Declaration

I hereby declare that this 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.

Li Juxin

7 Aug. 2012
Acknowledgements

First and foremost, I would like to express my sincere gratitude to my two supervisors, Associate Professor Lee Loo Hay and Associate Professor Chew Ek Peng. Their constructive advice, invaluable support and patient guidance throughout the whole course of my candidature have been of great value for me. The study reported in this thesis would not have been possible without their supervision. Deepest gratitude are also due to all the other faculty members of the Department of Industrial and Systems Engineering, from whom the knowledge and insights gained have helped in a number of ways in my research.

Special thanks to all my graduate friends, especially Zhou Qi, Wang Qiang, Chen Liqin, Fu Yinhui, Bae Minju and Nugroho Pujowidianto, for sharing the literature and ideas, and rendering invaluable assistance.

I am deeply indebted to my parents, for their understanding, unconditional love and support through the duration of my study. This dissertation is dedicated to them.
Contents

Declaration i
Acknowledgements ii
Summary vi
List of Tables viii
List of Figures ix
Symbols and Nomenclature x

1 Introduction 1
   1.1 Objectives of the Study . . . . . . . . . . . . . . . . . . . . . . . . 4
   1.2 Significance of the Research . . . . . . . . . . . . . . . . . . . . . 5
   1.3 Organization of the Thesis . . . . . . . . . . . . . . . . . . . . . . 6

2 Literature Review 8
   2.1 Simulation Optimization . . . . . . . . . . . . . . . . . . . . . . . . 8
       2.1.1 Ranking and Selection and Computing Budget Allocation 9
   2.2 Computing Budget Allocation Problems on Finite Sets . . . . . . 10
       2.2.1 Classification of Problems . . . . . . . . . . . . . . . . . . 10
       2.2.2 Solution Approaches . . . . . . . . . . . . . . . . . . . . . 12
   2.3 Computing Budget Allocation Strategies . . . . . . . . . . . . . . 15
       2.3.1 Problems with a Single Performance Measure . . . . . . 15
       2.3.2 Problems with Multiple Performance Measures . . . . . 19
       2.3.3 Summary of the Works . . . . . . . . . . . . . . . . . . . . 21
   2.4 Summary . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 23

3 Finding a Subset of Good Systems for Multi-objective Simulation Optimization on Finite Sets 25
### 3.1 Introduction

- 3.1.1 Problem Statement  
- 3.1.2 Organization

### 3.2 Preliminaries

### 3.3 Probability of Correct Selection

### 3.4 Computing Budget Allocation Strategy

- 3.4.1 An Approximate Closed-form Solution
- 3.4.2 A Sequential Allocation Procedure

### 3.5 Numerical Experiments

### 3.6 Conclusions

### 4 Optimal Computing Budget Allocation to Select the Non-dominated Systems: a Large Deviations Perspective

- 4.1 Introduction
- 4.1.1 Problem Statement
- 4.1.2 Organization

### 4.2 Notations and Assumptions

### 4.3 Rate Function of the Probability of False Selection

### 4.4 The Optimal Allocation Strategy

- 4.4.1 Optimal Allocation Strategy Using a Solver
- 4.4.2 Optimality Conditions

### 4.5 The Multivariate Normal Case

- 4.5.1 Optimal Sampling Allocation Using a Solver
- 4.5.2 An Approximate Closed-form Solution to Sampling Allocations
- 4.5.3 Closed-form Solutions to the Nested Optimization Problems

### 4.6 Numerical Experiments

### 4.7 Conclusions

### 5 Combining Computing Budget Allocation with Multi-objective Optimization via Simulation

- 5.1 Introduction
- 5.1.1 Objectives of This Study
- 5.1.2 Organization

### 5.2 Multi-objective Evolutionary Algorithms

- 5.2.1 Challenges for Multi-objective Optimization via Simulation
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.3</td>
<td>Combination of MOEAs and Computing Budget Allocation</td>
<td>89</td>
</tr>
<tr>
<td>5.3.1</td>
<td>Multi-objective Genetic Algorithms with Optimal Computing Budget Allocation</td>
<td>90</td>
</tr>
<tr>
<td>5.3.2</td>
<td>Multi-objective Estimation of Distribution Algorithms with Optimal Computing Budget Allocation</td>
<td>92</td>
</tr>
<tr>
<td>5.3.3</td>
<td>Discussions on the Convergence of the Combined Algorithms</td>
<td>93</td>
</tr>
<tr>
<td>5.4</td>
<td>Numerical Experiments</td>
<td>94</td>
</tr>
<tr>
<td>5.4.1</td>
<td>The Experiments Scheme</td>
<td>94</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Performance Metrics</td>
<td>95</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Test Problems</td>
<td>96</td>
</tr>
<tr>
<td>5.4.4</td>
<td>Results</td>
<td>98</td>
</tr>
<tr>
<td>5.5</td>
<td>Conclusions</td>
<td>105</td>
</tr>
<tr>
<td>6</td>
<td>Conclusions</td>
<td>107</td>
</tr>
<tr>
<td>6.1</td>
<td>Conclusions of the Study</td>
<td>107</td>
</tr>
<tr>
<td>6.2</td>
<td>Discussions and Future Research</td>
<td>109</td>
</tr>
</tbody>
</table>

**Bibliography** | 112
Summary

Complex systems are very common in real world situations and multiple performance measures are usually of interest. Simulation has been widely employed in evaluating these systems and selecting the desired ones. Performances of these systems are frequently stochastic in nature and therefore selection based on simulation output bears uncertainty. Correct selection would require considerable sampling from simulation models. However, simulation runs of complex systems tend to be expensive and simulation budget is often limited. It is therefore vital to determine an optimal sampling allocation strategy such that the desired systems can be correctly selected with the highest evidence.

This thesis describes how computing budget allocation concerns are addressed in the multi-objective simulation optimization context. The concept of Pareto optimality is incorporated to resolve the trade-offs among the multiple competing performance measures, where preferences of the decision maker are not required. Evidence of correct selection is maximized through mathematical programming models that are built from either a probability or a large deviations perspective. Finite time performance and asymptotic properties of the proposed strategies are both investigated.

The problem of finding a subset of good systems from a finite set is first studied under a multi-objective simulation optimization context. The alternative systems are measured by their ranks to be Pareto-optimal, often referred to as the domination counts within the finite set. Probability of correct selection is used as the evidence of correct selection, and the objective is to determine an optimal computing budget allocation that maximizes this probability. Bonferroni bounds are employed to provide estimates for the probability, from which asymptotic allocation strategies are derived assuming multivariate normally distributed samples. The efficacy of the proposed allocation schemes in finite time are illustrated through numerical examples.
To develop sampling laws in a general context and resolve the possible sub-optimality brought by probability bounds into the sampling laws, the problem of selecting the non-dominated systems is revisited from a large deviations perspective. Focusing on the asymptotic rate of decay of the probability of incorrect selection rather than the probability itself, a mathematically robust formulation of the problem is established to determine the optimal computing budget allocation that maximizes the rate of decay. Sampling correlations are explicitly modelled into the related rate functions. The optimal sampling allocation is proposed to be computed using numerical solvers in a general context. The formulation and the solution approach are then applied to problems under multivariate normal assumptions, for which rate functions are well-defined. An approximate closed-form solution to sampling allocation which is computationally more efficient is also suggested as an alternative to the solution approach using a solver, while both approaches explicitly characterize sampling correlations. Numerical examples illustrate the benefit gained in terms of convergence rate by the proposed solution approaches.

This study also deals with extending the optimal computing budget allocation strategies on finite sets to optimization via simulation problems with a relatively large solution space. Population-based search heuristics, for instance, evolutionary algorithms, are usually employed to drive the search for multi-objective optimization via simulation problems. Computing budget allocation techniques are embedded into iterations of the select population-based search algorithms, targeting for a higher confidence in selecting promising systems for reproduction. Efficacy and efficiency enhancement is demonstrated numerically in terms of convergence and coverage measures for these search heuristics. The findings may suggest the great potential in search quality and speed that can be gained from designing algorithm-specific sampling laws for population-based search heuristics.

Overall, the study reported in this thesis provides effective and efficient allocation strategies for decision makers who are faced with limited budget to simulate complex and stochastic systems. While these allocation strategies asymptotic in nature, numerical experiments illustrate that the proposed methods also provide robust and reliable performances in finite time.
List of Tables

2.1 A summary table of the literature on R&S .......................... 22

3.1 Computing budget allocation for Experiment 2 ....................... 44
3.2 Computing budget allocation for Experiment 3 ....................... 45
3.3 Computing budget allocation for Experiment 4 ....................... 47

4.1 Means for Experiment 1 ............................................. 75
4.2 Sampling allocations and rates for Experiment 1 ...................... 75
4.3 Means for Experiment 2 ............................................. 76
4.4 Sampling allocations and rates for Experiment 3 ...................... 78
4.5 Relative differences in rate and time for Experiment 4 .............. 79

5.1 Running settings of MOGAs for Test Problem 1 ..................... 99
5.2 Running settings of MOGAs for Test Problem 2 ..................... 100
5.3 Running settings of MOEDAs for Test Problem 1 ................... 102
5.4 Running settings of MOEDAs for Test Problem 2 ................... 103
List of Figures

3.1 Probability of correct selection for Experiment 1 . . . . . . . . . . . 40
3.2 Probability of correct selection for Experiment 1 with correlation 41
3.3 Spread of systems for Experiment 2 . . . . . . . . . . . . . . . . . 42
3.4 Probability of correct selection for Experiment 2 . . . . . . . . . . 43
3.5 Spread of systems for Experiment 3 . . . . . . . . . . . . . . . . . 45
3.6 Probability of correct selection for Experiment 3 . . . . . . . . . . 46
3.7 Spread of systems for Experiment 4 . . . . . . . . . . . . . . . . . 47
3.8 Probability of correct selection for Experiment 4 . . . . . . . . . . 48
3.9 Probability of correct selection for Experiment 5: the neutral case 49
3.10 Probability of correct selection for Experiment 5: the flat case 50
3.11 Probability of correct selection for Experiment 5: the steep case 51
4.1 Rate of decay for Experiment 2 . . . . . . . . . . . . . . . . . . . . 76
5.1 The flow chart for the MOGA + MOCBA framework . . . . . . . 91
5.2 The flow chart for the MOEDA + MOCBA-subset framework . . 93
5.3 Objective space and Pareto front for Test Problem 1 . . . . . . . . 97
5.4 Objective space and Pareto front for Test Problem 2 . . . . . . . . 98
5.5 Convergence measures of MOGAs for Test Problem 1 . . . . . . 99
5.6 Coverage measures of MOGAs for Test Problem 1 . . . . . . . . 100
5.7 Convergence measures of MOGAs for Test Problem 2 . . . . . . 101
5.8 Coverage measures of MOGAs for Test Problem 2 . . . . . . . . 101
5.9 Convergence measures of MOEDAs for Test Problem 1 . . . . . 102
5.10 Coverage measures of MOEDAs for Test Problem 1 . . . . . . . 103
5.11 Convergence measures of MOEDAs for Experiment 2 . . . . . . 104
5.12 Coverage measures of MOEDAs for Test Problem 2 . . . . . . 104
Symbols and Nomenclature

$S$ : the finite set of alternative systems

$r$ : number of alternative systems in $S$, $|S| = r$

$s$ : number of objective measures

$h_i$ : vector of objective measures of system $i$

$h_{ik}$ : mean of system $i$ at objective $k$

$\Sigma_{h_i}$ : variance-covariance matrix of objectives of system $i$

$\sigma_{h_{ik}}^2$ : variance of $k_{th}$ objective of system $i$

$\bar{H}_{ik}$ : sample mean of system $i$ at objective $k$

$\Lambda(\cdot)$ : log-moment generating function of a random variate

$I(\cdot)$ : rate function of a random variate

$S_p$ : subset of Pareto (non-dominated) systems in $S$

$m$ : size of subset $S_p$, $|S_p| = m$

$\overline{S}_p$ : non-Pareto set of systems

$CS$ : the event of correct selection

$P(CS)$ : probability of correct selection

$FS$ : the event of false or incorrect selection, $IS$

$P(FS)$ : probability of false (incorrect) selection, also referred to as $P(IS)$

$n$ : total computing budget (replicates)

$n_i$ : number of replicates allocated to system $i$
\( \alpha_i \): proportion of computing budget allocated to system \( i \)

\( R_i \): Pareto rank, or the domination count of system \( i \)

\( y \): cut-off (threshold) value of Pareto rank

\( S_y \): the subset of good systems

\( \bar{S}_y \): the observed subset of good systems

\( I(\cdot) \): indicator function

\( x_i \): parameters of system \( i \)

\( \bar{x} \): mean of parameters of given systems

\( \Sigma_x \): variance-covariance matrix of parameters of given systems

\( d(x_i, x_j) \): Euclidean distance between solutions \( x_i \) and \( x_j \) in the objective space

\( D_{\text{convergence}} \): convergence metric of a searching algorithm

\( D_{\text{coverage}} \): coverage metric of a searching algorithm

SO : Simulation Optimization

OvS : Optimization via Simulation

R & S : Ranking and Selection

IZ : Indifference-zone

OCBA : Optimal Computing Budget Allocation

MOEA : Multi-objective Evolutionary Algorithm

MOGA : Multi-objective Genetic Algorithm

MOEDA : Multi-objective Estimation of Distribution Algorithm
Chapter 1

Introduction

Decision makers in real-world situations are often faced with optimization scenarios where they need to find the systems of interest from a number of alternatives. These alternative systems are usually dynamic and complex in nature, making it difficult or even impossible to build analytical models for evaluation. With the advances of computer technology, computer simulation has been widely used as the tool to evaluate performances of these complex systems. Therefore optimization scenarios facing decision-makers tend to be ones on simulation models, where the paradigms of optimization and simulation are combined into the well-established concept of simulation optimization (Law and McComas, 2000). Simulation serves as a modelling tool for evaluating complex systems and optimization intends to find the systems of interest.

Simulation optimization problems arise in many engineering areas and have been drawing significant attention from researchers (Tekin and Sabuncuoglu, 2004). A variety of approaches and techniques have been proposed to solve various simulation optimization problems. In brief, the alternative systems form the solution space for the simulation optimization problem. When the solution space contains infinite or a finite but large enough number of alternatives, search algorithms are typically required for local or global optimality, where only selected systems are simulated and analysed. When the number of alternatives is finite and small enough, simulating each system is possible and the simulation optimization problem becomes a ranking and selection (R&S) problem. Simulation output provides statistical estimates of performances of interest for each alternative system, based on which ranking is performed for all systems in the finite set under problem-specific criteria. Selection of desired systems is then
conducted on top of the ranking.

It is noted that the output of simulated systems is stochastic in nature, and therefore ranking and selection bear uncertainty. The estimation accuracy of systems’ performances can be improved with increased sampling, and higher evidence of correct selection would require considerable sampling from simulation models. However, simulation runs of complex systems tend to be expensive and simulation budget is often limited. It is therefore vital to determine an optimal sampling allocation strategy such that the desired systems can be correctly selected with the highest evidence.

Ranking and selection problems can be categorized by the number of performance measures that serve either as objectives or as constraints, the desired systems to select, and the measures of selection quality. Typical measurements of selection quality include the probability of correctly selecting the desired systems and the expected opportunity cost of an incorrect selection.

Ranking and selection problems are usually modelled by the indifference zone (IZ) scheme (Kim and Nelson, 2006b) or in the optimal computing budget allocation (OCBA) framework (Chen et al., 2000a; Chen and Yücesan, 2005; Chen et al., 1997). The two formulation differs in whether the requirement is on selection quality, or on the simulation budget (Kim and Nelson, 2007). The indifference-zone ranking and selection approach seeks a sampling allocation that can provide a lower bound guarantee of the probability of correct selection, or an upper bound guarantee of the expected opportunity cost of an incorrect selection, subject to the constraint that the best system is better than other systems for at least an indifference-zone difference in performance measure. Correspondingly, stopping rules of sampling for indifference zone ranking and selection procedures are to continue sampling till the specified target of selection quality is satisfied. The OCBA framework, on the other hand, focuses on an allocation that maximizes the probability of correct selection, or minimizes the expected opportunity cost of incorrect selection, subject to a computing budget constraint. The natural stopping rules for procedures in the OCBA framework are to continue sampling till the computing budget is exhausted.

Sampling allocation solutions to ranking and selection problems are often called ranking and selection procedures. These procedures typically involve a sequential sampling process, where samples are allocated in more than one stage. R&S procedures are generally distinguished by their measures of selection quality, sampling assumptions, approximations, stopping rules, and most importantly,
the computing budget allocation strategy for each subsequent stage (Branke et al., 2007).

A number of studies on ranking and selection have been reported and a variety of sampling procedures have been proposed in this field (Goldsman and Nelson, 1994; Kim and Nelson, 2007). These studies usually feature different problem settings in terms of performance measures, the systems of interest and the measures of selection quality. Most studies deal with problems with a single objective measure, or a single objective measure with one or more constraint measures (Branke et al., 2007; Kim and Nelson, 2007). There are substantial cases in real life where systems need to be evaluated by multiple objective measures. Underlying differences exist in comparing designs with multiple objective measures from that with a single objective, thus the sampling allocation techniques for the latter cannot be simply extended and applied. Butler et al. (2001) and Morrice and Butler (2006) consider comparisons of systems with multiple performance measures and combine the multi-attribute utility theory (MAUT) with the indifference zone approach to develop a ranking and selection procedure. However, the MAUT approach transforms the problem into a single-objective one and cannot fully characterize the trade-off among the multiple performance measures. Pareto-optimality has been employed to model the trade-offs and initial studies on multi-objective ranking and selection with Pareto-optimality have been reported, examples include the work done by Lee et al. (2004), Lee et al. (2010b) and Lee et al. (2010c) that deal with selection of non-dominated systems under a multi-objective simulation optimization context.

The practical need of selecting a subset containing good designs for multi-objective simulation optimization is still unmet. This need is evident when the target systems are so complex that the simulation model of the actual system is built with assumptions that need to be considered in making subsequent decisions. Decision makers in such cases may seek a subset of good systems as the promising candidates (Wang et al., 2011). The advancing of population-based multi-objective evolutionary algorithms also drives studies on the subset selection problem. These algorithms often deal with deterministic problems and require a subset of systems in the intermediate iterations to reproduce more promising alternatives (Bosman and Thierens, 2006; Deb et al., 2002; Pelikan et al., 2006). When it comes to a stochastic simulation optimization context, there is the natural need to select the subset with highest confidence to facilitate reproduction of alternatives. It is therefore important to develop sampling al-
location rules for subset selection problems and provide trustworthy guidelines for simulation practitioners.

There are also concerns to address with the mathematical rigidity of the solution framework to derive computing budget allocation rules, where multi-objective problems are not exception. The mathematical development of sampling allocations often involves assumptions of probabilistic normal distributions, which may reduce the generality of the derived solution and thereby confine its application. Moreover, the solution framework usually introduces probability bounds into derivation, the looseness of which may result in sub-optimality of the final solution (Branke et al., 2007; Kim and Nelson, 2007). As a consequence, sampling correlations between multiple performance measures are not explicitly characterized in the probability bounds and thereby, the allocation rules. These concerns with single-objective problems with or without constraint measures are partially addressed by asymptotic analyses from a large deviations perspective (Glynn and Juneja, 2004, 2008; Hunter and Pasupathy, 2010; Hunter et al., 2011; Szechtman and Yücesan, 2008). The great potential of applying large deviation principles also motivates us to extend the asymptotic analysis to multi-objective settings and provide a more mathematically robust solution to the sampling allocation problems.

1.1 Objectives of the Study

In this study, we consider multi-objective simulation optimization problems on finite sets and focus specifically on sampling allocation across systems. In view of the existing literature, it is noted that most of the previous studies deal with single objective simulation optimization problems only, and there is the unmet practical need to develop efficient computing budget allocation rules for multi-objective simulation optimization problems. Moreover, investigation into generalization and optimality of the derived allocation rules is still lacking and a study in a rigorous mathematical framework is necessary.

The main objective of this study is to propose effective and efficient computing budget allocation rules for multi-objective simulation optimization problems on finite sets. More specifically, the aims of this research are to

1. study the problem of finding a subset of good systems in a multi-objective simulation optimization context, provide a computing budget allocation
that can maximize the probability of correct selection, subject to a limited computing budget constraint;

2. examine the performance of population-based multi-objective evolutionary algorithms in a stochastic simulation optimization context, by embedding optimal computing budget allocation on finite sets into the selection operator of these algorithms in each iteration;

3. revisit the problem of selecting non-dominated systems from a large deviations perspective, develop a general solution framework for sampling allocation and investigate the asymptotic optimality of the allocation rules;

4. suggest a sampling allocation scheme for selecting non-dominated systems that can explicitly characterize sampling correlations among performance measures, that is, an allocation as a function of sampling correlations;

5. apply the general solution framework to a multivariate normal context in particular and present effective and efficient sampling laws by using domain-specific knowledge.

1.2 Significance of the Research

This study deals with specific problem settings, where assumptions may be made if necessary. Firstly, constraint measures on systems are not explicitly considered and it is assumed that a finite set of feasible alternatives are given prior to determination of a sampling allocation. Another fundamental assumption is that the comparison and thereby the ranking of the alternatives are based on their expectation (mean) only, regardless of their variances. While variances may also be of interest for decision making under uncertainty, our analysis being asymptotic in nature partially address this concern. Moreover, systems are assumed to be independently simulated of each other and therefore sampling correlations between systems are not taken into account.

Nevertheless, this study has taken a major step towards allocating limited computing budget in an optimal manner for multi-objective simulation optimization problems on finite sets. The significance of this research is highlighted as below.

1. For decision-making scenarios of finding a subset of good systems, this
study would provide effective and efficient sampling laws and suggest implementation guidelines for practitioners.

2. This research would shed light on the potential of integrating the presented sampling laws with multi-objective search algorithms to enhance search efficiency. The proposed technique could provide a powerful technique for generating a set of seeding solutions for population-based evolutionary algorithms.

3. For problems of selecting non-dominated systems, this study should provide a strong theoretical basis for a robust framework of developing sampling laws, allowing for optimality analyses in a general context. Sampling correlations may also be explicitly featured in the optimal solution derived using the framework.

4. This study would present sampling laws for finding Pareto systems under a particular multivariate normal assumption and provide guidelines for implementing appropriate allocation procedures.

5. The findings may offer a clearer explanation for the allocation strategy in terms of the convergence rate of correct (or false) selection from a large deviations perspective.

In summary, findings of this study would provide guidelines to optimally allocate computing budget for practitioners carrying out real world simulation experiments. The proposed approach may have great potential in application since it does not require any interaction from the decision maker for finding the desired systems. The examination of optimality by employing large deviations principles would contribute to a mathematically rigorous framework and also contribute to a better understanding and interpretation of the rules derived.

1.3 Organization of the Thesis

The rest of the thesis is organized as follows.

In Chapter 2, we provide a comprehensive review of the existing literature on sampling allocations for simulation optimization problems on finite sets. A summary of the classifications of problems and the employed solution frameworks are also presented. Research gaps that exist between the up-to-date literature and the practical requirements are elaborated, suggesting motivations of this study.
In Chapter 3, we consider the problem of finding a subset of good systems for multi-objective simulation optimization problems and provide computing budget allocation strategies that is efficient and easy to implement. Numerical illustrations are also presented.

In Chapter 4, we revisit the problem of selecting the non-dominated systems from a large deviations perspective. A mathematically robust formulation of the problem is provided and an optimal solution framework explicitly characterizing sampling correlations are proposed in a general context. Detailed discussions follow on applying this solution framework to problems under a particular multivariate normal assumption.

In Chapter 5, we present numerical illustrations for optimization via simulation problems by adapting existing heuristics for deterministic optimization problems to a stochastic simulation optimization context. Computing budget allocation techniques on finite sets are embedded into iterations of population-based search algorithms. Efficiency boosting is demonstrated numerically in terms of performance indicators of interest.

Chapter 6 concludes this study by presenting significance and contributions of this research work. Limitations to this study, including problem-specific assumptions made and the solution approaches employed, are further discussed, suggesting future research directions to enriching and enhancing the work reported in this thesis.
Chapter 2

Literature Review

2.1 Simulation Optimization

Simulation optimization combines two well-established paradigms, namely, simulation and optimization (Fu et al., 2008; Tekin and Sabuncuoglu, 2004). Simulation intends to be a modelling tool for evaluating complex systems in practice, whereas optimization aims to find the system with the best decision variables (Fu et al., 2008). Simulation optimization involves optimization on a simulation model and it is therefore also referred to as simulation-based optimization (Law and McComas, 2000).

Without loss of generality, the simulation optimization problem can be formulated as

$$\min_{x \in \mathcal{X}} h(x) \equiv E[H(x, \epsilon)],$$

where $\mathcal{X}$ denotes the solution space, and $x$ is one particular system represented by a vector of system parameters. $H(x, \epsilon)$ is the sample performance and $\epsilon$ represents the system noise. $h(x)$ is the true objective measure for system $x$, which can be a scalar or vector for the single objective or multi-objective case respectively. It is noted that the solution space may also be explicitly specified by constraints like $g(x) \leq c$, where $g(x)$ are constraint measures and $c$ stands for constants. The objective of simulation optimization problems is to find the feasible $x$’s with the minimum true objectives, where performance measures of each system are usually estimated by sample mean via a Monte Carlo sampling procedure.

Simulation optimization problems usually assume a discrete state space and can be classified in terms of the number of alternatives to choose from, or the size of the solution space. When the number of alternatives is infinite or finite but large
enough, it would be practically impossible to simulate all the alternatives. This type of problem is often referred to as optimization via simulation (OvS) problem, for which search algorithms are usually required (Hong and Nelson, 2009). The major concerns with OvS are the search efficiency for optimization and the sampling allocation for simulation, where the trade-off between exploring potentially better alternatives and exploiting currently promising systems needs to be considered. When the solution space is finite and small enough, simulating each alternative is possible and the simulation optimization problem becomes a ranking and selection problem. Ranking is performed based on performance estimates for all systems in the finite set under problem-specific criteria. Selection of desired systems is then conducted on top of the ranking. Ranking and selection bear uncertainty due to the stochastic output of simulated systems and therefore the research interest would be to deal with the stochastic nature of systems. Many approaches to simulation optimization have been developed, examples include sample path optimization, response surface methods and searching heuristics. Among these approaches, simulation budget allocation or sampling allocation becomes vital in conducting efficient simulation experiments for a finite and small enough set of alternatives and is the research area of interest in this study.

The computing budget allocation problem falls in the well-established ranking and selection (R&S) problem settings. A comprehensive review of the problems and solutions is provided in the following sections.

2.1.1 Ranking and Selection and Computing Budget Allocation

Ranking and selection (R&S) problems are those that compare a finite number of simulated alternatives and select the systems that qualify under pre-specified criteria (Bechhofer et al., 1995). A number of studies on ranking and selection have been reported in the simulation field. Branke et al. (2005) and Kim and Nelson (2007) discuss recent advances made on R&S and reviews the issues and challenges existing in simulation optimization.

Ranking and selection problems focus on ordinal comparison of alternatives rather than accurate estimate of the cardinal performances of these systems (Ho et al., 1992, 2007). In brief, ordinal comparison considers whether system a
is better than system $b$ (or a standard) rather than the difference between systems $a$ and $b$ (or a standard) (Lee et al., 1999). Ordinal comparisons possess exponential convergence rates, whereas the convergence rate of the estimate of a cardinal value is no more than $1/\sqrt{N}$ (Dai, 1996; Ho et al., 2007). Therefore to guarantee the same level of statistical confidence, significant savings in the simulation budget can be gained for ordinal comparison.

Ranking and selection applies to simulation optimization problems where the search space of alternatives is small enough to simulate all the systems. R&S procedures aim to select the desired system, where a system being desirable can be either the best ones among all alternatives, the feasible ones under certain constraints, or the best feasible ones. The goal of ranking and selection is usually to find a computing budget allocation that maximizes the selection quality or maintain the selection quality above a certain confidence level. Therefore a ranking and selection problem of interest is also a computing budget allocation problem. In the following text, we use ranking and selection and optimal computing budget allocation interchangeably where necessary.

2.2 Computing Budget Allocation Problems on Finite Sets

In this section, we provide a summary of classifications of the computing budget allocation problems that appear in the simulation optimization literature and present a summary of the frameworks employed to solve these problems.

2.2.1 Classification of Problems

In general, problems considered in the literature can be classified based on the following characteristics.

1. Number of performance measures for simulated systems.

Many ranking and selection problems have focused on problems with a single performance measure. When the performance measure serves as an objective measure, the goal of the problem is then to select the best system(s) with the largest or smallest expected value of performance, where multiple comparison of systems are required (Kim, 2005; Kim and Nelson, 2003, 2007). When the performance measure acts as a constraint
measure, the alternative systems are compared with a threshold, and therefore the goal is to select those feasible systems (Nelson and Goldsman, 2001; Szechtman and Yücesan, 2008).

A number of studies have extended ranking and selection to problems with multiple performance measures. These performance measures can either be primary as objective measures, or be secondary as constraint measures. Development on problems with a primary performance measure and one or more secondary performance measures have been presented (Andradóttir et al., 2005; Batur and Kim, 2010; Kabirian and Ölafsson, 2009; Kim and Nelson, 2003; Osogami, 2009). Problems with multiple primary performance measures, also referred to as multi-objective simulation optimization problems, are also investigated (Chen and Lee, 2009; Lee et al., 2010b,c).

Multiple performance measures changes the nature of comparisons of systems a great deal (Kim and Nelson, 2007). Complexities arise in evaluating the overall probability of correct selection or other measures of evidence of correct selection. Hence we suggest that problems can be classified first by the number of performance measures for the simulated systems.

2. The desired systems to select.

The desired systems to select is directly connected with the number of performance measures. When there is at least one objective measure, the selection would require multiple comparisons across systems, and the goal can be to find the single best system (Kim and Nelson, 2003), a subset of systems containing or close to the best (Koenig and Law, 1985), or the optimal subset of top systems (Chen et al., 2008a). When there are only constraint measure(s), the goal of the selection is simply to identify the feasible systems (Szechtman and Yücesan, 2008).

Whether a system is desirable is problem-specific and depends highly on decision makers. For example, there may be conditions or constraints that are not built into simulation model but not negligible in the practical implementation. Decision makers under this scenario may seek for a subset of alternatives close to the best for further consideration (Wang et al., 2011). Decision maker’s knowledge of the simulation model and the real system would play a vital role in determining the desired system(s).

Measurement of the quality of a selection, also referred to as the evidence of correct selection in Branke et al. (2007), is dependent on the specific needs of decision makers. For instance, the decision makers may want to minimize the opportunity cost of an incorrect selection in a business environment.

The measures of selection quality are usually defined in terms of loss functions. The zero-one (0-1) loss function equals 1 if the desired system is not correctly selected, and equals 0 otherwise. In a similar manner, the linear loss function, also known as opportunity cost, is the difference between the desired system and the selected system if the desired system is not correctly selected and is 0 otherwise (Branke et al., 2007). Therefore the probability of correct selection (PCS) is defined in terms of the expected 0-1 loss and the expected opportunity cost (EOC) defined in terms of the expected linear loss (Chick and Inoue, 2001, 2002; Chick and Wu, 2005).

The probability of correct selection have prevailingly been the primary measure of choice as the evidence of correct selection. This measure, especially when selecting a subset, tends to be conservative in the sense of resulting in loss 1 with even one incorrectly-selected system, regardless of the difference of this system from the desired ones. The expected opportunity cost, on the other hand, helps to reduce or avoid this conservatism (Chick and Inoue, 2001; He et al., 2007).

Measures of selection quality can be evaluated from either a frequentist perspective assuming known parameters to calculate the losses, or from a Bayesian perspective where no prior knowledge of the parameters is available and the posterior information of the unknown parameters are used to measure the evidence of correct selection. Measures of selection quality are key in deriving selection procedures and determining when to stop sampling.

2.2.2 Solution Approaches

It is usually a sequential process to allocate simulation budget to alternative systems in contention, where being sequential means the allocation across systems
takes more than one stage. Solutions to ranking and selection problems that systematically allocate simulation budget are therefore often called ranking and selection procedures. These procedures are, in general, distinguished by their measure of evidence of correct selection, sampling assumptions, approximations, parameters with respect to stages, stopping rules, and most importantly, the computing budget allocation strategy per subsequent stage.

The computing budget allocation strategy is related directly to the statement and thereby the formulation of the ranking and selection problem. There are two main streams of formulations in this field, namely, the indifference zone (IZ) ranking and selection approach (Kim and Nelson, 2006b) and the optimal computing budget allocation (OCBA) framework (Chen et al., 2000a; Chen and Yücesan, 2005; Chen et al., 1997). The two formulations differs in whether the requirement is imposed on the evidence of correct selection, or on the simulation budget (Kim and Nelson, 2007).

The indifference-zone ranking and selection approaches attempt to allocate samples to provide a lower bound guarantee of the probability of correct selection, or to provide an upper bound guarantee of the expected opportunity cost of an incorrect selection, subject to the constraint that the best system is better than other systems for at least an indifference-zone difference in performance measures. Differences of less than the indifference-zone are considered insignificant and an alternative within the indifference zone of the best is called a good system (Nelson and Banerjee, 2001). The indifference-zone parameter is required to be positive and is usually set as the minimal detectable difference between the best system and others. Ranking and selection procedures equipped with allocation strategies derived from this type of formulation are classified as indifference-zone ranking and selection procedures (or strategies).

The OCBA framework, on the other hand, aims to find an allocation that maximizes the probability of correct selection, or minimizes the expected opportunity cost of incorrect selection, subject to a computing budget constraint (Lee et al., 2010a). OCBA procedures do not require a positive indifference-zone parameter. Selection procedures embedded with allocation strategies derived by the OCBA framework are classified as OCBA procedures (or strategies). When the probability of correct selection is the choice of evidence of correct selection in an OCBA framework, the major challenges in solving the problem include developing a tractable and differentiable estimate of the probability and deriving asymptotically analytic solution from optimality conditions.
An alternative measure of probability of correct selection using large deviations principle (LDP) has recently drawn great interest from the simulation field (Blanchet et al., 2008; Broadie et al., 2007; Glynn and Juneja, 2004, 2008; Szechtman and Yücesan, 2008). The large deviations principle relaxes the normality assumption and focuses on the asymptotic rate of decay associated with the probability of incorrect (false) selection, and therefore open a new avenue to simplifying the problem formulation and deriving asymptotically analytical solutions. Approaches from a large deviations perspective also have the potential to address concerns on sub-optimality of procedures derived from an estimate of the probability of correct selection (Kim and Nelson, 2007) and on an explicit characterization of sampling correlations among performance measures (Hunter and Pasupathy, 2010; Hunter et al., 2011).

Stopping rules relate directly to the formulation of the selection problems. For indifference zone ranking and selection procedures, the default stopping rule is to continue sampling till the specified target of selection quality is satisfied. Likewise, the default stopping rule for procedures by the OCBA framework is to continue sampling till the specified total computing budget is exhausted. It is evident that stopping rules for IZ procedures possess the flexibility to “stop earlier if the evidence for correct selection is sufficiently high and allow for additional sampling when the evidence is not sufficiently high” (Branke et al., 2007).

Branke et al. (2007) suggest that when the evidence of correct selection is measured from the Bayesian perspective, the posterior measure of selection quality for OCBA procedures can be quantified and therefore these procedures can stop when desired levels of selection quality is achieved.

Selection procedures can be evaluated in terms of (a) efficiency, measuring the ability to deliver the targeted level of selection quality with minimum number of samples, and (b) robustness, measuring the performance sensitivity with respect to variations of parameters, assumptions and problem characteristics (Branke et al., 2007; Kim and Nelson, 2007). These measurements, in principle, can be assessed from either a theoretical or an empirical perspective. Different selection approaches, however, often make different basic assumptions and approximations, which render a theoretical analysis difficult to develop. Empirical comparisons, as a consequence, become a more practical choice for comparing different selection procedures (Branke et al., 2005; Inoue et al., 1999).
2.3 Computing Budget Allocation Strategies

In this section, we present studies and findings on optimal computing budget allocation strategies in the literature. These studies are organized following the classifications by the number of performance measures for systems that are to be simulated.

2.3.1 Problems with a Single Performance Measure

The single performance measure can be used either as a primary objective measure, or as a secondary constraint measure (Goldsman et al., 1991). The objective is to find the desired systems with the largest or smallest means, or to determine feasibility of these alternatives, respectively.

Problems with a single performance measure have drawn great attention from researchers in the simulation field and a number of solutions have been proposed. The indifference zone ranking and selection procedures have their root in Bechhofer (1954) from the statistics community, where a single stage sampling procedure is proposed to find the best system with a guaranteed lower bound of the probability of correct selection. This sampling procedure assumes known common variance across all systems, which is usually not valid in practice (Gupta, 1965). Dudewicz and Dalal (1975) address this issue in the simulation context by presenting a two-stage sampling procedure, where sample variances from the first stage are used as surrogate to calculate the required number of samples for the second stage. Rinott (1978) further revises this IZ procedure to procedure R, which guarantees a higher probability of correct selection and would require more samples in consequence. The requirement on a large number of samples renders procedure R inapplicable to problems when the number of alternatives is large. To address this issue, Nelson et al. (2001) adjust the two-stage sampling procedure with screening after first stage. Systems that are not competitive are screened out at the end of first stage and thereby avoid sample allocations to these systems at the second stage. While this approach to allocating simulation budget is an additive decomposition in spreading the additive probability of correct selection into the screening stage and the ranking stage, Wilson (2001) proposes a multiplicative decomposition approach that establish a better lower bound of the probability of correct selection in a product form.
The indifference-zone ranking and selection procedure in Nelson et al. (2001) is extended to fully sequential ones in Kim and Nelson (2001) and Kim and Nelson (2006a), where being fully sequential refers to taking only a single basic observation for each alternative remaining in contention at each subsequent stage. Systems that are clearly inferior are immediately eliminated at the end of each stage till only the best alternative is left in contention, and hence reduce the total simulation effort spent to find the best system. Hong (2006) presents a new fully sequential procedures with variance-dependent sampling and shows improvement over existing sequential procedures for problems where systems have different variances. Chen and Kelton (2005) suggest an efficient sequential sampling procedure where the sample size depends on both the variance of systems and the difference between the sample means. Taking the sum of pairwise differences of the sample means as a Brownian motion process, Batur and Kim (2006) provide sequential indifference-zone procedures with Parabolic boundary. Tsai and Nelson (2009) also employ the Brownian motion process perspective and derive new fully sequential IZ procedures with a controlled sum of differences. Kim (2005) focuses on a problem of comparing performances of alternatives with a pre-determined system as a standard and develops fully sequential IZ procedures. Tsai and Wei (2011) suggest new multinomial selection procedures and practical parameters for comparison with a standard problems in a number of scenarios.

Issues on application scenarios and implementation efficiency of ranking and selection procedures are also addressed. In view of the fact that switching among simulation of alternatives occurs for multi-stage sequential ranking and selection procedures, Hong and Nelson (2005) discuss the efficiency of simulations by considering the trade-off between the sampling cost and the switching cost and then propose adaptive procedures to better characterize the simulation efficiency. Osogami (2009) presents an IZ procedure to reduce both the number generating samples and the frequency of changing system configurations during simulation. Hong and Nelson (2007) study an application scenario where alternative systems are sequentially revealed during the simulation experiments.

Many studies on ranking and selection assume that the alternative systems are independently simulated. This assumption can be justified when the simulations of different systems are driven by independent streams of random numbers. Since ranking and selection involves pairwise comparison of alternatives and the variance of the difference between the paired systems are influenced
by their covariance, positive correlation can reduce the variance and therefore make the comparison more sharper. Common random numbers (CRN) tend to introduce positive correlation and if correctly implemented, have the potential to improve the efficiency of comparisons. Another commonly made assumption is that outputs for each system are independently and identically distributed. This is usually true when the simulations are terminating ones where the initial and stopping conditions of each replication are inherent to the definition of the system (Kim and Nelson, 2007).

For steady-state simulations, however, the raw simulation output are often correlated and this autocorrelation invalidate the i.i.d assumption and requires adapting existing procedures or exploring of new procedures. One resolution is to simulate each alternative for multiple replicates, or use batch mean as the basic observation rather than the raw simulation output. This approach has disadvantages of either wasting observations of the transient state of the simulation, or wasting time to get sufficient batch data, rendering it practically inefficient. Selection procedures addressing these concerns are therefore required. Nakayama (1997) develops confidence intervals for multiple comparisons of systems with respect to the means of raw output from a single stage steady-state simulation. Damerdji and Nakayama (1999) extend the confidence intervals to two-stage steady-state simulations using a R-like heuristic. Goldsman et al. (2002) extend the existing R procedures to problems with general steady-state outputs. Kim and Nelson (2006a) provide a framework to examine the asymptotic validity of fully sequential ranking and selection procedures that are developed for steady-state simulations. Theoretical comparisons of different procedures can therefore be made, in addition to empirical comparisons of finite-time performances.

The key to resolve the autocorrelation of raw outputs from steady-state simulations is to provide an alternative variance estimator for the selection procedure that can handle the stationary and dependent simulation data. Kim and Nelson (2006a) establish general qualifications for this type of variance estimators and suggest variance updating to improve efficiency of selection procedures. Malone et al. (2005) extend the procedure in Kim and Nelson (2006a) by introducing common random numbers into simulation of different systems. Healey et al. (2007) and Healey et al. (2009) provide new variance estimators with statistically smaller biases and illustrate their performances in terms of significant savings in simulation budget.

While indifference-zone ranking and selection procedures aim to find the de-
sired systems with a guaranteed frequentist evidence of correct selection, procedures to maximize the evidence the correct selection under a simulation budget constraint are also investigated in the OCBA framework. Chen et al. (1997) develop a greedy heuristic to iteratively determine the most possibly promising system for further sampling. There is underlying difficulty for this approach in evaluating the probability of correct selection (PCS), and consequently the heuristic cannot guarantee the optimality of the sampling allocation. Chen et al. (2000b) present an approximation of the probability of correct selection using bound theory and provide an analytical solution to the problem. A better approximation of PCS is proposed in Chen et al. (2000a) and Chen and Yücesan (2005) and asymptotic allocation strategies are derived assuming the computing budget is not bounded. Fu et al. (2007) extend the OCBA approach by considering sampling correlation in simulation experiments. Employing the OCBA framework but using the expected value of information as an evidence of correct selection, Chick and Inoue (2001) study the computing budget allocation problem from a decision theoretic perspective and consider an allocation strategy to maximize the information gained from simulation output. He et al. (2007) develop an optimal sampling allocation scheme to minimize the expected opportunity cost. Frazier et al. (2008) and Frazier et al. (2009) introduce the knowledge gradient policy to solve the ranking and selection problem with an independent and correlated normally distributed belief (assumption) respectively. The knowledge gradient policy guides the sampling by choosing to simulate the system that would produce the highest reward with only one more measurement.

Approaches from a large deviations perspective are also reported. Glynn and Juneja (2004) study the single objective sampling allocation problem and provide mathematically rigorously optimality conditions to the original problem. The established optimality conditions also apply to problems with a general distribution of samples. The large deviations perspective is further employed to study single objective subset selection problems (Blanchet et al., 2008; Glynn and Juneja, 2008).

Computing budget allocation strategies are also extended to find a desired subset other than the single best. Gupta (1965) extends the ranking and selection procedures to select a subset assuming equal variances and zero indifference zone. Koenig and Law (1985) propose a two-stage allocation procedure to select a subset of $m$ designs which contain $l$ best ones. Sullivan and Wilson (1989) develop a heuristic procedure to select the good alternatives within the indifference-zone
distance from the best and finally select at most $m$ systems. Chen et al. (2008a) present an efficient asymptotic allocation approach in the OCBA framework to select an optimal subset containing best $m$ designs. Almomani and Rahman (2012) incorporate OCBA to select a promising subset as part of a sequential allocation to select a stochastically good design from a large number of alternatives. Wang et al. (2011) study the problem of finding the best-subset of all good systems and provide an IZ procedure with a guaranteed probability of correct selection.

When the single performance measure serves as a constraint measure, the focus of ranking and selection problems is then to determine feasibility rather than optimality of systems. Szechtman and Yücesan (2008) consider this problem from a large deviations perspective and present an asymptotically optimal allocation strategy and an algorithm for its deployment.

The systems being desirable are usually measured in terms of their means only. However, performance measures are stochastic in nature and their variances may also need to be taken into consideration to fully capture the risks. Concerns on the inadequate representation of the adhering risks are also addressed. Batur and Choobineh (2010b) propose comparisons of system in both means and variances where the best system has the best mean and smallest variance. Batur and Choobineh (2010a) employ the quantile of distributions of performance measures to better represent the underlying risk and suggest a more flexible quantile-based ranking and selection procedure.

### 2.3.2 Problems with Multiple Performance Measures

Many real-word ranking and selection problems involve more than one performance measure and these problems have also drawn great interest in the simulation field. The multiple performance measures can either be regarded primary as objective measures or be secondary as constraint measures.

Studies focusing on problems with one objective measure and one or more constraint measures have been reported. The goal of this type of ranking and selection problems is to find the best feasible solution from a finite set. Andradóttir et al. (2005) and Andradóttir and Kim (2010) present a sequential indifference-zone based selection procedure for problems with one primary objective measure and a secondary stochastic constraint measure where a promising set containing feasible or near-feasible systems is selected at the first phase, from which
the best is chosen at the second phase. Pujowidianto et al. (2009) employ the OCBA framework to provide an asymptotically approximate allocation strategy to the constrained simulation optimization problem, assuming that the objective measure and the constraint measure for each system are independently sampled. This problem is revisited in Hunter and Pasupathy (2010) by employing the large deviations principle and a better solution resolving the looseness of Bonferroni bounds is proposed. Sampling laws that can explicitly characterize the correlation between the objective and constraint measures is considered in Hunter et al. (2011) from a large deviations perspective. The solution using a solver and an analytically approximate allocation strategy are both suggested (Hunter et al., 2011). This work is further extended to problems with one objective measures and multiple constraint measure.

Feasibility detection problems are also investigated when the performance measures serve as secondary constraint measures. Batur and Kim (2005) and Batur and Kim (2010) study the problem of finding the feasible systems as an extension of the work by Andradóttir et al. (2005).

When all the performance measures act as objectives, the problems become multi-objective simulation optimization ones. A number of studies have been carried out to tackle such problems.

Butler et al. (2001) transform the multi-objective problem into a single objective one using multiple attribute utility theory and incorporating the R procedure for the ranking and selection. Prior information on decision-maker’s preference over the objectives is required which renders this method impractical. To address this concern, Chen and Lee (2009) employ the concept of Pareto optimality and extended the two-stage R procedure to select the non-dominated systems. Zhao et al. (2005) propose a method to determine the number of observed non-dominated layers to select, such that at least \( k \) systems in the true Pareto frontier are contained with a guaranteed probability \( \alpha \). Teng et al. (2007) extend the ordinal optimization technique to a multi-objective simulation optimization context and present lower-bound estimates of the associated alignment probabilities. Lee et al. (2004) study the problem of selecting all the non-dominated systems assuming a given number of non-dominated systems in the OCBA framework. Lee et al. (2010c) relax this assumption and suggest asymptotically analytical allocation rules to minimize the probability of two types of incorrect selection. Lee et al. (2007) explore the computing budget allocation problem for multi-objective simulation optimization using expected
opportunity cost as an evidence of correct selection. Allocation schemes with
gard to different evidence of correct selection are discussed and compared in
Lee et al. (2010b). Teng et al. (2010) deal with a multi-objective ranking and
selection problem where alternative have close performances by incorporating
the indifference zone concept for comparisons of systems.

2.3.3 Summary of the Works

A tabular summary with representative papers on sampling allocation for simu-
lation optimization on finite sets is provided in Table 2.1, under the classification
scheme of problems and solution approaches.
Table 2.1: A summary table of the literature on R&S

<table>
<thead>
<tr>
<th>Objective</th>
<th>unconstrained</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>OCBA</strong>: Szechtman and Yücesan (2008).</td>
</tr>
<tr>
<td>single objective</td>
<td><strong>IZ</strong>: Batur and Kim (2006); Chen and Kelton (2005); Goldsman et al. (2002);</td>
</tr>
<tr>
<td></td>
<td>Healey et al. (2007, 2009); Hong (2006); Hong and Nelson (2005, 2007); Kim</td>
</tr>
<tr>
<td></td>
<td>and Nelson (2001, 2006a,a); Malone et al. (2005); Nelson et al. (2001); Osogami</td>
</tr>
<tr>
<td></td>
<td>(2009); Tsai and Nelson (2009); Tsai and Wei (2011).</td>
</tr>
<tr>
<td>multi-objective</td>
<td><strong>IZ</strong>: Butler et al. (2001)</td>
</tr>
<tr>
<td></td>
<td><strong>IZ</strong>: Andradóttir et al. (2005); Andradóttir and Kim (2010); Batur and Kim</td>
</tr>
<tr>
<td></td>
<td>(2010); Kabirian and Ólafsson (2009); Kim and Nelson (2003); Osogami (2009).</td>
</tr>
<tr>
<td></td>
<td><strong>OCBA</strong>: Almomani and Rahman (2012); Blanchet et al. (2008); Chen et al.</td>
</tr>
<tr>
<td></td>
<td>(2008a, 2000a); Chen and Yücesan (2005); Chen et al. (2000b, 1997); Chick</td>
</tr>
<tr>
<td></td>
<td>and Inoue (2001); Frazier et al. (2008, 2009); Fu et al. (2007); Glynn and</td>
</tr>
<tr>
<td></td>
<td>Juneja (2004, 2008); He et al. (2007); Wang et al. (2011).</td>
</tr>
<tr>
<td></td>
<td><strong>OCBA</strong>: Hunter and Pasupathy (2010); Hunter et al. (2011); Pujowidianto et</td>
</tr>
<tr>
<td></td>
<td>al. (2009).</td>
</tr>
<tr>
<td></td>
<td><strong>IZ</strong>: Morrice and Butler (2006).</td>
</tr>
<tr>
<td></td>
<td><strong>OCBA</strong>: Chen and Lee (2009); Lee et al. (2007, 2010b, 2004, 2010c); Teng</td>
</tr>
<tr>
<td></td>
<td>et al. (2010).</td>
</tr>
</tbody>
</table>
2.4 Summary

The literature above deals with many simulation optimization scenarios of selecting desired systems to fulfil practical requirement. To reiterate, ranking and selection procedures directly fit in selecting the best, feasible or best feasible systems when the solution space contains only a finite set of alternatives. Concerns on relaxing the goal to select a subset of good systems or a best-subset are also addressed, especially when the problem is hard, or the simulation model is not adequate to reflect characteristics of the real system (Wang et al., 2011). For problems with a large number of alternatives, heuristics that iteratively search for the best systems are usually employed, among which population-based algorithms are mostly common. These algorithms are frequently developed for problems that are deterministic in nature and require a subset of systems in the intermediate iterations to reproduce more promising alternatives. When it comes to a simulation optimization context, ranking and selection procedures naturally meet the need of selecting the optimal subset and guarantee the selection quality in the stochastic environment (Chen et al., 2008a).

Most studies focus on problems with a single objective measure, or a single objective measure with one or more constraint measures (Branke et al., 2007; Kim and Nelson, 2007). Problems with multiple objective measures keep emerging in practice, where an arbitrary transformation into single objective problems are not justified to provide desired solutions (Deb, 2001). Considerations of the characteristics adherent to the multi-objective problems are necessary and these problems are largely unexplored. The work by Lee et al. (2004), Lee et al. (2010c) and Lee et al. (2010b) represents the initial and fundamental research effort in this field.

There are still important research problems to address. There is, on the one hand, the unmet need of selecting a subset of good systems for multi-objective simulation optimization practices. This need is evident when the target systems are so complex that the simulation models are not adequate to fully characterize these real systems. Compromises and assumptions may be made in building simulation models and decision makers in such cases would seek a subset of good alternatives for further consideration (Wang et al., 2011). The advancing of population-based multi-objective evolutionary algorithms also drives studies on the subset selection problem. Examples of such algorithms include multi-objective evolutionary algorithms (Deb et al., 2002; Zitzler and Thiele, 1999)
and estimation of distribution algorithms (Bosman and Thierens, 2002, 2006; Pelikan et al., 2006). These algorithms are often initially developed for deterministic problems and require a subset of good systems in the intermediate iterations to reproduce more promising alternatives (Bosman and Thierens, 2006; Deb et al., 2002). This subset usually contains good enough systems beyond the best (or non-dominated) ones, as the population size of the best systems may be too small and hence lead to premature convergence (Deb et al., 2002; Jin et al., 2008; Tan et al., 2001). When it comes to a stochastic simulation optimization context, there is the natural need to select the subset of good systems with highest confidence. It is therefore vital to develop sampling allocation rules for subset selections which would allow adapting these algorithms to a stochastic simulation optimization context and provide trustworthy guidelines for simulation practitioners.

On the other hand, critiques have been raised on the typical solution approach to deriving sampling laws, where multi-objective problems are not exception. The mathematical development of sampling allocations often involves assumptions of probabilistic normal distributions, which may reduce the generality of the derived solution and thereby confine its application. Moreover, the solution approach usually introduces bounded probability estimates, the looseness of which may result in sub-optimality and conservatism of the final solution (Branke et al., 2007; Kim and Nelson, 2007). As a consequence, sampling correlations between multiple performance measures are not explicitly characterized in the probability bounds and thereby, the allocation rules. These concerns with single-objective problems with or without constraint measures are partially addressed by asymptotic analyses from a large deviations perspective (Glynn and Juneja, 2004, 2008; Hunter and Pasupathy, 2010; Hunter et al., 2011; Szechtman and Yücesan, 2008). The Large deviations perspective focuses on the asymptotic rate of decay instead of the probability itself, which can facilitate a more robust mathematical formulation of the problem. The great potential of applying large deviation principles also motivates us to extend the asymptotic analysis to multi-objective problem settings and address the aforementioned concerns.
Chapter 3

Finding a Subset of Good Systems for Multi-objective Simulation Optimization on Finite Sets

3.1 Introduction

We consider a multi-objective simulation optimization problem where we aim to select the desired subset of systems under a stochastic environment. In particular, we focus on an optimal allocation of computing budget on finite sets, such that the probability of correct selection can be maximized. This problem falls in the well-established ranking and selection problem settings and a comprehensive survey on ranking and selection procedures developed in this field is provided in Chapter 2.

This study is motivated by the unmet need of selecting a subset of good systems in simulation practice. This need is evident when the target systems are so complex that the simulation model of the actual system is built with assumptions that need to be considered in making subsequent decisions. Decision makers in such cases may seek for a subset of good systems as the promising candidates (Wang et al., 2011). The advance of population-based multi-objective evolutionary algorithms also drives studies on the subset selection problem. These algorithms are often initially developed for deterministic problems and require a subset of good systems in the intermediate iterations to reproduce more promising alternatives (Bosman and Thierens, 2006; Deb et al., 2002). This subset usually contains good enough systems beyond the best ones, as the population
size of the best systems may be too small and hence lead to premature conver-
gence (Deb et al., 2002; Jin et al., 2008; Tan et al., 2001). When it comes to
a stochastic simulation optimization context, there is the natural need to select
the subset of good systems with highest confidence. This need is more evident
when the available simulation budget is limited and therefore the sampling al-
location is concerned. The subset selection procedure can be embedded into
iterations of search algorithms serving as the selection operator, which would
provide opportunities to extend existing heuristics to multi-objective optimiza-
tion via simulation context. It is therefore vital to develop sampling allocation
procedures and provide trustworthy guidelines for simulation practitioners.

Studies reported in this field have mainly focused on single objective problems.
For multi-objective problems, comparison of designs is significantly different
from that for single objective problems (Kim and Nelson, 2007). An arbitrary
transformation into single objective problems are not justified to provide desir-
able solutions (Deb, 2001). The problem of incorporating the nature of com-
parison of systems with multiple objectives needs to be addressed and yet these
problems are largely unexplored. Lee et al. (2004), Lee et al. (2010c) and Lee
et al. (2010b) incorporate the Pareto optimality concept and deal with the prob-
lem of finding the non-dominated systems under a multi-objective simulation
optimization context. The suggested techniques target Pareto-optimal systems
only, and therefore they are not applicable to problems of finding a general sub-
set, i.e., the subset of good systems that are beyond the Pareto-optimal ones.
Numerical tests also illustrate this infeasibility. It is thus important to develop
particular sampling allocation techniques for finding the subset of good systems
under a multi-objective simulation optimization setting.

3.1.1 Problem Statement

Consider a finite set $S$ consisting of $i = 1, \ldots, r$ systems where each system
has unknown performance values $h_i = (h_{i1}, \ldots, h_{is})$, where $h_{ik} \in \mathbb{R}$, for all $k = 1, \ldots, s$ and $i = 1, \ldots, r$. We aim to find a subset of systems with their means
qualified as being “good”. The means of each system can only be estimated
from stochastic simulation output, using sample means as the consistent esti-
mator. For system $i$, let $H_i = (H_{i1}, \ldots, H_{is})$ be the random vector output from
simulation. Let $\sigma_{ik}$ be the variance of objective $k$, $k \leq s$ for system $i$.

Consider a sampling allocation that allocates $\alpha_in$ amount of the total sampling
budget \( n \) to system \( i \), where \( \sum_{i=1}^{r} \alpha_i \leq 1 \) and \( \alpha_i > 0 \) for all \( i = 1, \ldots, r \). Let the systems having good performance estimates be selected as the estimated solution to the subset of good systems. Due to the uncertainties with these estimates, the selection based on estimation may result in a suboptimal (false) solution. Then the optimal sampling laws that can minimize the probability of false selection is of interest.

### 3.1.2 Organization

The rest of the study is organized as follows. In section 3.2, we introduce the preliminaries for multi-objective simulation optimization problems. In section 3.3, we formulate the simulation budget allocation problem into an optimization model and derive the asymptotic allocation rules using a lower bound estimate of the probability of correct selection. In section 3.5, numerical experiments are carried out to illustrate the improved efficiency of selection using our proposed methods. Section 3.6 concludes this chapter and provides some future research directions. Lastly, the appendices provide all the proofs appeared in this chapter.

### 3.2 Preliminaries

Let \( H_i = (H_{i1}, \ldots, H_{is}) \) be the output random vector from simulation, where \( H_i \)'s are samples observed from simulation experiments. The unknown expected value of \( H_i \) is \( h_i = (h_{i1}, \ldots, h_{is}) \).

For a minimization problem, a system \( i \) is said to dominate system \( l \), denoted as \( i < l \), if \( h_{ik} \leq h_{lk} \), for all \( k = 1, \ldots, s \) and for at least one \( k \), \( h_{ik} < h_{lk} \). If \( i < l \), then system \( i \) is said to be better than system \( l \).

Let \( \mathbb{I}(\cdot) \) be the indicator function. Let \( R_i \), the Pareto rank of system \( i \), be the number of systems in \( S \) that dominates \( i \). Therefore the Pareto rank is also referred to as the domination count. Mathematically

\[
R_i = \sum_{l \in S, l \neq i} \mathbb{I}(l < i).
\]  

(3.1)

The Pareto rank for any system within a set of \( r \) systems always takes an integer value from 0 to \( r - 1 \). Systems with Pareto ranks of 0 are not dominated by any other design and they are identified as the best within the finite set. These
systems construct the Pareto set and they are often referred to as non-dominated systems or Pareto-optimal systems.

Now we show that Pareto rank of a system can serve as the measure of being “good” in terms of domination.

It can be easily proven by the definition of dominance that 1) if \( i < l \), then \( R_i < R_l \); 2) if \( R_i \leq R_l \), then \( l \neq i \). It is therefore concluded that systems with lower ranks are, if not better than, as good as those with higher ranks in terms of dominance. Thus the Pareto rank can be used as the relative performance measure for systems in a given set and systems with lower ranks are preferable. A properly chosen threshold of the Pareto rank, \( \gamma \), can therefore be used to filtering those good systems. That is, the desired subset can be defined as \( S_\gamma = \{ i \mid R_i \leq \gamma \} \).

The requirement for the subset to contain the top \( m \) systems is usually not fit for the multi-objective simulation optimization context. It is highly probable that multiple systems may take the same Pareto rank, which makes them indifferent in terms of dominance and preference. While there could be secondary ranking criteria to further distinguish systems with the same rank, these criteria tend to be problem-specific and only applicable to deterministic problems (Jin et al., 2008; Zhang et al., 2008).

Therefore in general systems are possibly not distinct from each other and there simply does not exist the exact top \( m \) systems. For example, when the top 2 systems are required while there are actually 3 systems in the Pareto set (or with the Pareto rank \( \gamma = 0 \)), the subset of top 2 systems is not unique. Instead of making such a hard decision, we employ a similar concept to “goal softening” and relax the desired subset as the set of systems with ranks less than or equal to the smallest integer value \( \gamma \), where the subset contains at least than \( m \) systems. Then \( m \) systems can be randomly selected from \( S_\gamma \) and taken indifferently as an instance of the top \( m \) systems. In this study, we use \( S_\gamma \) as a general definition of the desired subset and the threshold \( \gamma \) can be specified.

When consistent estimators as sample means are used, the estimated domination is denoted as \( \hat{x} \). The estimated Pareto rank is denoted as \( \hat{R} \), and the estimated subset of systems is denoted as \( \hat{S}_\gamma \) accordingly.

In this study, we make the following assumptions, (1) for a given system and a given objective, the simulation output is following independent and identical
normal distribution; (2) observations of different objectives for each system are independent; (3) observations of different systems are independent.

### 3.3 Probability of Correct Selection

The objective is to find the optimal computing budget allocation that can maximize the probability that the desired subset is correctly selected based on estimators. The desired systems are those with ranks not higher than $\gamma$, therefore the event of correct selection ($CS$) occurs if each system in $S_\gamma$ has an estimated Pareto rank not higher than $\gamma$, and all other systems not in $S_\gamma$, each has a rank higher than $\gamma$.

Therefore the probability of correct selection, $P(CS)$, can be written as

$$P(CS) = P\left( \bigcap_{i \in S_\gamma} \hat{R}_i \leq \gamma, \bigcap_{j \notin S_\gamma} \hat{R}_j > \gamma \right) \quad (3.2)$$

The closed-form expression of $P(CS)$ is hardly tractable, due to the high correlations among estimated Pareto ranks. Here we aim to find an appropriate lower bound as a conservative estimate of $P(CS)$. The result is presented in Proposition 1.

**Proposition 1.** The probability of correctly selecting the desired subset has lower bound,

$$P(CS) \geq 1 - s(y + 1)(r - |S_y|) + s(y + 1) \sum_{j \notin S_\gamma} P(\bar{H}_{d,j,k} \leq \bar{H}_{jk}) - \binom{n - 1}{y + 1} \sum_{i \in S_y} P(\bar{H}_{d,i,k} \leq \bar{H}_{ik}) \quad (3.3)$$

where for all $i \in S_y, j \notin S_y$,

$$d_i = \arg\min_{l \in S_i} P(\hat{l} \leq i), \quad S_i = \arg\max_{S \subseteq S \mid |S| = |S_y|} P(i \text{ is dominated by all systems in } S'),$$

$$d_j = \arg\min_{l \in S_j} P(\hat{l} \leq j), \quad S_j = \arg\max_{S \subseteq S \mid |S| = |S_y|} P(j \text{ is dominated by all systems in } S'),$$

$$k_i = \arg\min_{k=1,...,s} P(\bar{H}_{d,i,k} \leq \bar{H}_{ik}), \quad k_j = \arg\min_{k=1,...,s} P(\bar{H}_{d,j,k} \leq \bar{H}_{jk}) \quad (3.4, 3.5, 3.6)$$
Proof. From the definition of $P(CS)$ and according to the probability inequalities, we have

$$P(CS) = P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y, \bigcap_{j \in S_y} \hat{R}_j > y\right) \geq 1 - \left[1 - P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y\right)\right] - \left[1 - P\left(\bigcap_{j \in S_y} \hat{R}_j > y\right)\right]$$

$$\geq P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y\right) + P\left(\bigcap_{j \in S_y} \hat{R}_j \geq y + 1\right) - 1. \quad (3.7)$$

We first investigate the lower bound of $P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y\right)$. From Bonferroni bounds, we have

$$P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y\right) = 1 - P\left(\bigcup_{i \in S_y} \hat{R}_i \geq y + 1\right) \geq 1 - \sum_{i \in S_y} P\left(\hat{R}_i \geq y + 1\right). \quad (3.8)$$

Since

$$P(\hat{R}_i \geq y + 1) = P\left(\bigcup_{S \subseteq S \mid |S'| = y + 1 \atop i \in S'} i \text{ is dominated by all systems in } S'\right) \leq \sum_{S' \subseteq S \mid |S'| = y + 1 \atop i \in S'} P(\text{i is dominated by all systems in } S') \leq \binom{r - 1}{y + 1} \cdot \max_{S' \subseteq S \mid |S'| = y + 1 \atop i \in S'} P(\text{i is dominated by all systems in } S'), \quad (3.9)$$

and

$$P(\text{i is dominated by all systems in } S' \text{ in observation}) = P\left(\bigcap_{i \in S'} l \hat{z}_i\right) \leq \min_{i \in S'} P(l \hat{z}_i), \quad (3.10)$$

and also

$$P(l \hat{z}_i) = P\left(\bigcap_{k = 1, \ldots, s} \overline{H}_{l,k} \leq \overline{H}_{l,k}\right) \leq \min_{k = 1, \ldots, s} P(\overline{H}_{l,k} \leq \overline{H}_{l,k}), \quad (3.11)$$

therefore we have

$$P\left(\bigcap_{i \in S_y} \hat{R}_i \leq y\right) \geq 1 - \sum_{i \in S_y} \binom{r - 1}{y + 1} \cdot \max_{S' \subseteq S \mid |S'| = y + 1 \atop i \in S'} \min_{k = 1, \ldots, s} P(\overline{H}_{l,k} \leq \overline{H}_{l,k})$$

$$= 1 - \binom{r - 1}{y + 1} \cdot \sum_{i \in S_y} P(\overline{H}_{d,k} \leq \overline{H}_{d,k}), \quad (3.12)$$

30
where

\[ S_i = \arg \max_{S' \subseteq S \mid |S'| = y+1} P(i \text{ is dominated by all systems in } S'), \quad (3.13) \]

\[ d_i = \arg \min_{l \in S'} P(l \not\leq i), \quad (3.14) \]

\[ k_i = \arg \min_{k=1, \ldots, s} P(\overline{H}_{d,k} \leq \overline{H}_{jk}). \quad (3.15) \]

Similarly,

\[ P(\bigcap_{j \in S'} \hat{R}_j \geq y + 1) \geq 1 - \sum_{j \notin S'} P(\hat{R}_j \leq y) \geq 1 - (r - |S'|) + \sum_{j \notin S'} P(\hat{R}_j \geq y + 1). \quad (3.16) \]

Since

\[ P(\hat{R}_j \geq y + 1) = P(\bigcap_{S' \subseteq S \mid |S'| = y+1} j \text{ is dominated by all systems in } S') \]

\[ = 1 - P\left( \bigcap_{S' \subseteq S \mid |S'| = y+1} (j \text{ is dominated by all systems in } S') \right) \]

\[ \geq 1 - \min_{S' \subseteq S \mid |S'| = y+1} P(\bigcap_{S' \subseteq S \mid |S'| = y+1} (j \text{ is dominated by all systems in } S')) \]

\[ = \max_{S' \subseteq S \mid |S'| = y+1} P(j \text{ is dominated by all systems in } S'), \quad (3.17) \]

and

\[ P(j \text{ is dominated by all systems in } S' \text{ in observation}) \]

\[ = P(\bigcap_{l \in S'} l \not\leq j) \]

\[ \geq 1 - \sum_{l \in S'} [1 - P(l \not\leq j)] \]

\[ \geq -y + (y + 1) \cdot \min_{l \in S'} P(l \not\leq j), \quad (3.18) \]

and also

\[ P(l \not\leq j) = P(\bigcap_{k=1, \ldots, s} \overline{H}_{lk} \leq \overline{H}_{jk}) \]

\[ \geq 1 - \sum_{k=1, \ldots, s} \left[1 - P(\overline{H}_{lk} \leq \overline{H}_{jk})\right] \]

\[ \geq 1 - s + s \cdot \min_{k=1, \ldots, s} P(\overline{H}_{lk} \leq \overline{H}_{jk}), \quad (3.19) \]
then we get

\[
P\left( \bigcap_{j \in S_j} \hat{R}_j \geq y + 1 \right) \\
\geq 1 - (y + 1)s(r - |S_j|) + (y + 1)s \cdot \sum_{j \in S_j \frac{S' \subseteq S}{|S'| = y}} \frac{\text{max} \text{ min} \text{ min}}{\text{P}}(H_{l,k} \leq \bar{H}_{jk}) \\
\geq 1 - (y + 1)s(r - |S_j|) + (y + 1)s \cdot \sum_{j \in S_j \frac{S' \subseteq S}{|S'| = y}} \text{P}(H_{d,j,k} \leq \bar{H}_{jk}) 
\]

(3.20)

where

\[
S_j = \arg \max \frac{\text{P}( j \text{ is dominated by all systems in } S')}{S' \subseteq S \frac{|S'| = y + 1}} \\
d_j = \arg \min_{l \in S_j} \text{P}(I \preceq j) \\
k_j = \arg \min_{k = 1, \ldots, s} \text{P}(H_{d,j,k} \leq \bar{H}_{jk}).
\]

(3.21)

(3.22)

(3.23)

From the above inequalities, we can get the lower bound of the probability of correct selection as stated in Proposition 1. We denote this lower bound as \( \text{LPCS} \).

\[\square\]

It can be seen from the above derivations that when the total computing budget \( n \) increases to infinity, the probability \( \text{P}(H_{d,j,k} \leq \bar{H}_{jk}) \) will converge to 1, whereas the probability \( \text{P}(H_{d,j,k} \leq \bar{H}_{ik}) \) will converge to 0, such that the right hand side of (3.3) will converge to 1, which justifies itself as a valid bound.

**Remark.** System \( d_i \) here is referred to as the *reference* system of system \( i \), which is, from the mathematical expressions above, the \( (y+1)_{th} \) most dominating system for system \( i \). Thus intuitively, to maximize the probability that system \( i \) is dominated by at most \( y \) systems in \( S \), we need only to minimize the probability \( \text{P}(d_{i} \preceq i) \), since as \( n \) goes to infinity, we will have \( \text{P}(d_{i} \preceq i) \) converging to 0, which means that system \( i \) is dominated by at most \( y \) systems in observation.

System \( d_j \) here is also called the *reference* system of system \( j \), and again, from the derivation, we can see that \( d_j \) is actually the \( (y+1)_{th} \) most dominating system for system \( j \) and we try to maximize the probability that system \( d_j \) dominates system \( j \) in observation. This probability will converge to 1 as \( n \) goes to in-
finity, inferring that system \( j \) would be dominated by at least \( y + 1 \) systems in observation.

### 3.4 Computing Budget Allocation Strategy

Using the lower bound estimate, \( LPCS \), for the probability of correct selection, the optimal computing budget allocation problem can be formulated as below.

\[
\begin{align*}
\text{max} & \quad LPCS \\
\text{s.t.} & \quad \sum_{l=1}^{r} n_l = n \quad (3.24) \\
& \quad n_l > 0, \ n_l \text{ is integer}
\end{align*}
\]

Here we also assume that the simulation running times and costs for different systems are approximately the same and thus the simulation budget can be denoted by the number of total replicates.

It is worth noting that when seeking to determine the asymptotic allocation of simulation budget, i.e., when \( n \) is asymptotically large (\( n \to \infty \)), we will also have \( n_l \) being asymptotically large for all \( l = 1, 2, \ldots, r \). Thus only the fraction of simulation budget \( \alpha_l \) for each system \( l \) is of interest. Since \( \alpha_l = n_l / n \), we will use \( n_l \) and \( \alpha_l n \) interchangeably in this chapter where necessary.

We temporarily relax the non-negativity constraints for \( n_l, \ l = 1, 2, \ldots, r \) and we ignore the minor issues with \( n_l \) not being integer. Now we solve the problem (3.24) and show the approximate closed-form solution below.

### 3.4.1 An Approximate Closed-form Solution

The following proposition presents an approximate closed-form solution to formulation (3.24), where the lower bound defined in Proposition 1 is used as an estimate of the probability of correct selection.

**Proposition 2.** Let all systems be categorized into two groups according to the definition below.

\[
S_A = \left\{ a \mid a \in S, \frac{(h_{ak} - h_{dk})^2}{\sigma_{h_{ak}}^2 / \alpha_a + \sigma_{h_{dk}}^2 / \alpha_{da}} < \min_{l \in S, d_l = a} \frac{(h_{lk} - h_{ak})^2}{\sigma_{h_{lk}}^2 / \alpha_l + \sigma_{h_{ak}}^2 / \alpha_a} \right\}, \quad (3.25)
\]
\[ S_B = S \setminus S_A. \]

Let \( \tau_a = \alpha_{d_a}/\alpha_a. \) If \( \alpha_i, i \leq n \) is the optimal solution that maximizes the lower bound estimate of \( P(\text{CS}) \), then the following conditions for \( \alpha \) hold.

For \( a \in S_A, \ o \in S_A, \)

\[
\frac{\alpha_a}{\alpha_o} = \frac{\sigma_{h_{ak}}^2 + \sigma_{h_{dka}}^2/\tau_a}{\sigma_{h_{ak}}^2 + \sigma_{h_{dka}}^2/\tau_o} \left( \frac{h_{ak_a} - h_{d_ka}}{h_{ok_a} - h_{d_ka}} \right)^2
\]  

(3.26)

For \( b \in S_B, \)

\[
\alpha_a^2 = \sum_{a \in S_A, d_a = b} \sigma_{h_{ak}}^2 \alpha_a^2
\]  

(3.27)

**Proof.** The Lagrangian function of (3.24) with multiplier \( \lambda \) is

\[
L = LPCS - \lambda \left( \sum_{i=1}^{n} n_i - n \right)
\]

Then we have the optimality conditions:

\[
\frac{\partial L}{\partial n_i} = \frac{\partial LPCS}{\partial n_i} - \lambda = 0
\]  

(3.28)

\[
\frac{\partial L}{\partial \lambda} = \sum_{i=1}^{n} n_i - n = 0
\]  

(3.29)

We first examine the derivatives in equation (3.28) for all \( a \in S_A \) and \( b \in S_B. \)

It is noted that \( H_{ik} \sim N(h_{ik}, \frac{\sigma_{h_{ik}}^2}{n_i}). \) Substituting the expression of \( LPCS \) in Proposition 1 into equation (3.28), we have, for \( a \in S_A, \)

if \( a \in S_y, \)

\[
\frac{\partial L}{\partial n_a} = \frac{(y + 1)H}{2\sqrt{2\pi}} \sum_{j \in S_y, d_j = a} \exp \left( -\frac{(h_{jk_j} - h_{ak_j})^2}{2(\sigma_{h_{jk_j}}^2/n_j + \sigma_{h_{ak_j}}^2/n_a)} \right) \frac{(h_{ak_j} - h_{jk_j})\sigma_{h_{ak_j}}^2}{(\sigma_{h_{ak_j}}^2/n_j + \sigma_{h_{dka}}^2/n_{d_ka})^{3/2}n_a^{3/2}}
\]

\[
\left( \frac{n - 1}{y + 1} \right) \frac{1}{2\sqrt{2\pi}} \exp \left( -\frac{(h_{ak_a} - h_{d_ka})^2}{2(\sigma_{h_{ak_a}}^2/n_a + \sigma_{h_{dka}}^2/n_{d_ka})} \right) \frac{(h_{d_ka} - h_{ak_a})\sigma_{h_{dka}}^2}{(\sigma_{h_{dka}}^2/n_a + \sigma_{h_{dka}}^2/n_{d_ka})^{3/2}n_a^{3/2}}
\]

34
\[
\begin{align*}
(n - 1) \frac{1}{2\sqrt{2\pi}} \sum_{i \in S_y} \exp \left(- \frac{(h_{ik_i} - h_{ak_i})^2}{2(\sigma_{h_{ik_i}}^2 / n_i + \sigma_{h_{ak_i}}^2 / n_a)}\right) & \left(\frac{h_{ak_i} - h_{ik_i}}{n_a + \sigma_{h_{ak_i}}^2 / n_a} \right)^2 - \lambda. \\
\end{align*}
\]

(3.30)

Denote
\[
C_1 = \left(\frac{n - 1}{y + 1}\right) \frac{1}{2\sqrt{2\pi}} \sum_{i \in S_y} \exp \left(- \frac{(h_{ak_i} - h_{dk_{ka}})^2}{2(\sigma_{h_{ak_i}}^2 / n_a + \sigma_{h_{dk_{ka}}}}^2 / n_{d_a})\right) \left(\frac{h_{dk_{ka}} - h_{ak_i}}{n_a + \sigma_{h_{dk_{ka}}}^2 / n_{d_a}} \right)^2 n_{d_a}^2 - \lambda, \\
\]
\[
D_1 = \left(\frac{n - 1}{y + 1}\right) \frac{1}{2\sqrt{2\pi}} \sum_{j \in S_y} \exp \left(- \frac{(h_{jk_j} - h_{ak_j})^2}{2(\sigma_{h_{jk_j}}^2 / n_j + \sigma_{h_{ak_j}}^2 / n_a)}\right) \left(\frac{h_{ak_j} - h_{jk_j}}{n_j + \sigma_{h_{ak_j}}^2 / n_a} \right)^2 n_{a}^2 - \lambda. \\
\]

From the definition of \(S_A\) (3.25), we have \(\lim_{n \to \infty} \frac{D_1}{C_1} = 0\), then asymptotically equation (3.30) can be simplified as \(C_1 - \lambda\), or
\[
\frac{\partial L}{\partial n_a} =
\left(\frac{n - 1}{y + 1}\right) \frac{1}{2\sqrt{2\pi}} \sum_{i \in S_y} \exp \left(- \frac{(h_{ak_i} - h_{dk_{ka}})^2}{2(\sigma_{h_{ak_i}}^2 / n_a + \sigma_{h_{dk_{ka}}}}^2 / n_{d_a})\right) \left(\frac{h_{dk_{ka}} - h_{ak_i}}{n_a + \sigma_{h_{dk_{ka}}}^2 / n_{d_a}} \right)^2 n_{d_a}^2 - \lambda,
\]

(3.31)

If \(a \notin S_y\), from a similar derivation, we have
\[
\frac{\partial L}{\partial n_a} = \frac{(y + 1)H}{2\sqrt{2\pi}} \sum_{j \in S_y} \exp \left(- \frac{(h_{jk_j} - h_{ak_j})^2}{2(\sigma_{h_{jk_j}}^2 / n_j + \sigma_{h_{ak_j}}^2 / n_a)}\right) \left(\frac{h_{ak_j} - h_{jk_j}}{n_j + \sigma_{h_{ak_j}}^2 / n_a} \right)^2 n_{a}^2 - \lambda. \\
\]

(3.32)

For \(b \in S_B\), following a similar procedure, we can get
\[
\frac{\partial L}{\partial n_b} = \left(\frac{n - 1}{y + 1}\right) \frac{1}{2\sqrt{2\pi}} \sum_{i \in S_y} \exp \left(- \frac{(h_{bk_i} - h_{ik_i})^2}{2(\sigma_{h_{bk_i}}^2 / n_i + \sigma_{h_{ik_i}}^2 / n_b)}\right) \left(\frac{h_{ik_i} - h_{bk_i}}{n_i + \sigma_{h_{ik_i}}^2 / n_b} \right)^2 n_{b}^2 - \lambda
\]
\[
- \frac{(y + 1)H}{2\sqrt{2\pi}} \sum_{j \in S_y} \exp \left(- \frac{(h_{jk_j} - h_{bk_j})^2}{2(\sigma_{h_{jk_j}}^2 / n_j + \sigma_{h_{bk_j}}^2 / n_b)}\right) \left(\frac{h_{bk_j} - h_{jk_j}}{n_j + \sigma_{h_{bk_j}}^2 / n_b} \right)^2 n_{b}^2 - \lambda. \\
\]

(3.33)
Thus for $a \in S_A, o \in S_A$, applying equation (3.28), we easily get

$$
\alpha_a \frac{(h_{ak_a} - h_{dk_a})^2}{\sigma_{h_{ak_a}}^2 + \sigma_{h_{dk_a}}^2 / \tau_a} = \alpha_o \frac{(h_{ok_o} - h_{dk_o})^2}{\sigma_{h_{ok_o}}^2 + \sigma_{h_{dk_o}}^2 / \tau_o},
$$

(3.34)

which implies

$$
\alpha_a = \frac{\sigma_{h_{ak_a}}^2 + \sigma_{h_{dk_a}}^2 / \tau_a}{\sigma_{h_{ok_o}}^2 + \sigma_{h_{dk_o}}^2 / \tau_o} \frac{(h_{ak_a} - h_{dk_a})^2}{(h_{ok_o} - h_{dk_o})^2}.
$$

(3.35)

For $q \in S_B$, applying equation (3.28) and substitution, we have

$$
n_b^2 = \sum_{a \in S_A, d_a = b} \frac{\sigma_{h_{ak_a}}^2}{\sigma_{h_{ak_a}}^2} n_a^2, \quad \text{or} \quad \alpha_b^2 = \sum_{a \in S_A, d_a = b} \frac{\sigma_{h_{ak_a}}^2}{\sigma_{h_{ak_a}}^2} \alpha_a^2.
$$

(3.36)

The computing budget allocated to each system can then be calculated by normalization. It can be seen from the expression of $\alpha$’s that the non-negativity constraints for $\alpha$’s hold.

**Remark.** There are actually 2 different types of allocation rules depending on the role that each system is playing in the sense of reference system. For systems which play the role of being dominated, the allocation rule will be ratio rule where the allocation quantity is inversely proportional to the signal to noise ratio. For those systems which play the role of dominating, the allocation rule will be the square root rule, where the allocation quantity for the system will be the square root of the sum of weighted square for those systems that it dominates. This is quite similar to the OCBA results for the single objective problems, where the best system is using the square root rule, while the other systems are using the ratio rule Chen et al. (2000a); Chen and Yücesan (2005). However, for the multi-objective problem, from the derivation of lower bound of probability of correct selection, we see that each system would have its own reference system for dominance comparison, where it plays a role of being dominated, and it can also be the reference system for one or more other systems, where it plays the role being dominating. Thus we need to establish some rules to determine the significant roles the systems are playing.

In general, systems in $S_A$ play the role of being dominated, whereas systems in...
S play the role of dominating. To determine which systems are in these sets, we need to use conditions in (3.25). The left hand side of the inequality is the signal to noise ratio for the system to play the role of being dominated, and the right hand side of the inequality is the signal to noise ratio when the system play the role of dominating. The smaller the signal to noise ratio is, the more significant the role it plays in determining the probability of correct selection. In order to maximize the probability of correct selection, we need to focus on the systems with the smaller signal to noise ratio.

The computation of the allocation quantity in proposition 2 is not trivial. The analytical solution is only approximate closed-form, as we need to check the condition in (3.25) to compute the allocation $\alpha$, but this condition also depends on the value of $\alpha$. Hence in practice, in order to solve this numerical problem, we need to iteratively search for the value of $\alpha$, that is, we first assume some initial values for $\alpha$, and then check the reference systems and conditions. After that compute the new values for $\alpha$ according the allocation rules. Repeat the process until $\alpha$ converges.

### 3.4.2 A Sequential Allocation Procedure

In this section, we propose a heuristic sequential sampling allocation procedure for the subset selection. Since the optimal allocation rules are derived from the frequentist perspective, sample means and sample variances are used as estimators. These sample information is updated during each stage which in the asymptotic sense will converge to the true responses. The sampling allocation procedure for the subset selection, denoted as MOCBA-subset, is outlined as below.

**Procedure MOCBA-subset**

1. Given the number of alternatives $r$, total computing budget $n$, specify a threshold of Pareto rank $\gamma$, an initial stage sample size $n_0 \geq 5$, a sampling increment $\Delta$ to allocate per subsequent stage, and an incremental sampling limit $\delta$ per system.

2. Initialize: Observe $n_0$ samples from system $l$, for all $l \leq r$. Update sample statistics $\overline{H}_{lk}$ and $\hat{\sigma}_{hlk}$ for all $l \leq r, k \leq s$. Determine the Pareto rank
estimate $\hat{R}_l$ for all $l \leq r$ and the subset estimate $\hat{S}_y$. Set $v \leftarrow 0$. Set $\alpha_l^y = 1/r, n_l^y = n_0$, for all $l \leq r$.

3. While $\sum_{l=1}^{r} n_l^v < n$ Do another stage:

(a) Calculate: Form Proposition 1, determine the reference system $d_i, d_j$, the most dominating objective $k_i, k_j$ for all $i \in \hat{S}_y, j \notin \hat{S}_y$. From Proposition 2, determine the grouping of all systems into $S_A$ and $S_B$. Compute the new budget allocation $\alpha_{a}^{v+1}$ for all $a \in S_A$, and $\alpha_{b}^{v+1}$ for all $b \in S_B$. Update accordingly $n_{a}^{v+1} = \alpha_{a}^{v+1} \cdot (\sum_{l=1}^{r} n_l^v + \Delta)$, $n_{b}^{v+1} = \alpha_{b}^{v+1} \cdot (\sum_{l=1}^{r} n_l^v + \Delta)$.

(b) Allocate: Observe $\min(\delta, \max(0, n_l^{v+1} - n_l^v))$ additional samples from system $l$, for all $l \leq r$.

(c) Update: update sample statistics $\overline{H}_{lk}$ and $\hat{\sigma}_{hk}$, determine $\hat{R}_l$ and $\hat{S}_y$ for all $l \leq r$. Set $v \leftarrow v + 1$.

4. Return $\hat{S}_y$ as the desired subset of good systems.

For the procedure above, $n_0$ is the initial number of replicates allocated to each system. Since it is a sequential allocation procedure where the subsequent allocation would depend on the current sampling information, $n_0$ cannot be too small to avoid the poor initial estimation (we suggest $n_0 \geq 5$). $\Delta$ is the fractional budget allocated in each iteration, and it cannot be too large for potential correction of allocation errors in the next iteration (we suggest $\Delta \leq 0.1$ when $r \leq 20$). $\delta$ is the maximum portion of budget that can be allocated to any individual system in each iteration, and its value cannot be too large either for the same purpose of allocation errors correction (we suggest $\delta \leq 10$). Numerical experiments show that the performance of the MOCBA-subset procedures are not sensitive to the choice of the parameter values in accordance with the guidelines above.

3.5 Numerical Experiments

In this section, we compare the performance of the proposed algorithm MOCBA-subset with the following procedures.

- Equal allocation, which simply allocates the same number of simulation replicates to each system. The performance of equal allocation is usually taken as the benchmark of allocation algorithms for comparison.
• The original MOCBA procedure to select the non-dominated systems in Lee et al. (2010c). It should be noted that the MOCBA procedure is derived to minimize two types of selection errors, where the selection errors can lead to the same bound of $P(CS)$ as in (3.3) with $\gamma = 0$. Thus MOCBA is a special case of MOCBA-subset with $\gamma = 0$, and the performance improvement of MOCBA over equal allocation is already comprehensively illustrated in Lee et al. (2010c). The numerical experiments below will focus only on selecting a general subset, that is, a subset of good systems that are beyond the Pareto-optimal ones.

The performance indicator used here is the empirical probability of correct selection, which is the percentage of the times that the desired subset is selected in observation out of 1000 independent experiments.

**Experiment 1.** We first test a general problem used in Lee et al. (2010c), whose result illustrates that MOCBA can achieve significant improvement of probability of correctly selecting the non-dominated systems. In this experiment, we run the same test problem shown in Table 1 of Lee et al. (2010c) for a general subset selection. There are 25 systems in total, and each system is evaluated by three objectives. The desired subset is set with $\gamma = 1$. Experiments for equal allocation, MOCBA, and the MOCBA-subset rules are carried out independently and the numerical result is shown in Figure 3.1. The X-axis denotes the number of computing budgets and the Y-axis denotes the corresponding empirical probability of correct selection for different budget.

In contrast to the result that MOCBA outperforms Equal allocation significantly in selecting the non-dominated systems ($\gamma = 0$) (Lee et al., 2010c), when the desired subset is more general, however, it is also noted that MOCBA performs fairly worse in this case than both equal allocation and MOCBA-subset. This is due to the fact that MOCBA is specifically designed for selecting the non-Pareto systems and it cannot be simply generalized and applied to subset selection problems. This result also justifies the need to develop efficient sampling schemes specifically for subset selection under a multi-objective simulation optimization setting.

When there are sampling correlations among the three objectives for each system, the general subset selection problem is also tested. Since this is a 3-objective problem, we first assume that any two of the three objectives are positively correlated with a correlation coefficient 0.9, and the numerical result is
shown in Figure 3.2(a). When there are negative correlation between the objectives, we assume that objective 1 is negatively correlated with objective 2 and objective 3 respectively with a correlation coefficient -0.9, and objective 2 is positively correlated with objective 3 with a correlation coefficient 0.9. The related numerical result is shown in Figure 3.2(b). With similar results to the test case with independent sampling, the results again indicate that MOCBA, which could intelligently control the computing budget allocation to identify the non-dominated systems, could not address the allocation intelligence in selecting a general subset. Thus in the subsequent numerical experiments, we will only compare MOCBA-subset and Equal allocation, which could pertain a higher convergence speed than MOCBA.

In the following experiments, we will test the allocation rules using three examples where the systems are distributed (or spread) in the objective space with typical patterns. Experiment 2 presents a case with systems are linearly spread, and Experiment 3 and 4 provide cases with flat and steep spread of systems respectively. The categorization of different types of spread is introduced in (Zhao et al., 2005). Any general test case can be a hybrid of the typical spread.

**Experiment 2.** In this experiment, we consider a problem with 20 systems in total, and the systems are spread in the 2-dimensional objective space as shown in Figure 3.3. Each system takes a unique Pareto rank in this case and this type of spread is referred to as being neutral (Zhao et al., 2005). In this test, the

![Figure 3.1: Probability of correct selection for Experiment 1](image-url)
Figure 3.2: Probability of correct selection for Experiment 1 with correlation
variance for each objective of each system is set to be $3^2$. The simulation output of each replicate for each system is generated as independent random numbers from corresponding normal distribution for each objective.

The desired subset is set with different $\gamma$ values ranging from 1 to 2. Independent experiments for equal allocation and the proposed MOCBA-subset rules are conducted. Performance of each allocation rule is tested under increasing number of total computing budgets, ranging from 200 to 2000 with a step increase of 200, and the performance of the two allocation rules are shown in Figure 3.4.

It can be clearly seen that the performances of both allocation rules are improved when the computing budget increases. This can be adequately explained by the increasing estimation accuracy of ordinal comparisons with more simulation replicates. The data also shows that with the same number of simulation budget, the empirical probability of correct selection of MOCBA-subset is significantly higher than that of equal allocation, and converges faster to 1 than equal allocation does. This result is due to the fact that MOCBA-subset can learn the intermediate sample information during sequential allocation procedures and, intelligently adjusts the allocation scheme accordingly, whereas equal allocation is allocating equally without considering the sample information or the domain knowledge involved in the specific problem.

The comparison can also be made in terms of the total computing budgets to achieve a certain level of $P(CS)$, and the result is shown in Table 3.1. The
Figure 3.4: Probability of correct selection for Experiment 2
speed-up factor is defined as the ratio between the average replicates needed by equal allocation and replicates needed by MOCBA-subset to achieve a certain level of probability of correct selection. We see that for a certain $\gamma$, the speed-up factor is up to 3, and this factor increases as the required level of probability of correct selection increases, which suggests that more savings of computing budget can be made when a higher level of selection quality is required. This result can be adequately explained by the higher convergence speed achieved by MOCBA-subset where the allocation facilitates the identification of the desired subset.

<table>
<thead>
<tr>
<th>$\gamma$</th>
<th>P(CS)</th>
<th>MOCBA-subset</th>
<th>Equal</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.900</td>
<td>240</td>
<td>960</td>
<td>4.00</td>
</tr>
<tr>
<td></td>
<td>0.950</td>
<td>320</td>
<td>1320</td>
<td>4.13</td>
</tr>
<tr>
<td></td>
<td>0.995</td>
<td>500</td>
<td>2700</td>
<td>5.40</td>
</tr>
<tr>
<td>2</td>
<td>0.900</td>
<td>280</td>
<td>960</td>
<td>3.43</td>
</tr>
<tr>
<td></td>
<td>0.950</td>
<td>320</td>
<td>1400</td>
<td>4.38</td>
</tr>
<tr>
<td></td>
<td>0.995</td>
<td>420</td>
<td>2600</td>
<td>6.19</td>
</tr>
</tbody>
</table>

The comparisons in both criteria provide clear evidence that MOCBA-subset can generally outperform equal allocation rule significantly.

**Experiment 3** Assume there are 16 systems in total and the systems spread in the objective space is illustrated in Figure 3.5. There are fewer systems when the Pareto rank gets larger, except that there is no system with a Pareto rank 2. This type of spread for systems is known as being flat (Zhao et al., 2005). The variance of each objective of each system is set to be $\frac{1}{2^x}$.

Numerical tests with $\gamma$ values set to be 1 and 3 are carried out and the corresponding results are shown in Figure 3.6.

All the results shown in Figure 3.6 clearly demonstrate the trend that generally for both algorithms, the selection quality would be increased as more computing budget is allocated, and that for any fixed number of computing budget, MOCBA-subset can always outperforms equal allocation with a significantly higher probability of correct selection. This result is consistent with that for the neutral cases tested above. The data shown in Table 3.2 in terms of computing budget savings also verifies the advantages gained by employing the proposed MOCBA-subset rules. It is also noted that when the value of $\gamma$ changes,
the achieved empirical probability of correct selection also changes, even with the same number of computing budget. This can be adequately explained by changes of the problem structure where different $\gamma$ values directly change the desired subset and subsequently affect the selection efficiency.

In terms of computing budget savings to maintain a pre-specified level of probability of correct selection, the numerical result is shown in Table 3.2. Similar to the result of the neutral test case, it can also be seen that the speed-up factor is up to 2, and keep increasing with a higher required $P(CS)$ for a certain $\gamma$. A higher value of speed-up factor implies more savings can be gained from implementation in practice.

Table 3.2: Computing budget allocation for Experiment 3

<table>
<thead>
<tr>
<th>$P(CS)$</th>
<th>MOCBA-subset</th>
<th>Equal</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\gamma=1$</td>
<td>0.80</td>
<td>460</td>
<td>2100</td>
</tr>
<tr>
<td></td>
<td>0.85</td>
<td>580</td>
<td>2700</td>
</tr>
<tr>
<td></td>
<td>0.90</td>
<td>700</td>
<td>3800</td>
</tr>
<tr>
<td>$\gamma=3$</td>
<td>0.5</td>
<td>520</td>
<td>1050</td>
</tr>
<tr>
<td></td>
<td>0.6</td>
<td>760</td>
<td>1800</td>
</tr>
<tr>
<td></td>
<td>0.7</td>
<td>1250</td>
<td>3800</td>
</tr>
</tbody>
</table>

The comparisons above both justify that MOCBA-subset can generally outperform equal allocation rule significantly for flat cases.
Figure 3.6: Probability of correct selection for Experiment 3
**Experiment 4** We consider a more general case where there are multiple systems with the same Pareto rank and the spread of the systems is sparser. We assume that there are 16 systems in total and the systems spread in the system space is illustrated in Figure 3.7. This type of spread is also referred to as being steep Zhao et al. (2005). The variance of each objective of each system is set to be $2^2$.

![Figure 3.7: Spread of systems for Experiment 4](image)

Similar simulation runs are conducted as previous experiments. There are no systems with Pareto ranks 1, 2 or 3. Simulation results featuring P(CS) is shown in Figure 3.8.

Simulation budget savings are presented in Table 3.3 respectively. Again the

![Table 3.3: Computing budget allocation for Experiment 4](table)

performance in term of P(CS) for both allocation rules are improved with the increased number of simulation budgets and the MOCBA-subset rule is always better than equal allocation in term of P(CS) or total simulation budget to achieve a certain level of probability of correct selection. Specifically for the speed-up factor, it generally increases as the required level of P(CS) increases except the case when $\gamma$ equals 0. However, the variations of speed-up factor
may not be significant due to the uncertainty involved. The data also suggests that the speed up factor may converge to some maximum value for a given $\gamma$ as studied in Chen and Yücesan (2005).

The experiments above are typical for multi-objective simulation optimization problems, and in all cases, the data proves that the simulation efficiency can be substantially improved by employing the proposed MOCBA-subset rules. Thus the results imply that in general, the MOCBA-subset rules can achieve a significantly higher performance for problems with independent objectives.

**Experiment 5** In this experiment, we examine the performance of MOCBA-subset in the presence of sampling correlations. Although we assume that there is no sampling correlation between sampled responses, the allocation rule should also work, since the correlation has no impact on deriving the bounds and consequently, the rules.

To examine the performance of the proposed method, we conduct similar numerical runs to the previous ones, with the existence of sampling correlations between objectives for each system. The test problems above with typical spread are used, and for the generated simulation output, we assume there is positive or negative linear correlation between objectives. For the bi-objective test problems, simulation samples are generated as Gaussian random variables with given means and standard deviation with correlation coefficients as 0.9 and -0.9 sepa-
rately. The results are shown in Figure 3.9, Figure 3.10, and Figure 3.11 respectively.

![Graph](image)

(a) Neutral case with positive correlation

![Graph](image)

(b) Neutral case with negative correlation

Figure 3.9: Probability of correct selection for Experiment 5: the neutral case

It can be seen from the results that, either for the positive correlation case or negative correlation case, the proposed allocation rules can always achieve a high probability of correct selection than the equal allocation does, with the same amount of computing budget. Or interpreting the result from another angle, to achieve the same level of probability of correct selection, MOCBA-subset can save a significant amount of computing budget compared with equal allocation.
Figure 3.10: Probability of correct selection for Experiment 5: the flat case
Figure 3.11: Probability of correct selection for Experiment 5: the steep case
The results also imply that sampling correlations have significant impact on the empirical PCS achieved by both MOCBA-subset and equal allocation. However, this effect is shown not to be consistent as we conduct substantial numerical testing with different type of problems and $\gamma$ values.

Numerical experiments are also carried out for cases with variances that are not common across designs as well as with different levels of correlations. The results share the same trend as presented above. For brevity, we present only examples of the results with detailed tables and illustrations.

Numerical results with different parameter settings for the MOCBA-subset procedure shows that, when the parameters are set following the guidelines, the proposed procedure proves to be robust and not sensitive to the parameters. Overall results demonstrate that MOCBA-subset can significantly outperform equal allocation in all cases, whether the samples are independent, positively correlated or negatively correlated. The proposed procedures involve computation for the sampling allocation. However, this computation time is usually negligible compared with the simulation time required for the alternative systems.

It is also worth noting that although the allocation rules are derived with the assumption of infinite computing budget, the allocation algorithm works well under limited number of simulation budget, which validates the real world implementation of this allocation scheme, if there are only limited computing budget available for practitioners.

### 3.6 Conclusions

In this study, we present an efficient computing budget allocation approach to find a desired subset for multi-objective ranking and selection problems. The sample allocation problem is formulated to maximize the probability of correct selection under a simulation budget constraint.

From the methodological perspective, we adopt the concept of Pareto optimality to measure the relative performance of systems. Another perspective often seen in subset selection is to select systems that are no more than a distance away from the best. This selection criterion may be reasonable under a single objective problem setting. However, to define the distance in a multi-objective
context, this criterion needs to assign a weight to each objective, which would implicitly transform the problem into a single objective one. The drawbacks of such transformations have been reported and well known in the literature (Butler et al., 2001; Deb, 2001). The suggested approach in this thesis employs Pareto-optimality to resolve the trade-offs among multiple objectives and provide a full picture of trade-offs (Pareto front) for decision makers, where no additional information on preferences over performance measures is required.

This study extends and generalizes the sampling allocation procedures for subset selection under the multi-objective simulation optimization setting. The MOCBA procedure that is specifically designed for selecting the non-Pareto systems (Lee et al., 2010c) becomes a special case of MOCBA-subset with the cut-off rank of 0.

Contribution of this study includes development of a tractable and differentiable lower bound estimate of the probability of correct selection, from which analytical allocation strategies are derived from an asymptotic analysis. Numerical experiments suggest that the proposed algorithm is more efficient than the naive equal allocation approach. Moreover, although the allocation algorithm is asymptotic in nature, numerical experiments reveal that the algorithm is also effective with finite and limited computing budget. There is the potential to incorporate our algorithm into the multi-objective search algorithms which require an elite set in each iteration for reproduction to further improve the overall search efficiency. Numerical illustrations for this combination are presented in Chapter 5.
Chapter 4

Optimal Computing Budget Allocation to Select the Non-dominated Systems: a Large Deviations Perspective

4.1 Introduction

We consider a stochastic problem setting where we aim to select the Pareto set for multi-objective simulation optimization problems. The Pareto set includes all the non-dominated systems in a given set and is regarded as the best among all alternatives. The selection of Pareto systems is based on the multi-objective simulation output and therefore bears uncertainty. In this study, we deal with the particular problem of optimally allocating limited computing budget among all systems, such that the probability of correct selection can be maximized, or equivalently, the probability of false selection can be minimized.

The Pareto set selection problem falls into the well-defined ranking and selection problem settings (Branke et al., 2007; Kim and Nelson, 2007; Swisher et al., 2003). Ranking and selection problems are usually modelled by the indifference zone (IZ) scheme (Kim and Nelson, 2006b) or in the optimal computing budget allocation (OCBA) framework (Chen et al., 2000a; Chen and Yücesan, 2005; Chen et al., 1997). The indifference-zone ranking and selection approach usually seeks for a sampling allocation that can provide a lower bound guarantee
of the probability of correct selection, subject to the constraint that the best system is better than other systems for at least an indifference-zone difference in performance measures. The OCBA framework, on the other hand, focuses on an allocation that maximizes the probability of correct selection, subject to a computing budget constraint.

There have been concerns with the mathematical rigidity of the solution framework employed to derive the sampling laws. Evaluation of the probability of correct (or false) selection is essential in determining the effectiveness and efficiency of consequent allocation schemes. In view of the literature on ranking and selection problems, it is noted that due to the complexity involved in the event of correct (or false) selection, an approximate mathematical framework is commonly employed where probability bounds are introduced to provide estimates of the desired probability. The looseness of these probability bounds may result in sub-optimality of the final solution (Branke et al., 2007; Kim and Nelson, 2007). For example, sampling correlations between multiple performance measures are not explicitly characterized in the probability bounds and consequently, the allocation rules. Since a variety of probability bounds can be developed in theory, the impact of these bounds on the sub-optimality of the derived solutions needs to be explored. Moreover, mathematical development of sampling allocations often involves assumptions of probabilistic normal distributions, which may reduce the generality of the derived solution and thereby limit its application. It is therefore of general concern whether a solution framework incorporating general distributions of samples can be established.

Studies attempting to address these concerns with single-objective problems have been reported. These studies tend to focus on the asymptotic rate of decay instead of the probability itself from a large deviations perspective. Glynn and Juneja (2004) study the single objective OCBA problem from a large deviation perspective where general distributions are allowed and optimality conditions to the problem are mathematically rigorously proven. The large deviations approach is further employed to study the single objective subset selection problems (Szechtmann and Yücesan, 2008), and problems with heavy tails (Blanchet et al., 2008; Broadie et al., 2007). Hunter and Pasupathy (2010) examine a constrained simulation optimization problem using the large deviations principle, assuming that the objective measure and the constraint measure for each system are independently sampled. Sampling laws that can explicitly characterize the correlation between the objective and constraint measure are further consid-
ered in Hunter et al. (2011). The idea behind is, when the total sample size is asymptotically large, false selection is actually a rare event, whose probability is decaying exponentially. Thus the large deviations techniques can be applied (Dembo and Zeitouni, 1998), focusing on the rate associated with the probability.

The aforementioned concerns also apply to multi-objective simulation optimization. In particular, for the computing budget allocation problem to select non-dominated systems under a multi-objective simulation optimization setting, the possible drawback of the existing sampling laws developed by the approximate mathematical framework (Lee et al., 2010c) is that the solution approach reduces comparison of systems on multiple objectives to that of systems on the most dominating objective, which may not explicitly or fully capture the intrinsic multi-objective feature. For instance, sampling correlations between multiple performance measures are not explicitly characterized in the allocation rules. Thus the question arises that whether a sampling allocation scheme explicitly characterizing sampling correlations among performance measures can be suggested. Asymptotic optimality of the allocation rules derived from the traditional approximate mathematical framework needs also to be investigated. The great potential of applying large deviations principles motivates us to explore these problems and provide a more mathematically robust solution framework for sampling allocations. The large deviations techniques would play a vital role in solving these problems. Briefly, this study aims to, 1) propose a general solution framework for multi-objective simulation optimization with generally distributed samples, and examine the optimality conditions of the proposed allocation scheme; 2) provide an efficient computing budget allocation scheme which can incorporate the multi-objective nature of the problem, explicitly characterizing sampling correlations among performance measures; 3) develop particular sampling laws for problems with the multivariate normality assumption; examine the asymptotic performance of the proposed scheme and other existing allocation rules and propose guidelines for simulation practices.

4.1.1 Problem Statement

Consider a finite set \( S \) containing \( r \) of systems, each with unknown objective means \( h_i = (h_{i1}, \ldots, h_{is}) \), where \( h_{ik} \in \mathbb{R} \), for all \( k = 1, \ldots, s \) and \( i = 1, \ldots, r \). Without loss of generality, we aim to find the non-dominated systems with the
lowest objective values, namely, the solution to $\arg\min_i h_i$. The means are observable only via statistical sampling. For instance, sample means are widely used as consistent estimators from the simulation output.

Consider a sampling allocation scheme that allocates $\alpha_i n$ amount of the total sampling budget $n$ to system $i$, where $\sum_{i=1}^r \alpha_i \leq 1$ and $\alpha_i > 0$ for all $i = 1, 2, \ldots, r$. Let the systems having the estimated non-dominated objectives be selected as the estimated solution to the aforementioned simulation optimization problem. The sampling allocation scheme has direct impact on the estimation accuracy and therefore the selection quality. Then an optimal sampling allocation is desired to minimize the probability of false selection.

### 4.1.2 Organization

The rest of the chapter is organized as follows. Section 4.2 describes the notations and assumptions for this study. Section 4.3 provides the derivation of the probability of false selection and the associated rate in the presence of sampling correlations. In section 4.4 the sampling allocation problem is formulated into an NLP model that maximizes the rate of decay of the probability of false selection. An optimal allocation strategy using NLP solvers is proposed and the optimality conditions for the NLP formulation is provided. Section 4.5 presents the allocation scheme specifically for problems under a multivariate normal assumption, explicitly characterizing the sampling correlations between performance measures. Section 4.6 provides numerical experiments to demonstrate the performance of the proposed allocation schemes and section 4.7 summarizes the findings and contributions of this study.

### 4.2 Notations and Assumptions

For system $i$, let $H_i = (H_{i1}, \ldots, H_{in})$ be the random vector output from simulation, where $H_i$’s are observed as samples from simulation experiments. Let $h_i = (h_{i1}, \ldots, h_{in})$ be the expected value of $H_i$.

We make the following assumptions throughout the paper.

- The systems are simulated independently of each other. That is, the random vectors $H_i$ are mutually independent for all $i = 1, 2, \ldots, r$. 
• Let $\Lambda^{H_{ik}}(\theta_{ik})$ and $\Lambda^{H_{i}}(\theta_{i})$ denote the log-moment (or cumulant) generating function of $H_{ik}$ and $H_{i}$ respectively and the corresponding Fenchel-Legendre transform be $I_{ik}(x) = \sup_{\theta_{ik} \in \mathbb{R}} \{\theta_{ik}x - \Lambda^{H_{ik}}(\theta_{ik})\}$ and $I_{i}(x) = \sup_{\theta_{i} \in \mathbb{R}} \{\langle \theta_{i}, x \rangle - \Lambda^{H_{i}}(\theta_{i})\}$, respectively, for all $k \leq s$, $i \leq r$.

Let the cumulant generating functions of the sample means $H_{ik} = \alpha_{i}^{n}/\sum_{v=1}^{n} H_{iv}$ and $H_{i} = (\sum_{v=1}^{n} H_{iv}, \ldots, \sum_{v=1}^{n} H_{iv})$ be denoted $\Lambda^{\overline{H}_{ik}}(\alpha_{i}^{n}\theta_{ik}) = \log E[e^{\alpha_{i}^{n}\overline{H}_{ik}}]$ and $\Lambda^{\overline{H}_{i}}(\theta_{i}) = \log E[e^{\langle \theta_{i}, \overline{H}_{i} \rangle}]$ respectively, where $\theta_{ik} \in \mathbb{R}$, $\theta_{i} \in \mathbb{R}^{s}$ and $\langle \cdot, \cdot \rangle$ denotes the dot product. Here we ignore the minor issues associated with $\alpha_{i}^{n}$ not being an integer.

Assume $\Lambda^{H_{ik}}(\theta_{ik}) = \lim_{n \to \infty} \frac{1}{\alpha_{i}^{n}} \Lambda^{\overline{H}_{ik}}(\alpha_{i}^{n}\theta_{ik})$ and the vector form $\Lambda^{H_{i}}(\theta_{i}) = \lim_{n \to \infty} \frac{1}{\alpha_{i}^{n}} \Lambda^{\overline{H}_{i}}(\alpha_{i}^{n}\theta_{i})$ are well defined for all $\theta_{ik}$ and $\theta_{i}$ and are strictly convex. Also as is typical in large deviations contexts, we assume $\overline{H}_{il}$ and $\overline{H}_{i}$ satisfies large deviations principle with good rate functions $I_{ik}(x), x \in \mathbb{R}$ and $I_{i}(x), x \in \mathbb{R}^{s}$, respectively (Dembo and Zeitouni, 1998).

• Assume the probability of any system being falsely classified based on the estimates of performances is non-zero. This assumption prevents a system from taking up all the sampling budget.

### 4.3 Rate Function of the Probability of False Selection

The objective is to find a computing budget allocation that minimizes the probability of falsely selecting the Pareto set of non-dominated systems. The concept of domination is defined as follows. Assuming a minimization problem, system $l$ dominates system $i$, denoted $l \succ i$, if $h_{lk} \leq h_{ik}$ for all $k = 1, \ldots, s$ and for at least one $k$, $h_{lk} < h_{ik}$. Otherwise, system $l$ does not dominate system $i$, denoted as $l \not\succ i$. We use $\hat{\succ}$ when the dominance is estimated by consistent estimators, say, sample means from simulation.

All the systems that are not dominated by others comprise the Pareto set $S_{p}$. Let $m$ denote the size of the Pareto set, that is, $|S_{p}| = m$. All the other systems are classified into the non-Pareto set $\overline{S}_{p}$.
Therefore the false selection occurs if either type of the following misclassification exists:

1. A Pareto system $i$ is estimated to be dominated by any other system $l$, or mathematically, $\bigcup_{l \in S, i \neq l} I^i_l$.

2. A non-Pareto system $j$ is estimated to be non-dominated by all other systems, or mathematically, $\bigcap_{l \in S, i \neq l} I^j_l$.

Thus the probability of false selection can be written as

$$P(FS) = P\left[\left(\bigcup_{i \in S_p, l \in S} I^i_l\right) \cup \left(\bigcup_{j \in S_p, l \in S} I^j_l\right)\right]$$  \hspace{1cm} (4.1)

From Bonferroni inequalities, $P(FS)$ is upper bounded by

$$[m(r - 1) + (r - m)] \max\left\{\max_{i \in S_p} \max_{l \in S} P(1^i_l), \max_{j \in S_p} \min_{l \in S} P(1^j_l)\right\},$$  \hspace{1cm} (4.2)

and is lower bounded by

$$\max\left\{\max_{i \in S_p} \max_{l \in S} P(1^i_l), \max_{j \in S_p} \prod_{l \in S} P(1^j_l)\right\}.$$  \hspace{1cm} (4.3)

**Proof.** By Bonferroni bounds, we have

$$P(FS) = P\left[\left(\bigcup_{i \in S_p, l \in S} I^i_l\right) \cup \left(\bigcup_{j \in S_p, l \in S} I^j_l\right)\right]$$

\[
\leq P\left(\bigcup_{i \in S_p, l \in S} I^i_l\right) + P\left(\bigcup_{j \in S_p, l \in S} I^j_l\right)
\leq \sum_{i \in S_p} P\left(\bigcup_{l \in S} I^i_l\right) + \sum_{j \in S_p} P\left(\bigcap_{l \in S} I^j_l\right)
\leq \sum_{i \in S_p} \sum_{l \in S} P(1^i_l) + \sum_{j \in S_p} \min_{l \in S} P(1^j_l)
\leq \sum_{i \in S_p} (n - 1) \max_{l \in S} P(1^i_l) + \sum_{j \in S_p} \min_{l \in S} P(1^j_l)
\leq m(n - 1) \max_{i \in S_p} \max_{l \in S} P(1^i_l) + (n - m) \max_{j \in S_p} \min_{l \in S} P(1^j_l)
\leq [m(n - 1) + (n - m)] \left\{\max_{i \in S_p} \max_{l \in S} P(1^i_l), \max_{j \in S_p} \min_{l \in S} P(1^j_l)\right\}.
\]
Similarly, we can get
\[
P(FS) \geq \max\{P(\bigcup_{i \in S} I_{zi}), P(\bigcup_{j \in \bar{S}} I_{zj})\}
\]
\[
\geq \max\{\max_{i \in S} \max_{l \in S} P(l_{zi}), \max_{j \in \bar{S}} \prod_{l \in \bar{S}} P(l_{zj})\}.
\]

Then we have the lower bound and upper bound of the rate of decay,
\[
\lim_{n \to \infty} -\frac{1}{n} \log P(FS) \geq \lim_{n \to \infty} -\frac{1}{n} \max\{\max_{i \in S} \max_{l \in S} P(l_{zi}), \min_{j \in \bar{S}} \prod_{l \in \bar{S}} P(l_{zj})\}, \quad (4.4)
\]
\[
\lim_{n \to \infty} -\frac{1}{n} \log P(FS) \leq \lim_{n \to \infty} -\frac{1}{n} \log \max\{\max_{i \in S} \max_{l \in S} P(l_{zi}), \max_{j \in \bar{S}} \prod_{l \in \bar{S}} P(l_{zj})\}. \quad (4.5)
\]

We use the lower bound in (4.4) as a conservative estimate of the rate of decay of the probability of false selection.

Let
\[
g_{il} = \lim_{n \to \infty} -\frac{1}{n} \log P(l_{zi}), \quad \text{for all } i \in S, l \in S, l \neq i, \quad (4.6)
\]
\[
\eta_{jl} = \lim_{n \to \infty} -\frac{1}{n} \log P(l_{zj}), \quad \text{for all } j \in \bar{S}, l \in S, l \neq j. \quad (4.7)
\]

The following proposition formally states that the overall rate function is lower bounded by the minimum rate function of the probabilities of misclassification.

**Proposition 3.** The rate function of \(P(FS)\) has the lower bound
\[
\lim_{n \to \infty} -\frac{1}{n} \log P(FS) \geq \min\{\min_{i \in S} \min_{l \in S} g_{il}, \min_{j \in \bar{S}} \min_{l \in \bar{S}} \eta_{jl}\}, \quad (4.8)
\]

where
\[
g_{il} = \inf_{x_i, x_{l}, x_{l} \in R^i} \left( \alpha_i I_i(x_i) + \alpha_l I_l(x_l) \right), \quad (4.9)
\]
\[
\eta_{jl} = \min_{k \leq j} \left[ \inf_{x_j, x_{l}, x_{l} \in R^j} \left( \alpha_j I_{jk}(x_j) + \alpha_l I_{lk}(x_l) \right) \right]. \quad (4.10)
\]

**Proof.** Consider first \(g_{il} = \lim_{n \to \infty} -\frac{1}{n} \log P(l_{zi}) = \lim_{n \to \infty} -\frac{1}{n} \log P(\overline{H}_i \geq H_i)\) for system \(i\) and system \(l\), where \(l \neq i\).
Let \( Z_n = (\overline{H}, \overline{H}) \) and denote the logarithmic moment generating function of \( Z_n \) by \( \Lambda_n(\theta_i, \theta_j) = \log E[e^{i(\theta_i, \theta_j)(\overline{H}, \overline{H})}] \) for \((\overline{\theta}_i, \overline{\theta}_j) \in \mathbb{R}^2 \).

For \( \theta_i, \theta_j \in \mathbb{R}^s \), By the independence of system \( i \) and system \( j \),

\[
\Lambda_n(\theta_i, \theta_j) = \log E[e^{i(\theta_i, \theta_j)(\overline{H}, \overline{H})}] = \log E[e^{i(\theta_i, \overline{H})}] \log E[e^{i(\theta_j, \overline{H})}] = \Lambda_n(\theta_i) + \Lambda_n(\theta_j)
\]

(4.11)

Under assumption 3,

\[
\lim_{n \to \infty} \frac{1}{n} \Lambda_n(n\theta_i, n\theta_j) = \lim_{n \to \infty} \frac{1}{n} \Lambda_n(\theta_i) + \frac{1}{n} \Lambda_n(\theta_j)
\]

\[
= \alpha_i \Lambda^H(\theta_i/\alpha_i) + \alpha_j \Lambda^H(\theta_j/\alpha_i)
\]

Then by the Gärtner-Ellis theorem,

\[
I(x_i, x_j) = \sup_{\theta_i, \theta_j} \left( (\theta_i, \theta_j), (x_i, x_j) \right) - \Lambda_n(\theta_i, \theta_j)
\]

\[
= \sup_{\theta_i, \theta_j} \left( (\theta_i, x_i) + (\theta_j, x_j) - \alpha_i \Lambda^H(\theta_i/\alpha_i) - \alpha_j \Lambda^H(\theta_j/\alpha_i) \right)
\]

\[
= \sup_{\theta_i} \left( (\theta_i, x_i) - \alpha_i \Lambda^H(\theta_i/\alpha_i) \right) + \sup_{\theta_j} \left( (\theta_j, x_j) - \alpha_j \Lambda^H(\theta_j/\alpha_i) \right)
\]

\[
= \alpha_i \sup_{\theta_i/\alpha_i} \left( (\theta_i/\alpha_i, x_i) - \Lambda^H(\theta_i/\alpha_i) \right) + \alpha_j \sup_{\theta_j/\alpha_i} \left( (\theta_j/\alpha_i, x_j) - \Lambda^H(\theta_j/\alpha_i) \right)
\]

\[
= \alpha_i I_i(x_i) + \alpha_j I_j(x_j)
\]

and hence

\[
g_{ij} = \inf_{x_i \leq x_j} \left( \alpha_i I_i(x_i) + \alpha_j I_j(x_j) \right)
\]

(4.12)

For \( \eta_{ij} = \lim_{n \to \infty} \frac{1}{n} \log P(I_k < j) \), for all \( j \in S_p, l \in S, l \neq j \), since the probability

\[
P(I_k < j) = P(\bigcup_{k < s} \overline{H}_{ik} > \overline{H}_{jk})
\]

is lower bounded by

\[
\max_{k < s} P(\overline{H}_{ik} > \overline{H}_{jk}),
\]

and is upper bounded by

\[
s \cdot \max_{k < s} P(\overline{H}_{ik} > \overline{H}_{jk}).
\]
Therefore by the squeeze theorem of limit and also according to Hunter and Pasupathy (2010),

\[
\lim_{n \to \infty} -\frac{1}{n} \log P(I^j > j) = \lim_{n \to \infty} -\frac{1}{n} \log \left[ \max_{k \leq s} P(\overline{h}_{lk} > \overline{h}_{jk}) \right]
\]

\[
= \min_{k \leq s} \lim_{n \to \infty} -\frac{1}{n} \log P(\overline{h}_{lk} > \overline{h}_{jk}).
\]

(4.13)

(4.14)

From the Gärtner-Ellis theorem, we can get

\[
\lim_{n \to \infty} -\frac{1}{n} \log P(\overline{h}_{lk} > \overline{h}_{jk}) = \inf_{x \geq x_j} (\alpha_j I_{jk}(x_j) + \alpha_l I_{lk}(x_l)).
\]

(4.15)

Therefore

\[
\eta_{jl} = \min_{k \leq s} \left[ \inf_{x \geq x_j} (\alpha_j I_{jk}(x_j) + \alpha_l I_{lk}(x_l)) \right].
\]

(4.16)

4.4 The Optimal Allocation Strategy

The problem of finding a sampling allocation that can minimize the probability of false selection is equivalent to one that can maximize the asymptotic rate of decay of the probability.

Therefore our problem can be formulated as

\[
\max \min \left\{ \min_{l \in S} \min_{i \in S} g_{il}, \min_{j \in S} \max_{l \in S} \eta_{jl} \right\}
\]

\[
s.t. \sum_{l \leq r} \alpha_l \leq 1, \quad \alpha_l \geq 0, \text{ for all } l = 1, \ldots, r.
\]

(4.17)
We re-expressed the problem in (4.17) as

\[
\text{Problem } P : \quad \max \quad z \\
\text{s.t.} \quad z \leq G_i, \quad \text{for all } i \in S_p \\
\quad \quad z \leq G_j, \quad \text{for all } j \in \overline{S}_p \\
G_i = \min_{l \leq r, l \neq i} g_{il}, \quad \text{for all } i \in S_p \\
G_j = \max_{l \leq r, l \neq j} \eta_{jl}, \quad \text{for all } j \in \overline{S}_p \\
\sum_{l \leq r} \alpha_l \leq 1 \\
\alpha_j \geq 0, \quad \text{for all } l \leq r,
\]

where \( g_{il} \) and \( \eta_{jl} \) are solved as nested optimization problems

\[
\text{Problem } Q_{il} : \quad \min \quad \alpha_i \cdot I_i(x_i) + \alpha_l \cdot I_l(x_l) \\
\text{s.t.} \quad x_l \leq x_i, x_l, x_i \in \mathbb{R}^s
\]

(4.19)

and

\[
\text{Problem } Q_{jl} : \quad \min \quad \alpha_j \cdot I_{jk}(x_j) + \alpha_l \cdot I_{lk}(x_l) \\
\text{s.t.} \quad x_l \geq x_j, x_l, x_j \in \mathbb{R}
\]

(4.20)

respectively for all systems \( i \in S_p \) and \( j \in \overline{S}_p \).

We now show that the solution to Problem P (4.18) exists and it can be obtained using an NLP solver.

### 4.4.1 Optimal Allocation Strategy Using a Solver

We first show that the solution to these nested problems exists by exploring the structure of the formulated problem.

It follows from our assumptions that each nested optimization problem \( Q_{il} \) or \( Q_{jl} \) is a strictly convex minimization problem over its convex feasible region and therefore a unique solution exists.

For Problem \( P \), it can be checked from definition that \( g_{il} \) is a concave function of \( (\alpha_i, \alpha_l) \), and the minimum of \( g_{il} \) is also concave. \( \eta_{jl} \) is also a concave function of \( (\alpha_j, \alpha_l) \). However, the maximum of \( \eta_{jl} \) is not necessarily concave. To resolve its effect on the concavity of the maximization problem, we can decompose
Problem $P$ into a set of sub-problems for each system $j \in \overline{S_p}$, namely

$$\text{Problem } P' : \quad \max \ z$$

$$s.t. \quad z \leq g_{il}, \quad \text{for all } i \in S_p, l \in S, l \neq i$$

$$z \leq \eta_{jl'}, \quad \text{for all } j \in \overline{S_p}$$

$$\sum_{l \leq r} \alpha_l \leq 1$$

$$\alpha_l \geq 0, \quad \text{for all } l \leq r.$$  \hspace{2cm} (4.21)

where $l'$ is a specific system for system $j \in \overline{S_p}$, $g_{il}$ and $\eta_{jl}$ are solved as nested optimization problems defined above.

Therefore each sub-problem $P'$ is a strictly concave maximization problem and at least one solution of $\alpha$ exists. The solution with the maximum $z$ value among all sub-problems is taken as the solution to Problem $P$.

We then propose using a solver to obtain the solution to Problem $P$, provided that the related rate functions, $I_{ik}(x), x \in \mathbb{R}$ and $I_i(x), x \in \mathbb{R}^s$, can be evaluated through well-established formulas for certain typical distributions or through statistical approximation methods (Szechtman and Yücesan, 2008). In practice, the solution to Problem $P$ may be directly returned by the employed solver.

We find that this solution approach using a solver is well fit for a small number of systems, where the size of the problems being small heavily depends on the computing resources available to implement the solver.

### 4.4.2 Optimality Conditions

We now exploit the structure of Problem $P$ (4.18) and investigate the optimality properties by applying Karush-Kuhn-Tucker analyses to the formulation.

The following theorem presents the optimality conditions of the solution to Problem $P$ (4.18).

**Theorem 1.** Let $d_i = \arg\min_{l \leq r, l \neq i} g_{il}, d_j = \arg\max_{l \leq r, l \neq j} \eta_{jl}$ for all $i \in S_p, j \in \overline{S_p}$. Hence $G_i = g_{id_i}, G_j = \eta_{jd_j}$. Let all systems be classified into the following two groups.

$$S_A = \left\{ a \mid a \in S, G_a < \min_{l \leq S, d_l = a} G_l \right\},$$

$$S_B = S \setminus S_A.$$  \hspace{2cm} (4.22)
If \( \alpha = \{ \alpha_1, \alpha_2, \ldots, \alpha_r \} \) is the optimal allocation that maximizes the lower bound estimate of the rate of decay, \( z \), then the following conditions hold.

\[
G_a = G_o, \quad \text{for all } a, o \in S_A, \tag{4.23}
\]

\[
\sum_{a \in S_A, \alpha_a = b} \frac{\partial G_a}{\partial \alpha_b} = 1, \quad \text{for all } b \in S_B. \tag{4.24}
\]

**Proof.** From (4.17), \( z = \min \{ G_i, G_j \} = \min \{ G_a, G_b \} \). From (4.22), for each \( b \in S_B \), there exists a system \( a, d_a = b \) that \( G_b \geq G_a \). Therefore we have an reduced form of \( z = \min_{a \in S_A} G_a \).

Now we consider the Karush-Kuhn-Tucker conditions for the formulation (4.18) with respect to the reduced \( z \). If \( \alpha = \{ \alpha_1, \alpha_2, \ldots, \alpha_r \} \) and \( z \) are the optimal solution to (4.18), then \( \alpha_i, i = 1, \ldots, r \), and \( z \) must satisfy the constraints in (4.18) and there must exist multipliers \( \lambda_a \)'s and \( \gamma \) satisfying

\[
\frac{\partial z}{\partial \alpha_a} - \sum_{a \in S_A} \lambda_a \frac{\partial [z - G_a]}{\partial \alpha_a} - \gamma \frac{\partial (\sum_{l=1}^r \alpha_l)}{\partial z} = 0 \tag{4.25}
\]

\[
\frac{\partial z}{\partial \alpha_a} - \lambda_a \frac{\partial [z - G_a]}{\partial \alpha_a} - \gamma \frac{\partial (\sum_{l=1}^r \alpha_l)}{\partial \alpha_a} = 0, \quad \text{for all } a \in S_A \tag{4.26}
\]

\[
\frac{\partial z}{\partial \alpha_b} - \lambda_a \frac{\partial [z - G_a]}{\partial \alpha_a} - \gamma \frac{\partial (\sum_{l=1}^r \alpha_l)}{\partial \alpha_b} = 0, \quad \text{for all } b \in S_B \tag{4.27}
\]

\[
\lambda_a [G_a - z] = 0, \quad \text{for all } a \in S_A \tag{4.28}
\]

\[
\gamma (1 - \sum_{l=1}^r \alpha_l) = 0 \tag{4.29}
\]

\[
\lambda_a \geq 0, \quad \text{for all } a \in S_A
\]

\[
\gamma \geq 0
\]

From (4.25), (4.26) and (4.27), we have

\[
\sum_{a \in S_A} \lambda_a = 1, \tag{4.30}
\]

\[
\lambda_a \frac{\partial G_a}{\partial \alpha_a} = \gamma, \quad \text{for all } a \in S_A, \tag{4.31}
\]

\[
\sum_{a \in S_A, \alpha_a = b} \lambda_a \frac{\partial G_a}{\partial \alpha_b} = \gamma, \quad \text{for all } b \in S_B. \tag{4.32}
\]

Equation (4.30) implies that \( \lambda_a > 0 \) for some \( a \). Since \( \frac{\partial G_a}{\partial \alpha_a} \) is strictly positive, it
follows that \( y > 0 \) and thus each \( \lambda_a > 0 \) from (4.31). Then from (4.28), we have

\[
G_a = G_o = z, \quad \text{for all } a, o \in S_A.
\]

From (4.29), we can get

\[
\sum_{l=1}^{k} a_l = 1. \tag{4.33}
\]

Substituting (4.31) into (4.32), we have

\[
\sum_{a \in S_A, d_a = b} \frac{\partial G_a}{\partial \alpha_b} = 1, \quad \text{for all } b \in S_B.
\]

It is worth noting that the problem formulation, the solution approach using a solver and the optimality conditions presented above apply to a general context.

In the next section, we investigate the sampling allocation problem under a multivariate normal assumption. This assumption is frequently made in the literature.

### 4.5 The Multivariate Normal Case

We deal with the case where the underlying random vector \( H_i, i \leq r \) follows a multivariate normal (MVN) distribution. Such distributions are typically characterized by the mean vectors and variance-covariance matrices.

Assume we can obtain i.i.d replicates of the multivariate normal random vector \( H_i \), and \( H_i \sim MVN(h_i, \Sigma_{h_i}) \), where \( \Sigma_{h_i} \) is the variance-covariance matrix

\[
\Sigma_{h_i} = \begin{pmatrix}
\sigma_{h_{i1}}^2 & \rho_{h_{i1}h_{i2}} \sigma_{h_{i1}} \sigma_{h_{i2}} & \cdots & \rho_{h_{i1}h_{is}} \sigma_{h_{i1}} \sigma_{h_{is}} \\
\rho_{h_{i1}h_{i2}} \sigma_{h_{i1}} \sigma_{h_{i2}} & \sigma_{h_{i2}}^2 & \cdots & \rho_{h_{i2}h_{is}} \sigma_{h_{i2}} \sigma_{h_{is}} \\
\vdots & \vdots & \ddots & \vdots \\
\rho_{h_{i1}h_{is}} \sigma_{h_{i1}} \sigma_{h_{is}} & \rho_{h_{i2}h_{is}} \sigma_{h_{i2}} \sigma_{h_{is}} & \cdots & \sigma_{h_{is}}^2
\end{pmatrix}, \tag{4.34}
\]

where \( \rho \) is the correlation coefficient between objectives and \( 0 < \sigma_{h_{ik}} < \infty \) for all \( i \leq r \) and \( k \leq s \).
According to the multidimensional version of Cramér’s theorem (Varadhan, 1984), \(\hat{H}_i\) follows the large deviations principle (LDP) with a good rate function

\[
I_i(x) = \frac{[x - \mathbf{h}_i]^T \Sigma_i^{-1}[x - \mathbf{h}_i]}{\sigma^2_{h_i}}, \text{ for all } i \leq r.
\] (4.35)

The marginal distribution for each replicate of \(H_{ik}\) is also normal, hence \(\hat{H}_{ik}\) satisfy the LDP with a good rate function

\[
I_{ik}(x) = \frac{(x - h_{ik})^2}{2\sigma^2_{h_{ik}}}, \text{ for all } i \leq r, k \leq s.
\] (4.36)

Substituting the rate functions above into \(g_{il}\) (4.9) and \(\eta_{jl}\) (4.10), we have

\[
g_{il} = \inf_{x_l \leq x_i} \left( \frac{\alpha_i}{2} [x_i - \mathbf{h}_i]^T \Sigma_i^{-1}[x_i - \mathbf{h}_i] + \frac{\alpha_l}{2} [x_l - \mathbf{h}_l]^T \Sigma_l^{-1}[x_l - \mathbf{h}_l] \right),
\] (4.37)

\[
\eta_{jl} = \min_{k \leq s} \left[ \inf_{x_l \geq x_j} \left( \frac{\alpha_j}{2} (x_j - h_{jk})^2 + \frac{\alpha_l}{2} (x_l - h_{lk})^2 \right) \right].
\] (4.38)

### 4.5.1 Optimal Sampling Allocation Using a Solver

Using the rates expressions (4.37) and (4.38) for the nested optimization problems \(Q_{il}\) (4.19) and \(Q_{jl}\) (4.20) respectively, we can obtain the optimal allocation to Problem \(P\) (4.18) under the MVN assumption using a solver. This approach is presented in the following definition.

**Definition 1.** MOCBA* is defined as the solution approach that determines the sampling allocation \(\alpha\) in the following steps.

1. Use \(g_{il}\) (4.37) and \(\eta_{jl}\) (4.38) for the nested problems \(Q_{il}\) (4.19) and \(Q_{jl}\) (4.20) and embed nested solvers;

2. Solve Problem \(P\) (4.18) using an NLP solver.

Solving the main problem \(P\) may not be trivial. The optimizer or the solver tends to treat the objective and constraints as black-boxes, knowing neither the function nor its structure. Hence these problems could be significantly more difficult. Typically, an NLP solver takes successive steps to find better solutions by determining a search direction from its current position. The efficacy of finding a promising search direction by the solver dictates the total solving time and solution qualify. It is verified by numerical experiments that solving Problem \(P\) using a solver tends to be computation-intensive.
The nested optimization problems $Q_{il}$ and $Q_{jl}$ under a multivariate normal assumption are quadratic programming ones with linear constraints. Solving these problems should require considerably fewer computations compared with solving Problem $P$. Numerical experiments also verify this finding.

We now investigate the problem structure and the optimality conditions to Problem $P$ under a particular MVN environment and propose an approximate closed-form solution that is computationally effective and more efficient.

### 4.5.2 An Approximate Closed-form Solution to Sampling Allocations

In view of the computing overhead inherent to solving Problem $P$ using a solver, in this section we suggest an alternative solution to problem $P$ under a multivariate assumption.

Using the well-defined rate functions for the MVN case, we can derive an allocation strategy directly from Theorem 1. The result is presented as Corollary 1.

**Corollary 1.** Assume there are $r$ systems that are independently sampled under a multivariate normal assumption. Let $d_i, d_j$ be defined as in Theorem 1 and all systems be classified into two groups $S_A$ and $S_B$.

Let

$$k_i = \arg\max_{k \leq s} \frac{|h_{d_i,k} - h_{i,k}|(h_{d_i,k} - h_{i,k})}{2\left(\sigma_{h_i,k}^2/\alpha_i + \sigma_{h_i,k}^2/\alpha_{d_i}\right)}, \text{ for all } i \in S_p,$$

$$k_j = \arg\max_{k \leq s} \frac{|h_{d_j,k} - h_{j,k}|(h_{d_j,k} - h_{j,k})}{2\left(\sigma_{h_j,k}^2/\alpha_j + \sigma_{h_j,k}^2/\alpha_{d_j}\right)}, \text{ for all } j \in S_p. \quad (4.39)$$

If $\alpha = \{\alpha_1, \alpha_2, \ldots, \alpha_r\}$ is the optimal allocation that maximizes the rate of decay of the probability of incorrectly selecting the non-dominated systems, then the following approximations for $\alpha$’s hold.

For $a \in S_A, \ o \in S_A$,

$$\frac{\alpha_a}{\alpha_o} = \frac{(G_a/\alpha_a)^{-1}}{(G_o/\alpha_o)^{-1}} \quad (4.40)$$
For \( b \in S_B \),
\[
\alpha_b^2 = \sum_{a \in S_A, da=b} \frac{\sigma_{h_{bka}}^2}{\sigma_{h_{aka}}^2} \alpha_a^2
\]  
(4.41)

Proof. It follows from equation (4.23) in Theorem 1 that equation (4.40) holds.

From equation (4.24), the derivatives are approximated as
\[
\frac{\partial G_a}{\partial \alpha_b} = \frac{(h_{bka} - h_{aka})^2}{2(\sigma_{h_{aka}}^2/\alpha_a + \sigma_{h_{bka}}^2/\alpha_b)^2} \sigma_{h_{bka}}^2/\alpha_b^2,
\]
\[
\frac{\partial G_a}{\partial \alpha_a} = \frac{(h_{bka} - h_{aka})^2}{2(\sigma_{h_{aka}}^2/\alpha_a + \sigma_{h_{bka}}^2/\alpha_b)^2} \sigma_{h_{aka}}^2/\alpha_a^2.
\]

By simple substitution, we get
\[
\alpha_b^2 = \sum_{a \in S_A, da=b} \frac{\sigma_{h_{bka}}^2}{\sigma_{h_{aka}}^2} \alpha_a^2
\]
(4.42)

It is noted that equations in Corollary 1 are not strictly closed-form. In practice, the \( \alpha \)'s can be recursively updated till convergence is achieved. This solution approach to sampling allocations is stated in Definition 2.

**Definition 2.** MOCBA+ is defined as the solution approach that iteratively determine the sampling allocation \( \alpha \)'s in the following steps.

1. Specify an initial sampling allocation \( \alpha^0 \). Equal allocation may serve as an alternative of this initial allocation.

2. While \( \alpha \) not converged Do another iteration:

   (a) Obtain \( g_{il} \) (4.37) and \( \eta_{jl} \) (4.38) by solving the nested problems.

   (b) Determine \( G_i, d_i, G_j, d_j \) as defined in Theorem 1. Determine the grouping of all systems into \( S_A \) and \( S_B \).

   (c) Determine \( k_i, k_j \) according to (4.39) in Corollary 1.

   (d) Compute the new allocation according to (4.40) and (4.41) in Corollary 1.

3. Return the current allocation.
We can see that sampling correlations between objectives are explicitly taken into account in both MOCBA* and MOCBA+, for $\Sigma_i$ and $\Sigma_l$ are characterized in the expression of $g_{il}$.

### 4.5.3 Closed-form Solutions to the Nested Optimization Problems

It is noted that for both MOCBA* and MOCBA, at each step of searching for the solution $\alpha$ (or the $\alpha$-step) to Problem $P$, a number of $r \times (r-1)$ nested optimization problems must be solved, where $r$ is the size of the finite set. These nested problems are quadratic programming ones in nature and should only require minimal time to be individually solved using optimizers. When the number of systems is large or the computation capacity is constrained, accelerating the solving process for the bulk of nested optimization problems may be desirable under a computation-sensitive environment.

Our purpose here is to provide closed-form expressions of the rates $g_{il}$ and $\eta_{jl}$ for some common cases. As an alternative to solving nested optimization problems using NLP optimizers, the proposed solutions can be directly embedded into MOCBA* and MOCBA+ for specific problem settings. Moreover, when the closed-form expressions are embedded into MOCBA+, we provide a solver-free solution approach to the sampling allocation problem, which should be computationally more efficient.

We first study the case where systems are simulated with no sampling correlations between objectives. The rates $g_{il}$ and $\eta_{jl}$ are evaluated explicitly in mathematical equations by exploring the infimum in expressions (4.37) and (4.38).

Let $\mathbb{1}_{(\cdot)}$ be the indicator function. Lemma 1 state the results formally.

**Lemma 1.** When systems are i.i.d sampled with no sampling correlations between objectives under a multivariate normal (MVN) assumption, the rates $g_{il}$ and $\eta_{jl}$ can be evaluated as below.

$$g_{il} = \sum_{k \leq s} \mathbb{1}_{(h_{ik} > h_{ik})} \cdot \frac{(h_{ik} - h_{ik})^2}{2(\sigma_{h_{ik}}^2/\alpha_i + \sigma_{h_{ik}}^2/\alpha_l)},$$  

$$\eta_{jl} = \mathbb{1}_{(l < j)} \cdot \min_{k \leq s} \frac{(h_{jk} - h_{lk})^2}{2(\sigma_{h_{jk}}^2/\alpha_j + \sigma_{h_{lk}}^2/\alpha_l)}. $$

*Proof.* Under the environment with no sampling correlations between systems.
Therefore it follows that 

\[ P(I \leq i) = P\left( \bigcap_{k \leq s} \overline{I}_{ik} \leq \overline{I}_{ik} \right) = \prod_{h \leq s} P(\overline{I}_{ih} \leq \overline{I}_{ih}). \]

From independence sampling, we get

\[
g_{il} = \lim_{n \to \infty} \frac{1}{n} \log P(I \leq i)
= \sum_{k \leq s} \lim_{n \to \infty} \frac{1}{n} \log P(\overline{I}_{ih} \leq \overline{I}_{ih})
= \sum_{k \leq s} \inf_{l_i \leq s} \left( \alpha_i \cdot I_{ih}(x_i) + \alpha_i \cdot I_{ik}(x_i) \right).\]

For all systems \( l \leq r \), we have \( \alpha_i \cdot I_{ih}(x_i) = \frac{\alpha_i(x_i - h_{ik})^2}{2\sigma^2_{hi}} \). Then we can easily find \( \inf_{x_i \leq s} \left( \alpha_i \cdot I_{ih}(x_i) + \alpha_i \cdot I_{ik}(x_i) \right) \) by applying Karush-Kuhn-Tucker conditions,

\[
\inf_{x_i \leq s} \left( \alpha_i \cdot I_{ih}(x_i) + \alpha_i \cdot I_{ik}(x_i) \right) = \begin{cases} 
\frac{(h_{ik} - h_{hk})^2}{2(\sigma^2_{hi} + \sigma^2_{hk}/\alpha_i)}, & \text{if } h_{ik} > h_{hk}, \\
0, & \text{otherwise.}
\end{cases}
\]

Therefore it follows

\[
g_{il} = \sum_{h=1}^{H} \mathbb{I}(h_{ik} > h_{hk}) \cdot \frac{(h_{ik} - h_{hk})^2}{2(\sigma^2_{hi} + \sigma^2_{hk}/\alpha_i)}.\]

Similarly for \( \eta_{jl} = \min_{k \leq r} \left[ \inf_{x_j \leq s} \left( \alpha_j I_{jk}(x_j) + \alpha_j I_{ik}(x_i) \right) \right] \), we have

\[
\inf_{x_j \leq s} \left( \alpha_j \cdot I_{jk}(x_j) + \alpha_j \cdot I_{ik}(x_i) \right) = \begin{cases} 
\frac{(h_{ik} - h_{jk})^2}{2(\sigma^2_{jk}/\alpha_j + \sigma^2_{ik}/\alpha_i)}, & \text{if } h_{ik} \leq h_{jk}, \\
0, & \text{otherwise.}
\end{cases}
\]

We note that when \( l \neq j \), there exists at least one objective \( k \) such that \( h_{ik} > h_{jk} \), and the related infimum term as defined above equals 0. Then it follows that \( \eta_{jl} = 0 \). When \( l < j \), \( h_{hk} \leq h_{jk} \) holds for all \( k \leq s \), and the related infimum terms are all positive. Thus we can rewrite \( \eta_{jl} \) as

\[
\eta_{jl} = \mathbb{I}(l < j) \cdot \min_{k \leq s} \frac{(h_{jk} - h_{ik})^2}{2(\sigma^2_{jk}/\alpha_j + \sigma^2_{ik}/\alpha_i)}.\]
It can be seen that the rate \( g_{il} \) characterize all those objectives that have a non-zero impact on the rate. Depending on the number of objectives that are active, there are \( \binom{1}{1} + \cdots + \binom{1}{1} = 2^1 - 1 \) possible scenarios and the indicator \( \mathbb{I}_{(h_{il} > h_{ik})} \) serves as a filter.

The rate \( \eta_{jl} \) involves a simple comparison of rates among all objectives, and consequently there is only one objective that is active. It is also noted that this rate is not affected by sampling correlations between objectives.

When sampling correlations between objectives exist, difficulties in explicitly expressing \( g_{il} \) into equations arise, which is due to the uncertainties with the number of effective objectives and the complexities with the correlations between these objectives.

Here we consider only the bivariate normal (BVN) case. Assume \((H_{i1}, H_{i2})^T \sim BVN \left((h_{i1}, h_{i2})^T, \Sigma_{h_i}\right)\), where \( \Sigma_{h_i} \) is the variance-covariance matrix for system \( i \). Suppose there are only linear correlations and the correlation coefficient is \( \rho \).

We further assume that the two performances have the same variances for each system.

We can obtain the rate functions from the Karush-Kuhn-Tucker (KKT) conditions on the infimum in expressions (4.37) and (4.38). The result is presented in Lemma 2.

**Lemma 2.** Suppose systems are i.i.d sampled under a bivariate normal (BVN) assumption with a sampling correlation \( \rho \). Assume the variances satisfy \( \sigma_{h_{i1}} = \sigma_{h_{i2}} = \sigma_{h_i} \) for any system \( i \). Then the rates \( g_{il} \) and \( \eta_{jl} \) can be evaluated as below.

\[
\begin{align*}
    g_{il} &= \begin{cases} 
        \frac{(h_{i1} - h_{i2})^2}{2(\sigma_{h_{i1}/\alpha_i}^2 + \sigma_{h_{i2}/\alpha_i}^2)}, & \text{condition 1,} \\
        \frac{1}{2}(h_{i1} - h_{i2})^2, & \text{condition 2,} \\
        \frac{1}{2}\left[h_{i1} - h_{i1}, h_{i2} - h_{i2}\right]\left[\frac{1}{\alpha_i} \Sigma_{h_i} + \frac{1}{\alpha_i} \Sigma_{h_i}\right]^{-1}\left[h_{i1} - h_{i1}, h_{i2} - h_{i2}\right]^T, & \text{otherwise.}
    \end{cases}
\end{align*}
\]

\[
\eta_{jl} = \mathbb{I}_{(l < j)} \cdot \min_{k \ge 2} \frac{(h_{jk} - h_{ik})^2}{2(\sigma_{h_{jk}/\alpha_i}^2 + \sigma_{h_{ik}/\alpha_i}^2)},
\]

where the conditions are defined as
condition 1:

\[
\begin{align*}
&\left( h_{l2} - h_{i2} > 0, h_{l1} - h_{i1} > h_{l2} - h_{i2}, \rho > \frac{h_{l1} - h_{i1}}{h_{l2} - h_{i2}} \right), \text{ or } \\
&\left( h_{l2} - h_{i2} < 0, h_{l1} - h_{i1} > - (h_{l2} - h_{i2}), \rho > \frac{h_{l2} - h_{i2}}{h_{l1} - h_{i1}} \right), \text{ or } \\
&\left( h_{l2} - h_{i2} < 0, 0 \leq h_{l1} - h_{i1} \leq -(h_{l2} - h_{i2}) \right).
\end{align*}
\]

(4.47)

condition 2:

\[
\begin{align*}
&\left( h_{l2} - h_{i2} > 0, -(h_{l2} - h_{i2}) \leq h_{l1} - h_{i1} \leq h_{l2} - h_{i2}, \rho > \frac{h_{l1} - h_{i1}}{h_{l2} - h_{i2}} \right), \text{ or } \\
&\left( h_{l2} - h_{i2} > 0, h_{l1} - h_{i1} \leq -(h_{l2} - h_{i2}) \right).
\end{align*}
\]

(4.48)

Condition 1 refers to the case when only objective 1 is actively contributing to the rate, whereas condition 2 refers to the case when only objective 2 is effective in computing the rate. The result in Lemma (2) above can be obtained by basic maths and the formal proof is omitted for brevity.

In summary, instead of solving nested optimization problems, we provide a direct approach to computing \(g_{jl}\) and \(\eta_{jl}\), which would further lessen the computation burden of finding solutions to the sample allocation problem.

4.6 Numerical Experiments

In this section, we present numerical experiments that illustrate the performance of our proposed sampling algorithms. The alternative sampling scheme for multi-objective simulation optimization on finite set is the MOCBA framework provided by Lee et al. (2010c), which is to be tested and compared with our algorithms.

It is noted that MOCBA is derived from a Bonferroni probability bound that approximates the probability of identifying each system based on the single objective that contributes most for each system. That is, only one objective is active in determining the sampling allocation for each system, and therefore sampling correlation between objectives is not explicitly characterized. The sub-optimality that may be introduced by this approximation is not addressed Lee et al. (2010c). Based on our analysis from a large deviations perspective,
we can point out that the main difference between MOCBA and MOCBA+ is
the calculation of rates $g_{il}$ (4.37) and thereby $G_{i}$, for all non-dominated systems.
We also show that there is no difference in calculating $\eta_{jl}$ (4.38). It is therefore
expected there will be sampling allocation differences when more than one ob-
jectives are active in determining the rates for non-dominated systems. The sub-
optimality by MOCBA should result in a decreased convergence rate of decay
of false selection.

While the MOCBA* approach employs a numerical solver, it is expected that
this approach will be more computation-intensive and therefore consume more
CPU time. MOCBA and MOCBA+ are both heuristics that iteratively update
the sampling allocation, for which the performance metrics of interest are the
solution quality and the convergence speed.

In brief, we are measuring the performance of the following sampling allocation
schemes:

- MOCBA*, the solver approach defined in Definition 1 in this paper. We
  implement the NLP solver using MatLab and the CPU time are given by
  the MatLab tic/toc functions.
- MOCBA+, the heuristic defined in Definition 2 in this paper, as an ap-
  proximate to MOCBA*;
- MOCBA, the approach introduced in Lee et al. (2010c);
- Equal allocation, which simply allocates samples evenly to all systems;

The key performance indicator of interest here is the asymptotic rate of decay
that can be achieved by these sampling schemes. We also provide a measure of
CPU time required by these allocation schemes to illustrate their computational
intensity.

**Experiment 1.** We first provide a simple numerical example to illustrate the
differences in sampling allocations and thereby convergence rates for these sam-
pling schemes.

Consider a 3-system, 3-objective simulation optimization problem, where the
replicates for each system are i.i.d. multivariate normal random vectors. As-
sume also there is no sampling correlation between objectives. The means of
the three systems are provided in Table 4.1. The variances are assumed to be 25
for all systems for all objectives.
It can be easily identified that system 1 and 3 are non-dominated, while system 2 is dominated by system 1. The result of solving for the sampling allocation is presented in Table 4.2.

The convergence rate for equal allocation, as expected, is the lowest among all allocation schemes. MOCBA achieves a significantly improved convergence rate compared with equal allocation. This improvement has been illustrated in terms of empirical PCS (or PFS) in finite time in Lee et al. (2010c). It is also noted that MOCBA allocates equally to system 2 and system 3. MOCBA+, on the other hand, returns a different sample allocation from MOCBA and achieve a significantly higher asymptotic rate. The different sampling allocation is due to the artifact that MOCBA uses only one active objective to compute allocation, while MOCBA+ considers all active objectives to determine the sampling allocation. Specifically for this example, MOCBA determines the allocation to system 3 by catering to its distance from system 1 on objective 2 only, which is 0.5 in this case. The active difference in the means of system 2 and system 1 is also 0.5, which leads to the same allocations of systems 2 and 3 under the MOCBA scheme. However, objective 3 is also active in identifying system 3 and thereby affecting the allocation. Taking all active objectives into consideration, MOCBA+ yield a sampling allocation that can return a better convergence rate. It is noted that MOCBA+, as a searching heuristic for sampling allocation, yields a convergence rate that is very close to the result by MOCBA* using a solver, which indicates that the approximate closed-form solution of MOCBA+ can return near optimal solution to sampling allocations.
The computation times of sampling allocation are also gauged in terms of average CPU time for 500 replications. It can be seen that the heuristics require considerably less time than the approach using a solver. Therefore MOCBA* is only fit for problems with a small number of systems. On the other hand, MOCBA+ consumes less time and provides a solution close to the solution by MOCBA*. The balance between solution quality and computing time may need to be dealt with in practical problem settings.

**Experiment 2.** In this experiment we investigate the robustness of the proposed sampling schemes over a dynamic problem structure. Assume the 3-system, 3-objective problems are having means as given in Table 4.3 and having universal variances of $5^2$. Assume also there is no sampling correlation between objectives.

<table>
<thead>
<tr>
<th>system</th>
<th>objective 1</th>
<th>objective 2</th>
<th>objective 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.0</td>
<td>4.0</td>
<td>[1.5, 2.8]</td>
</tr>
<tr>
<td>2</td>
<td>3.5</td>
<td>5.0</td>
<td>3.0</td>
</tr>
<tr>
<td>3</td>
<td>4.0</td>
<td>3.5</td>
<td>2.0</td>
</tr>
</tbody>
</table>

We vary the mean of objective 3 for system 1, $h_{13}$, and investigate the allocation dynamics of different sampling laws. The convergence rates of decay are presented in Figure 4.1.

![Figure 4.1: Rate of decay for Experiment 2](image)
It is firstly observed from Figure 4.1 that all MOCBA-family approaches out-perform equal allocation in returning higher rates of decay of false selection. The result also reveals that MOCBA+ can provide a performance with no distinguishable difference from MOCBA*, independent of the dynamic problem structure for this 3-system problem. This strongly indicates that our proposed heuristic of MOCBA+ is robust in searching for the optimal sampling allocation.

For this experiment, systems 1 and 3 are both non-dominated ones and system 2 is dominated by system 1. After examining the problem structure we know that the overall minimum rate is governed by the rate of systems 2. For equal allocation, when \( h_{13} \leq 2.5 \), The rate for system 2 is determined by its distance from system 1 on objective 1 only, which is a constant, 0.5. This explains why the overall rate of equal allocation keeps flat within this range. When \( h_{13} > 2.5 \), the rate of system 2 is dictated by its distance from system 1 on objective 3, which changes with \( h_{13} \). It is therefore observed that the overall rate for equal allocation decreases when \( h_{13} \) increases.

Now we demonstrate the impact of \( h_{13} \) on the allocation to systems and thereby the rates. When \( h_{13} \leq 2.0 \), actually only objective 2 is actively contributing to the rates of system 3 and affecting its allocation. Objective 3 turns out to be inactive. Therefore there is no difference in sampling allocation between MOCBA and MOCBA+ and the achieved rate is not affected by the changes of \( h_{13} \). However, when \( 2.0 < h_{13} \leq 2.5 \), objective 3 also becomes active in determining the rate and allocation for system 3, but MOCBA ignores it. That is why the rate of decay for MOCBA remains unchanged. By incorporating the contribution of objective 3 to the rate for system 3, MOCBA+ and MOCBA* are able to achieve a higher convergence rate of false selection than MOCBA. The difference between MOCBA+ and MOCBA is increasing when \( h_{13} \) is approaching 2.5.

When \( h_{13} > 2.5 \), the overall rate of decay is still constrained by the rate for system 2, which depends on its distance from system 1 on objective 3. Therefore we can see that the rates of all allocation schemes decrease with \( h_{13} \) increased. For MOCBA, objective 3 is the active one that determines the rate and we can examine that the rate for MOCBA also changes with \( h_{13} \). On the other hand, MOCBA+ and MOCBA* are able to capture the additional contribution of objective 2 to the convergence rate for system 3 and yields a higher rate of decay.

The result in Figure 4.1 also indicates that MOCBA+ and MOCBA* would reduce to MOCBA for problem settings where only one objective is active in determining the convergence rate for each system. For problem settings where more
than one objectives contribute to the convergence rate, MOCBA+ and MOCBA* is expected to yield higher rates of decay of false selection.

**Experiment 3.** In this experiment we examine the effect of sampling correlations between objectives on sample allocations. We reuse the test problem in Experiment 1, for which the means of systems are given in Table 4.1. Assume the sampling correlation coefficient is 0.9. The corresponding sampling allocations convergence rates are shown in Table 4.4.

Table 4.4: Sampling allocations and rates for Experiment 3

<table>
<thead>
<tr>
<th>system</th>
<th>Equal</th>
<th>MOCBA</th>
<th>MOCBA+</th>
<th>MOCBA*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.333</td>
<td>0.414</td>
<td>0.414</td>
<td>0.430</td>
</tr>
<tr>
<td>2</td>
<td>0.333</td>
<td>0.293</td>
<td>0.284</td>
<td>0.289</td>
</tr>
<tr>
<td>3</td>
<td>0.333</td>
<td>0.293</td>
<td>0.302</td>
<td>0.281</td>
</tr>
<tr>
<td><strong>Rate</strong> ($\times 10^{-4}$)</td>
<td>8.33</td>
<td>8.58</td>
<td>8.73</td>
<td>8.75</td>
</tr>
</tbody>
</table>

Similar to the result for Experiment 1, equal allocation yields the lowest convergence rate among all allocation schemes. MOCBA achieves a significantly higher rate compared to equal allocation. MOCBA+ and MOCBA* both return improved convergence rates while MOCBA* slightly outperforms MOCBA+.

It is noted that for this correlated case, MOCBA gives the same sampling allocation as for the independent case. It is attributed to the nature of MOCBA in considering only one active objective to determine the sampling allocation. Correlation therefore does not have any impact on the allocation scheme of MOCBA. On the contrary, MOCBA+ manages to take all active objectives and their correlations into consideration and results in a better result in terms of convergence rate. Being an approximate sampling solution, MOCBA+ again provides a sampling allocation that is very close to the optimal one from MOCBA*.

Another observation is that sampling correlations across means tend to degrade the convergence rate of decay of false selection, compared with the rates with independent sampling. This provides evidence that positive correlation, which is usually introduced by autocorrelation in simulation practices, may make it more difficult in correctly identifying systems.

**Experiment 4.** We now examine the efficacy and efficiency of the proposed sampling laws for problems with a larger number of systems. We extend the test problem in Experiment 1 and randomly generate more systems. System 1 and
3 from Experiment 1 are borrowed and kept non-dominated. 8 more systems that are dominated by the two non-dominated systems are randomly generated. Thus we have a finite set of 10 systems. The variance are assumed universally the same as 25 for each objective of all systems.

For problems with randomly generated systems, their problem structure can significantly differ and the rates of decay may also vary in orders of magnitude. This phenomenon renders cardinal (or absolute) differences of rates infeasible as performance indicators for such cases. Instead, we use the relative improvement of rates in terms of ratios to illustrate the benefit gained from using MOCBA+ and MOCBA*. From theoretical analyses and previous experiments, it becomes evident that in general MOCBA* and MOCBA+ outperform MOCBA, while equal allocation is the most inferior method. For comparing the rates of decay, we use the convergence rate for equal allocation as the base and present the ratio of rates by other sampling allocations over equal allocation. For comparing the computation time, since equal allocation takes no time, we use the computing time for MOCBA as the base and provide ratios of the time required for other allocation schemes over it.

For the randomly generated problems, solving for sampling allocations by the different allocation schemes gives the average results shown in Table 4.5.

<table>
<thead>
<tr>
<th>Equal</th>
<th>MOCBA</th>
<th>MOCBA+</th>
<th>MOCBA*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rate</td>
<td>1.00</td>
<td>3.38</td>
<td>3.62</td>
</tr>
<tr>
<td>CPU Time</td>
<td>-</td>
<td>1.00</td>
<td>0.99</td>
</tr>
</tbody>
</table>

It can be seen from Table 4.5 that on average, MOCBA can achieve a rate of decay that is 3.38 times as high as that achieved by equal allocation, which is significantly higher. This difference is more evident than that of Experiment 1, suggesting that further improvement on rates can be gained for larger size problems. This phenomenon can be explained by the fact that the inferior systems within the finite set tend to be more diversified. These inferior systems in such cases require only very few samples to be disqualified. However, equal allocation ignores the problem structure and allocates more samples than necessary to these inferior systems. MOCBA+, on the other hand, returns rates that are on average 3.66 times as high as that for equal allocation. This should be attributed to the nature of MOCBA+ in considering the effect of all objectives on sample allocation. It is also noted that in this case the MOCBA* yields the highest rates.
that are 3.66 times as high on average, which are slightly higher than that by MOCBA+. This result indicates that MOCBA+ can secure rates of decay that are very close to the optimal value.

In terms of computing time, there is no noticeable difference between the time consumed by MOCBA+ and MOCBA. This is due to the similar iterative structure of the two methods. It is also observed that the MOCBA* approach employing NLP solvers consumes about 99 times more time than MOCBA+ and MOCBA do, while MOCBA+ and MOCBA can return the rates within a few seconds for this 10-system experiment. This result indicates that MOCBA* is very computation-intensive, which becomes more evident for problems with a large number of systems. By contrast, MOCBA+ returns reliable solutions within a more acceptable time frame. The approximate closed-form solution approach turns out to be robustly effective and efficient for larger problems. It is acknowledged from the experiments that for certain problem settings, MOCBA* may give better results than MOCBA+, as shown in Experiment 1. However, the benefit is at a cost of considerably higher computing times. In practice, the trade-off between the solution quality and computing times need to be considered to better cater to practical needs.

It is also worth noting that since the probability of false selection is an exponential function of the rate of decay, the distinguishable gains in rates from using the suggested procedures are further amplified and become more evident when the differences are measured in terms of probabilities.

4.7 Conclusions

In this study, we consider a multi-objective simulation optimization problem where we aim to find an optimal computing budget allocation that can minimize the probability of false selection. By applying an asymptotic analysis to the problem from a large deviations perspective, we re-express the objective to maximize the rate of decay of the probability of false selection.

Our contribution is multi-fold. Firstly, we formulate the problem as a non-linear programming problem explicitly characterizing the correlations between performance measures and show that an asymptotically optimal solution exists. We then propose using a solver to find the asymptotically optimal solution in a general context, which is fit in the context of a small number of systems. Secondly,
we present the optimality conditions for sampling allocations by exploiting the problem structure. These conditions may result in explicit sampling laws when the related rate functions are readily available. Thirdly, in the multivariate normal context in particular, we present an approximate closed-form solution that iteratively searches for the sampling allocation, which significantly lessens the implementation complexity and the computing burden with a solver. Fourthly, we provide exact closed-form solutions to the nested optimization problems under an independent multivariate normal (MVN) assumption and a bivariate normal (BVN) assumption, which can be embedded into the solver approach and the heuristic approaches to enhance searching efficiency. Lastly, the performance of the suggested allocation strategies are demonstrated on a number of experiments, the results of which show significant gains over other allocation schemes in terms of asymptotic rates of decay of the probability of false selection. Although we provide an approximate closed-form allocation, the numerical experiments indicate that the proposed heuristic performs reliably and efficiently in giving allocations very close to those from using NLP solvers.

It is noted that rate functions are assumed existing in a general context and they are usually estimated from sample means and covariances. However, this estimation may only apply to problems where samples are following light-tailed distributions. For problem settings where heavy tails naturally arise, estimation errors of the rate functions may significantly offset the benefit gained from the large deviations analysis (Glynn and Juneja, 2011). From a practical viewpoint, estimation of the unknow rate functions and the impact of the estimates on the performance of the sampling allocation schemes provide promising venues for future research. The work by Glynn and Juneja (2011) considers this problem in a single objective context and it would be meaningful for future studies to extend the study to a more realistic and relevant multi-objective setting.
Chapter 5

Combining Computing Budget Allocation with Multi-objective Optimization via Simulation

5.1 Introduction

Multi-objective simulation optimization often involves a relatively large number of alternative systems, where the number of alternative systems can be finite and large enough, countably infinite, or uncountably infinite (Marler and Arora, 2004). Unlike problems with a finite and small enough number of alternatives, simulation of a large number of systems is computationally impractical, and it is therefore necessary to employ search heuristics to speed up search efficiency. These search heuristics are usually referred to as multi-objective optimization via simulation (OvS) techniques.

In the optimization context, the alternative systems with specific parameter settings are also referred to as solutions, which form the solution space or the parameter space. The terms of solution space and parameter space will be used interchangeably where appropriate in the following text. Objective values of these solutions form the objective space, correspondingly.

The ultimate goal of multi-objective optimization via simulation is to identify those non-dominated systems from the alternatives that are measured by multiple competing objectives via simulation.

Realizing that comparison of systems in terms of multiple measures is differ-
ent in nature from that of a single performance measure, many approaches have been developed to reduce the multi-objective optimization problems to a set of problems with an aggregated objective. These approaches include objective reduction approach, weight-allocation approach and sequential optimization approaches that focus on one objective only at each stage (Deb, 2001; Kim and de Weck, 2006). However, there are approach-specific drawbacks for these reduction techniques, in either not being able to fully capture those desirable non-dominated systems, or failing to detect the non-dominated systems in one optimization run.

The inadequacy with problem reduction techniques leads to the popular incorporation of Pareto-optimal concept into multi-objective optimization, which intrinsically deals with the trade-offs between performance measures equally, thus requires no prior information over the multiple objectives from decision-maker. The non-dominated systems construct the Pareto-optimal set in the solution space, and correspondingly define the Pareto-optimal front in the objective space.

Pareto-based multi-objective optimization techniques have been widely explored, among which the multi-objective evolutionary algorithms (MOEAs) have drawn great attention from researchers. Multi-objective evolutionary algorithms are population-based heuristics, which maintain a population of solutions in each iteration and improve the quality of updated populations during evolution. This population-based characteristic makes it the natural choice of Pareto-based approaches in covering a set of non-dominated solutions in a single optimization run. Many evolutionary algorithms have been proposed (Coello, 1999; Coello et al., 2007; Deb, 2001). These techniques are largely focusing on multi-objective optimization problems with deterministic performance measures and the goal is to provide a good representation of those non-dominated solutions by a finite set of candidates. The convergence metric that measures the difference between selected candidates and true Pareto-optimal solutions and the diversity metric that measures the spread of candidate solutions along the Pareto-optimal front are usually the performance of interest for these Pareto-based heuristics.

When it comes to the context of optimization via simulation (OvS), however, the problem of sampling allocation to candidate solutions arises and needs to be considered. There are often limitations on the available computing budget in practice, especially for expensive simulation of complex systems (Eskandari and Geiger, 2008; Nebro et al., 2008). The trade-off between exploring potentially
better alternatives (also referred to as breadth) and exploiting currently promising systems (also known as depth) exists in determining the sampling allocation. Searching algorithms for optimization via simulation (OvS) is therefore desirable. One approach would be to design new search algorithms that can explicitly balance the trade-off (He et al., 2010). Another approach is to extend current existing search heuristics to the stochastic simulation context by adding sampling allocation intelligence (Fu et al., 2008; Kim and Nelson, 2007). This extension separates exploring new candidates from exploiting current population by assigning the effort to the search heuristic and the sample allocation scheme respectively. The computing budget allocation techniques developed for problems with a finite and small enough number of systems serve as natural candidates for search algorithms that require an elite set either for elitism kept to next generation, or for reproduction of more promising solutions. Multi-objective genetic algorithms incorporating elitism and multi-objective estimation of distribution algorithms fall into these categories and require sampling allocation support to select the non-dominated systems and good systems respectively. In this chapter, we explore the potential of combining computing budget allocation techniques with these two typical family of search algorithms.

5.1.1 Objectives of This Study

This study attempts to adapt existing multi-objective evolutionary algorithms to a stochastic simulation context when there is practical limitation on the computing budget. The integration is implemented by embedding computing budget allocation into the selection process with each iteration (or generation) of the selected search heuristics. This approach may be naive in the sense that it does not explicitly characterize the trade-off between breadth and depth adherent to search algorithms in the stochastic simulation optimization context. However, this approach can be easily implemented without requiring significant changes to existing search algorithms.

The focus of this study is on the incorporation of sampling allocation strategies into multi-objective evolutionary algorithms. This incorporation simply aims to better identify and utilize information of promising solutions from a finite set of solutions in each iteration and does not require significant procedural changes to the original search algorithms. Empirical results are provided to illustrate the potential of this simple approach. It should be noted that designing
heuristic algorithms that can dynamically balance the search breadth and depth requirement is not the focus of the study. Moreover, analytical performance of heuristics combing search and sampling allocation is also beyond our scope and is therefore not dealt with. This may suggest future research directions to further enrich the literature.

5.1.2 Organization

The remaining of this chapter will be organized as below. In section 5.2, we introduce the context of multi-objective evolutionary algorithms, focusing specifically on two families of typical MOEA heuristics, namely, multi-objective genetic algorithms and multi-objective estimation of distribution algorithms. The challenges facing established MOEAs are also presented when these algorithms are extended to a stochastic simulation optimization context, with practical constraints on the simulation budget. The general framework for combining search algorithms with sampling laws are given in Section 5.3. Section 5.4 provides the experiment scheme and the performance indicators of interest. Test problems and numerical results for the combined algorithms are presented to illustrate the potential of employing OCBA in enhancing the search efficiency. Section 5.5 concludes this text while suggesting limitations and extensions of the study.

5.2 Multi-objective Evolutionary Algorithms

Multi-objective evolutionary algorithms have widely been explored and employed for multi-objective optimization problems (Chen et al., 2008b; Deb, 2001; Gregorio et al., 2007; Hart et al., 2005; Tan et al., 2005; Zitzler et al., 2001). In this section, we focus on two typical families of search heuristics that can potentially benefit from integrating with computing budget allocation techniques, when applied to a stochastic optimization via simulation context.

The first type of heuristic algorithms of interest is the class of multi-objective genetic algorithms (MOGAs). Genetic algorithms, in brief, mimic the natural selection and evolution procedure of species, where superior candidates possess a higher probability to survive and generate offspring, while those inferior candidates bears a higher risk of being eliminated. Genetic algorithms borrow this idea and implement this process by assigning fitness to candidate solutions and
using selection operators for reproduction of a new population. The reproduction operator refers to selection of a mating pool of good solutions as parents. Crossover operator is then applied to generating the offspring from two parents from the mating pool. Mutation operator follows to add diversity to the new population of candidates (Deb, 2001). New solutions are searched for directly based on previous population of solutions and thus genetic algorithms are also categorized as instance-based heuristics.

Many studies on multi-objective genetic algorithms focus on designing these operators and tuning related parameters (Deb, 2001; Eskandari and Geiger, 2008). For example, Tan et al. (2001) suggest a dynamic population size to avoid either the premature convergence for a small constant size or prolonged convergence of a too large constant size. Eskandari and Geiger (2008) proposes a new selection operator to better utilize information of Pareto dominance information and niching.

Elitism is found to be an important factor for improving the search efficiency of multi-objective evolutionary algorithms (Zitzler et al., 2000). Elitism simply refers to keeping the best systems of current population to the next generation. Multi-objective genetic algorithms also share this feature. The requirement of elitism provides an opportunity to incorporate computing budget allocation strategies into genetic algorithms under the stochastic simulation context. When there are practical constraints on the simulation budget, the noise with simulation models will have an impact on the elitism accuracy. This noise may mislead the selection of non-dominated systems and thus degrade the quality of the new population of candidates. The optimal computing budget allocation approach can maximize the evidence of a correct selection in each population and thus facilitates elitism identification with higher confidence.

The other family of multi-objective evolutionary algorithms of interest is the class of multi-objective estimation of distribution algorithms (MOEDAs). Instead of generating new candidates directly based on instances of previous solutions, this type of heuristics are model-based algorithms, which construct or update an intermediate probabilistic model of promising solutions from previous population and generate new solutions from this distribution (Bosman and Thierens, 2005, 2002; Jin et al., 2008; Mo et al., 2010; Zhang et al., 2008). These model-based approaches are shown to be able to explicitly characterize the domain knowledge like dependencies between the system parameters, or the variable linkages, for multi-objective (vector) optimization problems, where the
recombination operators of genetic algorithms are facing difficulties (Deb et al., 2006; Jin et al., 2008; Zhang et al., 2008; Zhou et al., 2005). New solutions that are sampled from the model then fully or in part replace the previous population.

The promising solutions from a population are usually beyond those non-dominated solutions and including the good ones to avoid premature local convergence (Bosman and Thierens, 2006; Mo et al., 2010; Zhang et al., 2008). Since statistical information is drawn from the selected solutions to build a posterior probabilistic model, the quality of promising solutions have a direct impact on the quality of newly generated solutions. The quality of solutions is usually measured by the domination count, which is the Pareto rank used in our study (Bosman and Thierens, 2006). An alternative measure is the non-dominated level, where designs with non-dominated level \( l \) are those that are non-dominated if all systems with levels less than \( l \) are not considered (Deb et al., 2002). It is observed that the difference of these two qualification metrics in practice is very small (Bosman and Thierens, 2003a, 2005, 2002, 2006).

A number of studies on multi-objective estimation of distribution algorithms have been reported, usually featuring different levels of complexities of the probabilistic models (Bosman and Thierens, 2005, 2002; Mo et al., 2010; Zhang et al., 2008). Nonetheless, Gaussian distribution are widely employed to model the promising solutions and generate new candidates.

Under a stochastic optimization via simulation context, the correct selection of promising solutions is more vital as the noise may mislead the detection of superior candidates and result in selection of inferior solutions (Bui et al., 2005). The inferiority of solutions, if selected, may lead to undesirable solutions in the next generation and bear the risk of accumulating degradation of solution qualities over generations. Computing budget allocation schemes can fit into this scenario and guarantee a highest confidence in selection quality under a constrained budget.

### 5.2.1 Challenges for Multi-objective Optimization via Simulation

Many studies reported on multi-objective evolutionary algorithms deal with deterministic problems only. These problems frequently feature a continuous solution space, where the Pareto-optimal front may also be continuous and map
to an infinite number of Pareto-optimal solutions. This phenomenon makes it impossible to select the exact Pareto-optimal solutions rather than a finite set of solution estimates that could only be close to the Pareto-optimal front. A good representation of the Pareto-optimal solutions is usually required for this finite set of candidates, where “being good” is usually measured by the convergence metric and the diversity metric. Convergence refers to the closeness of the candidates to the true Pareto-optimal front in the objective space, whereas diversity measures the spread of these candidates along the Pareto-optimal front (Bosman and Thierens, 2006; Deb et al., 2002). The balance between the two performance metrics of interest is usually characterized by the algorithm-specific operators of these search heuristics (Bosman and Thierens, 2003b). It should be noted that it is the diversity along the Pareto-optimal front that is to be preserved rather than the diversity in general. Diversity is not of equal importance as convergence (Bosman and Thierens, 2006). Hence convergence always precedes diversity as the basis of selection and serves as the primary or the only performance indicator of interest (Mo et al., 2010; Nebro et al., 2008; Zhang et al., 2008).

For optimization under a stochastic simulation context, the discrete solution spaces are more common and the performance measures of candidate solutions are dynamic in nature (Andradóttir, 2006; Hong and Nelson, 2009, 2006). Simulation noise has an adverse impact on the selection process and therefore the performance of the search algorithm. To resolve this effect, research interests have focused on combining search algorithms with selection procedures. Studies on embedding ranking and selection procedures to optimization via simulation algorithms have been reported. Boesel et al. (2003) employ the ranking and selection procedure as the last step of simulation optimization to select the best solution. Ranking and selection procedures are applied to neighbourhood search to obtain faster convergence (Pichitlamken and Nelson, 2002, 2003; Pichitlamken et al., 2006). Branke and Schmidt (2004) use sequential sampling to guarantee a pre-specified confidence level of the tournament selection operator. He et al. (2010) propose a cross-entropy algorithm that can explicitly balance the trade-off between sampling breadth of new candidates and sampling depth of current solutions.

Multi-objective evolutionary algorithms in noisy environments have also been studied. Extensive studies on the impact of noise on the performance of multi-objective evolutionary algorithms can be found in Goh et al. (2006), Goh and
Tan (2007) and Tan and Goh (2008). New stochastic or probabilistic dominance concepts and soft selections are usually suggested to reduce the negative effect of noises (Eskandari and Geiger, 2009; Siwik and Natanek, 2008).

The studies on multi-objective evolutionary algorithms in noisy environments do not explicitly consider a limit on the available computing budget for simulation optimization. Simulation models of real-word complex systems tend to be highly time-consuming or computationally expensive, hence the available computing budget is frequently constrained. There are practical needs of embedding simulation budget allocation techniques into evolutionary multi-objective optimization via simulation algorithms. Our study on optimal computing budget allocation provides opportunities to extend existing heuristics to the multi-objective optimization via simulation context, where the available simulation budget is limited and the optimal sampling allocation is concerned.

5.3 Combination of MOEAs and Computing Budget Allocation

In this study, we focus on multi-objective optimization via simulation problems with constraint computing budget. The evolutionary algorithms of interest are MOGAs with elitism and MOEDAs. It is assumed that there is a constraint on the available computing budget for simulating alternatives of a given population.

Specifically, for multi-objective genetic algorithms, we incorporate the computing budget allocation scheme in each iteration to select the Pareto-optimal set with the highest evidence, enhancing the contribution of fitness assignment and elitism to this family of evolutionary algorithms. For multi-objective estimation of distribution algorithms, the sampling allocation laws are employed to select a subset of good solutions with the highest confidence, so that more promising solutions can be generated from the sample distribution constructed on these good systems. In the following text, we use the terms of MOCBA and MOCBA-subset to refer to the family of multi-objective optimal computing budget allocation strategies to select the non-dominated systems and the strategy to select a subset of good systems from a finite set, respectively.
5.3.1 Multi-objective Genetic Algorithms with Optimal Computing Budget Allocation

The general framework for MOGAs combined with MOCBA are shown below. This framework applies to general instances of multi-objective genetic algorithms that employ elitism.

1. Specify necessary parameter settings for the given problem,

2. Initialize a population of $n$ points which are randomly sampled from the solution space,

3. While not terminated Do another iteration:
   
   (a) Apply the MOCBA family of sampling laws and determine the non-dominated systems,

   (b) Compute fitness values for systems in this population,

   (c) Find those elite systems by a specified fitness value threshold and keep them till the next generation, let the size of elite solutions be $n_e$,

   (d) Generate $n - n_e$ systems to replace those non-elite systems, using the selection, crossover and mutation operators.

4. Return the non-dominated solutions.

A flowchart for the MOGA + MOCBA framework is shown in Figure 5.1.

There are many variations of MOGAs reported in the literature, focusing either on designing more efficient operators or on optimizing running parameters like the population size and the crossover and mutation probabilities.

Fitness assignment is vital for MOGAs, which provides the basis for the selection operator. In the stochastic optimization via simulation context, since the ultimate goal is to select those non-dominated solutions, the non-dominated probability is the natural choice for the fitness assigned to each solution (Lee et al., 2009). The MOCBA family of sampling law for finding the non-dominated systems can play an important role in fitness assignment, for in nature it maximizes the non-dominated probability for true Pareto systems and minimize this probability for those inferior systems. This fitness can be easily calculated under a normal distribution assumption.
In this study, we employ the MOGA described in Deb (2001) to demonstrate the idea of embedding sampling allocation into search algorithms. For each solution that is to be replaced in each generation, we use the tournament selection method to select its parents. That is, we randomly select 2 solutions and return the one with a higher fitness value as one parent. The other parent is selected similarly. This simple method can guarantee that solutions with higher fitness values would have higher probabilities to generate off-springs.

Reproduction of solutions involves the crossover operator and the mutation operator. In this study, crossover is done using the blend-\(\alpha\) method with \(\alpha = 0.5\). Assume in generation \(t\), the to-be generated solution is \(x^{(t+1)}\) and its two parents are \(x^{(1,t)}\) and \(x^{(2,t)}\) respectively. Then the \(i_{th}\) gene of \(x^{(t+1)}\), \(x^{(t+1)}_i = (1-\gamma_i)x^{(1,t)}_i + \gamma_i x^{(2,t)}_i\), where \(\gamma_i = (1 + 2\alpha)u_i - \alpha\) and \(u_i\) is a random number from the standard uniform distribution. Crossover can be done with an optional probability \(P_c\) for crossover and in this study we set it as 1. We use the real-coding scheme here and the \(i_{th}\) gene of a solution is its parameter value on the \(i_{th}\) dimension in the solution space. Mutation for a solution occurs with a probability \(P_m\) where a randomly selected gene is replaced by a random value sampled from its range.
5.3.2 Multi-objective Estimation of Distribution Algorithms with Optimal Computing Budget Allocation

A general framework for combining MOEDAs with MOCBA-subset is provided as below. This framework is similar to that presented in Bosman and Thierens (2006) but extends to the stochastic optimization via simulation context.

1. Specify necessary parameter settings for the given problem,
2. Initialize a population of \( n \) points which are randomly sampled from the solution space,
3. While not terminated Do another iteration:
   (a) Apply the MOCBA-subset sampling law, compute the Pareto rank and determine the promising subset of solutions with ranks within a threshold limit,
   (b) Compute elitism metrics for systems in this population,
   (c) Find those elite systems by a specified elitism threshold and keep them till the next generation, let the size of elite solutions be \( n_e \),
   (d) Establish probabilistic distributions for the promising subset in the solution space,
   (e) Sample \( n - n_e \) points from the distribution to replace those non-elite systems.
4. Clean up and return the non-dominated solutions.

A flowchart for the MOEDA + MOCBA-subset framework is shown in Figure 5.2.

The promising subset in each iteration may be clustered to better model the spread of points and enable parallel search (Bosman and Thierens, 2006). The probabilistic distributions are then established for each cluster. In the last step, a clean-up is needed to find those non-dominated systems (Boesel et al., 2003).

In this study, we model the spread of promising points using a multi-variate normal distribution \( \text{MVN}(\mathbf{\mu}, \mathbf{\Sigma}) \) in the solution space. New solutions are sampled from this distribution to replace those inferior ones. The elitism metric, similar to the fitness value, are measured in terms of the non-dominated probability.
5.3.3 Discussions on the Convergence of the Combined Algorithms

Convergence properties for the combination of multi-objective evolutionary algorithms and sampling allocation algorithms involves the convergence of the search algorithms and the consistency of the optimal allocation estimators respectively.

The asymptotic convergence of many evolutionary algorithms has been reported for both genetic algorithms (Fogel, 1994; Lozano et al., 1999) and estimation of distribution algorithms (Zhang and Muhlenbein, 2004). A general outline to examine the convergence property is to model the search process, i.e., the probability distribution of the evolved population, as a Markovian process. The Markov chain is proven to be weakly and strongly ergodic and therefore the probability distribution will converge asymptotically to a distribution from which the optimal solutions can be sampled with a probability of 1.

For the optimal allocation estimator, consistency measures the convergence of the estimated sampling allocation to the true values, since estimation errors may be significant to misguide the allocation. The frequent argument for this consistency is that, when each systems is allocated a positive proportion of the total
simulation budget, the estimated allocation will converge asymptotically to the true optimal values. The general proof outline employs the law of large numbers that sample means will converge to the true means when the total computing budget is large. This convergence dictates the consistency of the probability distributions for each system and thereby the consistency of the estimated rate function of the decaying probability and the estimated allocation (Glynn and Juneja, 2004).

The search algorithms in this study are basic instances of the evolutionary algorithms and the convergence properties are well-established. For the sampling allocation algorithm, the assignment of computing budget for each system is also positive. Then we may assume with confidence the convergence and consistency and verify this assumption using the following numerical experiments.

5.4 Numerical Experiments

In this section, numerical experiments for search algorithms integrated with multi-objective optimal computing budget allocation are implemented to demonstrate the potential benefit gained under a stochastic simulation context.

5.4.1 The Experiments Scheme

Our aim is to illustrate the potential of embedding sampling allocation techniques into selection of desired solutions in each iteration of the heuristics of interest.

We consider the combination of sampling allocation with MOGA and MOEDA respectively. The general framework is employed to simply extend the search algorithms from a deterministic context to a stochastic context. Performance indicators and test problems for the combined algorithm are provided. Those benchmark problems, also known as test functions, usually feature certain difficulties for the search algorithm to search for the non-dominated solutions (Huband et al., 2005; Okabe et al., 2004).

Most test problems have a continuous solution space and also a continuous Pareto-optimal front, whereas in optimization via simulation, a solution space of
discrete candidates are more common. The benchmark problems that are commonly adopted in the literature are taken as the first choice and are discretized accordingly.

### 5.4.2 Performance Metrics

The solutions of interest are the subset of non-dominated systems found in the final population of the search algorithms. We call this subset the estimated set and denote it as $S$. Let $P$ denote the Pareto-optimal set.

Performance indicators are used to measure the quality of the estimated set. Distance metrics are commonly used for such indicators. We use the definition by Bosman and Thierens (2006) for our experiments. For Pareto-optimality is defined in the objective space, the distance between two solutions $x_i$ and $x_j$ is defined to be the Euclidean distance between their objective values $h_i$ and $h_j$, or mathematically

$$d(x_i, x_j) = \| h_i - h_j \|^2.$$

(5.1)

An alternative to $d(x_i, x_j)$ is to use the Euclidean distance scaled to the range in each objective (Deb and Jain, 2002). We now define the distance between a solution $x_i$ and the set $P$ as the minimum distance between $x_i$ and any solution $x_j$ in $P$. Then the distance between the estimated set $S$ and the Pareto set $P$ in the objective space can be defined by the average minimum distance between each solution in $S$ and $P$, or

$$D_{\text{convergence}}(S) = \frac{1}{|S|} \sum_{x_i \in S} \min_{x_j \in P} d(x_i, x_j).$$

(5.2)

This distance measures the convergence of the estimated set towards the Pareto-optimal set and a smaller value is favourable. The convergence metric can also be normalized within $[0, 1]$ by its maximum value for all generations (Deb and Jain, 2002).

The incorporation of computing budget allocation should improve the selection quality of desirable systems and thus could potentially result in a better convergence. It is noted that when a solution contained in $S$ is Pareto-optimal, its distance the Pareto-optimal set $P$ is 0. Therefore convergence metric only implicitly features the coverage of Pareto-optimal solutions for the estimated set $S$. As a secondary indicator, we use a coverage metric to measure the number
of non-dominated trade-offs along the Pareto-optimal front \( \mathcal{F} \) that is contained in the estimated set \( \mathcal{S} \) in the objective space for all iterations.

\[
\mathcal{D}_{\text{coverage}}(\mathcal{S}) = |\mathcal{S} \cap \mathcal{P}|_{\mathcal{F}}. \tag{5.3}
\]

It should be noted that the coverage metric \( \mathcal{D}_{\text{coverage}} \) is not equivalent to the diversity metric measuring the spread of the estimated solutions along the Pareto-optimal front for continuous multi-objective optimization problems.

### 5.4.3 Test Problems

Benchmark problems are usually used to test the performance of optimization algorithms. These problems usually feature different levels of difficulties to find the diverse Pareto-optimal solutions (Deb, 2001). Multi-modality, non-convexity and discreteness of the test problems are among those well-known characteristics that contribute to the difficulty. Specifically for optimization via simulation, the problems are usually discrete in nature and hence reveal underlying difficulties for optimization algorithms. In this study, we demonstrate the performance of the proposed procedures for two typical test problems that characterize multi-modality and non-convexity respectively.

We use the following test problems for the combined algorithms.

**Test problem 1.** This test problem is a variation of the test problem SCH (Deb et al., 2002) and it has the following objective functions,

\[
f_1(\mathbf{x}) = (x_1 - a_1)^2 + (x_2 - b_1)^2, \tag{5.4}
\]

\[
f_2(\mathbf{x}) = (x_1 - a_2)^2 + (x_2 - b_2)^2. \tag{5.5}
\]

The solution space is two-dimensional and its range can be arbitrary. In this study, the solution space is set as \([-5, 5]\) and is discretized at a 0.1 interval on each dimension to better fit the simulation optimization context. Hence there are in total \(101^2 = 10201\) systems in the solution space. We set \(a_1 = 0, a_2 = 1, b_1 = 0, b_2 = 1\). The Pareto-optimal set for such a discrete problem is \(\{(x_1, x_2) \mid 0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1, |x_2 - x_1| \leq 0.1\}\). While there are 31 non-dominated systems in the solution space, they are mapped to only 21 distinct trade-offs along the
Pareto-optimal front in the objective space. Figure 5.3 provides an illustration of the objective space and Pareto front.

![Objective Space and Pareto Front](image)

Figure 5.3: Objective space and Pareto front for Test Problem 1

Assume that simulation samples follow i.i.d normal distributions with mean 0 and standard deviation defined by the coefficient of variation, or the noise level.

**Test problem 2.** This test problem is also known as FON (Deb et al., 2002) and it has the following objective functions.

\[
\begin{align*}
  f_1(x) &= 1 - \exp \left( \sum_{i=1}^{p} \left( x_i - \frac{1}{\sqrt{3}} \right)^2 \right) \\
  f_2(x) &= 1 - \exp \left( \sum_{i=1}^{p} \left( x_i + \frac{1}{\sqrt{3}} \right)^2 \right)
\end{align*}
\]

The dimension of the solution space \( p \) can be arbitrary. For a continuous version of the problem where the decision variables take real values, the Pareto-optimal set \( P \) is

\[
P = \{(x_1, x_2, \ldots, x_p) \mid x_1 = \ldots x_p \in [-1/\sqrt{p}, 1/\sqrt{p}]\}
\]

The solution space for this test problem is also discretized at a 0.1 interval on each dimension. The corresponding Pareto-optimal set can be defined as \( \{(x_1, x_2, \ldots, x_p) \mid \max_{1 \leq p} x_i - \min_{1 \leq p} x_i \leq 0.1\} \). There are 85 non-dominated systems in the solution space, mapped to 37 unique trade-offs along the Pareto-optimal
front in the objective space. Figure 5.4 provides an illustration of the objective space and Pareto front.

![Figure 5.4: Objective space and Pareto front for Test Problem 2](image)

We assume $p = 3$, and the solution space is set to be $[-2, 2]^3$. Thus there are in total $4^3 = 68921$ systems in the solution space. Variances (or noises) are added to make this problem stochastic, which are assumed following normal distributions with mean 0 and standard deviation defined by the coefficient of variation.

### 5.4.4 Results

We integrate the MOGA described above with equal allocation and MOCBA family of sample laws respectively. For the tested MOGA, we implement MOCBA+, whereas for the tested MOEDA, we implement MOCBA-subset.

Now we present the numerical experiments for the MOEAs with sampling allocations with respect to the aforementioned test problems.

**Experiment 1.** We first test the performance of the combination of MOGA and MOCBA. The running parameters of MOGAs for test problem 1 are given in Table 5.1.

For the experiment, we progressively increase the simulation budget as the population would be more dense after reproduction.
Table 5.1: Running settings of MOGAs for Test Problem 1

<table>
<thead>
<tr>
<th>Search settings</th>
<th>Value</th>
<th>MOCBA settings</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimension</td>
<td>2</td>
<td>Noise level</td>
<td>0.1</td>
</tr>
<tr>
<td>Population size</td>
<td>30</td>
<td>Initial Budget</td>
<td>2000</td>
</tr>
<tr>
<td>Elitism threshold</td>
<td>0.8</td>
<td>Budget incremental</td>
<td>400</td>
</tr>
<tr>
<td>Generations</td>
<td>10</td>
<td>Initial allocation</td>
<td>20</td>
</tr>
<tr>
<td>Instances</td>
<td>500</td>
<td>Sequential allocation</td>
<td>200</td>
</tr>
</tbody>
</table>

We run the experiment for 500 times and compute the average performance metrics. The convergence measure of the MOGAs is shown in Figure 5.5.

![Figure 5.5: Convergence measures of MOGAs for Test Problem 1](image)

It can be seen from Figure 5.5 that the MOCBA approaches embedded into the MOGA facilitate search efficiency by finding solutions with smaller distance to the Pareto-optimal front. This improvement is more evident at the first generations, for the population is more diversified at the first stages. This allows MOCBA to fully explore the problem structure, assign fitness more reliably and eliminate those inferiors solutions more efficiently than Equal allocation does, resulting in more promising offspring in subsequent generations.

Figure 5.6 provides the coverage measure for this experiment.

It can be seen from Figure 5.6 that on average more solutions along the Pareto front are found when integrating MOGA with MOCBA approaches. It can be explained by the fact that MOCBA manages to yield more accurate fitness assignment, which consequently leads to better elitism and reproduction by those more promising solutions.
The performance metrics illustrate the trend that OCBA approaches can enhance search efficiency by exploring systems closer to the Pareto-optimal Front and exploiting more systems spread along the Pareto front. These results confirm that the MOCBA optimizes sampling allocations such that the non-dominated solutions are easier to distinguish with higher fitness values. Equal allocation does not exploit the problem structure and therefore utilize the total computing budget less efficiently.

**Experiment 2.** Table 5.2 presents the running parameters of MOGAs for test problem 2 (FON).

<table>
<thead>
<tr>
<th>Search settings</th>
<th>Value</th>
<th>MOCBA settings</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimension</td>
<td>3</td>
<td>Noise level</td>
<td>0.03</td>
</tr>
<tr>
<td>Population size</td>
<td>40</td>
<td>Initial Budget</td>
<td>4000</td>
</tr>
<tr>
<td>Elitism threshold</td>
<td>0.8</td>
<td>Budget incremental</td>
<td>500</td>
</tr>
<tr>
<td>Generations</td>
<td>10</td>
<td>Initial allocation</td>
<td>20</td>
</tr>
<tr>
<td>Instances</td>
<td>500</td>
<td>Sequential allocation</td>
<td>200</td>
</tr>
</tbody>
</table>

Similarly, we run the experiment for 500 times and compute the average performance metrics. Figure 5.7 shows the convergence measure of the MOGAs when integrated with MOCBA and equal allocation.

Figure 5.8 gives the convergence measure of the MOGAs.
Figure 5.7: Convergence measures of MOGAs for Test Problem 2

Figure 5.8: Coverage measures of MOGAs for Test Problem 2
Again the results verify our previous findings that the MOCBA procedures facilitate a fast convergence speed for MOGAs by obtaining solutions closer to the Pareto-optimal front. More trade-offs along the Pareto-optimal front are identified are found when MOCBA approaches are embedded in MOGAs. This result is consistent with that for Experiment 1, showing the same trend that the MOCBA procedures have the great potential of enhancing search efficiency when integrated with MOGAs.

**Experiment 3.** In this experiment, we examine the performance MOEDAs combined with the MOCBA-subset allocation scheme. The running parameters for test problem 1 are provided in Table 5.3.

<table>
<thead>
<tr>
<th>Search settings</th>
<th>Value</th>
<th>MOCBA settings</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimension</td>
<td>2</td>
<td>Noise level</td>
<td>0.1</td>
</tr>
<tr>
<td>Population size</td>
<td>30</td>
<td>Initial Budget</td>
<td>2000</td>
</tr>
<tr>
<td>Elitism threshold</td>
<td>0.8</td>
<td>Budget incremental</td>
<td>400</td>
</tr>
<tr>
<td>Pareto rank threshold</td>
<td>1</td>
<td>Initial allocation</td>
<td>20</td>
</tr>
<tr>
<td>Generations</td>
<td>10</td>
<td>Sequential allocation</td>
<td>200</td>
</tr>
</tbody>
</table>

We run 500 instances of the experiment and calculate the average performance metrics. Figure 5.9 and Figure 5.10 show the convergence measures and coverage measures respectively.

![Figure 5.9: Convergence measures of MOEDAs for Test Problem 1](image)

It is evident from Figure 5.9 that when integrated with sampling allocation techniques, the MOEDA can find solutions that are significantly closer to the Pareto-
optimal front. The improvement on the convergence speed is notable during all generations. This may suggest that the model-based algorithm fit this problem well in exploiting the problem structure using normally distributed variables. The observation on the coverage measures also justify the efficacy of MOEDA for this test problem in that almost all the Pareto-optimal trade-offs are detected in the final population, which is around 19 out of a total of 21 unique solutions. This finding implies that the probabilistic models built from a subset of solutions would be critical for the efficacy and efficiency of the model-based algorithms. Specifically for this test problem, a subset of good systems with a higher confidence yields more solutions spread along the Pareto-optimal front, thereby contributing to a faster convergence speed and a more comprehensive coverage of the desirable trade-offs.

**Experiment 4.** Table 5.4 lists the running parameters for the combined MOEDAs for test problem 2.

Table 5.4: Running settings of MOEDAs for Test Problem 2

<table>
<thead>
<tr>
<th>Search settings</th>
<th>Value</th>
<th>MOCBA settings</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimension</td>
<td>3</td>
<td>Noise level</td>
<td>0.03</td>
</tr>
<tr>
<td>Population size</td>
<td>40</td>
<td>Initial Budget</td>
<td>4000</td>
</tr>
<tr>
<td>Elitism threshold</td>
<td>0.8</td>
<td>Budget incremental</td>
<td>500</td>
</tr>
<tr>
<td>Pareto rank threshold</td>
<td>1</td>
<td>Initial allocation</td>
<td>20</td>
</tr>
<tr>
<td>Generations</td>
<td>10</td>
<td>Sequential allocation</td>
<td>200</td>
</tr>
</tbody>
</table>
We run the experiment 500 times and compute the average performance metrics, as given in Figure 5.11 and Figure 5.12 respectively.

![Figure 5.11: Convergence measures of MOEDAs for Experiment 2](image1)

![Figure 5.12: Coverage measures of MOEDAs for Test Problem 2](image2)

We can see from Figure 5.11 that the non-dominated solution estimate within each population is getting closer to the Pareto-optimal front. This characteristic is largely due to the search efficiency of MOEDA. When sampling allocation techniques are integrated, OCBA approaches help to achieve a shorter distance between the observed non-dominated trade-off to the Pareto front, especially at the first generations when the population is more diversified. This suggests that MOCBA-subset secures a more promising search direction (or distribution) by identifying the good enough subsets and establish probabilistic models pro-
gressively. The improved probabilistic models also contribute to more samples along the Pareto-optimal front, as indicated in Figure 5.12.

It is worth noting that running parameters for MOEAs are vital in dictating the performances of evolutionary algorithms. Tuning these parameters and finding the optimal settings may also be important in designing and implementing these algorithms (Deb, 2001; Eskandari and Geiger, 2008). However, in this study, our focus is to illustrate the potential of embedding sampling laws into search to find better solutions in a stochastic optimization via simulation context. It is therefore natural to assume the search heuristics are given, which provides a fair base to compare different sampling laws.

5.5 Conclusions

In this study, we demonstrate the potential of combining computing budget allocation techniques with evolutionary algorithms for multi-objective optimization via simulation problems. This straightforward combination does not require significant changes to the procedures developed for the deterministic case, and may serve as a technique of choice when dealing with stochastic simulation optimization problems with a constrained simulation budget. Numerical results illustrate that the computing budget allocation techniques can facilitate detection of promising solutions either for elitism preservation or for the updates of sampling distributions.

It is acknowledged that the combination presented in this study does not explicitly characterize the balance between sampling breadth and sampling depth. Designing algorithms featuring such a dynamic balance is an open research problem and provide the possibility for future research directions.

The proposed combined algorithms provides a general framework for extending multi-objective search algorithms to a optimization via simulation context. To assess the performance of the proposed algorithms, two typical benchmark problems are employed that characterize different level of search difficulties. It would be interesting to customize and apply the procedures to real-word discrete-event simulation models for future studies.

There are also concerns regarding the combination of simulation budget allocation with optimization via simulation algorithms. For example, the previously
visited solutions are possibly to be revisited in the current iteration. Reuse of the past information would be desirable. Most sampling allocation techniques assume no prior information, rendering them inapplicable to problems where past information of alternatives are retained (Bosman, 2009; Kim and Nelson, 2007). Addressing these issues may also be of interest for future studies.
Chapter 6

Conclusions

6.1 Conclusions of the Study

This study explores the sampling allocation strategy for multi-objective simulation optimization problems. In view of the practical needs within a multi-objective simulation optimization context, the desired systems are defined either as a good subset containing promising systems for reproduction, or as the non-dominated systems. The goal of the study is to find an optimal computing budget allocation that can maximize the evidence of correct selection. This evidence can either be expressed in a probability term or indirectly in terms of the rate of decay from a large deviations perspective.

Specifically for the subset selection problem, we employ the probability of correct (or false) selection as an evidence and aim to find a sampling allocation that can maximize a lower bound estimate of this probability. Asymptotic analyses are applied to establish approximate closed-form sampling allocation strategies. Numerical experiments illustrate that the proposed allocation schemes can generally obtain a significantly higher empirical probability of correct selection than the compared allocation does. In other words, to maintain the same pre-specified confidence level of correct selection, our rules can make substantial savings of computing budget than the compared alternative allocations. This observation provides clear evidence that the proposed allocation rules can utilize the available samples more efficiently, without significant compromise in computing the allocation. A plausible explanation of such findings is that the proposed OCBA rule can learn the sample information during the sequential allocation procedure and benefit from intelligently adjusting the allocation scheme with updated in-
formation. This study has taken a major step towards allocating limited computing resource in an optimal manner for multi-objective subset selection problems and has provided implementation guidelines for practitioners. Another contribution of this study is that it can enhance the search efficiency when integrated with multi-objective search algorithms, for which an elite set is needed in the intermediate iterations to reproduce promising solutions. The proposed methodology provides a powerful technique for generating a set of seeding solutions for genetic algorithms or evolutionary algorithms for problems with multiple performance measures.

This study also examines the Pareto set selection problem from a large deviations perspective. A robust mathematical framework is employed and the problem is formulated into an non-linear programming problem with nested optimization problems, targeting a sampling allocation that can maximize the rate of decay of the probability of false selection. The optimal solution to the formulated NLP problem can be secured from using solvers in a general context. Optimality conditions to the NLP formulation are also presented by exploiting the problem structure. For problems with a multivariate normal assumption in particular, an approximate closed-form solution is suggested by elaborating distribution-specific characteristics in the derivation. This approximate solution can serve as an alternative to the solver approach while providing non-compromising solutions efficiently and reliably. Moreover, closed-form solutions are provided to the nested optimization problems for the NLP formulation, which can further lessen the computing time when embedded into the solver approach or the approximate heuristic approach. Numerical results also justify the advantage of the proposed allocation schemes. The solutions from using a solver (MOCBA*) and the approximate MOCBA+ approach can significantly outperform other allocation schemes for a set of problems with multiple competing objectives. This is probably attributed to the fact that all the objectives are taken into consideration for comparison while using large deviations theory, whereas the MOCBA approach in Lee et al. (2010c) considers only the most dominating objective and thus loses certain information essential for identifying systems.

Another contribution is that we explicitly characterize the sampling correlations between performance measure by using large deviations. This correlation is usually dissolved by the Bonferroni bounds of probabilities and is therefore implicitly considered. By exploiting the rates of decay of the probability of false
selection from a large deviations perspective, sampling correlations appear in related rate terms and are therefore explicitly characterized in the problem formation and consequently, in the solution. By investigating sampling allocations using a mathematically more robust framework, this study is significant in that the commonly accepted assumption of independent sampling between objectives can be ruled out in theory and application. Numerical tests indicate that allocation strategies incorporating sampling allocations manage to guarantee a faster convergence rate, compared with those sampling rules that do not consider the effect of correlation on the sampling allocation.

The findings have also provided valuable insight into the interpretation of the allocation rules in terms of the rate of decay of the probability of false selection that is targeted to minimize. The underlying intelligence adherent to the allocation strategy can therefore be better explained. Moreover, the proposed approach may have great potential in application since it does not require any interaction from the decision maker to find the desired systems.

6.2 Discussions and Future Research

Being an exploratory study, this work makes several assumptions, which may not always hold in practice. For example, constraint measures are not considered for the targeted problem settings, which may restrict the application of the allocation scheme to some extent. Although the duality between constrained optimization and multi-objective optimization is well known, research work should take into consideration the deficiency of such dualities in term of problem size scaling and non-equivalence (Deb, 2001). In the aspect of generality of problem settings, further study is needed to incorporate constraints on system performances into modelling. To achieve this, the definition of evidence of correct selection should be systematically explored, due to the additional complexity introduced by the constraint measures in detecting feasibility.

The problem settings assume that all performance measures are following a certain sampling distribution. There are often cases that the performances of interest include both discrete and continuous ones and they are not necessarily following a joint distribution. To extend this study to more general cases, estimation of the sampling distribution is critical. Machine learning techniques may be employed to explore the problem structure. For example, feature selec-
tion can be applied to find those relevant measures and cluster them into groups. Pattern recognition techniques can then be used to identify the pattern or distributions within group and the correlations among groups. As a promising venue for further research, it would be interesting to extend the proposed approaches in this study to a more general context.

This study assumes that no systems are having objectives equal to that of other systems, since noises make it impossible to distinguish these systems from simulation output. Future studies may incorporate the indifference-zone (IZ) concept into a new problem formation to resolve this issue. The indifference zone parameter may be determined by the minimum detectable difference for the finite set of systems.

Another fundamental assumption is that the systems are ranked by means only. Variance may also be of interest for decision making under uncertainty. While our analysis being asymptotic in nature partially address this concern, there are also instances where a decision maker will prefer a balance between the projected mean and the variability from a finite time perspective. Ranking of systems considering both mean and variance information are reported for the indifference-zone ranking and selection problems (Batur and Choobineh, 2010a,b), and it would be interesting to incorporate this concept into multi-objective simulation optimization.

From a methodological perspective, it is noted that the suggested sampling allocation schemes are derived based on asymptotic analyses, or the a large number of computing budget, while the motivation of the sampling allocation comes from a limited computing budget context. For finite time analyses, the probability of correct selection is often guaranteed by very conservative bounds. Gradient-based heuristics are usually then developed to estimate a sampling allocation. For example, the indifference-zone approach requires a problem-specific parameter delta, or the minimum detectable difference, to derive the allocation procedures. Such procedures tend not to be robust and cannot provide insights or interpretation of the sampling scheme. On the other hand, the asymptotic analysis allows for a large deviations perspective to look into the decaying property of the probability of false selection. The optimal rate of decay can then be achieved. The asymptotic optimality separates the impact of finite-time factors and gives the trend of the sampling allocation when the computing budget is increased. This optimality also provides insights and interpretations of the sampling scheme. It is an intuitive philosophical testing to compare the
rules from asymptotic analyses with those heuristics and the suggested procedures prove to be both robust and efficient in finite-time scenarios. Empirical results of finite-time simulation optimization experiments justify this testing and verify the trend to the optimal rate. It is noted that for the suggested procedures to achieve the expected performance in carrying out practical experiments, the general guideline for choosing the proper parameters applies. If the budget is even not sufficient enough to initialize the samples with equal replicates, the suggested procedures would terminate prematurely and degrade to equal allocation in such cases.

Although we provide a general solution framework for sampling allocation, we do not give explicit sampling laws for general cases. The explicit sampling laws presented in this study apply to problems under a multi-variate assumption, which is a common practice in the literature. For problems with samples following other distributions, the proposed sampling rules for the MVN case need to be carefully adapted to the case by using batch means or other methodologies (Hart et al., 2005). It would also be interesting to examine explicit sampling laws for problems with other particular distributions or general distributions. The main challenge is to estimate the distribution pattern or the rate functions.

It is acknowledged that sampling correlations between systems are not taken into account due to the complexity of evaluating probabilities with highly correlated terms. Based on the simulation results for multi-objective objective ranking and selection problems with correlated objectives, we speculate that sampling correlations between individual systems would also have significant impact on the determination of the computing budget allocation. Thus future studies should incorporate this type of sampling correlation into modelling. The computing budget allocation rules applicable to more general contexts can then be provided.
Bibliography


113


Nelson, B. L., Swann, J., Goldsman, D., Song, W., 2001. Simple procedures for selecting the best simulated system when the number of alternatives is large. Operations Research 49 (6), 950–963.


