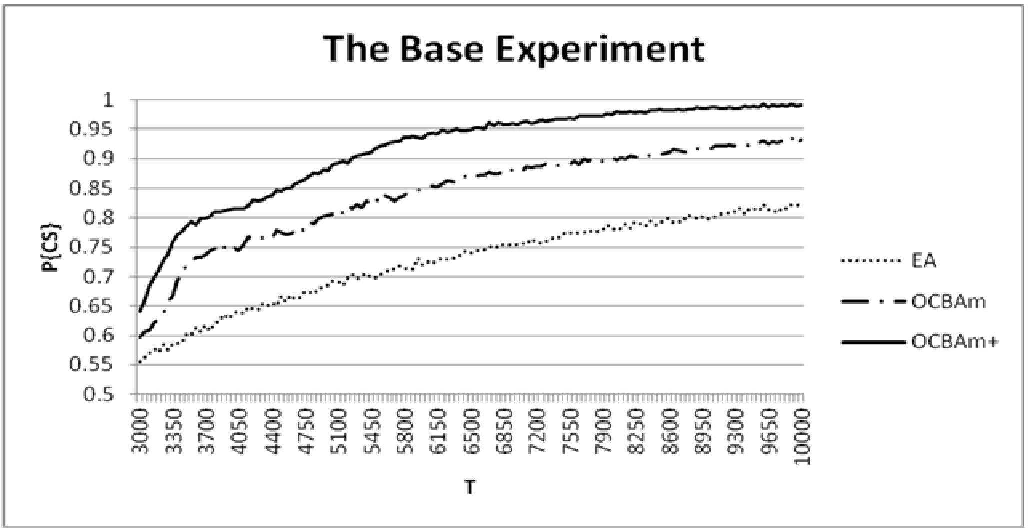


Table 3.1. a The speed-up factor with different values of P{CS} in the Base Experiment.

Probability of correct selection, $P\{CS\}$	Speedup factor of OCBAm over EA	Speedup factor of OCBAm+ over EA
90%	2.24	3.33
95%	2.78	5.30
99%	3.12	7.21

Table 3. 1. b Theoretical convergence rates in the Base Experiment.

Rule	EA	OCBAm	OCBAm+
Convergence Rate	0.50×10^{-4}	5.30×10^{-4}	6.59×10^{-4}

From figure 3.1 and table 3.1.a, we can see that the performance of OCBAm+ is the best and the performance of OCBAm is the second best among these three allocation rules. Moreover, the superiority of OCBAm+ over OCBAm and EA is significant. This experiment result is consistent with the theoretical comparison given in table 3.1.b.

3.7.2 Variants of the Base Experiment

We make some parameter changes in the Base Experiment, and build some different scenarios, whose parameter settings are shown in table 3.2.

Table 3. 2 Parameter settings for different scenarios.

Scenarios	m	k	Distribution of alternative *i*
Base Experiment	5	50	$N(i\ , 10^2)$
1 small size subset	2	50	$N(i\ , 10^2)$
2 small scale problem	5	10	$N(i\ , 10^2)$
3 monotone decreasing variance	5	50	$N(i, ((51\text{-}i)/4)^2)$
4 monotone increasing variance	5	50	$N(i,((i+10)/2)^2)$
5 convex decreasing means	5	50	$N(50-\sqrt{50}\times\sqrt{50-i}\ , 10^2)$
6 concave decreasing means	5	50	$N(50-\left((50-i)/\sqrt{50}\right)^2, 10^2)$
7 randomly generated means	5	50	$N(\text{rand}(0,50), 10^2)$

For every scenario in table 3.2, we run experiments and get the average total simulation replications needed for each allocation rule to make the probability of correct selection 90%. Based on these numbers of replications, we compute the speedup factor of OCBAm over EA and the speedup factor of OCBAm+ over EA in each scenario, which are given in table 3.3.a. Table 3.3.b shows the theoretical convergence rates of the three allocation rule under different scenarios.

Tables 3.3.a and 3.3.b show that OCBAm+ is the best performer among the three compared methods. Specifically, in Scenario 1 in which the value of *m* decreases from five to two, both the speedup factors and convergence rates of OCBAm and OCBAm+ become higher while the convergence rate of EA is still same. This indicates that OCBAm+ and OCBA can save more computing cost than EA as the size of optimal subset becomes higher. When the number of alternatives decreases in Scenario 2, the speedup factor of OCBAm+ lowers because a smaller alternative space allows the OCBAm+ algorithm less flexibility in allocating the computing budget.

Table 3.3. a Average Computing budget required for reaching 90% P{CS}

Scenarios	T for reaching 90% PCS			Speed-up factor of OCBAm over EA	Speed-up factor of OCBAm+ over EA
	EA	OCBAm	OCBAm+		
Base	17500	7800	5250	2.24	3.33
Scenario 1	17300	6150	4500	2.81	3.84
Scenario 2	4100	4050	2350	1.01	1.74
Scenario 3	21200	11750	6100	1.80	3.48
Scenario 4	10000	4650	3500	2.15	2.86
Scenario 5	60000	55500	16500	1.08	3.64
Scenario 6	5450	2950	2350	1.85	2.32
Scenario 7	140000	78500	22800	1.78	6.14

Table 3.3. b Theoretical convergence rates in different scenarios.

Scenarios	Convergence rate of EA	Convergence rate of OCBAm	Convergence rate of OCBAm+
Base Experiment	0.50×10^{-4}	5.30×10^{-4}	6.59×10^{-4}
Scenario 1	0.50×10^{-4}	5.46×10^{-4}	7.26×10^{-4}
Scenario 2	2.50×10^{-4}	6.44×10^{-4}	6.83×10^{-4}
Scenario 3	3.86×10^{-5}	4.13×10^{-4}	5.24×10^{-4}
Scenario 4	8.32×10^{-5}	8.40×10^{-4}	0.0010
Scenario 5	1.40×10^{-5}	1.48×10^{-4}	1.86×10^{-4}
Scenario 6	1.58×10^{-4}	0.0017	0.0021

Scenario 3 and Scenario 4 consider the different settings about alternatives variances. From table 3.3.a and table 3.3.b, we can see OCBAm+ is still the best one among these three allocation rules, regardless of variance increasing or decreasing. This indicates that the performance of OCBAm+ is quite robust to the changes of alternatives' variances.

Scenario 5, Scenario 6 and the Base Experiment are different settings about alternatives where the means for alternatives are convex, concave and linear functions with respect to the indices of alternatives. From table 3.3.b, in these three scenarios, convergence rates become lower in the convex case and higher in the concave case, relative to the linear case. This is because the means of alternatives within or near the optimal subset are closer to each other in the convex case than in the linear and concave cases. Thus, compared with the linear case, more computing budget is needed for the convex case to identify the alternatives belonging to the optimal subset, and less computing budget is needed for the concave case, which coincides with the result in table 3.3.a.

In scenario 7, the mean of each alternative sets to be a random number following the uniform distribution from 0 to 50. The performance is close to the performance in the base experiment, except it requires much more replications. In the tested scenarios with different settings of means (scenario 5, 6 and 7), OCBAm+ is always a better choice than OCBAm and EA.

From the numerical experiments in subsection 3.7.1 and 3.7.2, we can observe that both OCBAm+ and OCBAm are better than EA. Furthermore, OCBAm+ is the best allocation rule among these three allocation rules, not only in the linear mean and equal variance case, which has been shown in Theorem 3.3 and Theorem 3.4 from the perspective of the asymptotic convergence rate analysis, but also in some nonlinear mean situations and unequal variance situation such as scenario 3 to scenario 7. The superiority of OCBAm+ over OCBAm and EA is quite robust with the mean and variance settings of alternatives.

3.7.3 Numerical Results for Simulation Optimization

In this subsection, the OCBAm+ algorithm is tested under the simulation optimization setting, in which OCBAm+ is integrated with optimization methods, Cross-Entropy (CE) and Genetic Algorithm (GA). We apply OCBAm+ to allocate simulation runs to each solution at each iteration to select an elite subset which is used to generate new populations. The resulting performance is compared with the same optimization method using OCBAm and EA. We use the average true optimal function value obtained at each iteration over 200 independent experiments as a measurement of effectiveness.

The result is compared with algorithm combining CE and GA with OCBAm and EA. We use 2D Griewank function

$$f(X) = \frac{1}{4}\sum_{i=1}^{2} x_i^2 - \prod_{i=1}^{2}\cos\left(x_i / \sqrt{i}\right) + 1$$

and 2D Rosenbrock function

$$f(X) = 100\left(x_2 - x_1^2\right)^2 + \left(x_1 - 1\right)^2$$

as two testing functions. Both of these two functions have the optimal function value 0. The standard deviation of noise, set as 1, is added on these two functions. The searching result is shown by the following figure 3.2 and figure 3.3.

Figure 3. 2 Performance of CE and GA combining with allocation rules for 2D Griewank function.

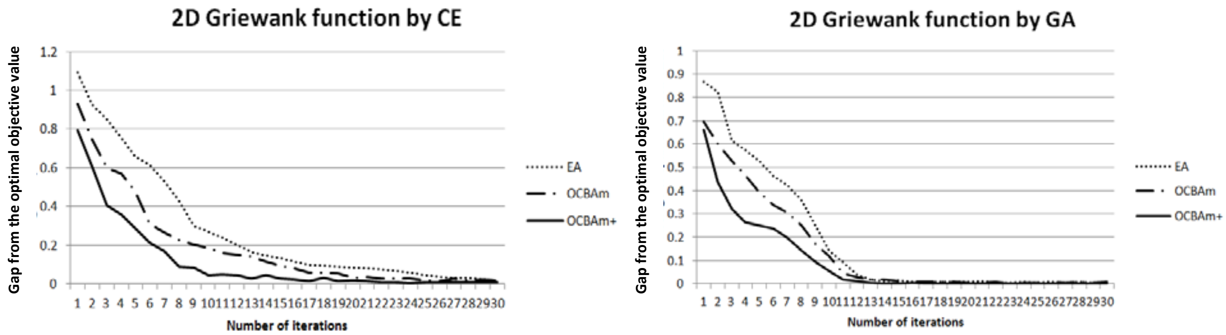
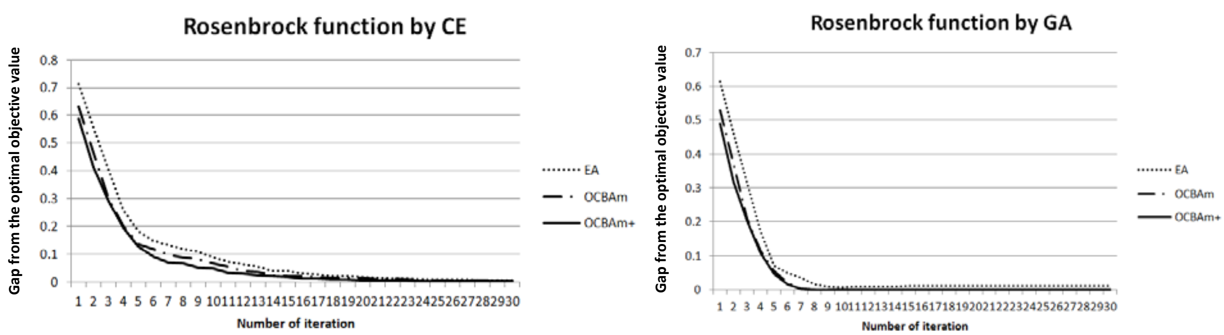


Figure 3. 3 Performance of CE and GA combining with allocation rules for Rosenbrock function.



From figure 3.2 and figure 3.3 we see that it is faster for the simulation optimization algorithms to obtain the global optimal value by integrating OCBAm+ compared with integrating OCBAm and EA. This implies that OCBAm+ enhances the efficiency of searching algorithms to find the best value of optimization problems when compared with OCBAm and EA for these two functions.

3.8 Conclusions and comments

Under the Optimal Computing Budget Allocation framework, we derived an improved allocation rule, OCBAm+, for optimal subset selection problems. Moreover, we presented a framework for asymptotic convergence rate analysis for optimal subset selection problems. This provided us with a theoretical tool for comparing different allocation rules besides traditional empirical testing. By numerical experiments, OCBAm+ seems to be the most efficient procedure for the optimal subset selection problem and its performance is quite good under many parameter settings.

However, the derivation for the allocation rule OCBAm+ is based on the assumption that the performance of each alternative in each replication is independent of each other. As the performance of each alternative sometimes are correlated such as the simulation with common random number, it is necessary for us to extend our study into the situation with correlation as described in the next chapter.

Chapter 4 Efficient computing budget allocation for optimal subset selection with correlated sampling

In this chapter, we generalize our work in chapter 3 into the problem with correlated sampling. Section 4.1 briefly introduces the problem and reviews the related literatures about R&S problems considering correlation. In section 4.2, we model the problem from the view of large deviation theory. Different allocation rules for different simplified cases are derived in section 4.3 and we test the performance of derived allocation rule in section 4.4. Section 4.5 concludes the whole chapter.

4.1 Introduction

In general, when we run simulation or design experiments, each replication of simulation or each trial is usually independent to each other. For the solutions or designs that with high variance, the total number of simulation replications or trials maybe very large to guarantee certain accuracy of estimation. Because the positive correlation can reduce the variance of the difference between two random variables, the correlation sometimes is introduced into simulation or design of experiments (DOE) to reduce the required number of simulation replications or trials. One popular technique is the one called common random numbers (CRN) which induces a positive correlation between the outputs of each system (Law and Kelton 2000, Banks et al. 2000). Because CRN provides more information during the comparisons between two systems without any computing cost of simulation, we apply it into simulation and study the ranking and selection problem with correlated sampling.

There are already some ranking and selection procedures developed for the best design selection problem incorporating common random numbers, such as Clark and Yang (1986), Nelson and Matejcik (1995), and Kim and Nelson (2001) all of which developed procedures based on the least favorable configuration (LFC), a common assumption for indifference zone procedures. However, this assumption will induce the high conservative property of the procedures because it cannot efficiently use the information of mean. Chick and Inoue (2001b) then considered the problem from the Bayesian framework and presented a two-stage procedure by using the value of information of measure which is further extended in Qu et al. (2012) by creating an optimal approximation of conjugacy and deriving a value of information procedure to capture the unknown correlation structures. Fu et al. (2007) studied the best design selection problem in the presence of correlated sampling under the OCBA framework proposed in Chen et al. (2000). The literature for the optimal subset selection problem under correlated sampling is little now. Since correlation usually exists in many real optimization problems and the optimal subset selection problem is worthy to be studied as shown in Chapter 3, we aim to extend the work in Chapter 3 to the more general situation considering correlation to fill this research gap.

In Fu et al. (2007), the study is for the best design selection and the allocation rule is derived based on the general OCBA framework that maximizes the probability of correct selection. Because of the presence of correlation, the derivation becomes more complex such as calculating the eigen-value of a matrix related to covariance. The value of information procedures in Chick and Inoue (2001) and Qu et al. (2012) from the Bayesian perspective is also not easily to implement. In this chapter, we want to not only extend the best design selection to the optimal subset selection under correlated sampling but also study the optimal computing budget allocation problem from the perspective of large deviation theory to simplify the complex derivation work induced by correlation.

4.2 Problem formulation from the perspective of large deviation theory

In this chapter, all notations have the same meaning with the definition in Chapter 3. The only difference is that we relax the assumption that the performance of each alternative in each replication is independent of each other and consider the correlated sampling here. We consider the optimal subset selection problem in the presence of correlated sampling case. Let X_{ij} denote the j^{th} simulation replication value of alternative i. We assume that $\{X_{ij}, i = 1, \dots, k, j = 1, \dots, N_i\}$ has a joint normal distribution, and

$$\operatorname{cov}\left(X_{is}, X_{jt}\right) = \begin{cases} 0, & \text{if } s \neq t \\ c_{ij}, & \text{if } s = t \end{cases}$$

in which $c_{ij} > 0$ to reduce the variance of the difference between two random variables.

Our aim is still to find the optimal allocation rule α^* such that the probability of correctly selecting m best solutions can be maximized under the total computing budget constraint. Thus, the problem can be formulated as follows.

$$\begin{aligned} &\max_{(\alpha_1, \alpha_2, \dots, \alpha_k)} \quad P\{CS\} \\ &s.t. \quad \sum_{i=1}^{m} \alpha_i = 1 \\ &\qquad\quad \alpha_i \geq 0 \end{aligned}$$

The goal maximizing the probability of correct selection is equivalent to minimize the probability of false selection, which goes to zero as $T \to \infty$ if $\alpha_i > 0$ for all i. For different allocation schemes of computing budget, the probability of incorrect selection approaches to zero with different speeds. Considering the computing efficiency, an allocation is preferred if it makes the probability of false selection converge to zero faster. It is therefore possible to use the convergence rate of the probability of false selection going to zero as a measure of the quality of allocation rules, which falls in the research area of large deviations theory. In chapter 3, we use large deviation theory to do analysis on the convergence rate of $P\{\text{IS}\}$. As a matter of fact, large deviation theory not only is a useful theory in the convergence rate analysis, but can also be used to derive the allocation rule for subset selection problem. The OCBA problems can be modeled from the large deviations perspective as below, where the objective is to find an allocation that can maximize the convergence rate of the probability of incorrect selection $P\{\text{IS}\}$ going to zero.

$$\begin{aligned} &\max_{(\alpha_1,\alpha_2,\dots,\alpha_k)} \quad \text{Convergence rate of P}\{\text{I}S\} \\ &s.t. \qquad \sum_{i=1}^{k}\alpha_i = 1 \\ &\qquad\qquad \alpha_i \geq 0 \end{aligned} \tag{4.1}$$

In model (4.1), the event incorrect selection means that the subset we selected based on sample means is not $\{1,2,\dots,m\}$. This event happens if the sample mean value of any designs from 1 to m is larger than the sample mean value of any designs from m+1 to k. So the probability of incorrect selection can be formulated as below.

$$P\{IS\} = P\left\{\bigcup_i\bigcup_j\left(\bar{X}_i \geq \bar{X}_j\right),\ \text{for i} = 1,2,\dots,m \text{ and j} = m+1, m+2,\dots,k\right\}.$$

As we discussed in chapter 3, the asymptotic convergence rate of $P\{\text{IS}\}$ have the following expression.

$$\lim_{T\to\infty}\frac{1}{T}\log P\{IS\} = -\min_{i\in S_1,\, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right).$$

This means that $P\{\text{IS}\}$ will decay exponentially with increasing T at a rate given by $-\min_{i\in S_1,\, j\in S_2} G_{ij}\left(\alpha_i,\alpha_j\right)$. The convergence rate of $P\{\text{IS}\}$ is represented by the slowest convergence rate among the many pair wise comparisons which could cause a false selection event. Therefore, model (4.1) can be transformed as the following expression from the perspective of large deviation theory.

$$\begin{aligned} \max \quad & z \\ s.t. \quad & G_{ij}\left(\alpha_i, \alpha_j\right) \geq z \\ & \sum_{i=1}^{k} \alpha_i = 1 \\ & \alpha_i \geq 0. \end{aligned} \tag{4.2}$$

Being different from the general OCBA model such as (3.5), the computing budget allocation model built from the perspective of large deviation theory avoids the approximation on the probability of correct selection. In addition, this formulation also simplifies the derivation work. If we build the OCBA model to maximize $P\{\text{CS}\}$, we need to develop the correlation matrix for designs' sample means and need to do the matrix calculation. It will be very complex. Fu et al. (2007) show the difficulty to get the allocation rule in general case even for the one best design selection problem.

4.3 Derivation of the allocation rules

In general, the expression of $G_{ij}\left(\alpha_i, \alpha_j\right)$ is difficult to be attained. Under the assumption of normal distribution, we can express it as follows by large deviation theory.

$$G_{ij}\left(\alpha_i, \alpha_j\right) = \frac{\left(\mu_i - \mu_j\right)^2}{2\left[\dfrac{\sigma_i^2}{\alpha_i} + \dfrac{\sigma_j^2}{\alpha_j} - 2\rho_{ij}\dfrac{\sigma_i \sigma_j}{\max\left(\alpha_i, \alpha_j\right)}\right]} \tag{4.3}$$

in which $\rho_{ij} = c_{ij} / \left(\sigma_i \sigma_j\right)$ is the correlation coefficient between alternative *i* and *j*.

We use Lagrangian method to derive the optimal asymptotical allocation rule for problem (4.2). The Lagrangian function of model (4.2) is

$$F(\alpha) = -z + \sum_{i=1}^{m} \sum_{j=m+1}^{k} \lambda_{ij} \left(z - G_{ij} \right) + v \left(\sum_{i=1}^{k} \alpha_i - 1 \right) - \sum_{i=1}^{k} h_i \alpha_i \ .$$

Applying KKT conditions, we can obtain the theorem below.

Theorem 4.1. *The allocation rule is asymptotically optimal for model (4.3) if it satisfies the following conditions:*

(a) $\sum_{j=m+1}^{k} \lambda_{ij} \frac{\partial G_{ij}}{\partial \alpha_i} = v$, $\forall i = 1,2,...,m$; $\sum_{i=1}^{m} \lambda_{ij} \frac{\partial G_{ij}}{\partial \alpha_j} = v$, $\forall j = m+1, m+2,...,k$.

(b) $\lambda_{ij} \left(z - G_{ij} \right) = 0$, $\forall i = 1,2,...,m$; $j = m+1, m+2,...,k$

(c) $\sum_{i=1}^{k} \alpha_i = 1$

(d) $\alpha_i > 0 \ \ \forall i = 1,2,...,k$

(e) $\lambda_{ij} \geq 0$, $\forall i = 1,2,...,m$; $j = m+1, m+2,...,k$.

We can find from the model and Theorem 4.1 that it is a multiple comparison problem and $G_{ij}\left(\alpha_i, \alpha_j\right)$ is a nonlinear function of allocation rule. Thus, it is very difficult, or even impossible, to get a closed form expression of the optimal allocation rule from this model. Some nonlinear programming solvers can be applied to get the numerical values of the optimal allocation rule for a given parameter setting.

However, with some assumptions and approximation made to the optimization models, we are able to derive the closed-form allocation rule and this rule will be easier to implement in practice.

In the next few subsections, we will show how these rules can be derived under different scenarios and assumptions.

4.3.1 Allocation rule for two alternatives

In the case of two alternatives, the model (4.2) can be simplified to

$$\max \quad \frac{(\mu_1-\mu_2)^2}{2\left[\frac{\sigma_1^2}{\alpha_1}+\frac{\sigma_2^2}{\alpha_2}-2\rho\frac{\sigma_1\sigma_2}{\max(\alpha_1,\alpha_2)}\right]} \quad \text{subject to } \alpha_1+\alpha_2=1,\ \alpha_i\ge 0. \tag{4.4}$$

in which ρ is the correlation coefficient between two alternatives.

For derivation convenience, we introduce the ratio $r=\sigma_1/\sigma_2$ and assume $r\ge 1$. If $\sigma_1<\sigma_2$, we just need to change the roles of alternative 1 and alternative 2. We make an assumptions that there exists the optimal rule for (4.4) that satisfies $\alpha_1\ge\alpha_2$. Take the first order derivative of the objective in (4.4) with respect to α_1,

$$\frac{d}{d\alpha_1}G_{12}=\frac{(\mu_1-\mu_2)^2\left[\frac{\sigma_1^2-2\sigma_1\sigma_2\rho_{12}}{\alpha_1^2}-\frac{\sigma_2^2}{\alpha_2^2}\right]}{2\left[\frac{\sigma_1^2}{\alpha_1}+\frac{\sigma_2^2}{\alpha_2}-2\rho_{12}\frac{\sigma_1\sigma_2}{\max(\alpha_1,\alpha_2)}\right]^2}.$$

Let it equal zero, we can get the formula below.

$$\frac{\alpha_1^2}{\alpha_2^2}=r^2-2r\rho_{12}. \tag{4.5}$$

Because $\alpha_1\ge\alpha_2$, the equation (4.5) exists only when $r^2-2r\rho_{12}\ge 1$, that is $r-\frac{1}{r}\ge 2\rho$. Substituting α_2 by $1-\alpha_1$, we can get

$$\alpha_1 = \frac{\sqrt{r(r-2\rho)}}{1+\sqrt{r(r-2\rho)}} \quad \text{when } r - \frac{1}{r} \geq 2\rho .$$

For the situation $r - \frac{1}{r} \leq 2\rho$, we have

$$\frac{d}{d\alpha_1} G_{12} \leq 0 .$$

Because the derivative is negative, G_{12} is an decreasing function of α_1. So the maximum value of G_{12} can be obtained when $\alpha_1 = \alpha_2$. Therefore, the assumption there exists the optimal rule for (4.4) that satisfies $\alpha_1 \geq \alpha_2$ is established. Based on the above analysis, we can get Lemma 4.1.

Lemma 4.1. The optimal allocation rule for the model (4.4) is

(a) For $r = \sigma_1/\sigma_2 \geq 1$

$$(\alpha_1, \alpha_2) = \begin{cases} \left(\frac{\sqrt{r(r-2\rho)}}{1+\sqrt{r(r-2\rho)}}, \frac{1}{1+\sqrt{r(r-2\rho)}} \right) & \text{if } r - \frac{1}{r} \geq 2\rho \\ \left(\frac{1}{2}, \frac{1}{2} \right) & \text{if } r - \frac{1}{r} \leq 2\rho \end{cases}$$

(b) For $r = \sigma_1/\sigma_2 \leq 1$

$$(\alpha_1, \alpha_2) = \begin{cases} \left(\frac{1}{1+\sqrt{\frac{1}{r}\left(\frac{1}{r}-2\rho\right)}}, \frac{\sqrt{\frac{1}{r}\left(\frac{1}{r}-2\rho\right)}}{1+\sqrt{\frac{1}{r}\left(\frac{1}{r}-2\rho\right)}} \right) & \text{if } r - \frac{1}{r} \geq 2\rho \\ \left(\frac{1}{2}, \frac{1}{2} \right) & \text{if } r - \frac{1}{r} \leq 2\rho \end{cases}$$

From Lemma 4.1, we also can conclude that the optimal allocation rule for two alternatives when there is no correlation (i.e. $\rho = 0$) is

$$\frac{\alpha_1}{\alpha_2} = \frac{\sigma_1}{\sigma_2}.$$

The allocation rule indicates that the computing budget allocation is only determined by the variance of each solution when the performance is independent to each other. The solution with higher variance should be given more simulation replications. When there exists correlated sampling between designs, the allocation rule depends both on the variance and covariance coefficient. One special thing for the correlated situation is that, if *r*=1, the simulation replications allocated to each one is always the same no matter what the value of ρ.

4.3.2 Allocation rule for best design selection (m=1)

When m equals one, the optimal subset selection problem reduces to the best design selection problem and the OCBA model (4.2) can be simplified as follows respectively.

$$\begin{aligned} \max \quad & z \\ s.t. \quad & G_{1i}\left(\alpha_1, \alpha_i\right) \geq z \\ & \sum_{i=1}^{k} \alpha_i = 1 \\ & \alpha_i \geq 0. \end{aligned} \tag{4.6}$$

From the model, we can see that alternative 1 is very important because all the other solutions are compared with it. So we make a reasonable assumption that there exists an optimal allocation rule for model (4.6) which satisfies $\alpha_1 > \alpha_i, \ \forall i \neq 1$.

Based on Theorem 4.1, we have the lemma below for the best design selection problem.

Lemma 4.2. *The allocation rule for model (4.6) is asymptotically optimal if it satisfies the following conditions:*

(a) $\sum_{i=2}^{k} \frac{\partial G_{1i} / \partial \alpha_1}{\partial G_{1i} / \partial \alpha_i} = 1$

(b) $G_{1i} = G_{1j} \;\; \forall i, j \neq 1$

(c) $\sum_{i=1}^{k} \alpha_i = 1$

(d) $\alpha_i > 0 \;\; \forall i = 1, 2, ..., k$

Under this assumption $\alpha_1 > \alpha_i \;\; \forall i \neq 1$, we have

$$G_{1i}\left(\alpha_1, \alpha_i\right) = \frac{\left(\mu_1 - \mu_i\right)^2}{2\left[\frac{\sigma_1^2 - 2\sigma_1\sigma_i\rho_{1i}}{\alpha_1} + \frac{\sigma_i^2}{\alpha_i}\right]}, \tag{4.7}$$

$$\frac{\partial G_{1i}}{\partial \alpha_1} = \frac{\left(\mu_1 - \mu_i\right)^2 \left(\frac{\sigma_1^2 - 2\sigma_1\sigma_i\rho_{1i}}{\alpha_1^2}\right)}{2\left[\frac{\sigma_1^2 - 2\sigma_1\sigma_i\rho_{1i}}{\alpha_1} + \frac{\sigma_i^2}{\alpha_i}\right]^2}, \tag{4.8}$$

$$\frac{\partial G_{1i}}{\partial \alpha_i} = \frac{\left(\mu_1 - \mu_i\right)^2 \left(\frac{\sigma_i^2}{\alpha_i^2}\right)}{2\left[\frac{\sigma_1^2 - 2\sigma_1\sigma_i\rho_{1i}}{\alpha_1} + \frac{\sigma_i^2}{\alpha_i}\right]^2}. \tag{4.9}$$

Substituting (4.8) and (4.9) into Lemma 4.2(a), the relationship between α_1 and others can be expressed by

$$\alpha_1 = \sqrt{\sum_{i=2}^{k} \frac{\sigma_1^2 - 2\sigma_1\sigma_i\rho_{1i}}{\sigma_i^2}\alpha_i^2} \quad . \tag{4.10}$$

From (4.10), we can see that the computing budget allocated to the best solution is the square root of the weighted sum of other solutions' square. Hence, our assumption is established. If we strengthen this assumption to $\alpha_1 >> \alpha_i \ \forall i \neq 1$, we can also find the closed-form expression for relationship among other designs by Lemma 4.2(b) and (4.7), that is,

$$\frac{\alpha_x}{\alpha_y} = \left(\frac{\sigma_x/\delta_x}{\sigma_y/\delta_y}\right)^2 \text{ in which } \delta_x = \mu_1 - \mu_x \text{ and } x, y \neq 1. \tag{4.11}$$

Therefore, we make the conclusion in Lemma 4.3.

Lemma 4.3. *Assuming $\alpha_1 >> \alpha_i \ \forall i \neq 1$, the optimal allocation rule for the best design selection under correlated sampling is (4.10) and (4.11).*

Note that, when there is no correlation applied, the optimal rule we derived above can be directly reduced to the OCBA1 allocation rule in Chen et al. (2000).

4.3.3 Allocation rule for the optimal subset selection (m>1)

The model (4.2) for general optimal subset selection problem contains multiple pair-wise comparisons between solutions. Therefore, it is difficult to develop the closed-form allocation rule for it. One way to tackle this difficulty is making some approximations to simplify the model.

Being inspired by the idea in deriving OCBAm+ in chapter 3 that employs solution m and m+1 as two thresholds to establish the approximated probability of correct selection, we can assume that $G_{ij}\left(\alpha_i,\alpha_j\right) \geq \min\left(G_{mj}\left(\alpha_m,\alpha_j\right), G_{i(m+1)}\left(\alpha_i,\alpha_{(m+1)}\right)\right) \quad \forall i, j \neq m, m+1$ and $\alpha_m, \alpha_{m+1} >> \alpha_i$ $\forall i \neq m, m+1$ because the false selection probability $P\left\{\bar{X}_i \geq \bar{X}_{m+1}\right\}$ for $i \leq m$ and $P\left\{\bar{X}_m \geq \bar{X}_j\right\}$ for $j \geq m+1$ are usually higher than other $P\left\{\bar{X}_i \geq \bar{X}_j, \text{ for i} = 1,2,\ldots,m-1 \text{ and j} = m+2,\ldots,k\right\}$ when the variances of solutions do not have very obvious difference. So the computing budget allocation model can be transformed into

$$\begin{aligned}
&\max \quad z \\
&s.t. \quad G_{i(m+1)}\left(\alpha_i,\alpha_{m+1}\right) \geq z \;\; \forall i = 1,2,...,m \\
&\qquad\; G_{mj}\left(\alpha_m,\alpha_j\right) \geq z \qquad \forall j = m+1, m+2,...,k \\
&\qquad\; \sum_{i=1}^{k} \alpha_i = 1, \;\; \alpha_i \geq 0.
\end{aligned} \tag{4.12}$$

Similarly, we can obtain the following lemma for model (4.12) based on Theorem 4.1.

Lemma 4.4. *The allocation rule is asymptotically optimal for problem (4.12) if it satisfies the following conditions*:

(a) $\sum_{j=m+2}^{k} \frac{\partial G_{mj} / \partial \alpha_m}{\partial G_{mj} / \partial \alpha_j} = 1$ and $\sum_{i=1}^{m-1} \frac{\partial G_{i,m+1} / \partial \alpha_{m+1}}{\partial G_{i,m+1} / \partial \alpha_i} = 1$

(b) $G_{mj} = G_{i(m+1)} \quad \forall i = 1,2,...,m \;\; \forall j = m+1, m+2,...,k$

(c) $\sum_{i=1}^{k} \alpha_i = 1$

(d) $\alpha_i > 0 \;\; \forall i = 1,2,...,k$

By taking the partial derivative of G_{ij} and substituting the result into Lemma 4.4, the following closed-form allocation rule, named as OCBAm-cov, can be gained.

Lemma 4.5. *The following allocation rule, named as OCBAm-cov, is asymptotically optimal for problem (4.12).*

(a) $\alpha_m = \sqrt{\sum_{j=m+2}^{k} \frac{\sigma_m^2 - 2\sigma_m \sigma_j \rho_{mj}}{\sigma_j^2} \alpha_j^2}$ and $\alpha_{m+1} = \sqrt{\sum_{i=1}^{m-1} \frac{\sigma_{m+1}^2 - 2\sigma_{m+1}\sigma_i \rho_{i,m+1}}{\sigma_i^2} \alpha_i^2}$

(b) $\frac{\alpha_x}{\alpha_y} = \left(\frac{\sigma_x / \delta_x}{\sigma_y / \delta_y} \right)^2$ in which $\delta_x = \mu_{m+1} - \mu_x$ if $x \le m-1$ and $\delta_x = \mu_x - \mu_m$ if $x \ge m+2$.

4.3.4 Sequential allocation procedure

The allocation rules in Lemma 4.1, Lemma 4.3 and Lemma 4.5 are functions of the means, variances and covariance coefficients, which are unknown in practice. A sequential procedure is developed in this section to approximately estimate these parameters and implement the allocation rules. Each design is initially simulated with n_0 replications in the first stage, and additional replications are allocated to individual designs incrementally from Δ replications to be allocated in each subsequent stage until the simulation budget T is exhausted. In summary, we have the following algorithm.

Algorithm OCBA Procedure for the optimal subset selection problem with correlated sampling

---

INTIALIZE Let n equal to $n_0 k$; Set $N_1^n = N_2^n = \cdots = N_k^n = n_0$ and $T^n = \sum_{i=1}^{k} N_i^n$; Perform n_0 replications for all alternatives. Calculate sample mean, sample variance and covariance of each alternative.

LOOP **WHILE** $T^n < T$ **DO**

UPDATE Calculate sample mean of each alternative to estimate its true mean.

ALLOCATE Add Δ replications to T^n; Calculate the new computing replications allocated to each design according to Lemma 4.1, Lemma 4.3, or Lemma 4.5 based on different situations; Get the value of $N_1^{n+1}, N_2^{n+1}, \ldots, N_k^{n+1}$ and round them to the integers nearest to their values.

SIMULATE Set $N_i^{n+1} = \max\left(N_i^n, N_i^{n+1}\right)$ and $T^{n+1} = \sum_{i=1}^{k} N_i^{n+1}$; Perform additional $N_i^{n+1} - N_i^n$ replications of design *i*, *i=1,…,k*; Set n=n+1;

END OF LOOP

OUTPUT Select the alternatives whose performances' means are less than the *(m+1)*th smallest sample mean into the optimal subset and end the procedure.

Note that sample means and sample variances are consistent estimators of means and variances, which means that sample means and sample variances goes the true mean and variance as the *T* goes to infinity. Consequently, the sample allocation based on the sequential algorithm is also a consistent estimator of the allocation rule we derived.

4.4 Numerical Experiments

In this section, we provide numerical results to demonstrate the effectiveness of the allocation rule OCBAm-cov in the previous section. The probability of correct selection $P\{CS\}$ is used as the performance measurement of these two methods and is estimated by the fraction of times the procedure successfully finds all the true m-best designs. We set Δ equals to 50 and n_0 equals to

20 in all numerical experiment. To compare OCBAm-cov with EA, we gradually increase T to a maximum of 1,000 simulation samples and report the value of $P\{\text{CS}\}$.

We want to select top-3 solutions from 10 alternatives, with distribution shown in table 4.1 for different scenarios. For each scenario, three level of covariance coefficient are tested. The value of $P\{\text{CS}\}$ for each scenario after the total computing budget are allocated is present in table 4.2.

Table 4. 1 Parameter settings for different scenarios.

Scenarios	Distribution of alternative *i*
1 Basic experiments	$N(10\text{-}i\ ,\ 6^2)$
2 convex decreasing means	$N(10-\sqrt{10}\times\sqrt{10-i}\ ,\ 6^2)$
3 concave decreasing means	$N(10-\left((10-i)/\sqrt{10}\right)^2,\ 6^2)$
4 randomly generated parameters	N(rand(0,10), rand(24,36))

Table 4. 2 The value of P{CS} after 1,000 replications.

Scenarios	ρ =50%		ρ =70%		ρ =90%	
	EA	OCBAm-cov	EA	OCBAm-cov	EA	OCBAm-cov
Scenario 1	0.825	0.921	*0.856*	*0.960*	*0.992*	*0.999*
Scenario 2	*0.762*	*0.845*	*0.841*	*0.923*	*0.947*	*0.971*
Scenario 3	*0.863*	*0.957*	*0.914*	*0.982*	*0.998*	*1.000*
Scenario 4	0.713	0.782	*0.827*	*0.905*	*0.912*	*0.945*

From table 4.2, we can see the performance of OCBAm-cov is always better for EA in all the tested scenarios. In addition, the higher level correlation between solutions, the higher value of $P\{\text{CS}\}$ can be attained. This shows the computing cost saving by applying common random number into simulation.

4.5 Conclusions

In this chapter, we generalize the problem of subset selection by considering correlation, and all the single best, subset and single best with correlation become a special case. The computing budget allocation model for this problem is built based on the large deviation theory. The objective of the model is maximizing the convergence rate of the incorrect selection probability decreasing to zero instead of maximizing the probability of correct selection in general OCBA model. Under this framework, we derived the closed form allocation rules OCBAm-cov based on some mild assumptions. The numerical result shows that OCBAm-cov does help in saving the computing cost compared with EA.

Chapter 5 Particle Swarm Optimization with Optimal Computing Budget Allocation for Stochastic Optimization

In this chapter, we integrate the OCBA framework into a population-based simulation optimization technique called particle swarm optimization (PSO) to demonstrate the way tackling the simulation optimization problems with continuous or enormous sized solution spaces by OCBA. The background is roughly reviewed in section 5.1. In section 5.2, we introduce the general simulation optimization problem setting and give a brief introduction to PSO. Section 5.3 formulates the PSOOCBA problem and proposes an optimal allocation for both versions of PSO. In section 5.4, we present some numerical experiments comparing the implementations with equal allocation, which is followed by the conclusion in section 5.5.

5.1 Introduction

The OCBA procedures are only suitable for simulation optimization problems whose solution spaces are discrete, bounded and within certain size. The reason is that every solution should be given before the implementation of OCBA procedures and OCBA procedures allocate every solution certain replications at the initial stage to get a general idea about these solutions. If the solution space is of enormous size, continuous, or even unbounded, the total required computing replications will be prohibitively high. On the other hand, many search algorithms have been proposed to search good solutions to tackle the simulation optimization problems with continuous or enormous sized solution spaces. However, these methods seldom consider the computing efficiency for executing them.

In the search process, search algorithms need to repeatedly evaluate and compare candidate solutions to decide the next search direction. In this evaluation and comparison step, we already know the solutions required to be compared and the total number of candidate solutions at each iteration is relatively small, so OCBA can be applied to enhance the simulation efficiency of this step. Therefore, the integration of OCBA and search algorithms is better than OCBA or search algorithm individually in dealing with difficult simulation optimization problems. We aim to do some contribution work about integrating OCBA with search algorithms to solve simulation optimization problems having huge solution space by using particle swam optimization.

Particle Swarm Optimization (PSO) is one of popular population-based evolutionary techniques for optimization problems. Inspired by the idea of swarm intelligence and the evolutionary computation concept, Kennedy and Eberhart (1995) developed the basic model for PSO and facilitated PSO's application in optimization problems. In this version of PSO, a swarm is formed by certain number of particles. Each particle moves from one solution in the search space to another based on the location information of both the best solution that it has visited personally (personal best) and the best solution that is visited by any of the particles that this particle can communicate with (global best). To control the balance between exploration and exploitation, Shi and Eberhart (1998) and Clerc and Kennedy (2002) introduced the inertia weight and the constriction factor respectively into the update equation of velocity to improve the basic PSO model. These three papers build the basic framework for the canonical PSO (Bratton and Kennedy 2007). Because of the advantages of derivative-free, black-box methods, PSO has become a popular research topic and has been studied from many aspects. Many excellent reviews are available (see, for instance, Bratton and Kennedy 2007, Branks et al. 2007, 2008).

For all this development work on PSO, the main body has concentrated on optimization in deterministic environment. However, many realistic optimization problems are stochastic. Although there is little theoretical research about stochastic PSO, several numerical experiments that apply PSO to real problems, such as power systems (AlRashidi and El-Hawary 2009; Valle et al. 2008), have been done in a stochastic environment. The primary challenge for stochastic problems is the stochastic nature of evaluating the fitness value. Unlike deterministic optimizations, "once" is not enough since the fitness function estimate is noisy in stochastic settings. A general way is to take more than one sample for each solution and employ the sample mean of the fitness value as a measure to evaluate the quality of the solution. Hence, the number of simulation samples taken for each solution becomes a key issue because it determines the accuracy of evaluation. To make the evaluation of fitness values accurate, a large number of samples is required, which is time consuming. On the other hand, if we relax the requirement on accuracy, the high noise may decrease the algorithm's ability to identify global best and personal best and then sacrifice the search efficiency of PSO.

Traditionally, a large but constant number of samples are taken for all the particles generated in an iteration. If we treat computing effort as a resource and particles as demanders, most current work on the application of PSO to stochastic problems use equal resource allocation. The focus of this chapter is to develop an effective way to intelligently determine the number of samples for all solutions such that the PSO algorithm can efficiently select the personal best and global best when stochastic estimation noise is present. Given the popularity of PSO in deterministic optimization and the efficiency of OCBA in stochastic sampling, some researchers have proposed the integration of PSO with OCBA for stochastic optimization problems. Pan et al. (2006) directly applied the OCBA allocation rule in Chen et al. (2000) to PSO and obtain some improvement in computational efficiency. Horng et al. (2012) also directly employed the OCBA in Chen et al. (2000) with PSO as a two-stage algorithm and apply it to a wafer probe testing problem in semiconductor manufacturing. However, the OCBA in Chen et al. (2000) is designed to select the best one from certain number of alternatives. In PSO, we need to select not only the best one (global best) but also the personal best for each particle. Therefore, the direct application of OCBA in Chen et al. (2000) into PSO as shown Pan et al. (2006) and Horng et al. (2012) may cannot satisfy the actual requirement of PSO. Instead of directly applying the existing OCBA, we want to satisfy the real demand of PSO by considering the selection of both global best and personal best in PSO. Our aim is to derive a new computing effort allocation rule specifically for PSO.

5.2 Problem Setting

5.2.1 Basic Notations

We introduce the following notation.

Θ: continuous search space.

X : a feasible solution in Θ.

X_i : the location of the *i*-th solution.

m: number of particles in the swarm.

$f(X)$: the mean fitness value of the solution of X .

$\omega_j(X)$: the simulation noise at the *j*-th sample. We assume $\omega_j(X)$ is independently and normally distributed with zero mean and finite variance σ_j^2.

$\hat{f}_j(X)$: the sampled fitness value of X estimated at the *j*-th replication, that is, $\hat{f}_j(X) = f(X) + \omega_j(X)$ and $E\left[\hat{f}_j(X)\right] = f(X)$.

$\bar{f}(X)$: the sample mean after N simulation replications, $\bar{f}(X) = (1/N)\sum_{j=1}^{N}\hat{f}_j(X)$.

The general optimization problem can be expressed as follows.

$$\min_{X \in \Theta} f(X).$$

In the stochastic problem, the mean performance of a solution, $f(X)$, is estimated by the sample mean $\bar{f}(X)$. As we take more samples, $\bar{f}(X)$ estimates $f(X)$ more accurately. While it is impossible to have an infinite number of samples taken in practice, we aim to investigate how we should allocate the finite computing budget in a more efficient way for PSO for simulation optimization problems. Although there are different versions of PSO, the main objective of this chapter is to show that the efficiency of PSO can be significantly enhanced via OCBA framework, rather than to identify a best PSO algorithm.

5.2.2 Particle Swarm Optimization

Particle Swarm Optimization (PSO) was originally inspired by the social behavior of bird flocking for a food source and then was extended for solving non-linear optimization problems. After that, different versions of PSO improvement methods have been developed for different requirements. Bratton and Kennedy (2007) summarize these versions of PSO and define a standard PSO algorithm for providing a baseline for performance testing of improvements. Therefore, we employ the standard PSO as the basic version in our study.

One basic concept in PSO is swarm, which is formed by a certain number (suppose *m*) of particles. It can be thought that each particle "flies" through the fitness landscape finding the minimum of the mean fitness function. We use $X_i^t = \left(x_{i1}^t, x_{i2}^t, \ldots, x_{iD}^t\right)$, $i = 1, 2, \ldots, m$, to denote the location of a particle *i* at the *t*-th iteration in the solution space with D dimensions. The location of particle *i* at the (*t+1*)-th iteration is determined by updating the velocity $V_i^{t+1} = \left(v_{i1}{}^{t+1}, v_{i2}{}^{t+1}, \ldots, v_{iD}{}^{t+1}\right)$, which is related to the velocity V_i^t, the personal best, denoted by $P_i^t = \left(p_{i1}{}^t, p_{i2}{}^t, \ldots, p_{iD}{}^t\right)$, and the global best, denoted by $P_g{}^t = \left(p_{g1}{}^t, p_{g2}{}^t, \ldots, p_{gD}{}^t\right)$, at the *t*-th iteration.

The personal best of particle *i* at the *t*-th iteration is defined as the location of this particle's own previous best performance, that is, $P_i^t = \arg\min_{X_i^l, l=1,2,\ldots,t} f\left(X_i^l\right)$ and the global best is defined as the best solution that any particle in the swarm has found, that is, $P_g^{\,t} = \arg\min_{X_i^l,\ \text{for } l=1,\ldots,t; i=1,\ldots,m} f\left(X_i^l\right)$ which is the same with $P_g^{\,t} = \arg\min_{p_i^t,\ i=1,\ldots,m} p_i^t$. For each dimension *d* ($d = 1,2,\ldots,D$), the standard PSO updated velocity and location are

$$v_{id}^{\;t+1} = \chi\left(v_{id}^{\;t} + c_1\varepsilon_1\left(p_{id}^{\;t} - x_{id}^{\;t}\right) + c_2\varepsilon_2\left(p_{gd}^{\;t} - x_{id}^{\;t}\right)\right) \tag{5.1}$$

$$x_{id}^{\;t+1} = x_{id}^{\;t} + v_{id}^{\;t+1} \tag{5.2}$$

In (5.1), χ is the constrictive factor to cause convergence and guarantee the particles moving within the range of the solution space. c_1 and c_2 are two constants to control the balance between convergence speed to local best and the convergence speed to global best. ε_1 and ε_2 are two independent uniformly distributed random numbers which add some level of randomness to the search in order to avoid getting stuck in local optimum. The whole algorithm of PSO for deterministic problems can be summarized as follows.

Algorithm.	Particle Swarm Optimization Algorithm
Initialization	Select *m* solutions throughout the search space in a uniform random manner as the initial starting locations for *m* particles; velocity is also randomly initialized. Based on their performance, get the initial personal best and global best. Set t=1;
Updating	For each particle *i* in the swarm do Update position for each $i = 1,2,\ldots,m$ using (5.1) and (5.2); Calculate these new particles' fitness values $f(X_i^{\,t})$;

Update P_g^t and P_i^t;

end for

STOP If stopping criteria is satisfied, stop; otherwise set t=t+1. Else loop to step Updating.

Based on the standard PSO, we introduce another version of PSO, called PSO with elite set method (PSOe). PSOe classifies all particles into the elite set and the non-elite set according to the fitness values of these particles. The elite set at t-th iteration, S_e^t (assume $|S_e| = h$), contains the best h particles among all m particles,

$$S_e^t \equiv \left\{ X_i^t \middle| f\left(X_i^t\right) \le f\left(X_j^t\right),\ \forall X_i^t \in S_e^t, X_j^t \notin S_e^t \right\}.$$

The personal best for each particle at t-th iteration has the following definition.

$$P_i^t = \begin{cases} X_i^t, & \text{if } X_i^t \in S_e^t \\ \arg\min_{X_j^t \in S_e^t} \left\| X_j^t - X_i^t \right\|, & \text{if } X_i^t \notin S_e^t \end{cases}$$

For a particle within the elite set, its personal best is itself while the personal best of a particle outside of S_e is the particle in the S_e nearest to it. The definition of global best is the same with standard PSO, that is, $P_g^t = \arg \min_{p_i^t,\ i=1,\dots,m} p_i^t$. The updating equations and the algorithm of PSOe is the same as the standard PSO except for the different definition of personal best.

Note that we do not introduce PSOe to make a direct comparison between PSOe and the standard PSO. Instead, our purpose is to demonstrate that efficiency can be significantly improved by using an optimal computing budget allocation no matter which version of PSO is employed.

5.3 PSOOCBA Formulation

Unlike deterministic problems in which a particle's true fitness value can be calculated using one single evaluation, the mean fitness value in stochastic problems is estimated via Monte Carlo sampling of multiple evaluations. Although the true mean value is usually unknown in a stochastic environment, the sample mean, an unbiased estimator, can be employed to estimate the mean fitness value of each particle. On each iteration, a certain number of samples will be allocated to particles to calculate their sample means and then determine the personal best and global best. If we do not have enough samples for particles, the sample mean may not be a good estimate of the true mean. As a result, the algorithm may select an incorrect global best and an incorrect personal best, which will lead all particles in wrong directions. Therefore, in applying PSO to stochastic problems, the correct selection of personal best and global best has significant impact on the performance of PSO. Because the accuracy of sample means determines the correctness of selecting global best and personal best, how to allocate these samples to each particle to improve the probability of correctly selecting personal best and global best is an important task for PSO in stochastic problems.

Intuitively, the particles that have the major effect on updating the velocity and location should be given more samples so as to ensure all particles moves in a correct direction. Instead of giving each particle equal samples, as most PSO algorithms do, we develop the optimal computing budget allocation scheme for PSO in this part.

For the stochastic case, a quantitative measure to evaluate the correctness of selection is the probability of correct selection. To ensure that PSO performs well on stochastic problems, we want the probability of correctly selecting global best and personal best to be as high as possible. The following proposed procedure tries to determine the allocation of samples that maximizes the probability of correctly selecting global best and personal, which is equivalent to minimizing the probability of incorrect selection.

$$\min_{N_1,\ldots,N_k} P\{\text{incorrect selection of personal best and global best}\} \text{ subject to } N_1 + N_2 + \ldots. + N_k = T$$

Because different versions of PSO have different definitions of personal best and global best, the expressions of $P\{\text{CS}\}$ (or $P\{\text{IS}\}$) are different, as are the optimal ways of allocating samples. In the next two sub-sections, we derive optimal allocation rules for two versions of PSO and propose an easy-to-implement heuristic sequential allocation procedure.

5.3.1 Computing budget allocation for Standard PSO

In standard PSO, the personal best of one particle is defined as the best among the solutions that this particle has visited, and the global best is the best among the solutions that all particles in the swarm have visited. Based on the updating of personal best and global best, we define three sets for research convenience. They are

$$S_A = \left\{X_i^{\,t} : f\left(X_i^{\,t}\right) < f\left(P_i^{t-1}\right)\right\},\ S_B = \left\{X_i^{\,t} : f\left(X_i^{\,t}\right) > f\left(P_i^{t-1}\right)\right\}, \text{ and } S_G = \left\{X_i^{\,t} : f\left(X_i^{\,t}\right) \le f\left(P_g^{\,t-1}\right)\right\}.$$

In the above subsets, S_A and S_B are mutually exclusive, denoting, respectively, the set of particles whose personal best should be changed and the set of particles whose personal best do not need to be updated at *t*-th iteration. The subset S_G indicates whether the global best should be changed or not. If S_G is empty, the global best of this iteration $P_g^{\,t}$ is the same as the last iteration $P_g^{\,t-1}$. If S_G is nonempty, the best particle at this iteration should be the new global best, that is, $P_g^{\,t} = X_b^{\,t}$ in which $X_b^{\,t}$ is the best particle at the *t*-th iteration, that is, $f\left(X_b^{\,t}\right) \le \min_{i \ne b} f\left(X_i^{\,t}\right)$.

To build the computing budget allocation model for the standard PSO, the expression of $P\{\text{IS}\}$ must be derived. We discuss it case by case.

We first consider the situation $S_G = \Phi$. The event $S_G = \Phi$ indicates that $P_g^{\,t}$ should be equal to $P_g^{\,t-1}$. If there is any particle X_i^t , whose sample mean value is less than the sample mean value of $P_g^{\,t-1}$, $P_g^{\,t}$ will be incorrectly updated by the particle with minimum sample mean value instead of $P_g^{\,t-1}$. In this case, the selection of global best is incorrect. All particles in the set S_A should update their personal best, while the particles in S_B , whose personal best is P_i^{t-1} should not update. If the sample mean value of any particles in S_A is larger than its previous personal best sample mean, or the sample mean of any particles in S_B is smaller than its personal best sample mean, the selection of personal best is incorrect. Hence, the probability of incorrect selection in the situation $S_G = \Phi$ can be formulated as

$$P\{IS\} = P\{\left[\bigcup_{i \in S_A}\left[\left(\bar{f}\left(X_i^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right) \cup \left(\bar{f}\left(X_i^{\,t}\right) \ge \tilde{f}\left(P_i^{t-1}\right)\right)\right]\right] \cup \left[\bigcup_{j \in S_B}\left[\left(\bar{f}\left(X_j^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right) \cup \left(\bar{f}\left(X_j^{\,t}\right) \le \tilde{f}\left(P_j^{\,t-1}\right)\right)\right]\right]\} \qquad (5.3)$$

in which $\bar{f}(\cdot)$ is a random variable, denoting the sample mean fitness, and $\tilde{f}(\cdot)$ is a realized value of a sample mean from a previous iteration.

By the (*t-1*)-th iteration, we have the observed values of the sample means of $P_g^{\,t-1}$ and P_i^{t-1}, but we have no information about the mean fitness values of particles in the current iteration. Therefore, the key issue is to allocate computing effort to these particles to obtain information about their sample means. On the other hand, the accuracy of the sample means of global best and personal best at the (*t-1*)-th iteration is also important. Hence, it is also necessary to allocate some additional samples to $P_g^{\,t-1}$ and P_i^{t-1} to make their sample means more accurate. However, the number of personal bests is usually large, so computing effort may be wasted if we allocate too many samples to them. Since we already have certain information about their sample means and our aim is to improve computing efficiency, we do not allocate computing efforts to them at the *t*-th iteration. We use their observed sample mean values at the (*t-1*)-th iteration.

While the $P\{\text{IS}\}$ given by (5.3) can then be estimated using Monte Carlo simulation, Monte Carlo simulation is time-consuming. Since the purpose of the budget allocation is to improve computational efficiency, we develop an analytical approach for determining sample allocation. Instead of working on $P\{\text{IS}\}$ directly, we investigate its asymptotic convergence rate by large deviation theory like the analysis in chapter 4. When $T \to \infty$, $P\{\text{IS}\}$ will converge to zero. We intend to find a sample allocation such that the asymptotic convergence rate of $P\{\text{IS}\}$ is maximized.

Let P^* be the maximum probability among the incorrect selection events. That is,

$$P^* = \max\left(\max_{i\in S_A} P\left\{\bar{f}\left(X_i^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right\}, \max_{i\in S_A} P\left\{\bar{f}\left(X_i^{\,t}\right) \ge \tilde{f}\left(P_i^{t-1}\right)\right\}, \max_{j\in S_B} P\left\{\bar{f}\left(X_j^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right\}, \max_{j\in S_B} P\left\{\bar{f}\left(X_j^{\,t}\right) \le \tilde{f}\left(P_j^{t-1}\right)\right\}\right)$$

Thus, $P\{\text{IS}\}$ in (5.3) can be bounded by $P^* \le P\{IS\} \le 2mP^*$. Because $P^* \le P\{IS\} \le 2mP^*$, the convergence rate of $P\{\text{IS}\}$ is equal to the convergence rate of P^*. Based on large deviation theory (Dembo and Zeitouni 1992; Szechtman and Yücesan 2008), we can obtain the rate functions of any element in incorrect selection events as follows.

For $X_i^t \in S_A$,

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_i^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right\} = -G_{ig}\left(\alpha_i, \alpha_g\right) = -\inf_y \left(\alpha_i I_i\left(y\right) + \alpha_g I_g\left(y\right)\right),$$

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_i^{\,t}\right) \ge \tilde{f}\left(P_i^{t-1}\right)\right\} = -\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right),$$

and for $X_j^{\,t} \in S_B$

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_j^{\,t}\right) \le \bar{f}\left(P_g^{\,t-1}\right)\right\} = -G_{jg}\left(\alpha_j, \alpha_g\right) = -\inf_y \left(\alpha_j I_j\left(y\right) + \alpha_g I_g\left(y\right)\right),$$

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_j^{\,t}\right) \le \tilde{f}\left(P_j^{t-1}\right)\right\} = -\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right),$$

in which $I_i(y)$ is defined in large deviation theory as the convergence rate function of $P\left\{\overline{f}\left(X_i^t\right) > y\right\}$ for $y > f\left(X_i^t\right)$ or $P\left\{\overline{f}\left(X_i^t\right) < y\right\}$ for $y < f\left(X_i^t\right)$.

So we have

$$\lim_{T\to\infty}\frac{1}{T}\log P\{IS\} = -\min_{i\in S_A,\, j\in S_B}\{G_{ig}\left(\alpha_i,\alpha_g\right),\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right),G_{jg}\left(\alpha_j,\alpha_g\right),\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right)\}.$$

This means that $P\{\text{IS}\}$ will decay exponentially with increasing T at a rate given by

$$\min_{i\in S_A,\, j\in S_B}\{G_{ig}\left(\alpha_i,\alpha_g\right),\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right),G_{jg}\left(\alpha_j,\alpha_g\right),\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right)\}.$$

Our computing budget allocation problem for the standard PSO is to maximize the convergence rate of $P\{\text{IS}\}$ as below,

$$\begin{aligned}
&\max \min_{i\in S_A,\, j\in S_B}\{G_{ig}\left(\alpha_i,\alpha_g\right),\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right),G_{jg}\left(\alpha_j,\alpha_g\right),\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right)\}\\
&s.t. \quad \sum_{i=1}^{m}\alpha_i+\alpha_g=1\\
&\qquad\quad \alpha_i \ge 0.
\end{aligned} \tag{5.4}$$

which can be equivalently rewritten as,

$$\begin{aligned}
&\max \quad z \quad s.t.\\
&\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right)\ge z, \quad \text{for } X_i\in S_A\\
&G_{ig}\left(\alpha_i,\alpha_g\right)\ge z, \quad \text{for } X_i\in S_A\\
&\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right)\ge z, \quad \text{for } X_j\in S_B\\
&G_{jg}\left(\alpha_j,\alpha_g\right)\ge z, \quad \text{for } X_j\in S_B\\
&\sum_{i=1}^{m}\alpha_i+\alpha_g=1\\
&\alpha_i\ge 0.
\end{aligned}$$

In model (5.4), a closed-form expression of $I_i\left(f\left(P_i^{t-1}\right)\right)$ and $I_j\left(f\left(P_j^{t-1}\right)\right)$ for certain distributions of $\hat{f}(X)$ is available. Because $\alpha_i I_i\left(f\left(P_i^{t-1}\right)\right)$ and $\alpha_j I_j\left(f\left(P_j^{t-1}\right)\right)$ are linear and strictly increasing with respect to α^T, model (5.4) is a concave optimization problem when G_{ig} and G_{jg}

are concave and strictly increasing functions. The Karush-Kuhn-Tucker conditions can be applied to develop the best allocation rule as shown in the following theorem.

Theorem 5.1. *The convergence rate of P{IS} in model (5.4) can be asymptotically maximized if the allocation rule* α^T *satisfies the following conditions:*

(a) $\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{t-1}\right)\right) = G_{i_2 g}\left(\alpha_{i_2}, \alpha_g\right) = \alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) = G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right)$;

(b) $\sum_{i_2} \frac{\partial G_{i_2 g} / \partial \alpha_g}{\partial G_{i_2 g} / \partial \alpha_{i_2}} + \sum_{j_2} \frac{\partial G_{j_2 g} / \partial \alpha_g}{\partial G_{j_2 g} / \partial \alpha_{j_2}} = 1$

(c) $\sum_{i=1}^{m} \alpha_i + \alpha_g = 1$;

(d) $\alpha_i > 0$.

in which

$i_1 \in \left\{ i_1 : X_i^{\,t} \in S_A \text{ and } \alpha_i I_i\left(f\left(P_i^{t-1}\right)\right) \le G_{ig}\left(\alpha_i, \alpha_g\right) \right\}$ $\quad i_2 \in \left\{ i_2 : X_i^{\,t} \in S_A \text{ and } \alpha_i I_i\left(f\left(P_i^{t-1}\right)\right) > G_{ig}\left(\alpha_i, \alpha_g\right) \right\}$

$j_1 \in \left\{ j_1 : X_j^{\,t} \in S_B \text{ and } \alpha_j I_j\left(f\left(P_j^{t-1}\right)\right) \le G_{jg}\left(\alpha_j, \alpha_g\right) \right\}$ $j_2 \in \left\{ j_2 : X_j^{\,t} \in S_B \text{ and } \alpha_j I_j\left(f\left(P_j^{t-1}\right)\right) > G_{jg}\left(\alpha_j, \alpha_g\right) \right\}$.

Proof. See Appendix K.

By using some numerical solvers, the optimal allocation rule satisfying Theorem 5.1 can be found with some computational effort. To further enhance computational efficiency, we develop an approximate closed-form solution, which is easy to implement and also has good computational efficiency. Suppose the performance of each particle follows a normal distribution, that is, $\hat{f}\left(X_i\right) \sim N\left(f\left(X_i\right), \sigma_i^2\right)$. Then

$$I_i\left(y\right) = \frac{\left(y - f\left(X_i\right)\right)^2}{2\sigma_i^2}.$$

Based on Theorem 5.1, we can, in this case, get a closed-form optimal allocation rule under some mild assumptions shown in Lemma 5.1.

Lemma 5.1. *When the performance of each particle is normally distributed and $\alpha_g \gg \alpha_i$, the optimal allocation rule for the standard PSO at each iteration, called PSOs_OCBA, is*

(a) $\alpha_{i_1} : \alpha_{i_2} : \alpha_{j_1} : \alpha_{j_2}$

$$= \frac{\sigma_{i_1}^2}{\left(f\left(X_{i_1}\right) - f\left(P_{i_1}^{t-1}\right)\right)^2} : \frac{\sigma_{i_2}^2}{\left(f\left(X_{i_2}\right) - f\left(P_{g}^{t-1}\right)\right)^2} : \frac{\sigma_{j_1}^2}{\left(f\left(X_{j_1}\right) - f\left(P_{j_1}^{t-1}\right)\right)^2} : \frac{\sigma_{j_2}^2}{\left(f\left(X_{j_2}\right) - f\left(P_{g}^{t-1}\right)\right)^2}$$

(b) $\alpha_g = \sigma_g \sqrt{\sum_{i_2} \frac{\alpha_{i_2}^2}{\sigma_{i_2}^2} + \sum_{j_2} \frac{\alpha_{j_2}^2}{\sigma_{j_2}^2}}$.

Proof. See Appendix L.

In Lemma 5.1, the samples allocated to each particle and personal best are different. For the particles in the current iteration, the samples allocated to them depend on the variance of fitness values and the differences between their mean values for personal best or global best. The one with the highest variance and the one closest to personal best or global best will be given more samples. The number of samples allocated to the global best is the square root of the sum related to other particles allocation. This allocation rule clearly indicates which particles are critical and should be allocated more samples, as well as how many they should receive in order to efficiently decrease the probability of incorrect selection.

Following a similar step, we get the allocation rules for standard PSO in the case where $S_G \neq \Phi$. In this case, the global best will be updated using the one with minimum sample mean value among current particles, denoted as particle *b*. The probability of incorrect selection can be formulated as follows.

$$P\{IS\} = P\{\left[\overline{f}(X_b) \geq \overline{f}(P_g^{t-1})\right] \cup \left[\bigcup_{i \in S_A} \left[\left(\overline{f}(X_b) \geq \overline{f}(X_i)\right) \cup \left(\overline{f}(X_i) > \tilde{f}(P_i^{t-1})\right)\right]\right] \cup \left[\bigcup_{j \in S_B} \left[\left(\overline{f}(X_b) \geq \overline{f}(X_j)\right) \cup \left(\overline{f}(X_j) < \tilde{f}(P_j^{t-1})\right)\right]\right]\}, \tag{5.5}$$

Similarly, the computing budget allocation problem for maximizing convergence rates when $S_G \neq \Phi$ is given as follows.

$$\begin{aligned} &\max \min_{i \in S_A, j \in S_B} \{G_{bg}(\alpha_b, \alpha_g), G_{bi}(\alpha_b, \alpha_i), \alpha_i I_i\left(f(P_i^{t-1})\right), G_{bj}(\alpha_b, \alpha_j), \alpha_j I_j\left(f(P_j^{t-1})\right)\} \\ &s.t. \quad \sum_{i=1}^{m} \alpha_i + \alpha_g = 1 \\ &\qquad \alpha_i \geq 0. \end{aligned} \tag{5.6}$$

Similarly, an asymptotically optimal solution to problem (5.6) is given in Theorem 5.2 for the case $S_G \neq \Phi$. Its approximate closed-form analytic solution is offered in Lemma 1b.

Theorem 5.2. *The allocation rule* $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)$ *is asymptotically optimal for model (5.6) if it satisfies the following conditions:*

(a) $G_{bg}(\alpha_b, \alpha_g) = \alpha_{i_1} I_{i_1}\left(f(P_{i_1}^{t-1})\right) = G_{i_2 b}(\alpha_{i_2}, \alpha_b) = \alpha_{j_1} I_{j_1}\left(f(P_{j_1}^{t-1})\right) = G_{j_2 b}(\alpha_{j_2}, \alpha_b)$;

(b) $\dfrac{\partial G_{bg} / \partial \alpha_b}{\partial G_{bg} / \partial \alpha_g} + \sum_{i_2} \dfrac{\partial G_{i_2 b} / \partial \alpha_b}{\partial G_{i_2 b} / \partial \alpha_{i_2}} + \sum_{j_2} \dfrac{\partial G_{j_2 b} / \partial \alpha_b}{\partial G_{j_2 b} / \partial \alpha_{j_2}} = 1$

(b) $\sum_{i=1}^{m} \alpha_i + \alpha_g = 1$;

(c) $\alpha_i > 0$.

Lemma 5.2. *When the simulation noise of each particle is normally distributed and* $\alpha_g \gg \alpha_i$, *the optimal allocation rule for the standard PSO at each iteration, PSOs_OCBA, is*

(a) $$\alpha_g : \alpha_{i_1} : \alpha_{i_2} : \alpha_{j_1} : \alpha_{j_2} = \frac{\sigma_g^2}{\left(f(P_g^{t-1}) - f(X_b)\right)^2} : \frac{\sigma_{i_1}^2}{\left(f(X_{i_1}) - f(P_{i_1}^{t-1})\right)^2} : \frac{\sigma_{i_2}^2}{\left(f(X_{i_2}) - f(X_b)\right)^2} : \frac{\sigma_{j_1}^2}{\left(f(X_{j_1}) - f(P_{j_1}^{t-1})\right)^2} : \frac{\sigma_{j_2}^2}{\left(f(X_{j_2}) - f(X_b)\right)^2}$$

(b) $\alpha_b = \sigma_b \sqrt{\frac{\alpha_g^2}{\sigma_g^2} + \sum_{i_2} \frac{\alpha_{i2}^2}{\sigma_{i2}^2} + \sum_{j_2} \frac{\alpha_{j2}^2}{\sigma_{j2}^2}}$.

5.3.2 Computing budget allocation for PSOe

PSOe uses different information to update the velocity and location of each particle. In order to provide the best information for PSOe, the computing budget allocation will be different from that for the standard PSO. The primary difference of PSOe is its setting of the personal best. At any iteration *t*, particles are classified into the elite set $S_e{}^t \equiv \left\{ X_i^t \middle| f\left(X_i^t\right) \le f\left(X_j^t\right),\ \forall X_i^t \in S_e{}^t, X_j^t \notin S_e{}^t \right\}$ and the non-elite set $S_{ne} = \left\{ X_i^t \middle| X_i^t \notin S_e \right\}$ based on their mean fitness values. If a particle belongs to the elite set, its personal best is defined as itself. Otherwise, its personal best is defined as the nearest particle in the S_e. Note that the personal best is determined from the current iteration, not previous ones. Therefore, only the particle in the current iteration should be allocated the computing budget.

In order to update the velocity and location of each particle correctly, we should minimize the probability of incorrectly selecting the global best or the personal best for each particle, which is formulated as below.

$$P\{IS\} = P\{\left[\bigcup_{X_i \in S_e, X_i \ne X_b} \left(\bar{f}\left(X_b{}^t\right) > \bar{f}\left(X_i{}^t\right)\right)\right] \cup \left[\bigcup_{X_i \in S_e, X_j \in S_{ne}} \left(\bar{f}\left(X_i{}^t\right) > \bar{f}\left(X_j{}^t\right)\right)\right]\} \tag{5.7}$$

Based on the large deviation theory, we have

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_b{}^t\right) > \bar{f}\left(X_i{}^t\right)\right\} = -G_{bi}\left(\alpha_b, \alpha_i\right) = -\inf_y \left(\alpha_b I_b(y) + \alpha_i I_i(y)\right) \quad \text{for } X_i{}^t \in S_e \text{, and}$$

$$\lim_{T\to\infty} \frac{1}{T} \log P\left\{\bar{f}\left(X_i{}^t\right) > \bar{f}\left(X_j{}^t\right)\right\} = -G_{ij}\left(\alpha_i, \alpha_j\right) = -\inf_y \left(\alpha_i I_i(y) + \alpha_j I_j(y)\right) \text{ for } X_i{}^t \in S_e \text{ and } X_j{}^t \in S_{ne}.$$

Thus,

$$\lim_{T\to\infty}\frac{1}{T}\log P\{IS\} = -\min_{i\in S_e,\, j\in S_{ne}}\left\{G_{bi}\left(\alpha_b,\alpha_i\right), G_{ij}\left(\alpha_i,\alpha_j\right)\right\}.$$

The computing budget allocation model for PSOe is given as follows.

$$\begin{aligned} &\max \min_{i\in S_e,\, j\in S_{ne}}\left\{G_{bi}\left(\alpha_b,\alpha_i\right), G_{ij}\left(\alpha_b,\alpha_i\right)\right\} \\ &s.t. \quad \sum_{i=1}^{m}\alpha_i = 1 \\ &\qquad\quad \alpha_i \ge 0. \end{aligned} \tag{5.8}$$

In the same way, model (5.8) is equivalent to the following model:

$$\begin{aligned} &\max \quad z \\ &s.t. \quad z \le G_{bi}\left(\alpha_b,\alpha_i\right), \quad \text{for } X_i^t \in S_e \\ &\qquad\ \ z \le G_{ij}\left(\alpha_b,\alpha_i\right), \quad \text{for } X_i^t \in S_e, X_j^t \in S_{ne} \\ &\qquad\ \ \sum_{i=1}^{m}\alpha_i = 1 \\ &\qquad\ \ \alpha_i \ge 0. \end{aligned}$$

Similarly, the maximizing problem in model (5.8) for PSOe also has the property of concavity when $G_{bi}\left(\alpha_b,\alpha_i\right)$ and $G_{ij}\left(\alpha_i,\alpha_j\right)$ are concave and strictly increasing with respect to α^T. Applying the Karush-Kuhn Tucker conditions, we can get the conditions for the optimal allocation rule.

Theorem 5.3. *An allocation rule is asymptotically optimal for model (5.8) if we can find non-negatives values for* $\lambda_{bi},\lambda_{ij}$ *and* ν *for all* $X_i^t \in S_e, X_j^t \in S_{ne}$ *.such that it satisfies the following conditions:*

(a) $\lambda_{bi}\left[G_{bi}\left(\alpha_b,\alpha_i\right) - z\right] = 0$ $\lambda_{ij}\left[G_{ij}\left(\alpha_i,\alpha_j\right) - z\right] = 0$;

(b) For X_b^t, $\displaystyle\sum_{X_i^t\in S_e, X_i^t\ne X_b^t}\lambda_{bi}\frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right)}{\partial\alpha_b} + \sum_{X_j^t\in S_{ne}}\lambda_{bj}\frac{\partial G_{bj}\left(\alpha_b,\alpha_j\right)}{\partial\alpha_b} = \nu$;

For $X_i^t \in S_e, X_i^t \neq X_b^t$, $\lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b, \alpha_i\right)}{\partial \alpha_i} + \sum_{X_j^t \in S_{ne}} \lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i, \alpha_j\right)}{\partial \alpha_i} = \nu$;

For $X_j^t \in S_{ne}$, $\sum_{X_i^t \in S_e} \lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i, \alpha_j\right)}{\partial \alpha_j} = \nu$.

(c) $\sum_{i=1}^{m} \alpha_i = 1$;

(d) $\alpha_i > 0$.

Proof. See Appendix M.

The equations in Theorem 5.3 are difficult to solve because the expression of $G(\cdot)$ is unknown in general. Similar to Lemma 5.2, to enhance computational efficiency, we develop a closed-form approximate analytical optimal solution under some assumptions. For ease of notation, we categorize particles into different subsets:

S_e^0: the set of particles belonging to S_e and are not the personal best of any particles in the set S_{ne},

S_e^1: the set of particles belonging to S_e and are the personal best of at least one particle in the set S_{ne},

S_{ne}^i: the set of particles belonging to S_{ne} who treat particle *i* as its personal best.

Lemma 5.3. *When the simulation noise of each particle is normally distributed, under assumptions: (i)* $\alpha_b \gg \alpha_i \gg \alpha_j$ *for* $X_i^t \in S_e, X_j^t \in S_{ne}$ *; and (ii)* $\max_{X_k^t \in S_e^0} f\left(X_k^t\right) < \min_{X_i^t \in S_e^1} f\left(X_i^t\right)$ *, an asymptotically optimal allocation rule for model (8), called PSOe_OCBA, is*

(a) $\alpha_k : \alpha_i : \alpha_j = \frac{\sigma_k^2}{\left(f\left(X_b^{\,t}\right) - f\left(P_k^{t-1}\right)\right)^2} : \frac{\sigma_i^2}{\left(f\left(X_b^{\,t}\right) - f\left(X_i^{\,t}\right)\right)^2} : \frac{\sigma_j^2}{\left(f\left(X_i^{\,t}\right) - f\left(X_j^{\,t}\right)\right)^2}$

(b) $\alpha_b = \sigma_b \sqrt{\sum_{X_k^t \in S_e^0} \frac{\alpha_k^2}{\sigma_k^2} + \sum_{X_i^t \in S_e^1} \left(\frac{\alpha_i^2}{\sigma_i^2} - \sum_{X_j^t \in S_{ne}^i} \frac{\alpha_j^2}{\sigma_j^2} \right)}$

in which $X_k^{\,t} \in S_e^0$, $X_i^{\,t} \in S_e^1$ *and* $X_j^{\,t} \in S_{ne}^i$.

Proof. See Appendix N.

The allocation given by Lemma 5.1, 5.2 and 5.3 assumes known parameters of the distributions. In practice, a sequential algorithm is used to estimate these quantities using the updated sample values. With a set of new locations for all particles, the procedure will be applied to obtain the sample mean value of each particle and select the personal best and global best. A new set of particles can be generated using the newly obtained personal best and global best. Each particle is sampled n_0 times in the initial stage, and additional samples are allocated incrementally from Δ samples at each subsequent stage until the computing budget T is exhausted. The sequential algorithm is similar with the procedure in chapter 4 except that the allocation rule applied is the one in Lemma 5.1, 5.2 or 5.3 depending on different situations. In the end, the selected personal best and global best based on particles' sample mean values will update (5.1) and (5.2) in the PSO algorithms.

5.4 Numerical Experiments

In this section we present numerical results to demonstrate the efficiency improvement of PSO by using the proposed computing budget allocation scheme. The testing functions and their parameters are shown at table 5.1.

Table 5. 1 Formulas and parameter settings of the tested functions.

Function name	D	Formula	Minimal value	Feasible range
Sphere	10	$f(X)=\sum_{i=1}^{D} x_i^2$	0	$[-100,100]^D$
Rosenbrock	10	$f(X)=\sum_{i=1}^{D-1}\left\{100\left(x_{i+1}-x_i^2\right)^2+\left(x_i-1\right)^2\right\}$	0	$[-100,100]^D$
Griewank	10	$f(X)=\frac{1}{4}\sum_{i=1}^{D} x_i^2-\prod_{i=1}^{D}\cos\left(x_i/\sqrt{i}\right)+1$	0	$[-100,100]^D$
Printer function	2	$f(X)=\sum_{i=1}^{d} ix_i^2+\sum_{i=1}^{d} 20i\sin^2\left(x_{i-1}\sin x_i-x_i+\sin x_{i+1}\right)+\sum_{i=1}^{d} i\log_{10}\left(1+i\left(x_{i-1}^2-2x_i+3x_{i+1}-\cos x_i+1\right)^2\right)$	0	$[-100,100]^D$

To simulate the stochastic environment, noise following a normal distribution with zero mean value and variance of 5^2 is added to these functions. The aim is to find the optimal solutions. We assume the number of particles in a swarm is 20 for both the standard PSO and PSOe. The size of elite set is 2 in PSOe. The values of c_1 and c_2 in (5.1) are set to be 2.05 based on the recommendation of Bratton and Kennedy (2007). The constrictive factor χ is set to be a decreasing function of the iteration number, that is,

$$\chi=\frac{\max\_iter+1-i}{\max\_iter+1}\cdot\frac{2}{\left|2-c1-c2-\sqrt{\left(c1+c2\right)^2-4\left(c1+c2\right)}\right|}$$

in which max_iter is the maximal number of iterations, set as 50. For the computing budget allocation algorithm, the parameter Δ is set to be 100 and n_0 is set to be 20. The total computing budget in one iteration of PSO is 5000 at the first iteration and increases by 100 at the following iterations.

In addition, we also test PSO and PSOe without using our computing budget allocation scheme. In this case, the computing budget is equally allocated to all particles. The performances of equal allocation, called PSOe_EA and PSOs_EA, serve as benchmarks for comparison. The performances are shown in figure 5.1 to figure 5.4.

Figure 5.1. a Result of 10 D Sphere function by PSOs_EA and PSOs_OCBA.

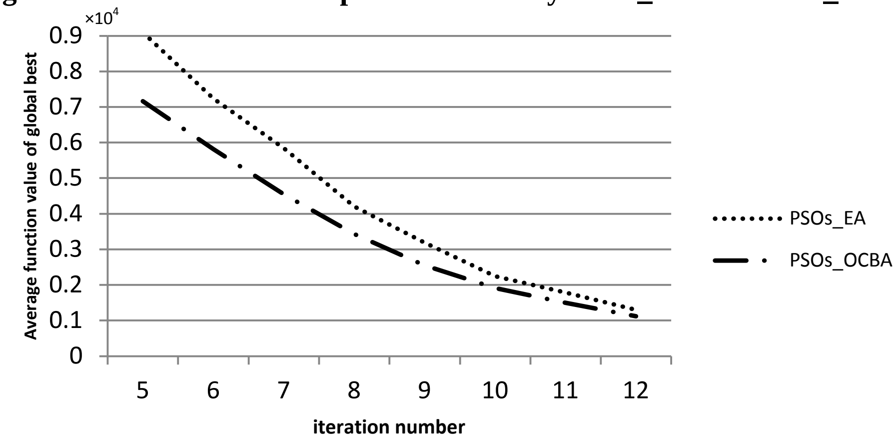


Figure 5.1. b Result of 10 D Sphere function by PSOe_EA and PSOe_OCBA.

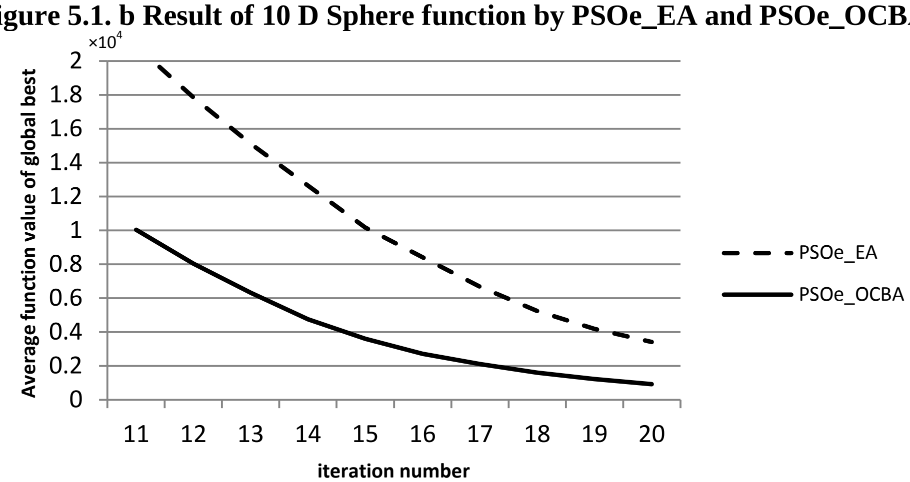


Figure 5.2. a Result of 10 D Rosenbrock function by PSOs_EA and PSOs_OCBA.

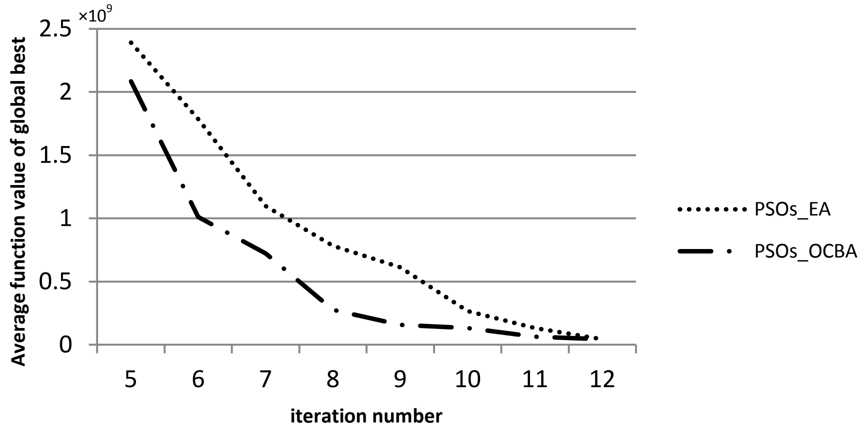


Figure 5.2. b Result of 10 D Rosenbrock function by PSOe_EA and PSOe_OCBA.

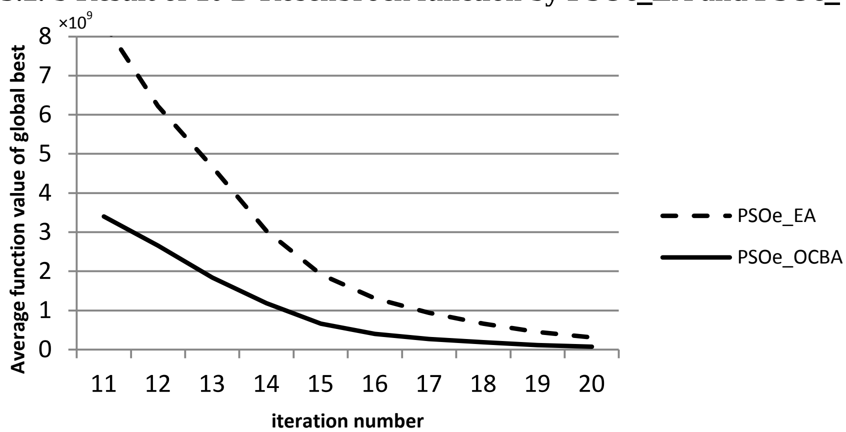


Figure 5.3. a Result of 10 D Griewank function by PSOs_EA and PSOs_OCBA.

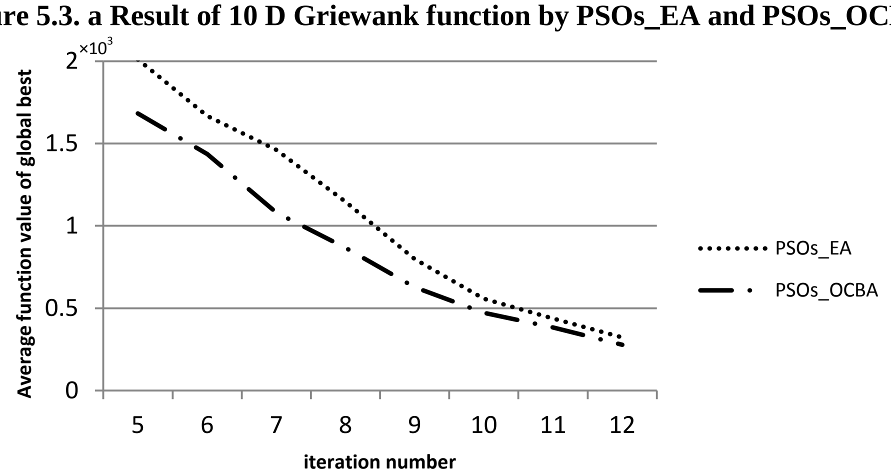


Figure 5.3. b Result of 10 D Griewank function by PSOe_EA and PSOe_OCBA.

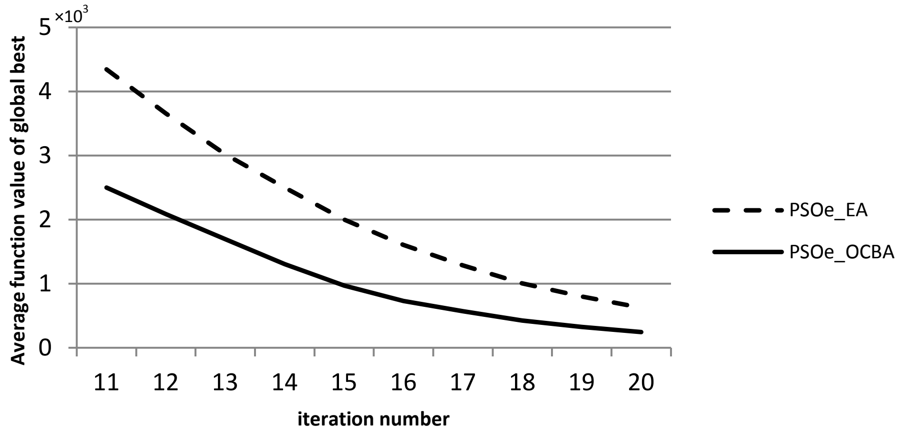


Figure 5.4. a Result of Printer function by PSOs_EA and PSOs_OCBA.

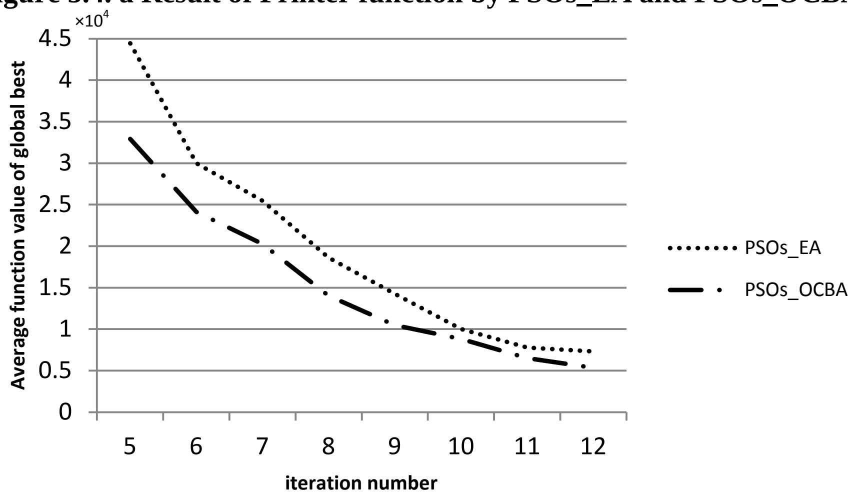
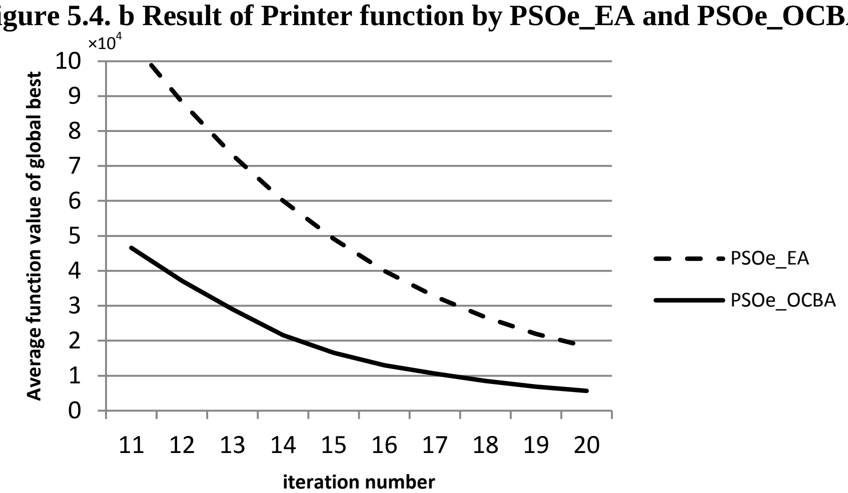


Figure 5.4. b Result of Printer function by PSOe_EA and PSOe_OCBA.



From the figures, we see that PSOs_OCBA performs much better than PSOs_EA, and PSOe_OCBA performs much better than PSOe_EA. The PSO with our allocation scheme can attain better results for the same amount of computing budget. Based on these numerical experiments, it can be concluded that the developed computing budget allocation for PSO does cause PSO to converge to the optimal solution faster in the above experiments and improves the computational efficiency of PSO for stochastic problems, for the standard one and for PSOe.

5.5 Conclusions

We propose an intelligent computing budget allocation scheme to improve the efficiency of the PSO method when applied to stochastic optimization problems. The conditions for the asymptotically optimal allocation rules are derived for the standard PSO and PSOe. Under some assumptions we derive closed-form analytical allocation rules PSOs_OCBA and PSOe_OCBA, which can be easily implemented. The numerical result indicates that the new computing effort allocation approach for PSO is promising, resulting in substantial computational efficiency gains over PSO with equal allocation.

Chapter 6 Enhancing the Efficiency of the Analytic hierarchy Process (AHP) by OCBA framework

In the previous chapters, we mainly study OCBA for the simulation optimization problems. From a more general perspective, if we treat the computing run as a resource, the OCBA framework considers the problem how to allocate the limited resources to each alternative such that we can get the best outcome. Therefore, the OCBA framework can also be applied to problems beyond the simulation optimization. In this chapter, we extend the application of OCBA framework from the simulation optimization problems to the choice decision problem beyond simulation optimization. We integrate the OCBA framework with a popular decision making method, the analytic hierarchy process (AHP), to demonstrate the performance improvement of AHP by using OCBA framework. The rest of this chapter is organized as follows. Section 6.1 briefly introduces the development of AHP and presents our motivation. In section 6.2, we build the expert resource allocation model for AHP in choice decision problem based on the general OCBA framework. Section 6.3 finds the optimal allocation of experts to each criteria in the model by using the Karush-Kuhn-Tucker (KKT) conditions and asymptotic analysis. Numerical experiments comparing the implementations with equal allocation and proportional allocation are provided in section 6.4. Section 6.5 concludes the whole chapter.

6.1 Introduction

The OCBA framework, as a popular ranking and selection technique, is mainly developed and applied to tackle simulation optimization problems. If we treat the computing budget as a budget of one resource, each alternative is allocated to certain resource budget and obtain the output by processor. By synthesize the output of each alternative, a final outcome can be attained to support decision making. Usually, the more budget allocated to an alternative, the higher quality of output obtained by this alternative. The allocation scheme of resource will affect the quality of output, and hence the final outcome. Therefore, the OCBA framework can be generalized as an optimization model which determines the best allocation scheme to maximize a certain objective which is related to the quality of the outcome (Chen and Lee, 2011). From this generalized perspective of OCBA framework, OCBA can also be applied to problems or domains beyond simulation optimization.

The choice decision among alternatives with qualitative goals is a common problem that almost all organizations need to face with, such as product selection, vendor selection, policy decision and so on. It involves the selection of one alternative from a given set of alternatives, usually in a multi-criteria environment. Some techniques have been developed for the choice decision problems, such as ELECTRE (Roy, 1968) and Multi-Attribute Utility Theory (Keeney, and Raiffa, 1976). The Analytic Hierarchy process (AHP) is one of these technique and has been widely applied because of its technical validity and practical usefulness. In this chapter, we aim to do some contributions on improving the implementing efficiency of AHP by the OCBA framework.

The framework of AHP is originally developed by Saaty (1977, 1980, 1986) and used to solve choice problems in a multi-criteria environment and other problems in evaluation, resource allocation, benchmarking, quality management, public policy and so on. It generally contains four steps: problem modeling, weights evaluation, weights aggregation and sensitivity analysis (Ishizaka and Labib, 2011).

The problem modeling is the process of building the hierarchical structure of the criteria. Saaty and Forman (1992) summarized hierarchies in different applications. A detailed discussion about building the hierarchical structure of a problem is provided in Brugha (2004). For the weights evaluation process, experts are consulted to build the pair-wise comparison matrix which is used to calculate the local priority for each alternative of each criteria. Different scales for comparing two alternatives are proposed such as linear (Satty, 1977), Geometric (Lootsma, 1989), Logarithmic (Ishizaka, Balkenborg and Laplan, 2010) and so on. To compute the local priority, Saaty (1977) proposed to use the principal eigenvalue based on the support from the perturbation theory. However, this method may result the rank reversal problem. To avoid this shortcoming, Crawford and Williams (1985) applied the approach in minimizing the multiplicative error by geometric mean to obtain the local priority. There are also a lot research work to study the consistency check on the pair-wise comparison matrices (e.g. Peláez and Lamata, 2003, Crawford and Williams, 1985, Stein and Mizzi, 2007). The last step for AHP is aggregation which synthesize the local priorities of all criteria for each alternative in order to determine each alternative's global priority. The common way for aggregation is the weighted additive aggregation. Another way for aggregation called the multiplicative aggregation is proposed in Barzilai and Lootsma (1997). A comprehensive review of the AHP and its application is provided by Forman and Gass (2001), while Ishizaka and Labib (2011) summarized the main developments of the AHP in the methodology part. All these papers focus on the improvement of AHP method itself.

In the application of AHP to choice decision, experts specialized in different areas will be invited when the knowledge about criteria in the hierarchy are belong to very different areas. Moreover, to avoid the probable bias from a single expert, we also require more than one expert in each criteria to evaluate each alternative's performance with respect to this criteria. These experts can be treated as a kind of resource and the invitation of them is a cost to implement the AHP. From the cost efficiency perspective, we want to make rational use of these experts to make a good choice by the AHP with a low cost. Since the OCBA framework study the best resource allocation problem, the efficiency problem in the implementation of the AHP can be tackled by applying OCBA concept.

In this chapter, we focus on the efficiency issue of the AHP and aims to find rational number of experts for each criteria such that we can make a good choice from alternatives by the AHP. We reiterate that our main objective is not to improve the AHP methodology, but rather to demonstrate the AHP implementation's efficiency improvement via a proper control of experts' allocation based on OCBA framework.

6.2 Formulation for expert allocation problem in AHP

We consider the choice decision problem having a hierarchy with two levels, because the two-level hierarchy is the basic unit in the hierarchy structure. For the hierarchy with more levels, we can treat is as a group of these unit hierarchy. In the two-level hierarchy, the first level is the overall objective while the second level contains multiple criteria. Assume there are *h* criteria in the second level and the weight of criteria *l* is given as w_l, l=1,…,h.

The choice decision problem is to select the best alternative, denoted as alternative *b*, from *k* candidate alternatives. To evaluate alternatives, experts are invited to give their judgments on each alternative. As different criteria may belong to different domains, the invited experts should also be specified on different domains respectively. We consider the situation that each expert just give the judgment on the criteria that he (she) is best at and use N_l to denote the number of invited experts with respect to criteria *l*. Let p_{iln} denote the local priority of alternative *i* with respect to the criteria *l* given by expert *n* responsible for criteria *l*. The local priority is a real value obtained by the pair-wise comparison matrix and denotes the score of this alternative in this criterion obtained from one expert. The high local priority means this expert think this alternative is good in this criterion. Because different experts have their own evaluations on each alternative, the local priorities for one alternative with respect to one criteria varies expert by expert. So we can treat p_{iln} as a random variable following certain distribution. The average of these local priorities $\overline{p}_{il} = \left(\sum_{n=1}^{N_l} p_{i\ln} \right) \Big/ N_l$ is used to calculate the global priority. In this paper, we choose the additive aggregation as the way of aggregation. So the global priority for one alternative is

$$gp_i = \sum_{l=1}^{h} w_l \overline{p}_{il} \ , \ i = 1, \ldots, k \quad .$$

The alternative with the highest global priority is the best alternative.

Suppose T is the total number of experts we can afford to invite. In implementing the AHP, we need to make a decision on how to allocate the T number of experts to each criteria. Usually, the decision makers just find equal number of experts for each criteria. However, to efficiently use the recourse of experts, intuitively, more experts are required for the criteria with respect to which the alternatives' performance is not easy to judge or the judgment incurs large subjectivity. And more experts are required in the criteria which has higher weight compared with other criteria. Therefore, we aim to tackle the expert allocation problem in the AHP to improve the efficiency of implementing the AHP.

Based on the OCBA framework, the expert allocation problem in AHP can be modeled as the one that we want to find the optimal way to determine the number of experts required for each criteria to maximizing the probability of correctly selecting the alternative with highest global priority (P\{CS\}), which is shown as follows.

$$\max P\{CS\}$$
$$s.t. \quad \sum_{j=1}^{m} N_j = T$$
$$N_j \geq 0;\ j = 1, 2, \ldots, m$$

This is equivalent to minimizing the probability of incorrectly selecting the best alternative (P{IS}). Similar to the discussion in chapter 4, P{IS} approaches to zero as $T \to \infty$ if $\alpha_i > 0$ for all i. For different allocation schemes of experts, the probability of incorrect selection approaches to zero with different speeds. An allocation is preferred if it makes the probability of false selection converge to zero faster. Therefore we can use the convergence rate of the probability of false selection going to zero as a measure of the quality of allocation rules and model the problem as below.

$$\begin{aligned} \max \quad & \text{Convergence rate of } P\{IS\} \\ s.t. \quad & \sum_{i=1}^{m} \alpha_i = 1 \\ & \alpha_i \geq 0 \end{aligned} \tag{6.1}$$

In the model (6.1), P{IS} means the probability of incorrect selection which happens if the global priority of the alternative b is smaller than the global priority of any one alternative. So

$$P\{IS\} = P\left\{\bigcup_{i \neq b} \left(gp_b \leq gp_i \right)\right\}. \tag{6.2}$$

Being similar to the discussion in section 3.4, $P\{IS\}$ in (6.2) can be bounded by

$$\max_{i \neq b} P\{gp_b \leq gp_i\} \leq P\{IS\} \leq (k-1) \max_{i \neq b} P\{gp_b \leq gp_i\}.$$

As T increases, the convergence rate of $P\{IS\}$ approaches the convergence rate of $\max_{i \neq b} P\{gp_b \leq gp_i\}$.

For any given $i \neq b$, there exists a rate function G_{bi} such that

$$\lim_{T\to\infty}\frac{1}{T}\log P\{gp_b \le gp_i\} = -G_{bi}\left(\vec{\alpha}\right),$$

so we have

$$\lim_{T\to\infty}\frac{1}{T}\log\left(\max_{i\neq b} P\{gp_b \le gp_i\}\right) = -\min_{i\neq b} G_{bi}\left(\vec{\alpha}\right).$$

Hence,

$$\lim_{T\to\infty}\frac{1}{T}\log P\{IS\} = -\min_{i\neq b} G_{bi}\left(\vec{\alpha}\right).$$

So the convergence rate of $P\{IS\}$ is $\min_{i\neq b} G_{bi}\left(\vec{\alpha}\right)$.

The model (6.1) can then be transferred to

$$\begin{aligned} \max\quad & z \\ s.t.\quad & G_{bi} \ge z \\ & \sum_{i=1}^{k}\alpha_i = 1 \\ & \alpha_i \ge 0. \end{aligned} \tag{6.2}$$

6.3 Derivation of the allocation rule AHP_OCBA

In this section, we derive the optimal allocation rule for model (6.2). The Lagrangian method is applied to derive the optimal asymptotical allocation rule. The Lagrangian function of model (6.2) is

$$F\left(\alpha\right) = -z + \sum_{i\neq b}^{k}\lambda_i\left(z - G_{bi}\right) + v\left(\sum_{i=1}^{k}\alpha_i - 1\right) - \sum_{i=1}^{k}h_i\alpha_i \quad .$$

Applying KKT conditions, we can obtain the theorem below.

Theorem 6.1. *The allocation rule is asymptotically optimal for model (6.2) if it satisfies the following conditions:*

(a) $\sum_{i \neq b}^{k} \lambda_i \frac{\partial G_{bi}}{\partial \alpha_l} = v \quad \forall l = 1, 2, ..., h$.

(b) $\lambda_i \left(z - G_{bi} \right) = 0 \quad \forall \ i = 1, 2, ..., k$ and $i \neq b$.

(c) $\sum_{i=1}^{k} \alpha_i = 1$

(d) $\alpha_i > 0 \quad \forall i = 1, 2, ..., k$

(e) $\lambda_i \geq 0 \quad \forall i = 1, 2, ..., k$.

In general, the expression of $G_{bi}\left(\vec{\alpha}\right)$ is difficult to be attained. Under the assumption of normal distribution, we can express it in closed form by large deviation theory. Assume the local priorities for all alternatives given by each expert for one criteria follows the multivariate normal distribution, that is, the vector $\vec{p}_{ln} = \left(p_{1ln}, ..., p_{iln}, ..., p_{kln} \right)$ is multivariate normally distributed with mean $\vec{\mu}_l = \left(\mu_{1l}, ..., \mu_{il}, ..., \mu_{kl} \right)$ and covariance matrix Σ_l as below.

$$\Sigma_l = \begin{bmatrix} \sigma_{1l}^2 & \cdots & \rho_{1i}\sigma_{1l}\sigma_{il} & \cdots & \rho_{1k}\sigma_{1l}\sigma_{kl} \\ \vdots & \ddots & & & \vdots \\ \rho_{1i}\sigma_{1l}\sigma_{il} & & \sigma_{il}^2 & & \rho_{ik}\sigma_{il}\sigma_{kl} \\ \vdots & & & \ddots & \vdots \\ \rho_{1k}\sigma_{1l}\sigma_{kl} & \cdots & \rho_{ik}\sigma_{il}\sigma_{kl} & \cdots & \sigma_{kl}^2 \end{bmatrix}$$

in which ρ_{ij} is the correlation coefficient between the local priority of alternative *i* and the local priority of alternative *j*. The existence of correlation is because the local priorities are calculated by the pair-wise comparison matrices which are determined by doing pair-wise comparisons between each two alternatives. Based on the assumption of normal distribution, we have

$$G_{bi}\left(\vec{\alpha}\right)=\frac{\left(\sum_{l=1}^{h} w_l\mu_{bl}-\sum_{l=1}^{h} w_l\mu_{bi}\right)^2}{2\left[\sum_{l=1}^{h} w_l^2\frac{\sigma_{bl}^2}{\alpha_l}+\sum_{l=1}^{h} w_l^2\frac{\sigma_{il}^2}{\alpha_l}-2\rho_{bi}\sum_{l=1}^{h} w_l^2\frac{\sigma_{bl}\sigma_{il}}{\alpha_l}\right]} \tag{6.3}$$

From (6.3) and Theorem 6.1, it is difficult to get the optimal allocation rule for model (6.2) in formula. Although we can calculate it by some solver, it is also necessary to get some closed-form formula for the optimal allocation rule in order to simplify the implementation. Hence, for easier implementation, we derive some good closed-form allocation rules for (6.2) under some cases or approximations.

We firstly consider the special case with equal variance for each criteria and equal covariance coefficient. For this case, we have $\sigma_{il}^2=\sigma_i^2\ \forall l=1,2,...,h$ and $\rho_{bi}=\rho\ \forall\ i=1,2,...,k$. The $G_{bi}\left(\vec{\alpha}\right)$ can be simplified as

$$G_{bi}\left(\vec{\alpha}\right)=\frac{\left(\sum_{l=1}^{h} w_l\mu_{bl}-\sum_{l=1}^{h} w_l\mu_{bi}\right)^2}{2\left[\sum_{l=1}^{h} w_l^2\frac{\left(\sigma_b^2+\sigma_i^2-\rho\sigma_b\sigma_i\right)}{\alpha_l}\right]}.$$

Based on theorem 6.1, we can have the following lemma.

Lemma 6.1. The asymptotically optimal allocation rules for model (6.2) with equal variance and equal covariance are given as follows:

$$\frac{\alpha_l}{\alpha_s}=\frac{w_l}{w_s},\ \forall l,s=1,2,...,h \text{ and } l\neq s. \tag{6.4}$$

In this situation, the allocation of experts to each criteria is only related to the weight of each criteria. The number of experts assigned to each criterion is purely depending on the importance of that criterion. The higher weight, the more experts are allocated.

For the general cases, we have the following equation based on (6.3).

$$\frac{\partial G_{bi}}{\partial \alpha_l} = \frac{\left(\sum_{l=1}^{h} w_l \mu_{bl} - \sum_{l=1}^{h} w_l \mu_{bi}\right)^2 \left(\sigma_{bl}^2 + \sigma_{il}^2 - 2\rho_{bi}\sigma_{bl}\sigma_{il}\right)}{2\left[\sum_{l=1}^{h} w_l^2 \frac{\sigma_{bl}^2}{\alpha_l} + \sum_{l=1}^{h} w_l^2 \frac{\sigma_{il}^2}{\alpha_l} - 2\rho_{bi}\sum_{l=1}^{h} w_l^2 \frac{\sigma_{bl}\sigma_{il}}{\alpha_l}\right]^2} \cdot \frac{w_l^2}{\alpha_l^2}. \tag{6.5}$$

Substituting (6.5) into condition (a) in theorem 6.1, we can get the equation below.

$$\frac{w_l^2}{\alpha_l^2} \sum_{i \neq b} \frac{\lambda_i \left(\sum_{l=1}^{h} w_l \left(\mu_{bl} - \mu_{bi}\right)\right)^2 \left(\sigma_{bl}^2 + \sigma_{il}^2 - 2\rho_{bi}\sigma_{bl}\sigma_{il}\right)}{2\left[\sum_{l=1}^{h} w_l^2 \frac{\left(\sigma_{bl}^2 + \sigma_{il}^2 - 2\rho_{bi}\sigma_{bl}\sigma_{il}\right)}{\alpha_l}\right]^2} = v \quad \forall l = 1, 2, ..., h \tag{6.6}$$

Let $d_l = \arg\max_{i \neq b}\left(\sigma_{bl}^2 + \sigma_{il}^2 - 2\rho_{bi}\sigma_{bl}\sigma_{il}\right)$ to denote alternative with highest variance of the difference between this alternative to the best alternative. To get the closed-form allocation rule, we ignore the less important elements in the summation part of (6.6) and approximate the summation part by the maximal element related to alternative d_l. Under this approximation, we have the lemma as below.

Lemma 6.2. The approximated asymptotically optimal allocation rules for model (6.2), named as AHP_OCBA, are given as follows:

$$\frac{\alpha_l}{\alpha_s} = \frac{w_l \sqrt{\sigma_{bl}^2 + \sigma_{d_l l}^2 - 2\rho_{bd_l}\sigma_{bl}\sigma_{d_l l}}}{w_s \sqrt{\sigma_{bs}^2 + \sigma_{d_s s}^2 - 2\rho_{bd_s}\sigma_{bs}\sigma_{d_s s}}}, \ \forall l, s = 1, 2, ..., h \text{ and } l \neq s. \tag{6.4}$$

Lemma 6.2 indicates that the number of experts allocated to a criterion should be related to the importance of that criterion and the variance of the experts' opinions on the best alternative and the dominant alternative with respect to that criterion. If we have a more important criterion and the experts have more varying opinions on the best and dominant alternatives regarding to that criterion, we will assign more experts to that criterion.

The allocation rules in lemma 6.1 and 6.2 depend on the function of distributions. In practice, a sequential procedure similar with the sequential procedure in chapter 4 can be applied to implement the allocation rule AHP_OCBA. In the end, we select the alternative with the highest final priority as the final decision.

6.4 Numerical experiments

In this section, AHP_OCBA algorithm is compared with Proportional and Equal allocation rules to see the efficiency improvement by integrating the OCBA concept into the AHP. In equal allocation rule (EA) $N_l = T/m$, and in proportional rule, $N_l/N_s = w_l/w_s$. In all numerical experiments, the procedure is run 10,000 independent times. We estimate P {CS} (probability of correct selection) by dividing the number of times we successfully find the true best alternative with 1,000 to represent the correct selection frequency.

6.4.1 The Base Experiment

We want to select the best alternative from 10 alternatives which are evaluated in terms of 10 criteria. The local priority of alternative *i* with respect to criteria *l* following the distribution $N\left(i/5,(l/2)^2\right)$, $i =$ 1, …, 10 and $l =$ 1, …, 10. Assume there is no correlation among the local priorities of alternatives. The weight of the l^{th} criteria, $w_l = (l+5)/105$. We want to find the alternative with the maximum mean. The solution 10 is the actual best alternative. The performances of AHP-OCBA, proportional and uniform with an increasing *T* are shown in figure 6.1.

From figure 6.1, we can see, P {CS} increases as T increases for all three allocation procedures. Figure 6.1 also shows that the performance of AHP-OCBA is the best and the performance of proportional is the second best among these three allocation rules.

Figure 6. 1 Performance comparison of P{CS} in the Base Experiment.

6.4.2 Variants of the Base Experiment

To further analyze the performance of AHP-OCBA, we also make some parameter changes in the base experiment and build some different scenarios. The detailed parameter settings are shown in table 6.1.

For every scenario in table 6.1, we run experiments and get the average total number of experts needed for each allocation rule to make the probability of correct selection 90%. Based on these numbers of experts, we compute the speedup factor of AHP-OCBA over Uniform and the speedup factor of Proportional over Uniform in each scenario, which are given in table 6.2.

Table 6. 1 Parameter settings for different scenarios.

Scenarios	k	h	w_l	Distribution of alternative i
Base Experiment	10	10	$(l+5)/105$	$N\left(i/5,(l/2)^2\right)$
Scenario 1	10	10	$(l+10)/155$	$N\left(i/5,(l/2)^2\right)$
Scenario 2	10	10	$(l+5)/105$	$N\left(i/5,l^2\right)$
Scenario 3	5	10	$(l+5)/105$	$N\left(i/5,(l/2)^2\right)$
Scenario 4	10	5	$(l+5)/40$	$N\left(i/5,(l/2)^2\right)$

Table 6. 2 The speed-up factor to attain P{CS}=90% in different scenarios.

Scenarios	Speed-up factor of AHP-OCBA over Uniform		Speed-up factor of Proportional over Uniform	
	ρ=0	ρ=-20%	ρ=0	ρ=-20%
Base Experiment	1.50	1.45	1.14	1.10
Scenario 1	1.59	1.47	1.16	1.12
Scenario 2	1.15	1.10	1.06	1.03
Scenario 3	1.60	1.57	1.20	1.15
Scenario 4	1.71	1.62	1.19	1.14

Table 6.2 shows that AHP-OCBA is the best performer among the three compared methods. Specifically, in Scenario 1 in which the difference between the weights of criteria goes larger, the speedup factors become higher. When the variance of experts' opinions increases in scenario 2, the speedup factors becomes lower. In scenario 3 and 4, we decrease the number of alternatives or decrease the number of criteria, all the speedup factors increase. Compared

scenario 3 and scenario 4, we also can find that the number of alternatives influence the performance of allocation rules more than the number of criteria.

In summary, from the numerical experiments, we can observe that both Proportional and AHP-OCBA are better than Uniform. Furthermore, AHP-OCBA is the best allocation rule among these three allocation rules. This indicates that the efficiency of implementing the AHP does improved by integrating the OCBA concept.

One thing need to note is that the numerical experiments here are still relatively rough. One possible way to improve is using some AHP problems in practice to test the property of local priorities and the correlation among them. In future research, we may use the validated problem settings to test the performance of AHPOCBA compared with other allocation rules.

6.5 Conclusions

The application of OCBA into simulation optimization has been discussed by many researchers while the application of OCBA into the decision making techniques is seldom studied. In this chapter, we integrate the concept of OCBA into AHP, a method being widely used in choice decision problem. The condition for the optimal allocation rule is derived. Under some assumptions, we manage to get the allocation rule AHP-OCBA in closed form and easily to be implemented. The numerical result shows AHP-OCBA are better than Proportional and Uniform allocation rule. The integration of OCBA concept into AHP does improve the efficiency of AHP.

One thing need to note that we derive the allocation rule under the asymptotic environment. Although Figure 6.1 shows OCBA rule still outperforms than equal allocation when the total number of experts is not large, we still need to study the effect of asymptotic assumption on the real implementation efficiency of AHP. In addition, we only consider the simplest structure of hierarchy in AHP and simply assume the local priority as random variable following certain distribution. In future work, we need to improve it to be more suitable for more practical and general implementation of AHP.

Chapter 7 Conclusions

This study explored the optimal computing budget allocation for simulation based optimization. The framework of optimal computing budget allocation was studied in detail and improved from both theoretical aspect and practical aspect.

From the perspective of problem setting, we extended OCBA to optimal subset selection problem which studied the problem of maximizing the probability of correctly selecting the top-m designs out of k designs under a computing budget constraint. Under the Optimal Computing Budget Allocation framework, we developed a new procedure OCBAm+ which is more efficient and robust than currently existing procedures in the literature. We also provide a framework for analyzing its asymptotic convergence rate. Based on this framework, we show that our new procedure achieves a higher convergence rate than other procedures under certain conditions. Numerical testing supports our analytical analysis and shows that the new procedure is significantly more efficient and robust.

From the perspective of OCBA framework, another way for modeling computing budget allocation problems was proposed. Instead of using the probability of correct selection as a measure of selection quality, we employed the large deviation theory to formulate the computing budget allocation problem for the optimal subset selection to avoid the hardness in building the expression of probability of correct selection. More importantly, we relaxed the assumption of independence in most OCBA procedures and considered the correlated sampling during the formulation of problems. Although we can just obtain the optimal allocation rules in closed form under some assumptions due to the difficulty of solving the model, this modeling at least provides a more general model and shows positive potential in obtaining the true optimal allocation rules under correlated situation.

From the perspective of OCBA application, we integrated OCBA with the searching algorithm Particle Swarm Optimization (PSO), to solve complicated simulation optimization problems with large solution space. The conditions for the asymptotically optimal allocation rules were derived for both versions of PSO. Under some assumptions, we managed to obtain the allocation rules PSOs_OCBA and PSOe_OCBA in closed form so that algorithms can be implemented easily. From the numerical result, it can be concluded that PSOs_OCBA and PSOe_OCBA use much less computing replications than PSOs_EA and PSObw_EA in finding the optimal solutions for simulation optimization problems. The integration of OCBA concept into PSO can improve the efficiency of PSO significantly. The combination of searching mechanism, which is the main focus of searching algorithms, and computing efficiency, which is the advantage of OCBA, results in the tremendous improvement on simulation optimization approaches. In addition, the application of OCBA into decision making problems outside the simulation optimization area was also studied. The resource allocation problem in AHP was modeled from the perspective of OCBA framework. An asymptotically optimal allocation rule AHP_OCBA was specifically derived to improve the efficiency of AHP in selecting the best alternative from many candidates. It should help the extension work of OCBA into more general areas.

In our study, some common assumptions were made to make the problem tractable. Firstly, the allocation rules were derived under the asymptotic environment. Although the assumption about infinite computing budget cannot be fulfilled in practice, the numerical result showed that the allocation rule derived under this assumption still performs well in the numerical experiments with finite computing budget. The other assumption is the normally distributed observation of each individual design. This assumption can be partially justified by the Law of Large Numbers, where the batch mean can be used as a single observation.

Although OCBA framework has bright potential in dealing with simulation optimization problems, there still exist some challenges in this field. It is observed that OCBA procedures evaluate the goodness of a design by its mean. However, another metric of designs' performance quantile (Batur and Choobineh, 2010) may be a more proper criterion because it is flexible to adjust the performance metric among the downside risk, the central tendency, and upside risk. Hence, developing the allocation rule when the selection is based on quantile instead of mean is an interesting area for future research.

Another possible direction of future study is customizing OCBA to facilitate its integration with search algorithms leading to an improved efficiency in tackling simulation optimization problems with large solution space. It can be studied from two perspectives. In Chapter 5, we have shown that the integration of OCBA and search algorithms can efficient improve the simulation efficiency of search algorithms. So the first perspective is to consider deriving the specified OCBA rule for other meta-heuristic algorithms to improve the simulation efficiency of them. One the other hand, one shortcoming of the proposed algorithm in Chapter 5 is that it can do nothing on the search part about the algorithm. It is still an open challenge to develop more customized framework for integrating OCBA with search algorithms which can improve the overall simulation efficiency of searching algorithms by optimally balancing the exploration and exploitation. This is the other perspective of future research for improving efficiency of search algorithms.

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Appendix A. Proof of Lemma 3.1

The new lower bound can be derived as follows.

$$P\{CS\} \geq \max(P\left\{\left[\bigcap_{i=1}^{m-1}\left(\bar{X}_i \leq \bar{X}_m\right)\right]\bigcap\left[\bigcap_{j=m+1}^{k}\left(\bar{X}_j \geq \bar{X}_m\right)\right]\right\}, P\left\{\left[\bigcap_{i=1}^{m}\left(\bar{X}_i \leq \bar{X}_{m+1}\right)\right]\bigcap\left[\bigcap_{j=m+2}^{k}\left(\bar{X}_{m+1} \leq \bar{X}_j\right)\right]\right\})$$
$$= \max\left(P\left\{A\bigcap B\right\}, P\left\{C\bigcap D\right\}\right),$$

in which A, B, C and D define the events $\bigcap_{i=1}^{m-1}\left(\bar{X}_i \leq \bar{X}_m\right)$, $\bigcap_{j=m+1}^{k}\left(\bar{X}_j \geq \bar{X}_m\right)$, $\bigcap_{i=1}^{m}\left(\bar{X}_i \leq \bar{X}_{m+1}\right)$ and $\bigcap_{j=m+2}^{k}\left(\bar{X}_{m+1} \leq \bar{X}_j\right)$ respectively. Based on Boole's inequality, we know

$$P\left\{A\bigcap B\right\} = 1 - P\left\{\bar{A}\bigcup\bar{B}\right\} \geq 1 - P\left\{\bar{A}\right\} - P\left\{\bar{B}\right\},$$

$$P\left\{C\bigcap D\right\} = 1 - P\left\{\bar{C}\bigcup\bar{D}\right\} \geq 1 - P\left\{\bar{C}\right\} - P\left\{\bar{D}\right\}, \text{ and}$$

$$P\left\{\bar{A}\right\} = P\left\{\bigcup_{i=1}^{m-1}\left(\bar{X}_i \geq \bar{X}_m\right)\right\} \leq \sum_{i=1}^{m-1} P\left\{\bar{X}_i \geq \bar{X}_m\right\}.$$

For $P\left\{\bar{B}\right\}$, $P\left\{\bar{C}\right\}$ and $P\left\{\bar{D}\right\}$, we have similar inequalities.

We use $APCSm_1$ denote $1-\sum_{i=1}^{m-1} P\left\{\bar{X}_i \geq \bar{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\bar{X}_m \geq \bar{X}_j\right\}$ and use $APCSm_2$ denote $1-\sum_{i=1}^{m} P\left\{\bar{X}_i \geq \bar{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\bar{X}_{m+1} \geq \bar{X}_j\right\}$. Based on the above inequalities, $APCSm+$ can be derived as follows.

$$
\begin{aligned}
P\{CS\} &\geq \max\left(P\left\{A\bigcap B\right\}, P\left\{C\bigcap D\right\}\right) \\
&\geq \max\left(1 - P\left\{\overline{A}\right\} - P\left\{\overline{B}\right\}, 1 - P\left\{\overline{C}\right\} - P\left\{\overline{D}\right\}\right) \\
&\geq \max(1 - \sum_{i=1}^{m-1} P\left\{\overline{X}_i \geq \overline{X}_m\right\} - \sum_{j=m+1}^{k} P\left\{\overline{X}_m \geq \overline{X}_j\right\},\ 1 - \sum_{i=1}^{m} P\left\{\overline{X}_i \geq \overline{X}_{m+1}\right\} - \sum_{j=m+2}^{k} P\left\{\overline{X}_{m+1} \geq \overline{X}_j\right\}) \\
&= \max\left(APCSm_1, APCSm_2\right) \equiv APCSm+.
\end{aligned}
$$

□

Appendix B. Proof of Lemma 3.2

Since the two sub-problems have similar structure, we only show the proof of the convexity for sub-problem 1.

If all constraints are affine and the objective is a concave function, sub-problem 1 is convex with respect to the vector α.

Since the linear constraints in (3.6) satisfy the affine requirement, we only need to show $f \equiv \sum_{i=1}^{m-1} P\left\{\overline{X}_i \geq \overline{X}_m\right\} + \sum_{j=m+1}^{k} P\left\{\overline{X}_m \geq \overline{X}_j\right\}$ is convex, or specifically, each term in the summation is convex. Assume α^* is strictly positive. Define

$$
g\left(\alpha_i, \alpha_m\right) = \begin{cases} P\left\{\overline{X}_m \leq \overline{X}_i\right\}, \text{ if } 1 \leq i \leq (m-1) \\ P\left\{\overline{X}_i \leq \overline{X}_m\right\}, \text{ if } (m+1) \leq i \leq k \end{cases}.
$$

We have

$$
P\left\{\overline{X}_i \leq \overline{X}_j\right\} = \int_{-\infty}^{-\frac{\delta_{ij}}{\sigma_{ij}}} \frac{1}{\sqrt{2\pi}} e^{-\frac{t^2}{2}} dt, \tag{B.1}
$$

in which $\sigma_{ij}^2 = \frac{1}{T}\left(\frac{\sigma_i^2}{\alpha_i} + \frac{\sigma_j^2}{\alpha_j}\right)$, and $\delta_{ij} = \mu_i - \mu_j$. The second order partial derivatives of (B.1) with respect to α_i and α_j can be obtained.

$$\frac{\partial^2 g(\alpha_i, \alpha_m)}{\partial \alpha_i{}^2} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[\frac{\delta_{im}}{\sigma_{im}^5 T^2}\frac{\sigma_i^4}{\alpha_i^4}\left(\frac{1}{2}\frac{\delta_{im}^2}{\sigma_{im}^2} - 3\right) + 2\frac{\delta_{im}}{\sigma_{im}^3 T}\frac{\sigma_i^2}{\alpha_i^3}\right],$$

$$\frac{\partial^2 g(\alpha_i, \alpha_m)}{\partial \alpha_m{}^2} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[\frac{\delta_{im}}{\sigma_{im}^5 T^2}\frac{\sigma_m^4}{\alpha_m^4}\left(\frac{1}{2}\frac{\delta_{im}^2}{\sigma_{im}^2} - 3\right) + 2\frac{\delta_{im}}{\sigma_{im}^3 T}\frac{\sigma_m^2}{\alpha_m^3}\right],$$

$$\frac{\partial^2 g(\alpha_i, \alpha_m)}{\partial \alpha_i \partial \alpha_m} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[\frac{\delta_{im}}{\sigma_{im}^5 T^2}\frac{\sigma_i^2}{\alpha_i^2}\frac{\sigma_m^2}{\alpha_m^2}\left(\frac{1}{2}\frac{\delta_{im}^2}{\sigma_{im}^2} - 3\right)\right],$$

$$\frac{\partial^2 g(\alpha_i, \alpha_m)}{\partial \alpha_p \partial \alpha_q} = 0 \text{ for } p, q \neq i \text{ and } p, q \neq m.$$

For simplicity, let

$$a_{im} = \frac{\partial^2 g(\alpha_i, \alpha_m)}{\partial \alpha_i \partial \alpha_m},\ a_{ii} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[\frac{\delta_{im}}{\sigma_{im}^5 T^2}\frac{\sigma_i^4}{\alpha_i^4}\left(\frac{1}{2}\frac{\delta_{im}^2}{\sigma_{im}^2} - 3\right)\right],\ b_{ii} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[2\frac{\delta_{im}}{\sigma_{im}^3 T}\frac{\sigma_i^2}{\alpha_i^3}\right],$$

$$a_{mm} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[\frac{\delta_{im}}{\sigma_{im}^5 T^2}\frac{\sigma_m^4}{\alpha_m^4}\left(\frac{1}{2}\frac{\delta_{im}^2}{\sigma_{im}^2} - 3\right)\right], \text{ and } b_{mm} = \frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right)\left[2\frac{\delta_{im}}{\sigma_{im}^3 T}\frac{\sigma_m^2}{\alpha_m^3}\right].$$

Therefore,

$$\begin{aligned}\alpha^T \nabla^2 g(\alpha_i, \alpha_m)\alpha &= (a_{ii} + b_{ii})\alpha_i{}^2 + (a_{mm} + b_{mm})\alpha_m{}^2 + 2a_{im}\alpha_i\alpha_m \\ &= \left[\frac{a_{im}}{\sqrt{(a_{mm} + b_{mm})}}\alpha_{i_r} + \sqrt{(a_{mm} + b_{mm})}\alpha_m\right]^2 + \left[(a_{ii} + b_{ii}) - \frac{a_{im}{}^2}{(a_{ii} + b_{ii})}\right]\alpha_i{}^2.\end{aligned} \quad \text{(B.2)}$$

We know that b_{ii} and b_{mm} are strictly positive for every $T > 0$. For the term a_{im} in (B.2), we have $a_{im} > 0$ when $T > T_{im} = 6\left(\sigma_i^2/\alpha_i + \sigma_m^2/\alpha_m\right)/\delta_{im}^2$. We can find that a_{ii} and a_{mm} are also strictly positive when $T > T_{im}$. Besides, these terms also have the following relationship.

$$a_{im} = \left(\frac{\alpha_i}{\alpha_m}\right)^2 \left(\frac{\sigma_m}{\sigma_i}\right)^2 a_{ii}, \ a_{mm} = \left(\frac{\alpha_i}{\alpha_m}\right)^4 \left(\frac{\sigma_m}{\sigma_i}\right)^4 a_{ii}, \text{ and } b_{mm} = \left(\frac{\alpha_i}{\alpha_m}\right)^3 \left(\frac{\sigma_m}{\sigma_i}\right)^2 b_{ii}.$$

Thus, when $T > T_{im}$, we can also obtain

$$\frac{{a_{im}}^2}{\left(a_{mm} + b_{mm}\right)} = \frac{a_{ii}}{1 + b_{mm}/a_{mm}} < a_{ii}.$$

and $\alpha^T \nabla^2 g\left(\alpha_i, \alpha_m\right)\alpha \geq 0$ for any $\alpha > 0^T$. This means that the hessian matrix with respect to α is positive semi-definite, so the function $g\left(\alpha_i, \alpha_m\right)$ is convex when $T > T_{im}$ .Let $T_1^* = \max\left\{T_{im} \middle| i \neq m\right\}$. The function *f* is a convex function when $T > T_1^*$, and so sub-problem 1 is a convex problem for any *T* greater than T_1^* . □

Appendix C. Proof of Lemma 3.3

Similar with the proof of Lemma 3.2, we only show how to derive the conditions for the optimal allocation rule of sub-problem 1. Assume α^* is strictly positive. The KKT conditions of sub-problem 1 can be stated as follows by using (3.8).

$$\frac{\partial F_1}{\partial \alpha_i} = -\frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2}\right) \frac{\delta_{im}}{\sigma_{im}^3} \frac{\sigma_i^2}{T\alpha_i^2} - \lambda - \nu_i = 0, \text{for } i = 1, 2, \ldots, m-1. \tag{C.1}$$

$$\frac{\partial F_1}{\partial \alpha_j} = -\frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{mj}^2}{2\sigma_{mj}^2}\right) \frac{\delta_{mj}}{\sigma_{mj}^3} \frac{\sigma_j^2}{T\alpha_j^2} - \lambda - \nu_j = 0, \text{for } j = m+1, m+2, \ldots, k. \tag{C.2}$$

$$\frac{\partial F_1}{\partial \alpha_m} = -\frac{1}{2\sqrt{2\pi}} \frac{\sigma_m^2}{T\alpha_m^2} \left[\sum_{i=1}^{m-1} \exp\left(-\frac{\delta_{im}^2}{2\sigma_{im}^2} \right) \frac{\delta_{im}}{\sigma_{im}^3} + \sum_{j=m+1}^{k} \exp\left(-\frac{\delta_{mj}^2}{2\sigma_{mj}^2} \right) \frac{\delta_{mj}}{\sigma_{mj}^3} \right] - \lambda - \nu_m = 0. \tag{C.3}$$

$$\nu_i \alpha_i = 0, \text{for } i = 1, 2, \ldots, k. \tag{C.4}$$

Since $\alpha_i > 0,\ \forall\ i = 1, 2, \ldots, k$, it can be attained that $\nu_i = 0,\ \forall\ i = 1, 2, \ldots, k$ by (C.4). From (C.1) and (C.2), we know

$$-\frac{1}{2\sqrt{2\pi}} \exp\left(-\frac{\delta_{rm}^2}{2\sigma_{rm}^2} \right) \frac{|\delta_{rm}|}{\sigma_{rm}^3} = \lambda \frac{T\alpha_r^2}{\sigma_r^2}, \text{for } r \neq m. \tag{C.5}$$

Substituting (C.5) into (C.3), we obtain

$$\alpha_m = \sigma_m \sqrt{\sum_{r \neq m}^{k} \frac{\alpha_r^2}{\sigma_r^2}}.$$

For any $x, y \neq m$, the following equation also can be derived by (C.1) and (C.2)

$$\exp\left(\frac{T}{2} \left(\frac{\delta_{ym}^2}{\left(\frac{\sigma_y^2}{\alpha_y} + \frac{\sigma_m^2}{\alpha_m} \right)} - \frac{\delta_{xm}^2}{\left(\frac{\sigma_x^2}{\alpha_x} + \frac{\sigma_m^2}{\alpha_m} \right)} \right) \right) = \frac{|\delta_{ym}|}{|\delta_{xm}|} \frac{\left(\frac{\sigma_x^2}{\alpha_x} + \frac{\sigma_m^2}{\alpha_m} \right)^{3/2}}{\left(\frac{\sigma_y^2}{\alpha_y} + \frac{\sigma_m^2}{\alpha_m} \right)^{3/2}} \frac{\sigma_y^2}{\sigma_x^2} \frac{\alpha_x^2}{\alpha_y^2}.$$

Considering the asymptotic limit $T \to \infty$, we obtain

$$\frac{\delta_{xm}^2}{\left(\frac{\sigma_x^2}{\alpha_x} + \frac{\sigma_m^2}{\alpha_m} \right)} = \frac{\delta_{ym}^2}{\left(\frac{\sigma_y^2}{\alpha_y} + \frac{\sigma_m^2}{\alpha_m} \right)}.$$

Thus, the allocation rule $\alpha^{*1} = \left(\alpha_1^{*1}, \alpha_2^{*1}, \ldots, \alpha_k^{*1} \right)$ satisfying the following conditions is the asymptotically optimal allocation rule for sub-problem 1.

(i) $\alpha_m = \sigma_m \sqrt{\sum_{i \neq m}^{k} \frac{\alpha_i^2}{\sigma_i^2}}$;

(ii) $\frac{(\mu_x - \mu_m)^2}{\sigma_x^2/\alpha_x + \sigma_m^2/\alpha_m} = \frac{(\mu_y - \mu_m)^2}{\sigma_y^2/\alpha_y + \sigma_m^2/\alpha_m}$, $x, y \neq m$;

(iii) $\sum_{i=1}^{k} \alpha_i = 1$;

(iiii) $\alpha_i > 0$. □

Appendix D. Proof of Proposition 3.1

We show the proof related to $\alpha^{*1} = (\alpha_1^{*1}, \alpha_2^{*1}, \ldots, \alpha_k^{*1})$. The proof related to $\alpha^{*2} = (\alpha_1^{*2}, \alpha_2^{*2}, \ldots, \alpha_k^{*2})$ will follow the same procedure.

Because we have $\mu_1 < \mu_2 < \cdots < \mu_k$, there exist two constants w_l and w_u such that $0 < w_l < \min_{i \neq m} |\mu_i - \mu_m|$ and $\max_{i \neq m} |\mu_i - \mu_m| < w_u < \infty$. For all designs' variances, we can also find two constants v_l and v_u such that $0 < v_l < \min\{\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2\}$ and $\max\{\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2\} < v_u < \infty$.

By condition (ii) at lemma 3.3(a), we have

$$\frac{\sigma_j^2 (\mu_i - \mu_m)^2}{\alpha_j} + \frac{\sigma_m^2 (\mu_i - \mu_m)^2}{\alpha_m} = \frac{\sigma_i^2 (\mu_j - \mu_m)^2}{\alpha_i} + \frac{\sigma_m^2 (\mu_j - \mu_m)^2}{\alpha_m} \text{ for } i, j \neq m. \quad \text{(D.1)}$$

Case 1. $|\mu_i - \mu_m| \leq |\mu_j - \mu_m|$

In this case, by (D.1), we have

$$\frac{\sigma_i^2\left(\mu_j-\mu_m\right)^2}{\alpha_i}\le\frac{\sigma_j^2\left(\mu_i-\mu_m\right)^2}{\alpha_j},$$

And hence

$$\alpha_j\le\frac{\sigma_j^2}{\sigma_i^2}\frac{\left(\mu_i-\mu_m\right)^2}{\left(\mu_j-\mu_m\right)^2}\alpha_i<\frac{v_u}{v_l}\frac{w_u}{w_l}\alpha_i\,. \tag{D.2}$$

Case 2. $|\mu_i-\mu_m|>|\mu_j-\mu_m|$

It can be obtained by (D.1) that

$$\frac{\sigma_i^2\left(\mu_j-\mu_m\right)^2}{\alpha_i}=\frac{\sigma_j^2\left(\mu_i-\mu_m\right)^2}{\alpha_j}+\frac{\sigma_m^2\left(\mu_i-\mu_j\right)\left(\mu_i+\mu_j-2\mu_m\right)}{\alpha_m}.$$

By condition (i) at lemma 3.3(a), we have $(\alpha_m/\sigma_m)>\max_i(\alpha_i/\sigma_i)$. Thus,

$$\frac{\sigma_i^2\left(\mu_j-\mu_m\right)^2}{\alpha_i}<\frac{\sigma_j^2\left(\mu_i-\mu_m\right)^2}{\alpha_j}+\frac{\sigma_m\sigma_j\left(\mu_i-\mu_j\right)\left(\mu_i+\mu_j-2\mu_m\right)}{\alpha_j}.$$

So, we can get that

$$\alpha_j<\alpha_i\frac{\sigma_j^2\left(\mu_i-\mu_m\right)^2+\sigma_m\sigma_j\left(\mu_i-\mu_j\right)\left(\mu_i+\mu_j-2\mu_m\right)}{\sigma_i^2\left(\mu_j-\mu_m\right)^2}<\alpha_i\frac{v_u^2\left(2w_u^2-w_l^2\right)}{v_l^2w_l^2}. \tag{D.3}$$

Combing (D.2) and (D.3), it can be proved that there exists a constant c_{ij}>0 such that $\alpha_j<c_{ij}\alpha_i$, $\forall i,j\neq m$. Let $\alpha_{\min}=\min_{i\neq m}\{\alpha_i\}$. So, we can conclude that there exists a constant c>0 such that $\alpha_i<c\alpha_{\min}$, $\forall i\neq m$.

By condition (i) at lemma 3(a),

$$\left(1/v_l\right) > \left(\alpha_m/\sigma_m\right) = \sqrt{\sum_{i\neq m}^{k}\left(\alpha_i/\sigma_i\right)^2} > \left(\alpha_{\min}\sqrt{k-1}/\sqrt{v_u}\right). \tag{D.4}$$

Therefore, as $k \to \infty$, $\alpha_{\min} \to 0$. Because $\alpha_i < c\alpha_{\min}$, it can be concluded that $\lim_{k\to\infty}\alpha_i^{*1} = 0,\ i \neq m$.

By (D.4) and $\alpha_i < c\alpha_{\min}$, we have

$$\frac{\alpha_i}{\alpha_m} < \frac{c\sqrt{v_u}}{\sigma_m\sqrt{k-1}} < \frac{c\sqrt{v_u}}{\sqrt{v_l}\sqrt{k-1}}. \tag{D.5}$$

Thus, as $k \to \infty$, $\alpha_i/\alpha_m \to 0$, $\forall i \neq m$. So we have $\lim_{k\to\infty}\left(\alpha_i^{*1}/\alpha_m^{*1}\right) = 0,\ \forall\ i \neq m$.

Let $\alpha_{\max} = \max_{i\neq m}\{\alpha_i\}$. By (D.5),

$$\sqrt{\frac{v_l}{v_u}}\frac{1}{\sqrt{k-1}}\frac{1}{c} < \frac{\alpha_{\min}}{\sigma_m\sqrt{(k-1)\alpha_{\max}{}^2/v_l}} < \frac{\alpha_i}{\alpha_m} < \sqrt{\frac{v_u}{v_l}}\frac{c}{\sqrt{k-1}}.$$

As $k \to \infty$, this yields $\left(\alpha_i/\alpha_m\right) = \mathrm{O}\left(1/\sqrt{k}\right)$. So we have $\left(\alpha_i^{*1}/\alpha_m^{*1}\right) = \mathrm{O}\left(1/\sqrt{k}\right),\ \forall\ i \neq m$. □

Appendix E. Illustration of simplified conditions in Remark 3.1

We know

$$\begin{aligned}
&APCSm_1\left(\alpha^{*1}\right) - APCSm_2\left(\alpha^{*2}\right) \\
&= 1 - \sum_{i=1}^{m-1} P\left\{\bar{X}_i\left(\alpha^{*1}\right) \geq \bar{X}_m\left(\alpha^{*1}\right)\right\} - \sum_{j=m+1}^{k} P\left\{\bar{X}_m\left(\alpha^{*1}\right) \geq \bar{X}_j\left(\alpha^{*1}\right)\right\} \\
&- \left(1 - \sum_{i=1}^{m} P\left\{\bar{X}_i\left(\alpha^{*2}\right) \geq \bar{X}_{m+1}\left(\alpha^{*2}\right)\right\} - \sum_{j=m+2}^{k} P\left\{\bar{X}_{m+1}\left(\alpha^{*2}\right) \geq \bar{X}_j\left(\alpha^{*2}\right)\right\}\right)
\end{aligned}$$

Since $\left(\bar{X}_i - \bar{X}_j\right) \sim N\left(\mu_i - \mu_j, \left(\sigma_i^2 / \alpha_i + \sigma_j^2 / \alpha_j\right) / T\right)$, we have

$$P\left\{\bar{X}_i - \bar{X}_j \geq 0\right\} = \Phi\left(\left(\mu_i - \mu_j\right) \Big/ \sqrt{\frac{1}{T}\left(\frac{\sigma_i^2}{\alpha_i} + \frac{\sigma_j^2}{\alpha_j}\right)}\right).$$

For the allocation rule α^{*1} in (3.10), let $A_{21} = \sum_{i \neq m}^{k} \frac{\sigma_i^2}{\left(\mu_i - \mu_m\right)^2} + \sigma_m \sqrt{\sum_{i \neq m}^{k} \frac{\sigma_i^2}{\left(\mu_i - \mu_m\right)^4}}$. Then, for $i \leq m-1$ and $j \geq m+1$, we can get

$$P\left\{\bar{X}_i - \bar{X}_m \geq 0\right\} == \Phi\left(-\sqrt{T} \Big/ \sqrt{\left(A_{21} + \frac{\sigma_m^2}{\alpha_m\left(\mu_m - \mu_i\right)^2}\right)}\right),$$

$$P\left\{\bar{X}_m - \bar{X}_j \geq 0\right\} = \Phi\left(-\sqrt{T} \Big/ \sqrt{\left(A_{21} + \frac{\sigma_m^2}{\alpha_m\left(\mu_j - \mu_m\right)^2}\right)}\right).$$

The maximal value of all $P\left\{\bar{X}_i - \bar{X}_m \geq 0\right\}$ and all $P\left\{\bar{X}_m - \bar{X}_j \geq 0\right\}$ is the one in which the mean of two random variables' difference equals to $\min\left\{\mu_m - \mu_{m-1}, \mu_{m+1} - \mu_m\right\}$. Besides, $P\left\{\bar{X}_1 \geq \bar{X}_m\right\} < \cdots < P\left\{\bar{X}_{m-1} \geq \bar{X}_m\right\}$ and $P\left\{\bar{X}_m \geq \bar{X}_{m+1}\right\} > \cdots > P\left\{\bar{X}_m \geq \bar{X}_k\right\}$.

In the same way, for the allocation rule α^{*2} , we have the inequalities $P\left\{\bar{X}_1 \geq \bar{X}_{m+1}\right\} < \cdots < P\left\{\bar{X}_m \geq \bar{X}_{m+1}\right\}$ and $P\left\{\bar{X}_{m+1} \geq \bar{X}_{m+2}\right\} > \cdots > P\left\{\bar{X}_{m+1} \geq \bar{X}_k\right\}$. And the most largest one among all these probabilities is the one with $\min\left\{\mu_{m+1} - \mu_m, \mu_{m+2} - \mu_{m+1}\right\}$.

The difference between $APCSm_1$ and $APCSm_2$ can be approximated as follows by ignoring other unimportant elements and only considering the largest elements.

$$APCSm_1\left(\alpha^{*1}\right)-APCSm_2\left(\alpha^{*2}\right)$$
$$\approx\Phi\left(-\sqrt{T}\Big/\sqrt{\left(A_{22}+\frac{\sigma_{m+1}^2}{\alpha_{m+1}b^2}\right)}\right)-\Phi\left(-\sqrt{T}\Big/\sqrt{\left(A_{21}+\frac{\sigma_m^2}{\alpha_m a^2}\right)}\right)$$

in which $a=\min\{\mu_m-\mu_{m-1},\mu_{m+1}-\mu_m\}$ and $b=\min\{\mu_{m+1}-\mu_m,\mu_{m+2}-\mu_{m+1}\}$.

When the means and the variances of design *m* and design *(m+1)* do not have very huge difference, we can assume $A_{21}\approx A_{22}$ and $\sigma_m^2/\alpha_m^{*1}\approx\sigma_{m+1}^2/\alpha_{m+1}^{*2}$. In this case, if $a\geq b$, we have $APCSm_1\left(\alpha^{*1}\right)\geq APCSm_2\left(\alpha^{*2}\right)$, and otherwise versa. □

Appendix F. Proof of Corollary 3.1

If we can prove $APCSm_1\left(\alpha^{*2}\right)>APCSm_2\left(\alpha^{*2}\right)$, corollary 3.1 can be proved because $APCSm_1\left(\alpha^{*1}\right)\geq APCSm_1\left(\alpha^{*2}\right)$.

We have

$$APCSm_1\left(\alpha^{*2}\right)-APCSm_2\left(\alpha^{*2}\right)=\sum_{i=3}^{k}\left(P\left\{\bar{X}_2\left(\alpha^{*2}\right)\geq\bar{X}_i\left(\alpha^{*2}\right)\right\}-P\left\{\bar{X}_1\left(\alpha^{*2}\right)\geq\bar{X}_i\left(\alpha^{*2}\right)\right\}\right).$$

In the equal variance case, the allocation rule α^{*2} is

$$\alpha_x^{*2}=\frac{1\big/\left(\mu_x-\mu_2\right)^2}{B}\ \text{ for }x\neq 2\text{, and }\ \alpha_2^{*2}=\frac{\sqrt{\sum_{x\neq 2}^{k}1\big/\left(\mu_x-\mu_2\right)^4}}{B}$$

in which $B=\sum_{x\neq 2}^{k}1\big/\left(\mu_x-\mu_2\right)^2+\sqrt{\sum_{x\neq 2}^{k}1\big/\left(\mu_x-\mu_2\right)^4}$.

Thus, for every design i,

$$P\left\{\bar{X}_2\left(\alpha^{*2}\right) \geq \bar{X}_i\left(\alpha^{*2}\right)\right\} = \phi\left(-\sigma\sqrt{\frac{T}{B}} \cdot \frac{\mu_i - \mu_2}{\sqrt{\left(\mu_i - \mu_2\right)^2 + 1 \Big/ \sqrt{\sum_{i \neq 2}^{k} \frac{1}{\left(\mu_i - \mu_2\right)^4}}}}\right)$$

and

$$P\left\{\bar{X}_1\left(\alpha^{*2}\right) \geq \bar{X}_i\left(\alpha^{*2}\right)\right\} = \phi\left(-\sigma\sqrt{\frac{T}{B}} \cdot \frac{\mu_i - \mu_1}{\sqrt{\left(\mu_i - \mu_2\right)^2 + \left(\mu_1 - \mu_2\right)^2}}\right).$$

Because

$$\frac{\mu_i - \mu_2}{\sqrt{\left(\mu_i - \mu_2\right)^2 + 1 \Big/ \sqrt{\sum_{i \neq 2}^{k} \frac{1}{\left(\mu_i - \mu_2\right)^4}}}} < 1 < \frac{\mu_i - \mu_1}{\sqrt{\left(\mu_i - \mu_2\right)^2 + \left(\mu_1 - \mu_2\right)^2}},$$

we have

$$P\left\{\bar{X}_2\left(\alpha^{*2}\right) \geq \bar{X}_i\left(\alpha^{*2}\right)\right\} > P\left\{\bar{X}_1\left(\alpha^{*2}\right) \geq \bar{X}_i\left(\alpha^{*2}\right)\right\}.$$

Then, the inequality $APCSm_1\left(\alpha^{*2}\right) > APCSm_2\left(\alpha^{*2}\right)$ can be proved. □

Appendix G. Proof of Theorem 3.2

The limit condition $T \to \infty$ is equivalent to the iteration number in the procedure $n \to \infty$. In the procedure, the vector $\alpha^n \equiv \left(\alpha_1^n, \alpha_2^n, \cdots, \alpha_k^n\right)$ states the proportion of computing replications allocated to each design based on the OCBAm+ allocation rule until the n[th] replication. Because $\alpha^n \equiv \left(\alpha_1^n, \alpha_2^n, \cdots, \alpha_k^n\right)$ is the function of sample means of designs, it is also a statistic. The sample value of $\alpha^n \equiv \left(\alpha_1^n, \alpha_2^n, \cdots, \alpha_k^n\right)$ is updated iteration by iteration based on sample means. Let

$$\beta_i^n = \frac{\hat{\sigma}_i^2}{\left(\bar{X}_i - \bar{X}_m\right)^2} \ \ \forall i \neq m \text{ and } \beta_m^n = \hat{\sigma}_m \sqrt{\sum_{i \neq m}^{k} \left(\beta_i^n / \hat{\sigma}_i\right)^2}, \text{ if } APCSm_1\left(\alpha^{n-1}\right) \geq APCSm_2\left(\alpha^{n-1}\right), \text{ and}$$

$$\beta_i^n = \frac{\hat{\sigma}_i^2}{\left(\bar{X}_i - \bar{X}_{m+1}\right)^2} \ \ \forall i \neq m+1 \text{ and } \beta_{m+1}^n = \hat{\sigma}_{m+1} \sqrt{\sum_{i \neq m+1}^{k} \left(\beta_i^n / \hat{\sigma}_i\right)^2}, \text{ if } APCSm_1\left(\alpha^{n-1}\right) < APCSm_2\left(\alpha^{n-1}\right).$$

So the proportion of computing budget allocated to design i at the n^{th} iteration in the procedure is $\alpha_i^n = \beta_i^n \Big/ \sum_{j=1}^{k} \beta_j^n$. Let $\gamma_i^n = \dfrac{N_i^n}{T^n}$. So we have the following expression for the procedure.

$$\gamma_i^{n+1} = \gamma_i^n + \frac{I\left(s_n = i\right) - \gamma_i^n}{n+1}, \tag{G.1}$$

in which s_n is a random variable with sample space {1,2,…k} and P{ $s_n = i | i = 1,2,\ldots,k$ }$= \alpha_i^{\,n}$, and $I(\cdot)$ is the indicator function. We can re-write the recursion for $\gamma_{i,n}$ in the following way.

$$\gamma_i^{n+1} = \gamma_i^n + \frac{\alpha_i^* - \gamma_i^n}{n+1} + \frac{I\left(s_n = i\right) - \alpha_i^n}{n+1} + \frac{\alpha_i^n - \alpha_i^*}{n+1}. \tag{G.2}$$

Because $E\left[I\left(s_n = i\right) \middle| \text{all sample values until replicate } n\right] = \alpha_i^n$, the sequence $\left\{I\left(s_n = i\right) - \alpha_i^n\right\}$ is a martingale difference with respect to the sequence of σ-algebras generated by all sample values generated until the replicate n. Therefore, the sequence $\left\{I\left(s_n = i\right) - \alpha_i^n\right\}$ will be asymptotically negligible.

We know $\sum_{n=0}^{\infty} 1/(n+1) = \infty$, $\sum_{n=0}^{\infty} 1/(n+1)^2 < \infty$, and γ_i^{n+1} <1. Based on the Theorem 5.2.1 of Kushner and Yin (2003), to prove $\frac{N_i^n}{T} \to \alpha^*$ almost surely in our case, we only need to show that $\sum_n \frac{\left|\alpha_i^n - \alpha_i^*\right|}{n+1} < \infty$ with probability one.

For the term $\frac{\alpha_i^n - \alpha_i^*}{n+1}$ in (G.2), we have

$$\sum_n \frac{\left|\alpha_i^n - \alpha_i^*\right|}{n+1} \le \sum_n \frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(n+1)\right)}{n+1} + \sum_n \frac{1}{(n+1)^2} \tag{G.3}$$

We know $\sum_{n=0}^{\infty} 1/(n+1)^2 < \infty$, so $\sum_n \frac{\left|\alpha_i^n - \alpha_i^*\right|}{n+1} < \infty$ almost surely can be proved if $\sum_{n=0}^{\infty} \frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(n+1)\right)}{n+1} < \infty$ with probability one.

The set $\left\{\sum_n \frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(n+1)\right)}{n+1} = \infty\right\}$ is the subset of $\bigcup_{h=0}^{\infty} \left\{\frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(h+1)\right)}{n+1} = \infty\right\}$. Because β_i^n >0 $\forall i = 1,\dots,k$ and k is a constant, we can always find a positive value c such that $\alpha_i^n > c \quad \forall n \in N^{++}$. In addition, the sample mean and sample variance are consistent estimators of its real mean and variance, so we have $\alpha_i^n \to \alpha_i^*$ as n goes to infinity. Because $\alpha_i^n \to \alpha_i^*$ almost surely, we have $P\left\{\sum_n \frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(h+1)\right)}{n+1} = \infty\right\} = 0$. So $\sum_{n=0}^{\infty} \frac{I\left(\left|\alpha_i^n - \alpha_i^*\right| > 1/(n+1)\right)}{n+1} < \infty$ w.p.1. Hence, $\sum_n \frac{\left|\alpha_i^n - \alpha_i^*\right|}{n+1} < \infty$ almost surely.

Therefore, all the assumptions of Theorem 5.2.1 of Kushner and Yin (2003) satisfied. This results in $\frac{N_i^n}{T} \to \alpha^*$ almost surely. □

Appendix H. Proof of Lemma 3.5

Proof of Lemma 3.5(a)

The computing budget allocated to every design by OCBAm in the equal variance situation is

$$\frac{\alpha_x}{\alpha_y} = \left(\frac{1/\delta_x}{1/\delta_y}\right)^2,$$

in which $\delta_x = \mu_x - c$ for all $x = 1, 2, \ldots, k$ and $c = \frac{\mu_m + \mu_{m+1}}{2}$.

Let $A_1 = \sum_{i=1}^{k} \frac{1}{(\mu_i - c)^2}$. Then, it follows that $\alpha_i = \frac{1}{A_1} \cdot \frac{1}{(\mu_i - c)^2}$, for $i = 1, 2, \ldots, k$. Thus,

$$G_{ij}(\alpha_i, \alpha_j) = \frac{(\mu_i - \mu_j)^2}{2\sigma^2 A_1\left((\mu_i - c)^2 + (\mu_j - c)^2\right)} = \frac{1}{2\sigma^2 A_1} \cdot \left(1 + \frac{2}{x + \frac{1}{x}}\right),$$

in which $x = \frac{(c - \mu_i)}{(\mu_j - c)}$.

For $0 < x \le 1$, $G_{ij}(\alpha_i, \alpha_j)$ is an increasing function of *x*, while $G_{ij}(\alpha_i, \alpha_j)$ is a decreasing function of *x* when $x > 1$. Thus, the minimum of $G_{ij}(\alpha_i, \alpha_j)$ will be at the minimum value of *x* for $0 < x \le 1$

or the maximum value of x for $x>1$. Since $\mu_1<\mu_2<\cdots<\mu_k$ and $c=\frac{\mu_m+\mu_{m+1}}{2}$, it follows that $\min x=\frac{c-\mu_m}{\mu_k-c}$ for $0<x\le 1$ and $\max x=\frac{c-\mu_1}{\mu_{m+1}-c}$ for $x>1$. Therefore, it is proved that

$$\min_{i\le m,\, j\ge m+1} G_{ij}\left(\alpha_i,\alpha_j\right)=\min\left\{G_{mk}\left(\alpha_m,\alpha_k\right),G_{1(m+1)}\left(\alpha_1,\alpha_{(m+1)}\right)\right\}.$$

Proof of Lemma 3.5(b)

Suppose $\left(\alpha_1{}^L,\alpha_2{}^L,\cdots,\alpha_k{}^L\right)$ is the computing proportions allocated to all designs by OCBAm+.

When $APCSm_1\left(\alpha^{*1}\right)\ge APCSm_2\left(\alpha^{*2}\right)$,

$$\frac{\alpha_x^L}{\alpha_y^L}=\frac{1/\left(\mu_i-\mu_m\right)^2}{1/\left(\mu_j-\mu_m\right)^2}\text{, for } x,y\ne m\text{, and } \alpha_m^L=\sqrt{\sum_{i\ne m}\left(\alpha_i^L\right)^2};$$

and when $APCSm_1\left(\alpha^{*1}\right)\le APCSm_2\left(\alpha^{*2}\right)$,

$$\frac{\alpha_x^L}{\alpha_y^L}=\frac{1/\left(\mu_i-\mu_{m+1}\right)^2}{1/\left(\mu_j-\mu_{m+1}\right)^2}\text{, for } x,y\ne m+1\text{, and } \alpha_{m+1}^L=\sqrt{\sum_{i\ne m+1}\left(\alpha_i^L\right)^2}.$$

So we prove Lemma 3.5(b) by classifying it into two cases.

Case 1. $APCSm_1\left(\alpha^{*1}\right)\ge APCSm_2\left(\alpha^{*2}\right)$

Let $A_{21}=\sum_{i\ne m}\frac{1}{\left(\mu_i-\mu_m\right)^2}+\sqrt{\sum_{i\ne m}\frac{1}{\left(\mu_i-\mu_m\right)^4}}$. Then, we have $\alpha_i^L=\frac{1}{A_{21}}\cdot\frac{1}{\left(\mu_i-\mu_m\right)^2}$, for $i\ne m$, and $\alpha_m^L=\frac{1}{A_{21}}\sqrt{\sum_{i\ne m}\frac{1}{\left(\mu_i-\mu_m\right)^4}}$.

(1) For $i=1,2,\ldots,m-1$ and $j=m+1,\ldots,k$

We know that

$$\frac{1/\alpha_i^L + 1/\alpha_j^L}{1/\alpha_m^L + 1/\alpha_{m+1}^L} = \frac{(\mu_i - \mu_m)^2 + (\mu_j - \mu_m)^2}{\dfrac{1}{\sqrt{\sum_{i \neq m} \dfrac{1}{(\mu_i - \mu_m)^4}}} + (\mu_m - \mu_{m+1})^2}.$$

Because $(\mu_i - \mu_j)^2 \geq (\mu_i - \mu_m)^2 + (\mu_j - \mu_m)^2$ and $\dfrac{1}{\sqrt{\sum_{i \neq m} \dfrac{1}{(\mu_i - \mu_m)^4}}}$ >0, it can be proved that

$$\frac{(\mu_i - \mu_j)^2}{(\mu_m - \mu_{m+1})^2} \geq \frac{1/\alpha_i^L + 1/\alpha_j^L}{1/\alpha_m^L + 1/\alpha_{m+1}^L}.$$

Therefore,

$$G_{ij}\left(\alpha_i^L, \alpha_j^L\right) \geq G_{m(m+1)}\left(\alpha_m^L, \alpha_{m+1}^L\right) \quad \forall i < m,\ j \geq m+1.$$

(2) For $i = m$ and $j = m+1, \ldots, k$

$$G_{mj}\left(\alpha_m^L, \alpha_j^L\right) = \frac{1}{2\sigma^2 A_{21}} \cdot \frac{1}{1/\left[(\mu_m - \mu_j)^2 \alpha_m^L\right] + 1},$$

$$G_{m(m+1)}\left(\alpha_m^L, \alpha_{m+1}^L\right) = \frac{1}{2\sigma^2 A_{21}} \cdot \frac{1}{1/\left[(\mu_m - \mu_{m+1})^2 \alpha_m^L\right] + 1}.$$

Since $(\mu_{m+1} - \mu_m) \leq (\mu_j - \mu_m)$, it can be concluded that

$$G_{m(m+1)}\left(\alpha_m^L, \alpha_{m+1}^L\right) \leq G_{mj}\left(\alpha_m^L, \alpha_j^L\right).$$

Case 2. $APCSm_1\left(\alpha^{*1}\right) \leq APCSm_2\left(\alpha^{*2}\right)$

The proof in case 2 is similar with case 1. Let $A_{22} = \sum_{i \neq m+1} \frac{1}{(\mu_i - \mu_{m+1})^2} + \sqrt{\sum_{i \neq m+1} \frac{1}{(\mu_i - \mu_{m+1})^4}}$. So,

$\alpha_i^L = \frac{1}{A_{22}} \cdot \frac{1}{(\mu_i - \mu_{m+1})^2}$, for $i \neq m+1$, and $\alpha_{m+1}^L = \frac{1}{A_{22}} \sqrt{\sum_{i \neq m+1} \frac{1}{(\mu_i - \mu_{m+1})^4}}$.

(3) For $i = 1, 2, \ldots, m$ and $j = m+2, \ldots, k$

We know that

$$\frac{1/\alpha_i^L + 1/\alpha_j^L}{1/\alpha_m^L + 1/\alpha_{m+1}^L} = \frac{(\mu_i - \mu_{m+1})^2 + (\mu_j - \mu_{m+1})^2}{(\mu_m - \mu_{m+1})^2 + \frac{1}{\sqrt{\sum_{i \neq m+1} \frac{1}{(\mu_i - \mu_{m+1})^4}}}} .$$

Since $(\mu_i - \mu_j)^2 \geq (\mu_i - \mu_{m+1})^2 + (\mu_j - \mu_{m+1})^2$ and $\frac{1}{\sqrt{\sum_{i \neq m+1} \frac{1}{(\mu_i - \mu_{m+1})^4}}}$ >0, it follows that

$$\frac{(\mu_i - \mu_j)^2}{(\mu_m - \mu_{m+1})^2} \geq \frac{1/\alpha_i^L + 1/\alpha_j^L}{1/\alpha_m^L + 1/\alpha_{m+1}^L} .$$

Therefore, we have

$$G_{ij}(\alpha_i^L, \alpha_j^L) \geq G_{m(m+1)}(\alpha_m^L, \alpha_{m+1}^L) \quad \forall i \leq m,\, j > m+1 .$$

(4) For $i = 1, 2, \ldots, m$ and $j = m+1$

$$G_{i(m+1)}(\alpha_i^L, \alpha_{m+1}^L) = \frac{1}{2\sigma^2 A_{22}} \cdot \frac{(\mu_i - \mu_{m+1})^2}{(\mu_m - \mu_{m+1})^2 + 1/\alpha_{m+1}^L} = \frac{1}{2\sigma^2 A_{22}} \cdot \frac{1}{1 + 1/\left[(\mu_i - \mu_{m+1})^2 \alpha_{m+1}^L\right]},$$

$$G_{m(m+1)}(\alpha_m^L, \alpha_{m+1}^L) = \frac{1}{2\sigma^2 A_{22}} \cdot \frac{(\mu_m - \mu_{m+1})^2}{(\mu_m - \mu_{m+1})^2 + 1/\alpha_{m+1}^L} = \frac{1}{2\sigma^2 A_{22}} \cdot \frac{1}{1 + 1/\left[(\mu_m - \mu_{m+1})^2 \alpha_{m+1}^L\right]} .$$

Since $(\mu_{m+1}-\mu_m)\le(\mu_{m+1}-\mu_i)$, it can be concluded that

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)\le G_{i(m+1)}\left(\alpha_i^L,\alpha_{m+1}^L\right). \qquad \square$$

Appendix I. Proof of Theorem 3.3

When all designs have a common variance, the asymptotic convergence rate obtained by OCBAm+ is

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)=\begin{cases}\dfrac{\left(\mu_{m+1}-\mu_m\right)^2}{2A_{21}\sigma^2\left[1\Big/\sqrt{\sum\limits_{i\neq m}\dfrac{1}{\left(\mu_i-\mu_m\right)^4}}+\left(\mu_{m+1}-\mu_m\right)^2\right]}, & \text{if } APCSm_1\left(\alpha^{*1}\right)\ge APCSm_2\left(\alpha^{*2}\right)\\ \dfrac{\left(\mu_{m+1}-\mu_m\right)^2}{2A_{22}\sigma^2\left[1\Big/\sqrt{\sum\limits_{i\neq m+1}\dfrac{1}{\left(\mu_i-\mu_{m+1}\right)^4}}+\left(\mu_{m+1}-\mu_m\right)^2\right]}, & \text{if } APCSm_1\left(\alpha^{*1}\right)\le APCSm_2\left(\alpha^{*2}\right)\end{cases}. \qquad (I.1)$$

And the asymptotic convergence rate obtained by the equal allocation rule (EA) is

$$G_{m(m+1)}\left(\alpha_m^E,\alpha_{m+1}^E\right)=\frac{\left(\mu_m-\mu_{m+1}\right)^2}{4k\sigma^2}, \qquad (I.2)$$

When m equals one, OCBAm+ will reduce to OCBA in Chen et al. (2000), which has been proved own the highest rate for the best design selection problem in Glynn and Juneja (2004). Hence, we only need to consider the situation $m\ge 2$ and $k\ge m+1$.

By (I.1) and (I.2), we only need to prove the following two inequities when $(\mu_{m+1}-\mu_m)\le\min(\mu_{m+2}-\mu_{m+1},\mu_m-\mu_{m-1})$.

$$\left(\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^2}+\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)\cdot\left((\mu_{m+1}-\mu_m)^2+1\Big/\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)<2k\,, \tag{I.3}$$

$$\left(\sum_{i\neq m+1}\frac{1}{(\mu_i-\mu_{m+1})^2}+\sqrt{\sum_{i\neq m+1}\frac{1}{(\mu_i-\mu_{m+1})^4}}\right)\cdot\left((\mu_{m+1}-\mu_m)^2+1\Big/\sqrt{\sum_{i\neq m+1}\frac{1}{(\mu_i-\mu_{m+1})^4}}\right)<2k\,.$$

Because the proofs of these two inequalities are similar, we only show the proof of (I.3) here.

Since $\mu_1<\mu_2<\cdots<\mu_m<\mu_{m+1}<\cdots<\mu_{k-1}<\mu_k$ and $(\mu_{m+1}-\mu_m)\leq\min(\mu_{m+2}-\mu_{m+1},\mu_m-\mu_{m-1})$, the inequalities below is true.

$$(\mu_{m+1}-\mu_m)^2\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^2}<k-1, \tag{I.4}$$

$$\sum_{i\neq m}\left(\frac{1}{(\mu_i-\mu_m)^2}\Big/\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)<k-1. \tag{I.5}$$

Combining (I.4) and (I.5), we can get

$$\begin{aligned}&\left(\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^2}+\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)\cdot\left((\mu_{m+1}-\mu_m)^2+1\Big/\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)\\&=(\mu_{m+1}-\mu_m)^2\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^2}+(\mu_{m+1}-\mu_m)^2\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}+\sum_{i\neq m}\left(\frac{1}{(\mu_i-\mu_m)^2}\Big/\sqrt{\sum_{i\neq m}\frac{1}{(\mu_i-\mu_m)^4}}\right)+1<2k\end{aligned}$$

□

Appendix J. Proof of Theorem 3.4

When $\mu_{i+1}-\mu_i=d$, for $i=1,2,\ldots,k-1$, and all designs have a common variance, the convergence rate obtained by OCBAm+ is

i) If $APCSm_1\left(\alpha^{*1}\right)\geq APCSm_2\left(\alpha^{*2}\right)$

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)=\frac{d^2}{2\sigma^2}\cdot\frac{1}{\sum_{i\neq m}\frac{1}{(m-i)^2}+\sqrt{\sum_{i\neq m}\frac{1}{(m-i)^4}}}\cdot\frac{1}{\left(1+1\Big/\sqrt{\sum_{i\neq m}\frac{1}{(m-i)^4}}\right)}; \tag{J.1}$$

ii) If $APCSm_1\left(\alpha^{*1}\right)\leq APCSm_2\left(\alpha^{*2}\right)$

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)=\frac{d^2}{2\sigma^2}\cdot\frac{1}{\sum_{i\neq m+1}\frac{1}{(m+1-i)^2}+\sqrt{\sum_{i\neq m+1}\frac{1}{(m+1-i)^4}}}\cdot\frac{1}{\left(1+1\Big/\sqrt{\sum_{i\neq m+1}\frac{1}{(m+1-i)^4}}\right)}.$$

And the convergence rate obtained by OCBAm is

$$\begin{aligned}&\min\left\{G_{mk}\left(\alpha_m,\alpha_k\right),G_{1(m+1)}\left(\alpha_1,\alpha_{(m+1)}\right)\right\}\\&=\frac{d^2}{2\sigma^2}\cdot\frac{1}{\sum_{i=1}^{k}\frac{1}{\left(i-m-\frac{1}{2}\right)^2}}\cdot\min\left\{1+\frac{2}{2\left(k-m-\frac{1}{2}\right)+1\Big/2\left(k-m-\frac{1}{2}\right)},1+\frac{2}{2\left(m-\frac{1}{2}\right)+1\Big/2\left(m-\frac{1}{2}\right)}\right\}.\end{aligned} \tag{J.2}$$

When m equals one, OCBAm+ goes to the OCBA. In this situation, OCBAm+ is no worse than OCBAm. For m greater than one, we show the proof when $m\geq 4$ and $k\geq m+6$.

a) A lower bound of the convergence rate for OCBAm+ when $m\geq 4$ and $k\geq m+6$

If $APCSm_1\left(\alpha^{*1}\right) \geq APCSm_2\left(\alpha^{*2}\right)$, the asymptotic convergence rate for OCBAm+ is (J.1). When $m \geq 4$ and $k \geq m+6$, it is true that

$$2\times\left(1+\frac{1}{2^4}+\frac{1}{3^4}\right) < \sum_{i\neq m}\frac{1}{\left(m-i\right)^4} < 2\sum_{n=1}^{\infty}\frac{1}{n^4}\ . \tag{J.3}$$

The right part in this inequality (J.3) is a series whose sum is Riemann's zeta function, denoted as

$$\zeta\left(s\right)=\sum_{n=1}^{\infty}\left(1/n^s\right). \text{ When } s=4,\ \zeta\left(4\right)=\sum_{n=1}^{\infty}\left(1/n^4\right)=\frac{\pi^4}{90}\approx 1.0823\ .$$

So we have

$$1.466 < \sqrt{\sum_{i\neq m}\frac{1}{\left(m-i\right)^4}} < 1.472\ . \tag{J.4}$$

For $i \leq m-3$,

$$\frac{1}{\left(m-i\right)^2}=\frac{1}{\left(m-i-1\right)^2+2\left(m-i-1\right)+1}<\frac{1}{\left(m-i-1\right)^2+2\left(m-i-1\right)}=\frac{1}{2}\left(\frac{1}{m-i-1}-\frac{1}{m-i+1}\right).$$

Therefore, it is true that

$$\sum_{i=1}^{m-3}\frac{1}{\left(m-i\right)^2}<\frac{1}{2}\sum_{i=1}^{m-3}\left(\frac{1}{m-i-1}-\frac{1}{m-i+1}\right)=\frac{1}{2}\cdot\left(\frac{5}{6}-\frac{1}{m-1}-\frac{1}{m}\right). \tag{J.5}$$

Similarly,

$$\sum_{i=m+3}^{k}\frac{1}{\left(i-m\right)^2}<\frac{1}{2}\sum_{i=m+3}^{k}\left(\frac{1}{i-\left(m+1\right)}-\frac{1}{i-m+1}\right)<\frac{1}{2}\cdot\left(\frac{5}{6}-\frac{1}{k-m}-\frac{1}{k-m+1}\right). \tag{J.6}$$

Combining (J.5) and (J.6), an upper bound of $\sum_{i\neq m}\frac{1}{(m-i)^2}$ is

$$\sum_{i\neq m}\frac{1}{(m-i)^2}<\frac{1}{2}\cdot\left(\frac{5}{3}-\frac{1}{m-1}-\frac{1}{m}-\frac{1}{k-m}-\frac{1}{k-m+1}\right)+2.5. \tag{J.7}$$

Consequently,

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)>\frac{d^2}{2\sigma^2}\cdot\frac{1}{a_1+3.972}\cdot\frac{1}{1.683}, \tag{J.8}$$

in which $a_1=\frac{1}{2}\cdot\left(\frac{5}{3}-\frac{1}{m-1}-\frac{1}{m}-\frac{1}{k-m}-\frac{1}{k-m+1}\right)$.

Similarly, if $APCSm_1\left(\alpha^{*1}\right)\leq APCSm_2\left(\alpha^{*2}\right)$,

$$G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)>\frac{d^2}{2\sigma^2}\cdot\frac{1}{a_2+3.972}\cdot\frac{1}{1.683}, \tag{J.9}$$

in which $a_2=\frac{1}{2}\cdot\left(\frac{5}{3}-\frac{1}{m}-\frac{1}{m+1}-\frac{1}{k-m-1}-\frac{1}{k-m}\right)$.

b) An upper bound of the convergence rate for OCBAm when $m\geq 4$ and $k\geq m+6$

Because $m\geq 4$ and $k\geq m+6$, there exist $\left(k-m-\frac{1}{2}\right)\geq\frac{11}{2}$ and $\left(m-\frac{1}{2}\right)\geq\frac{7}{2}$. So,

$$\min\left\{1+\frac{2}{2\left(k-m-\frac{1}{2}\right)+1\Big/2\left(k-m-\frac{1}{2}\right)},1+\frac{2}{2\left(m-\frac{1}{2}\right)+1\Big/2\left(m-\frac{1}{2}\right)}\right\}\leq\frac{72}{61}. \tag{J.10}$$

For each $i\leq m-2$,

$$\frac{1}{\left(i-m-\frac{1}{2}\right)^2} > \frac{1}{(m-i)^2+2(m-i)} = \frac{1}{2}\left(\frac{1}{m-i}-\frac{1}{m-i+2}\right),$$

and for each $i \geq m+3$,

$$\frac{1}{\left(i-m-\frac{1}{2}\right)^2} > \frac{1}{\left[i-(m+1)\right]^2+2\left[i-(m+1)\right]} = \frac{1}{2}\left(\frac{1}{i-(m+1)}-\frac{1}{i-(m-1)}\right).$$

Therefore, we have

$$\sum_{i=1}^{k}\frac{1}{\left(i-m-\frac{1}{2}\right)^2} = \sum_{i=1}^{m-2}\frac{1}{\left(m+\frac{1}{2}-i\right)^2} + \sum_{i=m+3}^{k}\frac{1}{\left(i-m-\frac{1}{2}\right)^2} + 8 + \frac{8}{9} > \left(\frac{5}{3}-\frac{1}{m}-\frac{1}{m+1}-\frac{1}{k-m}-\frac{1}{k-m+1}\right)+\frac{80}{9}. \quad \text{(J.11)}$$

Combing inequalities (J.10) and (J.11), we have

$$\min\left\{G_{mk}\left(\alpha_m,\alpha_k\right),G_{1(m+1)}\left(\alpha_1,\alpha_{(m+1)}\right)\right\} < \frac{d^2}{2\sigma^2}\cdot\frac{1}{b+\frac{80}{9}}\cdot\frac{72}{61} < \frac{d^2}{2\sigma^2}\cdot\frac{1.1804}{b+8.88}, \quad \text{(J.12)}$$

in which $b=\frac{1}{2}\left(\frac{5}{3}-\frac{1}{m}-\frac{1}{m+1}-\frac{1}{k-m}-\frac{1}{k-m+1}\right)$.

c) The difference between OCBAm+'s convergence rate and OCBAm's convergence rate when $m \geq 4$ and $k \geq m+6$

Because $a_1 < b$ and $a_2 < b$, we can get the following inequality by (J.8), (J.9), and (J.12).

$$\begin{aligned}
&G_{m(m+1)}\left(\alpha_m^L,\alpha_{m+1}^L\right)-\min\left\{G_{mk}\left(\alpha_m,\alpha_k\right),G_{1(m+1)}\left(\alpha_1,\alpha_{(m+1)}\right)\right\}\\
&>\frac{d^2}{2\sigma^2}\cdot\frac{1}{b+3.972}\cdot\frac{1}{1.683}-\frac{d^2}{2\sigma^2}\cdot\frac{1.1804}{b+8.88}\\
&>\frac{d^2}{2\sigma^2}\left[\frac{0.987-0.987b}{1.683(b+3.972)(b+8.88)}\right].
\end{aligned}$$

Since $b < \frac{5}{6}$, it can be proved that

$$G_{m(m+1)}\left(\alpha_m^L, \alpha_{m+1}^L\right) - \min\left\{G_{mk}\left(\alpha_m, \alpha_k\right), G_{1(m+1)}\left(\alpha_1, \alpha_{(m+1)}\right)\right\} > \frac{d^2}{2\sigma^2}\left[\frac{0.987 - 0.987b}{1.683(b+3.972)(b+8.88)}\right] > 0.$$

For the case $m \geq 4$ and $k = m+5$ and the cases that m equals 2 and 3, the proof is easier and follows in similar fashion. □

Appendix K. Proof for Theorem 5.1

We firstly define four sets

$$S_{A_1} = \left\{i : X_i^{\,t} \in S_A \text{ and } \alpha_i I_i\left(f\left(P_i^{t-1}\right)\right) \leq G_{ig}\left(\alpha_i, \alpha_g\right)\right\}$$

$$S_{A_2}\left\{i : X_i^{\,t} \in S_A \text{ and } \alpha_i I_i\left(f\left(P_i^{t-1}\right)\right) > G_{ig}\left(\alpha_i, \alpha_g\right)\right\},$$

$$S_{B_1} = \left\{j : X_j^{\,t} \in S_B \text{ and } \alpha_j I_j\left(f\left(P_j^{t-1}\right)\right) \leq G_{jg}\left(\alpha_j, \alpha_g\right)\right\},$$

$$S_{B_2} = \left\{j : X_j^{\,t} \in S_B \text{ and } \alpha_j I_j\left(f\left(P_j^{t-1}\right)\right) > G_{jg}\left(\alpha_j, \alpha_g\right)\right\}.$$

Based on the definition, model (5.4) can be simplified as

$$
\begin{aligned}
&\max \quad z \quad s.t. \\
&\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{t-1}\right)\right) \geq z, \quad \text{for } X_{i_1} \in S_{A_1} \\
&G_{i_1 g}\left(\alpha_{i_2}, \alpha_g\right) \geq z, \quad \text{for } X_{i_2} \in S_{A_2} \\
&\alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) \geq z, \quad \text{for } X_{j_1} \in S_{B_1} \\
&G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right) \geq z, \quad \text{for } X_{j_2} \in S_{B_2} \\
&\sum_{i=1}^{m} \alpha_i + \alpha_g = 1 \\
&\alpha_i \geq 0.
\end{aligned}
\tag{K.1}
$$

Let F be the Lagrangian functions of model (K.1). Then, we have

$$
\begin{aligned}
F = z - &\sum_{X_{i_1} \in S_{A_1}} \lambda_{i_1}\left(\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{t-1}\right)\right) - z\right) - \sum_{X_{i_2} \in S_{A_2}} \lambda_{i_2}\left(G_{i_2 g}\left(\alpha_{i_2}, \alpha_g\right) - z\right) - \\
&\sum_{X_{j_1} \in S_{B_1}} \lambda_{j_1}\left(\alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) - z\right) - \sum_{X_{j_2} \in S_{B_2}} \lambda_{j_2}\left(G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right) - z\right) - \\
&\nu\left(1 - \left(\sum_{i=1}^{m} \alpha_i + \alpha_g\right)\right) - \sum_{i=1,\ldots,m \text{ or } i=g} \gamma_i \alpha_i
\end{aligned}
$$

The Karush-Kuhn-Tucker conditions are

i. The primal constraints:

$$
\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{t-1}\right)\right) \geq z, \quad \text{for } X_{i_1} \in S_{A_1} \qquad G_{i_2 g}\left(\alpha_{i_2}, \alpha_g\right) \geq z, \quad \text{for } X_{i_2} \in S_{A_2}
$$

$$
\alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) \geq z, \quad \text{for } X_{j_1} \in S_{B_1} \qquad G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right) \geq z, \quad \text{for } X_{j_2} \in S_{B_2}
$$

$$
\sum_{i=1}^{m} \alpha_i + \alpha_g = 1, \ \alpha_i \geq 0.
$$

ii. The dual constraints:

$$
\lambda_i \geq 0, \ \nu \geq 0 \text{ and } \gamma_i \geq 0 \text{ for all } i = 1, \ldots, m, g.
$$

iii. Complementary slackness:

$$\lambda_{i_1}\left(\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{\ t-1}\right)\right)-z\right)=0\,, \quad \lambda_{i_2}\left(G_{i_2 g}\left(\alpha_{i_2},\alpha_g\right)-z\right)=0\,,$$

$$\lambda_{j_1}\left(\alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{\ t-1}\right)\right)-z\right)=0\,, \quad \lambda_{j_2}\left(G_{j_2 g}\left(\alpha_{j_2},\alpha_g\right)-z\right)=0\,,$$

$$\nu\left(\sum_{i=1}^{m}\alpha_i+\alpha_g-1\right)=0\,,\ \gamma_i\alpha_i=0\,.$$

iv. Gradient of Lagrangian with respect to decision variables vanishes:

$$\nabla F=0\,.$$

Based on condition (iv), the following equations can be obtained.

$$\lambda_{i_1}\frac{\partial\alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{\ t-1}\right)\right)}{\partial\alpha_{i_1}}-\nu+\gamma_{i_1}=0 \quad \forall X_{i_1}\in S_{A_1} \tag{K.2}$$

$$\lambda_{i_2}\frac{\partial G_{i_2 g}\left(\alpha_{i_2},\alpha_g\right)}{\partial\alpha_{i_2}}-\nu+\gamma_{i_2}=0 \quad \forall X_{i}\ \in S_{A_2} \tag{K.3}$$

$$\lambda_{j_1}\frac{\partial\alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{\ t-1}\right)\right)}{\partial\alpha_{j_1}}-\nu+\gamma_{j_1}=0 \quad \forall X_{j_1}\in S_{B_1} \tag{K.4}$$

$$\lambda_{j_2}\frac{\partial G_{j_2 g}\left(\alpha_{j_2},\alpha_g\right)}{\partial\alpha_{j_2}}-\nu+\gamma_{j_2}=0 \quad \forall X_{j_2}\in S_{B_2} \tag{K.5}$$

$$\sum_{X_{i_2}\in S_{A_2}}\lambda_{i_2}\frac{\partial G_{i_2 g}\left(\alpha_{i_2},\alpha_g\right)}{\partial\alpha_g}+\sum_{X_{j_2}\in S_{B_2}}\lambda_{j_2}\frac{\partial G_{j_2 g}\left(\alpha_{j_2},\alpha_g\right)}{\partial\alpha_g}-\nu+\gamma_g=0 \tag{K.6}$$

In stochastic situation, each solution has a noise and will be given no less than one sample to evaluate its performance. That is, $\alpha_i>0$, $\forall i=1,\ldots,m,g$. So we have $\gamma_i=0\ \forall i=1,\ldots,m,g$. Let $\lambda_i>0$, $\nu>0$ for all $i=1,\ldots,m,g$. Based on (iii), we have

$$\alpha_{i_1} I_{i_1}\left(f\left(P^{t-1}{}_{i_1}\right)\right) = G_{i_2 g}\left(\alpha_{i_2}, \alpha_g\right) = \alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) = G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right),$$

and

$$\lambda_{i_1} = \frac{v}{\partial \alpha_{i_1} I_{i_1}\left(f\left(P_{i_1}^{t-1}\right)\right) \Big/ \partial \alpha_{i_1}} \quad \forall X_{i_1} \in S_{A_1}, \quad \lambda_{i_2} = \frac{v}{\partial G_{i_2 g}\left(\alpha_{i_2}, \alpha_g\right) \Big/ \partial \alpha_{i_2}} \quad \forall X_{i_2} \in S_{A_2},$$

$$\lambda_{j_1} = \frac{v}{\partial \alpha_{j_1} I_{j_1}\left(f\left(P_{j_1}^{t-1}\right)\right) \Big/ \partial \alpha_{j_1}} \quad \forall X_{j_1} \in S_{B_1}, \quad \lambda_{j_2} = \frac{v}{\partial G_{j_2 g}\left(\alpha_{j_2}, \alpha_g\right) \Big/ \partial \alpha_{j_2}} \quad \forall X_{j_2} \in S_{B_2}.$$

Substituting them into (K.6), the following equation can be obtained.

$$\sum_{i_2} \frac{\partial G_{i_2 g} / \partial \alpha_g}{\partial G_{i_2 g} / \partial \alpha_{i_2}} + \sum_{j_2} \frac{\partial G_{j_2 g} / \partial \alpha_g}{\partial G_{j_2 g} / \partial \alpha_{j_2}} = 1 .$$

Therefore, if a solution satisfies the conditions in theorem 5.1, we can find the values of γ_i, λ_i and v such that it also satisfies the KKT conditions. Because of the concavity of the maximization problem, the KKT condition is the sufficient and necessary condition for optimality. Therefore, the rule satisfying Theorem 5.1 is an optimal allocation rule for model (5.4). □

Appendix L. Proof for Lemma 5.1

When the performance of each particle follows a normal distribution, we can obtain the following equation based on large deviation theory.

$$I_{i_1}\left(f\left(P^{t-1}{}_{i_1}\right)\right) = \frac{\left(f\left(P^{t-1}{}_{i_1}\right) - f\left(X_{i_1}\right)\right)^2}{2\sigma_{i_1}^2} \quad \forall X_{i_1} \in S_{A_1} \tag{L.1}$$

$$I_{j_1}\left(f\left(P^{t-1}{}_{j_1}\right)\right)=\frac{\left(f\left(P^{t-1}{}_{j_1}\right)-f\left(X_{j_1}\right)\right)^2}{2\sigma_{j_1}^2}\ \forall X_{j_1}\in S_{B_1} \quad \text{(L.2)}$$

$$G_{i_2g}\left(\alpha_{i_2},\alpha_g\right)=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{i_2}\right)\right)^2}{\sigma_g^2/\alpha_g+\sigma_{i_2}^2/\alpha_{i_2}}\ \forall X_{i_2}\in S_{A_2} \quad \text{(L.3)}$$

$$G_{j_2g}\left(\alpha_{j_2},\alpha_g\right)=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{j_2}\right)\right)^2}{\sigma_g^2/\alpha_g+\sigma_{j_2}^2/\alpha_{j_2}}\ \forall X_{j_2}\in S_{B_2} \quad \text{(L.4)}$$

For $X_{i_2}\in S_{A_2}$,

$$\frac{\partial G_{i_2g}\left(\alpha_{i_2},\alpha_g\right)}{\partial\alpha_{i_2}}=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{i_2}\right)\right)^2}{\left(\sigma_g^2/\alpha_g+\sigma_{i_2}^2/\alpha_{i_2}\right)^2}\cdot\frac{\sigma_{i_2}^2}{\alpha_{i_2}^2}\ \text{and}\ \frac{\partial G_{i_2g}\left(\alpha_{i_2},\alpha_g\right)}{\partial\alpha_g}=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{i_2}\right)\right)^2}{\left(\sigma_g^2/\alpha_g+\sigma_{i_2}^2/\alpha_{i_2}\right)^2}\cdot\frac{\sigma_g^2}{\alpha_g^2}. \quad \text{(L.5)}$$

For $X_{j_2}\in S_{B_2}$

$$\frac{\partial G_{j_2g}\left(\alpha_{j_2},\alpha_g\right)}{\partial\alpha_{j_2}}=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{j_2}\right)\right)^2}{\left(\sigma_g^2/\alpha_g+\sigma_{j_2}^2/\alpha_{j_2}\right)^2}\cdot\frac{\sigma_{j_2}^2}{\alpha_{j_2}^2}\ \text{and}\ \frac{\partial G_{j_2g}\left(\alpha_{j_2},\alpha_g\right)}{\partial\alpha_g}=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{j_2}\right)\right)^2}{\left(\sigma_g^2/\alpha_g+\sigma_{j_2}^2/\alpha_{j_2}\right)^2}\cdot\frac{\sigma_g^2}{\alpha_g^2}. \quad \text{(L.6)}$$

Substituting (L.5) and (L.6) into (b) in Theorem 5.1,

$$\sum_{i_2}\frac{\sigma_g^2/\alpha_g^2}{\sigma_{i_2}^2/\alpha_{i_2}^2}+\sum_{j_2}\frac{\sigma_g^2/\alpha_g^2}{\sigma_{j_2}^2/\alpha_{j_2}^2}=1.$$

Hence,

$$\alpha_g=\sigma_g\sqrt{\sum_{i_2}\frac{\alpha_{i_2}^2}{\sigma_{i_2}^2}+\sum_{j_2}\frac{\alpha_{j_2}^2}{\sigma_{j_2}^2}}\ .$$

Under the assumption $\alpha_g \gg \alpha_i$, (L.3) and (L.4) can be simplified as

$$G_{i_2 g}\left(\alpha_{i_2},\alpha_g\right)=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{i_2}\right)\right)^2}{\sigma_{i_2}^2/\alpha_{i_2}}, \text{ and } G_{j_2 g}\left(\alpha_{j_2},\alpha_g\right)=\frac{\left(f\left(P^{t-1}{}_g\right)-f\left(X_{j_2}\right)\right)^2}{\sigma_{j_2}^2/\alpha_{j_2}}.$$

Substituting into (a) in Theorem 5.1 yields

$$\begin{aligned}&\alpha_{i_1}:\alpha_{i_2}:\alpha_{j_1}:\alpha_{j_2}\\ &=\frac{\sigma_{i_1}^2}{\left(f\left(X_{i_1}\right)-f\left(P_{i_1}^{t-1}\right)\right)^2}:\frac{\sigma_{i_2}^2}{\left(f\left(X_{i_2}\right)-f\left(P_g^{t-1}\right)\right)^2}:\frac{\sigma_{j_1}^2}{\left(f\left(X_{j_1}\right)-f\left(P_{j_1}^{t-1}\right)\right)^2}:\frac{\sigma_{j_2}^2}{\left(f\left(X_{j_2}\right)-f\left(P_g^{t-1}\right)\right)^2}\end{aligned}$$

□

Appendix M. Proof for Theorem 5.3

Being similar to the proof of Theorem 5.1, let F be the Lagrangian functions of model (5.8). Then, we have

$$F=z-\sum_{X_i^t\in S_e,X_i^t\neq X_b^t}\lambda_{bi}\left[G_{bi}\left(\alpha_b,\alpha_i\right)-z\right]-\sum_{X_i^t\in S_e,X_j^t\in S_{ne}}\lambda_{ij}\left[G_{ij}\left(\alpha_i,\alpha_j\right)-z\right]-\nu\left(1-\sum_{i=1}^m\alpha_i\right)-\sum_{i=1,\ldots,m}\gamma_i\alpha_i$$

Hence, the Karush-Kuhn-Tucker conditions are

i. The primal constraints:

$$z\le G_{bi}\left(\alpha_b,\alpha_i\right),\quad \text{for } X_i^t\in S_e,$$

$$z\le G_{ij}\left(\alpha_i,\alpha_j\right),\quad \text{for } X_i^t\in S_e, X_j^t\in S_{ne},$$

$$\sum_{i=1}^m\alpha_i=1,\ \alpha_i\ge 0.$$

ii. The dual constraints:

$$\lambda_{bi} \geq 0, \lambda_{ij} \geq 0, \ \nu \geq 0 \ \text{and} \ \gamma_i \geq 0 \ \text{for all} \ X_i^t \in S_e, \ X_j^t \in S_{ne} \ .$$

iii. Complementary slackness:

$$\lambda_{bi}\left[G_{bi}\left(\alpha_b, \alpha_i\right) - z\right] = 0 \quad \lambda_{ij}\left[G_{ij}\left(\alpha_i, \alpha_j\right) - z\right] = 0 \quad \nu\left(1 - \sum_{i=1}^{m} \alpha_i\right) = 0 \quad \gamma_i \alpha_i = 0$$

iv. Gradient of Lagrangian with respect to decision variables vanishes:

$$\nabla F = 0 \, .$$

Based on condition (iv), the following equations can be obtained.

$$\frac{\partial F}{\partial \alpha_b} = -\sum_{X_i^t \in S_e, X_i^t \neq X_b^t} \lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b, \alpha_i\right)}{\partial \alpha_b} - \sum_{X_j^t \in S_{ne}} \lambda_{bj} \frac{\partial G_{bj}\left(\alpha_b, \alpha_j\right)}{\partial \alpha_b} + \nu - \gamma_b = 0 \qquad \text{(M.1)}$$

$$\frac{\partial F}{\partial \alpha_i} = -\lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b, \alpha_i\right)}{\partial \alpha_i} - \sum_{X_j^t \in S_{ne}} \lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i, \alpha_j\right)}{\partial \alpha_i} + \nu - \gamma_i = 0, \ \text{for} \ X_i^t \in S_e, X_i^t \neq X_b^t \qquad \text{(M.2)}$$

$$\frac{\partial F}{\partial \alpha_j} = -\sum_{X_i^t \in S_e} \lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i, \alpha_j\right)}{\partial \alpha_j} + \nu - \gamma_j = 0, \ \text{for} \ X_j^t \in S_{ne} \qquad \text{(M.3)}$$

In stochastic situation, each solution has a noise and will be given no less than one sample to evaluate its performance. That is, $\alpha_i > 0$, $\forall i = 1, ..., m, g$. So (M.1) to (M.3) can be simplified as follows.

$$\sum_{X_i^t \in S_e, X_i^t \neq X_b^t} \lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b, \alpha_i\right)}{\partial \alpha_b} + \sum_{X_j^t \in S_{ne}} \lambda_{bj} \frac{\partial G_{bj}\left(\alpha_b, \alpha_j\right)}{\partial \alpha_b} = \nu$$

$$\lambda_{bi}\frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right)}{\partial\alpha_i}+\sum_{X_j^t\in S_{ne}}\lambda_{ij}\frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right)}{\partial\alpha_i}=\nu\text{ , for } X_i^t\in S_e, X_i^t\neq X_b^t;$$

$$\sum_{X_i^t\in S_e}\lambda_{ij}\frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right)}{\partial\alpha_j}=\nu\text{ , for } X_j^t\in S_{ne}.$$

Therefore, if we can find the non-negative values of λ_{ij} and ν such that one allocation rule can satisfies the above conditions, the rule is an optimal allocation rule for model (8). □

Appendix N. Proof for Lemma 5.3

Under the assumption of normality, Glynn and Juneja (2004) show that

$$G_{ij}\left(\alpha_i,\alpha_j\right)=\frac{\left(f\left(X_i\right)-f\left(X_i\right)\right)^2}{\sigma_i^2/\alpha_i+\sigma_j^2/\alpha_j}\ .$$

For X_b^t ,

$$G_{bi}\left(\alpha_b,\alpha_i\right)=\frac{\left(f\left(X_b^t\right)-f\left(X_i^t\right)\right)^2}{\sigma_b^2/\alpha_b+\sigma_i^2/\alpha_i}\text{ , for } X_i^t\in S_e, X_i^t\neq X_b^t.$$

$$G_{bj}\left(\alpha_b,\alpha_j\right)=\frac{\left(f\left(X_b^t\right)-f\left(X_j^t\right)\right)^2}{\sigma_b^2/\alpha_b+\sigma_j^2/\alpha_j}\text{ , for } X_j^t\in S_{ne}\ .$$

Because $\left|f\left(X_b^t\right)-f\left(X_i^t\right)\right|<\left|f\left(X_b^t\right)-f\left(X_j^t\right)\right|$ and $\alpha_i\gg\alpha_j$, we have $G_{bi}\left(\alpha_b,\alpha_i\right)<G_{bj}\left(\alpha_b,\alpha_j\right)$. Hence, $\lambda_{bj}=0$ for $X_j^t\in S_{ne}$. Similarly, because $\max_{X_k^t\in S_e^0}f\left(X_k{}^t\right)<\min_{X_i^t\in S_e^1}f\left(X_i{}^t\right)$ and $\alpha_k,\alpha_i\gg\alpha_j$, we have

$G_{kj}\left(\alpha_k,\alpha_j\right) > G_{ij}\left(\alpha_i,\alpha_j\right)$. Hence, $\lambda_{kj}=0$ for $X_j^t \in S_{ne}$. In the same way, we can get the inequality that $G_{i'j}\left(\alpha_{i'},\alpha_j\right) > G_{ij}\left(\alpha_i,\alpha_j\right)$ for $X_j^t \in S_{ne}^i$ and $X_j^t \notin S_{ne}^{i'}$. So, $\lambda_{ij}=0$ for $X_j^t \notin S_{ne}^i$.

Based on the above analysis, the condition (b) in Theorem 5.3 can be simplified as follows.

$$\sum_{X_k^t \in S_e^0} \lambda_{bk} \frac{\partial G_{bk}\left(\alpha_b,\alpha_k\right)}{\partial \alpha_b} + \sum_{X_i^t \in S_e^1} \lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right)}{\partial \alpha_b} = \nu \qquad \text{(N.1)}$$

$$\lambda_{bk} \frac{\partial G_{bk}\left(\alpha_b,\alpha_k\right)}{\partial \alpha_k} = \nu \ \text{ for } X_k^t \in S_e^0 \qquad \text{(N.2)}$$

$$\lambda_{bi} \frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right)}{\partial \alpha_i} + \sum_{X_j^t \in S_{ne}^i} \lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right)}{\partial \alpha_i} = \nu \ \text{ for } X_i^t \in S_e^1 \qquad \text{(N.3)}$$

$$\lambda_{ij} \frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right)}{\partial \alpha_j} = \nu \ \text{ for } \left\{ i \middle| X_j^t \in S_{ne}^i \right\} \qquad \text{(N.4)}$$

Substituting the expression of λ_{ij} in (N.4) into (N.3), for $X_i^t \in S_e^1$

$$\lambda_{bi} = \left(\nu - \sum_{X_j^t \in S_{ne}^i} \nu \frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right) / \partial \alpha_i}{\partial G_{ij}\left(\alpha_i,\alpha_j\right) / \partial \alpha_j} \right) \Bigg/ \left(\frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right)}{\partial \alpha_i} \right) \qquad \text{(N.5)}$$

By (N.1), (N.2) and (N.5), we have

$$\sum_{X_k^t \in S_e^0} \frac{\partial G_{bk}\left(\alpha_b,\alpha_k\right) / \partial \alpha_b}{\partial G_{bk}\left(\alpha_b,\alpha_k\right) / \partial \alpha_k} + \sum_{X_i^t \in S_e^1} \left[\frac{\partial G_{bi}\left(\alpha_b,\alpha_i\right) / \partial \alpha_b}{\partial G_{bi}\left(\alpha_b,\alpha_i\right) / \partial \alpha_i} \left(1 - \sum_{X_j^t \in S_{ne}^i} \frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right) / \partial \alpha_i}{\partial G_{ij}\left(\alpha_i,\alpha_j\right) / \partial \alpha_j} \right) \right] = 1$$

Because $\frac{\partial G_{ij}\left(\alpha_i,\alpha_j\right)}{\partial \alpha_i} = \frac{\left(f\left(X_i\right) - f\left(X_j\right) \right)^2}{\left(\sigma_i^2 / \alpha_i + \sigma_j^2 / \alpha_j \right)^2} \cdot \frac{\sigma_i^2}{\alpha_i^2}$, we have

$$\sum_{X_k^t \in S_e^0} \frac{\sigma_b^2/\alpha_b^2}{\sigma_k^2/\alpha_k^2} + \sum_{X_i^t \in S_e^1} \left[\frac{\sigma_b^2/\alpha_b^2}{\sigma_i^2/\alpha_i^2} \left(1 - \sum_{X_j^t \in S_{ne}^i} \frac{\sigma_i^2/\alpha_i^2}{\sigma_j^2/\alpha_j^2} \right) \right] = 1 \ .$$

Therefore,

$$\alpha_b = \sigma_b \sqrt{\sum_{X_k^t \in S_e^0} \frac{\alpha_k^2}{\sigma_k^2} + \sum_{X_i^t \in S_e^1} \left(\frac{\alpha_i^2}{\sigma_i^2} - \sum_{X_j^t \in S_{ne}^i} \frac{\alpha_j^2}{\sigma_j^2} \right)} \ .$$

Condition (a) in Theorem 5.3 also can be simplified as

$$G_{bk}\left(\alpha_b, \alpha_k\right) = G_{bi}\left(\alpha_b, \alpha_i\right) = G_{ij}\left(\alpha_i, \alpha_j\right) \ \text{for } X_k^t \in S_e^0, X_i^t \in S_e^1, X_j^t \in S_{ne}^i .$$

Under the assumption $\alpha_b \gg \alpha_i \gg \alpha_j$ for $X_i^t \in S_e, X_j^t \in S_{ne}$, we have the following approximation result.

$$\frac{\left(f\left(X_b^t\right) - f\left(X_k^t\right)\right)^2}{\sigma_k^2/\alpha_k} = \frac{\left(f\left(X_b^t\right) - f\left(X_i^t\right)\right)^2}{\sigma_i^2/\alpha_i} = \frac{\left(f\left(X_i^t\right) - f\left(X_j^t\right)\right)^2}{\sigma_j^2/\alpha_i} \text{for } X_k^t \in S_e^0, X_i^t \in S_e^1, X_j^t \in S_{ne}^i.$$

Therefore,

$$\alpha_k : \alpha_i : \alpha_j = \frac{\sigma_k^2}{\left(f\left(X_b^t\right) - f\left(X_k^t\right)\right)^2} : \frac{\sigma_i^2}{\left(f\left(X_b^t\right) - f\left(X_i^t\right)\right)^2} : \frac{\sigma_j^2}{\left(f\left(X_i^t\right) - f\left(X_j^t\right)\right)^2} \qquad \square$$