RANKING AND SELECTION PROCEDURES FOR FEASIBILITY DETERMINATION

By

Xiufeng Shao

A dissertation submitted in partial fulfillment of the

requirements for the degree of

Doctor of Philosophy

(Industrial and Systems Engineering)

at the

UNIVERSITY OF WISCONSIN – MADISON

2017

Date of final oral examination: August 4, 2017

The dissertation is approved by the following members of the Final Oral Committee:

Professor Leyuan Shi, Professor, Industrial Engineering

Professor Jingshan Li, Professor, Industrial Engineering

Professor Kaibo Liu, Assistant Professor, Industrial Engineering

Professor Zhengjun Zhang, Professor, Statistics

To my parents, Baoqun Shao and Xingui Wang

Abstract

The feasibility determination problem involves deciding whether a design meets certain criteria based on a performance measure estimated through Monte Carlo simulation. It typically comes into play when the decision-maker faces the problem of selecting a subset of designs according to some prescribed standards. Feasibility determination of a finite set of alternative designs is a special case of the classical multiple comparisons with a control problem, in the sense that the control that we compare with here is modeled as known.

Ranking and selection procedure focuses on intelligently allocating the total simulation budget to each design to better support the decisions when comparing a set of alternative designs. It is an issue of critical importance when the decision-maker faces a limited simulation budget. The ranking and selection procedure for feasibility determination provides the potential for significant simulation budget reduction while obtaining decisions with greater accuracy.

In this thesis, we first investigate the performance of current asymptotically optimal allocation methods. We prove that under certain conditions, current methods perform no better than the naive equal allocation method. To achieve better performance when the total simulation budget is limited, we propose a new allocation method that is based on a finite simulation budget perspective. We prove that the simulation budget allocated by our method converges to the optimal value. We also provide a proof that our method always performs no worse than current asymptotically optimal allocation methods. Numerical experiments of three illustrative examples, a facility-sizing problem, and

an emergency department setup problem are conducted to demonstrate the effectiveness of our method.

The majority of the research in ranking and selection formulate the budget allocation problem as a static optimization problem. We demonstrate the inadequacy of this formulation. In Bayesian setting, we formulate the budget allocation as a stochastic control problem and provide a one-step lookahead policy. We also illustrate the stochastic control implementation of previous proposed finite budget allocation method. Numerical examples are provided to demonstrate the differences between static and dynamic methods.

In simulation practice, different designs with close parameters often have similar performances. In this situation, we propose a new allocation method that takes the relationships between different designs into consideration. We use the kriging metamodel to capture the inter-design relationships and incorporate the information obtained from kriging into our allocation procedure based on the Bayesian framework. Computational results demonstrate the efficacy of this methodology.

Acknowledgements

I would like to express my sincere gratitude and thanks to my advisor Professor Leyuan Shi. Without her, I can never have this opportunity to join ISyE Dept. at UW-Madison. Her guidance, counsel and encouragement have always propelled me to be a better researcher.

I would also like to express my gratitude to Professor Jingshan Li and Zhengjun Zhang for their valuable suggestions and friendly encouragements. I am grateful to Professor Kaibo Liu for serving on my final examination committee.

I would thank Zhuang Wu and Wei Zheng for their friendship and invaluable help in my life. I would also thank Zhongshun Shi and Yijie Peng for their collaborative work.

During my PhD study, I am lucky to have my colleagues Chao Ma, Hongbo Meng, Jinglu Wang, Siyang Gao, Xiaolei Xie, Cong Zhao and Xiang Zhong. They are all friends to me and we have had a great time together, which has made my stay in Madison enjoyable.

Lastly, I would thank my parents for their unconditional love and deep caring, which always give me strength facing challenges in my life. The dissertation is lovingly dedicated to them.

Table of Contents

List of Tables

List of Figures

Chapter 1

Introduction

1.1 Overview and Research Motivation

Simulation is widely applied to the design and analysis of complex discrete-event systems such as health care systems, telecommunication systems, financial forecasting, and supply chain management. One common task of simulation is to aid in identifying the optimal system design from among a finite set of alternative designs. However, in real life, such a decision can be hard to make for various reasons.

One possible reason is that a decision-maker often has to face different objectives and constraints. In many cases, it is difficult to include all objectives and constraints to form one single criterion by which the decision-maker can compare the performance of different designs. For instance, suppose we want to use simulation to find an optimal ordering policy that has the lowest expected cost in inventory management. For complex inventory models, we can approximate the optimal policy by using threshold policies. In general, the more thresholds we set, the better we can approximate the optimal policy. However, the increasing number of thresholds in a policy clearly makes it harder to implement in practice. Therefore, we take at least two factors into consideration: the expected cost and the complexity of ordering policies (Yan et al. [88]).

Another possible reason is that the design space can be extremely large, which renders the total simulation cost prohibitively high. The simulation of complex systems allows for free configuration of a great number of parameters, which could easily result in a vast design space. For instance, the design of chip multiprocessors requires tuning a wide range of customizable parameters that are mainly related to microarchitecture, memory hierarchy, and interconnection network. The design space is so large that a full exploration is infeasible (Palermo et al. [67]).

To tackle these situations, feasibility determination (FD) is sometimes preferred. In FD, the designs have performance measures that must be estimated using Monte Carlo simulation, and thresholds for each performance measure are given. In this thesis, without loss of generality we define a design as feasible if all its performance measures are under corresponding thresholds. For multi-objective problems, we can deem one performance measure as primary and other measures as secondary. Thresholds are set on the secondary performance measures and the feasibility of each design is then determined. We then identify a feasible design with the best primary performance measure as the optimal one. For large design space problems, a common method is to first apply a simplified model and detect the feasibility of each design based on an appropriate criterion (Yan et al. [88]). Then we can carefully explore this much smaller design space consisting of all feasible designs.

FD is highly useful in a wide variety of simulation optimization problems. We endeavor to detect the feasibility of each design under a fixed total simulation budget. This FD problem is a special case of the classical multiple comparisons with a control (MCC) problem, in the sense that the control that we compare with here is modeled as known (Nelson and Goldsman [65]). The MCC problem is one of the four classes of comparison problems that arise in ranking and selection (R&S) studies (Kim and Nelson [55]).

The main focus of this thesis is on how to allocate a given simulation budget intelligently among the alternative designs to best support the feasibility decisions. The most straightforward and widely used way is to allocate the total budget equally to each design. This is inefficient because it is possible that some designs have performance far from the threshold. We can draw conclusions about their feasibility with a certain confidence and avoid consuming further budget. Other designs that need more simulation effort to make an accurate decision can then be assigned more simulation budget. This motivates the effort to design more intelligent ways to allocate the simulation budget.

This allocation problem can be addressed via frequentist or Bayesian approach. The current intelligent allocation methods from frequentist perspective aim to allocate a finite total simulation budget optimally. However, to make their derivation tractable they make approximations assuming the total simulation budget is infinite. The method has asymptotically optimal property may not perform well in finite budget situation. Xie and Frazier [87] have shown in their numerical experiments that it performs even worse than the equal allocation procedure, which undermines its value in practical applications. Gao et al. [42] have also pointed out the importance of designing allocation procedures under finite budget conditions in R&S studies.

The Bayesian approach in R&S usually models the budget allocation process as a stochastic control problem (SCP). Peng et al. [71] state that for selecting the best design problem, SCP framework is a better approach than the previous frequentist approach. Xie and Frazier [87] address the FD in the SCP framework. However, as stated in their paper, their method cannot be applied to the fixed budget scenario directly. To the author's best knowledge, currently there is no work solves the FD in the fixed budget scenario through SCP approach.

The current existing allocation methods do not take into consideration the relationships between different designs. The performance of each design is only evaluated via results of repeated simulation runs of the design itself. In real life simulation problems, it is often the case that different designs with close parameters have similar performance. In this situation, when we assess the performance of a design, the simulation results of its neighboring designs could be highly informative. Taking the relationships between different designs into consideration in the FD procedure has the potential to further enhance simulation efficiency.

In this thesis, we first propose our Finite simulation budget Large Deviations-based (FLD) allocation method, which is a frequentist approach based on a finite budget perspective. We investigate the limitations of current existing frequentist approach methods and provide a proof to show the superiority of our method. Secondly, we compare the SCP approach with the frequentist approach to demonstrate that in FD the SCP framework is more realistic. We then formulate the FD problem as a SCP, and provide a one-step lookahead policy. We also illustrate the dynamic implementation of our FLD method. At last, we propose our Optima simulation budget Allocation with Kriging (OAK) method, which applies kriging models to capture the relationships between different designs. Numerical experiments are conducted to demonstrate the effectiveness of the three methods in this thesis.

1.2 Organization of the Thesis

The rest of this document is organized as follows. In Chapter 2, a review of existing literature on ranking and selection is presented. Several R&S procedures for FD problem are briefly introduced, and we also review several simulation budget allocation procedures that using metamodels to facilitate the procedure development.

In Chapter 3, we investigate the performance of current existing asymptotically optimal allocation method under finite simulation budget condition. We then propose our

FLD allocation method and demonstrate its superiority compared to current existing methods theoretically. Three illustrative numerical examples, one facility-sizing problem, and an emergency department setup problem are presented to show the efficiency of our method.

In Chapter 4, we demonstrate the inadequacy of static optimization formulation for FD allocation. In Bayesian setting, we formulate the allocation problem as a SCP. We provide a one-step lookahead policy for this SCP. We also demonstrate the dynamic implementation of FLD. Numerical examples are provided to demonstrate the differences of static and dynamic methods.

In Chapter 5, the kriging model is introduced to capture the relationships between different designs. We incorporate the information provided by kriging model in our FD procedure using Bayesian framework and devise a corresponding simulation budget allocation method. Computational tests are conducted to illustrate the effectiveness of the method.

In Chapter 6, future research works on practical application of feasibility determination and risk averse feasibility determination based on robust optimization techniques are discussed.

Chapter 2

Literature Review

Much research effort has been devoted to ranking and selection procedures for different classes of problems that arise in simulation studies. The following literature review focuses on both the R&S studies about the FD problem, discussed in Section 2.1, and using metamodels to aid R&S procedures, introduced in Section 2.2.

2.1 Ranking and Selection Studies about Feasibility Determination

Ranking and selection procedures are to compare a finite number of simulated alternatives. Over the past few decades, there have been fruitful efforts in developing R&S procedures for finding the best among a finite set of alternative designs.

For example, Dudewicz and Dalal [28], Rinott [75], Nelson et al. [66], Kim and Nelson [53], and Kim and Nelson [54] propose indifferent zone based screening procedures, which attempt to correctly detect the best design whose performance is at least a user-specified amount better than the other designs with a guaranteed probability. Gupta and Miescke [47], Chen et al. [21] and Chick and Inoue [22] exemplify the value of information approach, which uses a Bayesian framework to describe the evidence for correct selection and focuses on allocating a simulation budget to maximize the expected value of information. Chen [17], Chen et al. [19], Chen and Lee [18], and Gao and Shi [41] present the

Optimal Computing Budget Allocation (OCBA) method, which intelligently allocates the simulation budget to asymptotically maximize the expected probability of correct selection or the expected opportunity cost, assuming the design output is normally distributed. Glynn and Juneja [44] introduced the large deviations (LD) framework to R&S community and generalized this approach to general distribution scenarios. Frazier et al. [34] model the budget allocation process as a SCP problem, and present the knowledge-gradient policy. Fu et al. [37],Goldsman et al. [46] and Branke et al. [13] provide extensive reviews and comparisons of some of the aforementioned methods.

Other possible selection tasks include selecting several top designs instead of the single best design (Koenig and Law [56], Chen et al. [20], Gao and Chen [38], Zhang et al. [89], Gao and Chen [39]) and selecting the alternative with the largest quantile (Batur and Choobineh [6], Shin et al. [78]). All of the aforementioned procedures focus on only one performance measure. In reality, we often face designs with multiple performance measures or constraints (Butler et al. [16], Andradóttir et al. [3]). It is possible that these measures are independent of each other. However, it also frequently happens that some of these measures are correlated or even in conflict with one another. For example, suppose we want to determine how many receptionists, doctors, lab technicians and nurses should be hired when setting up an emergency department. Our goal is to minimize total cost while making sure that average total waiting time for critical patients does not exceed a prescribed value (Ahmed and Alkhamis [1]).

The practical problems with multiple performance measures or constraints have inspired R&S studies in the presence of stochastic constraints. That is developing R&S procedures to select the best design based on a primary performance measure from the feasible designs whose feasibility is determined according to the secondary performance measures. Andradóttir and Kim [2], Lee et al. [58], Hunter and Pasupathy [52], Healey et al. [49], and Pasupathy et al. [68] all work through this research line. FD is a critical ingredient in these procedures and has received increasing attention in simulation optimization. FD can also find applications in many other scenarios. Yan et al. [88], and Xie and Frazier [87] have demonstrated some practical applications in which FD is highly useful.

FD can also find its origin from the classical multiple comparisons with a control (MCC) problem. In MCC, the control against which we compare is usually the performance of a specific design that we also need to estimate via simulation. Paulson [69], Dunnett [30], Dudewicz and Ramberg [27], Dudewicz and Dalal [29], Bofinger and Lewis [10], and Damerdji and Nakayama [24] propose various sampling procedures concentrating on creating simultaneous confidence intervals for the differences between the performance of each design and the control. The readers interested in MCC can refer to several books and review papers, Hochberg and Tamhane [50], Fu [36], Goldsman and Nelson [45], and Hsu [51]. When the control is modeled as known we recover FD problem.

For an FD problem, a requirement is imposed either on the determination quality or on the simulation budget. Batur and Kim [7] follow the former approach. Assuming the distribution of outputs of each design is normal, they provide fully sequential procedures to identify a set of feasible or near-feasible designs with a statistical guarantee on the determination quality. Szechtman and Yücesan [84] also provide a guarantee on the probability of correct decisions for each design. Based on the Bayesian approach, the paper proposes a screening procedure and if when the budget is depleted, the paper determines the number of additional samples required to make the feasibility decision for each unclassified design.

We are interested in the second approach. Gao and Chen [40] solve the fixed budget

FD problem following OCBA approach. The derivation of OCBA approach assumes the distribution of observations of each design is normal. In reality, this may not be the case (Law and Kelton [57], Gao and Chen [40]). Szechtman and Yücesan [83] employ the LD framework to address the FD problem under a fixed simulation budget, which relaxes the normal assumption to general light-tailed distribution. Their paper concentrates on maximizing the asymptotic decay rate of the expected number of incorrect determinations. In another related work, Xie and Frazier [87] model the FD problem as a stochastic control problem (SCP). They assume the total simulation budget is geometrically distributed and then turn the budget allocation problem to a multi-armed bandit problem (Mahajan and Teneketzis [60]). Based on Gittins index (Gittins [43]), they then develop Bayes-optimal fully sequential policies for the FD problem.

2.2 Ranking and Selection Studies with Metamodels

If the performance measure of different designs exhibits spatial correlation, the efficiency of R&S can be further improved by incorporating information from neighboring designs when we estimate the performance of each design. One approach to utilize information from all the designs is to build metamodels to approximate the performance measures, which can be used to tackle large-scale R&S problems (Barton and Meckesheimer [5]).

One major issue in metamodeling includes the choice of a functional form (Barton and Meckesheimer [5]). The popular choices include polynomial response surface metamodels (Box [11], Chih [23]), Myers et al. [64], multivariate adaptive regression splines (Friedman [35]), kriging metamodels (Santner et al. [77], Ankenman et al. [4]), radial basis functions (Franke [33], Shin et al. [79]), and artificial neural networks (Masson and Wang [61], Sabuncuoglu and Touhami [76]). Simpson et al. [80] and Li et al. [59] provide a review of these metamodel performances.

Using metamodels to aid the R&S procedure has drawn some attention in the simulation optimization community. Brantley et al. [14] demonstrated that if the performance measure is quadratic or near quadratic, R&S efficiency can be enhanced by incorporating simulation information from across the domain into a quadratic regression metamodel. Brantley et al. [15] and Xiao et al. [86] partitioned the domain into small local areas and then applied the quadratic regression model in each area to aid the simulation budget allocation.

We are interested in the kriging metamodel because it assumes less structure than the quadratic models. It also tends to be more resistant to overfitting than artificial neural network (Ankenman et al. [4]). Li et al. [59] applied the aforementioned metamodels to four popular test functions with different degrees of noise, and the kriging metamodel performed well compared to others. The kriging metamodel was first developed in the field of geostatistics and has been applied extensively to various fields since then. Readers may refer to Ankenman et al. [4], Quan et al. [73] and Sun et al. [82] for more details on kriging metamodeling in stochastic settings.

Chapter 3

Finite Simulation Budget Large Deviations-based Allocation Procedure

Existing intelligent budget allocation methods make approximations assuming the total simulation budget is infinite and achieve asymptotically optimal property. In real life, however, the total simulation budget is certainly finite. In this chapter, we first investigate the performance of the current methods under finite budget condition. We then propose our Finite budget Large Deviations-based (FLD) allocation method. We provide a proof that FLD is superior to the current methods. Numerical experiments are conducted to demonstrate the effectiveness of the FLD method.

3.1 Problem Formulation

In this section, we precisely define the budget allocation problem of interest. Consider a finite set $i = 1, ..., r$ of designs. Each design i has a performance measure $\mu_i \in \mathbb{R}$, $\boldsymbol{\mu} = [\mu_1, ..., \mu_r]^{\mathrm{T}}$. Given a constant $\gamma \in \mathbb{R}$, a design i is defined to be feasible if $\mu_i \leq \gamma$. Let $X_{i,j}$ for $i = 1, ..., r, j = 1, 2, ...$ denote an observation from jth replication of the ith design, $E[X_{i,j}] = \mu_i$. We assume the simulationist use $\bar{X}_i(N_i) = N_i^{-1} \sum_{j=1}^{N_i} X_{i,j}$ to estimate μ_i, where N_i is the number of samples of design i. We wish to use limited total simulation budget to determine for each design i whether it is feasible or not effectively.

The total simulation budget n is allocated to each alternative design in order to maximize the expected number of correct determinations. Let α_i represent the proportion of simulation budget that is allocated to sampling from design i. In this research we ignore the minor technicalities associated with $n\alpha_i$ not being an integer.

We make the following assumptions in our analysis.

Assumption 1. The simulation output replicates are independent from replication to replication as well as independent across different designs.

Common random numbers (CRN) technique is used in simulation to improve efficiency. However, our task is to determine the feasibility of the designs, which does not require comparison among designs. Consequently the efficiency will not be benefited by the use of CRN. The assumption of independence across different designs is thus plausible.

Assumption 2. No design has the performance measure that lies exactly at the boundary, that is, $\mu_i \neq \gamma$, for $i = 1, 2, ..., r$

This assumption also appears in (Szechtman and Yücesan [83]) and (Hunter and Pasupathy [52]). It ensures no design requires consuming all the simulation budget.

Assumption 3. For all designs, the moment generating function $M_i(\theta) = E[\exp(\theta X_{i,j})] < \infty$ for $\theta \in \mathbb{R}$

As was presented in (Szechtman and Yücesan [83]), this assumption holds in situations where underlying distribution is light-tailed, such as normal, Bernoulli, Poisson and gamma family.

Let g_n denote the expected number of correct determinations under total budget n. We use $\mathcal{S}_Y = \{i : \mu_i \leq \gamma\}$ to denote the set consisting of feasible designs, and

$\mathcal{S}_N = \{i : \mu_i > \gamma\}$ to denote the set consisting of infeasible designs. The FD budget allocation problem is to

$$\begin{aligned} Problem\ \mathcal{P} : \max_{\alpha_1,...,\alpha_r} & \ g_n(\alpha_1, ..., \alpha_r) \\ s.t. \sum_{i=1}^{r} & \alpha_i = 1 \\ & \alpha_i \geq 0, i = 1, ..., r \end{aligned}$$

where

$$g_n(\alpha_1, ..., \alpha_r) = \sum_{i \in \mathcal{S}_Y} P(\bar{X}_i(n\alpha_i) < \gamma) + \sum_{i \in \mathcal{S}_N} P(\bar{X}_i(n\alpha_i) > \gamma)$$

3.2 Current Asymptotically Optimal Allocation Methods

In this subsection, we assume the designs have normal distributed outputs, $X_{i,j} \sim N(\mu_i, \sigma_i^2)$, for $i = 1, 2, ..., r, j = 1, 2, ...$ Currently there are mainly two asymptotically optimal allocation rules, ALD and OCBA. In the normal environment the two allocation rules are identical. We first briefly derive these two rules and then discuss their performance under finite budget condition.

3.2.1 Derivation of ALD/OCBA Allocation Rule

In the normal environment we can express $g_n(\alpha_1, ..., \alpha_r)$ in closed form,

$$g_n(\alpha_1,...,\alpha_r) = \sum_{i\in\mathcal{S}_Y} P(\bar{X}_i(n\alpha_i) < \gamma) + \sum_{i\in\mathcal{S}_N} P(\bar{X}_i(n\alpha_i) > \gamma)$$
$$= \sum_{i\in\mathcal{S}_Y} \int_{-\infty}^{\frac{(\gamma-\mu_i)\sqrt{n\alpha_i}}{\sigma_i}} e^{-\frac{x^2}{2}} dx + \sum_{i\in\mathcal{S}_N} \int_{\frac{(\gamma-\mu_i)\sqrt{n\alpha_i}}{\sigma_i}}^{\infty} e^{-\frac{x^2}{2}} dx$$

Remember that for a random variable $X_{i,j} \sim N(\mu_i, \sigma_i^2)$, its LD rate function (see Dembo and Zeitouni [26]) $I_i(x) = \frac{1}{2}(\frac{\mu_i - x}{\sigma_i})^2$. Since we have assumption 2, $\mu_i \neq \gamma$, $I_i(\gamma) > 0$, $i = 1,..,r$. For design i, given budget N_i the probability that we make a correct decision is $\int_{-\infty}^{\sqrt{2N_iI_i(\gamma)}} e^{-\frac{x^2}{2}} dx$. If $I_i(\gamma)$ is large, this probability is relatively high and vice versa. Therefore $I_i(\gamma)$ could be seen as an indicator that indicates how difficult we can correctly determine the feasibility of design i. The larger $I_i(\gamma)$ is, the more easily we detect its feasibility. WLOG, from now on we assume $I_1(\gamma) \leq I_2(\gamma) \leq ... \leq I_r(\gamma)$. $g_n(\alpha_1,...,\alpha_r)$ can be expressed as

$$g_n(\alpha_1,...,\alpha_r) = \sum_{i=1}^{r}(1 - \int_{\sqrt{2nI_i(\gamma)\alpha_i}}^{\infty} e^{-\frac{x^2}{2}} dx)$$

Therefore, the original problem $\mathcal{P}$ can be transformed to

$$Problem\ \mathcal{P}1 : \min_{\alpha_1,...,\alpha_r} \sum_{i=1}^{r} \int_{\sqrt{2nI_i(\gamma)\alpha_i}}^{\infty} e^{-\frac{x^2}{2}} dx \tag{3.1}$$
$$s.t. \sum_{i=1}^{r} \alpha_i = 1 \tag{3.2}$$
$$\alpha_i \geq 0, i = 1, ..., r \tag{3.3}$$

$\int_{\sqrt{2nI_i(\gamma)\alpha_i}}^{\infty} e^{-\frac{x^2}{2}} dx$ is convex since it's twice differentiable and its second derivative with respect to α_i is $n^2 I_i(\gamma)^2 e^{-nI_i(\gamma)\alpha_i}(2nI_i(\gamma)\alpha_i)^{-\frac{3}{2}}(1+2nI_i(\gamma)\alpha_i)$, which is nonnegative. The objective function of problem $\mathcal{P}1$ is sum of convex functions, thus it is also a convex function. Since all the constraints are linear, we can conclude that problem $\mathcal{P}1$ is a convex optimization problem. We first omit constraint (3.3) and consider the problem $\widetilde{\mathcal{P}1}$

$$\textit{Problem } \widetilde{\mathcal{P}1} : \min_{\alpha_1,\ldots,\alpha_r} \sum_{i=1}^{r} \int_{\sqrt{2nI_i(\gamma)\alpha_i}}^{\infty} e^{-\frac{x^2}{2}} dx$$
$$s.t. \sum_{i=1}^{r} \alpha_i = 1$$

This is still a convex optimization problem, thus the solution satisfying the Karush-Kuhn-Tucker (KKT) conditions is the optimal solution to this problem (Boyd and Vandenberghe [12]). We use λ to represent a constant. The KKT conditions are stated as follows:

$$e^{-nI_i(\gamma)\alpha_i}(2nI_i(\gamma)\alpha_i)^{-\frac{1}{2}} nI_i(\gamma) = \lambda, i = 1, 2, ..., r \tag{3.4}$$
$$\sum_{i=1}^{r} \alpha_i = 1$$

Taking log function of both sides of condition (3.4) and performing some arithmetic operations, the KKT conditions are equivalent to

$$\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log \alpha_i - nI_i(\gamma)\alpha_i = \lambda, i = 1, 2, ..., r \tag{3.5}$$
$$\sum_{i=1}^{r} \alpha_i = 1$$

When n tends to infinity, the term $\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log \alpha_i$ in condition (3.5) becomes much smaller than $nI_i(\gamma)\alpha$ and is negligible. We can then simplify condition (3.5) to

$-nI_i(\gamma)\alpha_i = \lambda$. Since we have assumption 2, $I_i(\gamma)$ is positive. The solution of the conditions are then derived as $\alpha_i = \frac{1/I_i(\gamma)}{\sum_{i=1}^{r} 1/I_i(\gamma)}, i = 1, 2, ..., r$, which is the limit the optimal solution of problem $\widetilde{\mathcal{P}1}$ converges to when the total simulation budget n tends to infinity.

Let $p_i^* = \frac{1/I_i(\gamma)}{\sum_{i=1}^{r} 1/I_i(\gamma)}, i = 1, 2, ..., r$, $\boldsymbol{p}^* = (p_1^*, p_2^*, ..., p_r^*)^{\mathrm{T}}$. $p_i^* > 0$, p_i^* satisfies constraint (3.3). Therefore the optimal solution of problem $\mathcal{P}1$ approaches $\boldsymbol{p}^*$ when the total simulation budget n tends to infinity.

$\boldsymbol{p}^*$ is exactly the ALD/OCBA allocation rule. Szechtman and Yücesan [83] has established that $\lim_{n\to\infty} \frac{1}{n} \log(r - g_n(\alpha_1, ..., \alpha_r))$ is minimized when $\alpha_i = p_i^*, i = 1, ..., r$. That means when the total simulation budget n tends to infinity, allocation rule $\boldsymbol{p}^*$ can make the expected number of correct determinations g_n converge to r at highest rate of convergence.

3.2.2 Performance of ALD/OCBA under Finite Budget Condition

ALD/OCBA achieves asymptotically optimal property. However, in reality the total simulation budget n is always finite. If we apply the ALD/OCBA allocation rule $\boldsymbol{p}^*$ directly in finite budget situation, the performance may not be satisfying. We now prove the following property of allocation rule $\boldsymbol{p}^*$:

Proposition 3.1 *For any set of designs and any threshold, there exists an $n_t > 0$, when the total simulation budget $n \le n_t$, the performance of allocation rule $\boldsymbol{p}^*$ is always no better than the equal allocation (EA) rule, $\alpha_i = \frac{1}{r}, i = 1, 2, ..., r$.*

Proof: If $I_1(\gamma) = I_2(\gamma) = ... = I_r(\gamma)$, the ALD/OCBA allocation rule $\boldsymbol{p}^*$ is identical to the equal allocation, we can select any positive number as n_t.

Assume we have at least i, j, $I_i(\gamma) \neq I_j(\gamma)$. Let $f_1(n) = g_n(p_1^*, ..., p_r^*) - g_n(1/r, ..., 1/r)$,

$$f_1(n) = \sum_{i=1}^{r} \int_{\sqrt{2nI_i(\gamma)\frac{1}{r}}}^{\infty} e^{-\frac{x^2}{2}} dx - \sum_{i=1}^{r} \int_{\sqrt{2nI_i(\gamma)p_i^*}}^{\infty} e^{-\frac{x^2}{2}} dx$$

We have $f_1(0) = 0$. $f_1(n)$ is differentiable. Taking derivative,

$$\begin{aligned} f_1'(n) &= -\sum_{i=1}^{r} e^{-nI_i(\gamma)\frac{1}{r}} (2nI_i(\gamma)\frac{1}{r})^{-\frac{1}{2}} I_i(\gamma)\frac{1}{r} + \sum_{i=1}^{r} e^{-nI_i(\gamma)p_i^*} (2nI_i(\gamma)p_i^*)^{-\frac{1}{2}} I_i(\gamma)p_i^* \\ &= (2n)^{-\frac{1}{2}} \sum_{i=1}^{r} (e^{-nI_i(\gamma)p_i^*} (I_i(\gamma)p_i^*)^{\frac{1}{2}} - e^{-nI_i(\gamma)\frac{1}{r}} (I_i(\gamma)\frac{1}{r})^{\frac{1}{2}}) \end{aligned}$$

Let $h(n) = \sum_{i=1}^{r} (e^{-nI_i(\gamma)p_i^*} (I_i(\gamma)p_i^*)^{\frac{1}{2}} - e^{-nI_i(\gamma)\frac{1}{r}} (I_i(\gamma)\frac{1}{r})^{\frac{1}{2}})$. We next show $h(0) < 0$.

$$h(0) = \sum_{i=1}^{r} (I_i(\gamma)p_i^*)^{\frac{1}{2}} - \sum_{i=1}^{r} (I_i(\gamma)\frac{1}{r})^{\frac{1}{2}}$$

Plug in $p_i^* = \frac{1/I_i(\gamma)}{\sum_{i=1}^{r} 1/I_i(\gamma)}$,

$$h(0) = r(\sum_{i=1}^{r} \frac{1}{I_i(\gamma)})^{-\frac{1}{2}} - \sum_{i=1}^{r} (\frac{r}{I_i(\gamma)})^{-\frac{1}{2}}$$

Consider the function $x^{-\frac{1}{2}}, x \in (0, \infty)$. It is twice differentiable and its second derivative $\frac{3}{4}x^{-\frac{5}{2}} > 0$, which indicates that $x^{-\frac{1}{2}}, x \in (0, \infty)$ is a strictly convex function. By Jensen's inequality,

$$(\frac{1}{r}\frac{1}{I_1(\gamma)} + ... + \frac{1}{r}\frac{1}{I_r(\gamma)})^{-\frac{1}{2}} \leq \frac{1}{r}(\frac{1}{I_1(\gamma)})^{-\frac{1}{2}} + ... + \frac{1}{r}(\frac{1}{I_r(\gamma)})^{-\frac{1}{2}}$$

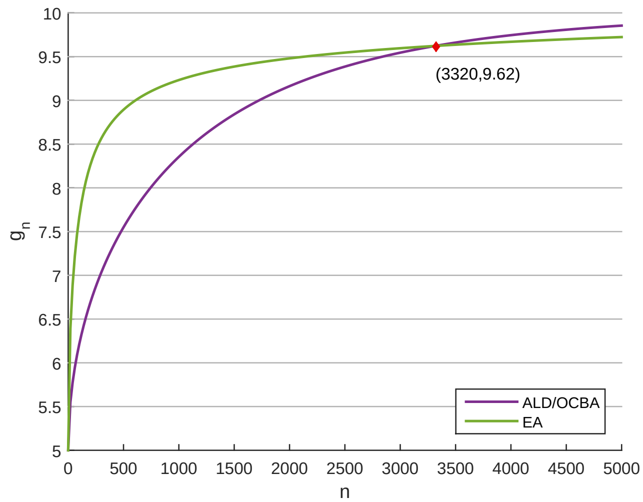
which is equivalent to $r(\sum_{i=1}^{r} \frac{1}{I_i(\gamma)})^{-\frac{1}{2}} \leq \sum_{i=1}^{r} (\frac{r}{I_i(\gamma)})^{-\frac{1}{2}}$. The equality holds only when $I_1(\gamma) = ... = I_r(\gamma)$. By assumption we have i, j that $I_i(\gamma) \neq I_j(\gamma)$. Hence here we have strict less than relationship, $h(0) < 0$.

$h(n)$ is a continuous function. Thus there exists an $n_t > 0$, when $n \leq n_t$ we have $h(n) < 0$. This implies when $n \leq n_t$, $f_1'(n) < 0$, $f_1(n)$ is a decreasing function. Remember that $f_1(0) = 0$, hence in $(0, n_t]$, $f_1(n) < 0$, $g_n(p_1^*, ..., p_r^*) \leq g_n(1/r, ..., 1/r)$. ■

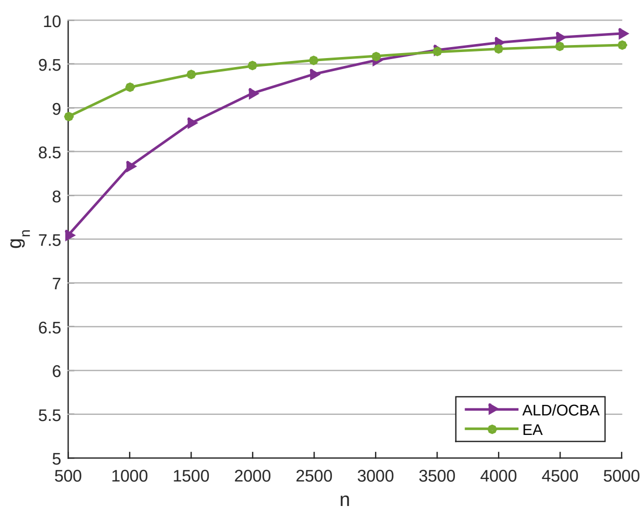
Proposition 3.1 indicates that there exists an $n_t > 0$, if the total simulation budget n falls within the interval $(0, n_t)$, the performance of ALD/OCBA is actually inferior to the equal allocation. The range of this interval depends on concrete cases. We now use a numerical example to illustrate this interval. Assume we have ten designs with $X_{i,j} \sim N(i, 10^2)$, $i = 1, 2, ..., 10$. The threshold $\gamma = 6.4$. The comparison of ALD/OCBA with EA under different budgets is displayed in Figure 3.1.

In Figure 3.1 (a), g_n is calculated by theoretical formula. Due to the factors such as rounding to integer when allocating the total budget to each design, the performance of each allocation rule would not be in the full accord with the theoretical result. We also use simulation to estimate the value of g_n. The estimation is based on 10000 independent experiments and the result is shown in Figure 3.1 (b). From the figure we can see the performance of ALD/OCBA could not surpass EA until the total budget exceeds 3000. At that moment both methods could achieve the g_n level 9.62.

Unfortunately, intelligent budget allocation method is often applied in the background that the budget is quite limited. The scenario $n <= n_t$ could happen easily in this situation, which undermines the value of ALD/OCBA method in realistic application. This motivates us to seek improvements on current allocation methods. Next section we propose our FLD allocation method, which is our effort along this research direction.



(a)



(b)

Figure 3.1: Comparison of ALD/OCBA with EA.

3.3 FLD Allocation Method

In this section, we discuss our FLD allocation rule. Remember that small $I_i(\gamma)$ value indicates design i is relatively more difficult to determine its feasibility. If we see difficult designs as critical, ALD/OCBA rule $p_i^* = \frac{1/I_i(\gamma)}{\sum_{i=1}^r 1/I_i(\gamma)}$ implies that critical designs obtain larger budget fraction.

In the previous section, we have derived an equivalent expression of KKT conditions of problem $\widetilde{\mathcal{P}1}$:

$$\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log \alpha_i - nI_i(\gamma)\alpha_i = \lambda, i = 1, 2, ..., r \tag{3.5}$$
$$\sum_{i=1}^{r} \alpha_i = 1$$

In constraint (3.5) if the total simulation budget n is sufficient large, we drop the term $\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log \alpha_i$ and derive the ALD/OCBA rule. However, if n is sufficient small, we could ignore the effect of $nI_i(\gamma)\alpha_i$. We then get $\alpha_i = \frac{I_i(\gamma)}{\sum_{i=1}^r I_i(\gamma)}$. This implies when the total simulation budget is very limited, the optimal allocation rule has the property that critical designs receive less budget fraction, which is contrary to the ALD/OCBA rule. This may explain for FD problem why it is possibly inappropriate to apply the ALD/OCBA rule directly given the total simulation budget is limited.

This is very different from the problem of selecting the best design from among a number of alternative designs via simulation. In that problem we define the design that is optimal or near optimal as critical and in actual practice the critical designs always receive relatively high budget fraction no matter what the total simulation budget is. Here the optimal budget allocation rule changes drastically when n changes, which indicates that we should consider the effect of n in our allocation rule.

3.3.1 Derivation of $\boldsymbol{p}$ Allocation Rule

Suppose the design outputs are normally distributed. We now consider the effect of the term $\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log\alpha_i$ in condition (3.5). Since $\boldsymbol{p^*}$ is the asymptotically optimal allocation ratio, we expect that the optimal allocation ratio should not deviate too far from $\boldsymbol{p^*}$. Therefore we approximate $\log\alpha_i$ by its first order Taylor expansion at p_i^*, $\log\alpha_i \doteq \log p_i^* + (\alpha_i - p_i^*)/p_i^*$. Let $T = \sum_{i=1}^r \frac{1}{I_i(\gamma)}$. Remember $p_i^* = \frac{1/I_i(\gamma)}{T}$, the KKT conditions of problem $\widetilde{\mathcal{P}1}$ could be approximated by

$$\log I_i(\gamma) - \frac{\alpha_i}{2p_i^*} - nI_i(\gamma)\alpha_i = \lambda, i = 1, 2, ..., r \tag{3.6}$$

$$\sum_{i=1}^r \alpha_i = 1 \tag{3.2}$$

Let $c_i = \log I_i(\gamma)T - \sum_{i=1}^r \frac{\log I_i(\gamma)}{I_i(\gamma)}, i = 1, ..., r$. Note $\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = T\sum_{i=1}^r \frac{\log I_i(\gamma)}{I_i(\gamma)} - \sum_{i=1}^r \frac{\log I_i(\gamma)}{I_i(\gamma)}T = 0$. Let $p_i = p_i^*(1 + \frac{c_i}{n+T/2}), i = 1, ..., r$, $\boldsymbol{p} = [p_1, p_2, ..., p_r]^{\mathrm{T}}$. We have

Proposition 3.2 *Allocation rule* $\boldsymbol{p}$ *satisfies constraint (3.6) and constraint (3.2).*

Proof:

$$\begin{aligned}
\sum_{i=1}^r p_i &= \sum_{i=1}^r p_i^*(1 + \frac{c_i}{n+T/2}) \\
&= 1 + \sum_{i=1}^r \frac{p_i^* c_i}{n+T/2} \\
&= 1 + \frac{1}{T(n+T/2)}\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} \\
&= 1
\end{aligned}$$

$\boldsymbol{p}$ satisfies constraint (3.2).

$$\begin{aligned}
&\log I_i(\gamma) - \frac{p_i}{2p_i^*} - nI_i(\gamma)p_i \\
&= \log I_i(\gamma) - \frac{1}{2}(1+\frac{c_i}{n+T/2}) - \frac{n}{T}(1+\frac{c_i}{n+T/2}) \\
&= \log I_i(\gamma) - \frac{1}{2} - \frac{n}{T} - \frac{c_i}{T} \\
&= \log I_i(\gamma) - \log I_i(\gamma) + \frac{1}{T}\sum_{i=1}^{r}\frac{\log I_i(\gamma)}{I_i(\gamma)} - \frac{1}{2} - \frac{n}{T} \\
&= \frac{1}{T}\sum_{i=1}^{r}\frac{\log I_i(\gamma)}{I_i(\gamma)} - \frac{1}{2} - \frac{n}{T}
\end{aligned}$$

$\frac{1}{T}\sum_{i=1}^{r}\frac{\log I_i(\gamma)}{I_i(\gamma)} - \frac{1}{2} - \frac{n}{T}$ does not depend on specific i. Hence $\boldsymbol{p}$ satisfies constraint (3.6).

■

Since $I_1(\gamma) \leq I_2(\gamma) \leq ... \leq I_r(\gamma)$, $c_1 \leq c_2 \leq ... \leq c_r$. For design i that $c_i \geq 0$, p_i is always positive. For the designs with $c_i < 0$, when $n > -c_1 - \frac{T}{2}$, $p_i = p_i^*(1+\frac{c_i}{n+T/2}) > p_i^*(1+\frac{c_i}{-c_1}) \geq 0$. Therefore when $n > -c_1 - \frac{T}{2}$, $\boldsymbol{p}$ satisfies constraint (3.3). We can see $\boldsymbol{p}$ as a good approximation of exact optimal allocation ratio.

If all $I_i(\gamma)$'s are equal, $c_i = 0$, $p_i^* = p_i = \frac{1}{r}$. Otherwise comparing with constraint (3.5), we observe that

$$\begin{aligned}
\lambda_1 &= \frac{1}{2}\log I_1(\gamma) - \frac{1}{2}\log p_1 - nI_1(\gamma)p_1 \\
&= \log I_1(\gamma) + \log(\sum_{i=1}^{r}\frac{1}{I_i(\gamma)}) - \frac{n}{\sum_{i=1}^{r}\frac{1}{I_i(\gamma)}} \\
&< \log I_r(\gamma) + \log(\sum_{i=1}^{r}\frac{1}{I_i(\gamma)}) - \frac{n}{\sum_{i=1}^{r}\frac{1}{I_i(\gamma)}} \\
&= \frac{1}{2}\log I_r(\gamma) - \frac{1}{2}\log p_r - nI_r(\gamma)p_r \\
&= \lambda_r
\end{aligned}$$

λ in constraint (3.5) must lie in the interval (λ_1, λ_r). To make constraint (3.5) valid, for design i with $I_i(\gamma)$ relatively small we should decrease p_i^* and for design i with large

$I_i(\gamma)$ we should increase p_i^*. This means ALD/OCBA allocation rule tends to allocate too small budget to the designs that are relatively easy to detect the feasibility and allocate too large budget to those relatively difficult designs.

$p_i = p_i^*(1 + \frac{c_i}{n+T/2})$, we can see $\frac{c_i}{n+T/2}$ as a modification coefficient to alleviate the aforementioned drawback of ALD/OCBA allocation rule. For the easy designs, $I_i(\gamma)$ is large, hence c_i tends to be positive. In this case $p_i > p_i^*$, $\boldsymbol{p}$ allocates more budget than allocation rule $\boldsymbol{p}$. For the difficult designs, $I_i(\gamma)$ is small, hence c_i tends to be negative. $p_i < p_i^*$, $\boldsymbol{p}$ allocates less budget than $\boldsymbol{p}$.

3.3.2 Convergence of $\boldsymbol{p}$ Allocation Rule

When $n \to \infty$, $p_i \to p_i^*$. $\boldsymbol{p}$ converges to $\boldsymbol{p^*}$ at rate $O(\frac{1}{n})$ when n tends to infinity. This indicates that $\boldsymbol{p}$ is also asymptotically optimal. However, $\lim\limits_{n\to\infty}(np_i - np_i^*) = \lim\limits_{n\to\infty} \frac{n}{n+T/2} p_i^* c_i = p_i^* c_i$. That means although our rule converges to $\boldsymbol{p}$, there always exists a difference between the budget assigned to each design by the two rules even when the total simulation budget tends to infinity. We now use a numerical example to show this phenomenon. Suppose we have two designs, $X_{1,j} \sim N(2, 2^2)$, $X_{2,j} \sim N(4, 2^2)$. The threshold $\gamma = 3.7$. The comparison of budget allocated to design 1 is illustrated in Figure 3.2.

In Figure 3.2 the 'Optimal' line represents the optimal value of N_1, denoted by N_1^*, which is obtained by using numerical methods. From the figure we can see budget allocated to design 1 by $\boldsymbol{p}$ converges quickly to N_1^*. Meanwhile there is a gap between budget allocated by ALD/OCBA rule and N_1^*. Instead of decreasing, this gap seems to become larger when the total simulation budget increases. This observation can be validated by $|np_i - np_i^*| = |p_i^* c_i|(1 - \frac{T}{2n+T})$, which is increasing as n increases. The gap converges to $|p_i^* c_i|$, in this example $|p_1 c_1| \doteq 9$. The figure indicates that compared with

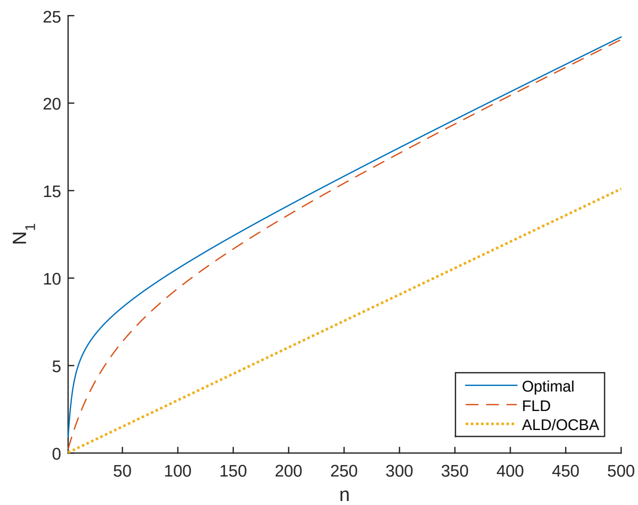


Figure 3.2: Comparison of budget allocated to design 1.

N_1^* this gap is significant even when the total simulation budget achieves 500.

Let $N_i^*(n)$ be the optimal budget that should be allocated to design i given total simulation budget n. We now prove the convergence of budget allocated by FLD rule to optimal value – as observed in the previous example – always holds.

Proposition 3.3 $\lim_{n\to\infty} (N_i^*(n) - np_i) = 0,\ i = 1, ..., r.$

Proof: Suppose there exists a design i, $\lim_{n\to\infty} (N_i^*(n) - np_i) \neq 0$. That means there exists an $\epsilon > 0$, for any natural number N, we can find an n such that $n \geq N$ and $|N_i^*(n) - np_i| \geq \epsilon$. Note that $\sum_{i=1}^r N_i^*(n) = \sum_{i=1}^r np_i = n$. Case 1, if $N_i^*(n) - np_i \geq \epsilon$, there must exists a design j, $N_j^*(n) - np_j \leq -\frac{\epsilon}{r}$. Otherwise $0 = \sum_{i=1}^r N_i^*(n) - \sum_{i=1}^r np_i \geq \epsilon - \frac{\epsilon}{r}(r-1) = \frac{\epsilon}{r} > 0$, which is impossible. Similarly, case 2, if $N_i^*(n) - np_i \leq -\epsilon$, there must exists a design j, $N_j^*(n) - np_j \geq \frac{\epsilon}{r}$.

From constraint (3.5), we can see for any design a, b, $\frac{1}{2}\log I_a(\gamma) - \frac{1}{2}\log N_a^*(n) - N_a^*(n) I_a(\gamma) = \frac{1}{2}\log I_b(\gamma) - \frac{1}{2}\log N_b^*(n) - N_b^*(n) I_b(\gamma)$. By assumption no matter what N

is, we can always find an $n \geq N$ and a design j that satisfies case 1 or case 2. For case 1,

$$
\begin{aligned}
&|\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log(np_i) - np_iI_i(\gamma) - (\frac{1}{2}\log I_j(\gamma) - \frac{1}{2}\log(np_j) - np_jI_j(\gamma))| \\
&= |\frac{1}{2}\log N_i^*(n) + N_i^*(n)I_i(\gamma) - \frac{1}{2}\log(np_i) - np_iI_i(\gamma) \\
&\ - (\frac{1}{2}\log N_j^*(n) + N_j^*(n)I_j(\gamma) - \frac{1}{2}\log(np_j) - np_jI_j(\gamma))| \\
&\geq \frac{1}{2}\log(np_i + \epsilon) + \epsilon I_i(\gamma) - \frac{1}{2}\log(np_i) - (\frac{1}{2}\log(np_j - \frac{\epsilon}{r}) - \frac{\epsilon}{r}I_j(\gamma) - \frac{1}{2}\log(np_j)) \\
&= \frac{1}{2}(\log(\frac{np_i + \epsilon}{np_i}) - \log(\frac{np_j - \epsilon/r}{np_j})) + \epsilon I_i(\gamma) + \epsilon\frac{1}{r}I_j(\gamma) \\
&> \epsilon I_i(\gamma) + \epsilon\frac{1}{r}I_j(\gamma) \\
&> 0
\end{aligned}
$$

Similarly, for case 2, we can derive $|\frac{1}{2}\log I_i(\gamma) - \frac{1}{2}\log(np_i) - np_iI_i(\gamma) - (\frac{1}{2}\log I_j(\gamma) - \frac{1}{2}\log(np_j) - np_jI_j(\gamma))| > \epsilon I_i(\gamma) + \epsilon\frac{1}{r}I_j(\gamma) > 0$. However, for any a, b,

$$
\begin{aligned}
&\lim_{n\to\infty}(\frac{1}{2}\log I_a(\gamma) - \frac{1}{2}\log(np_a) - np_aI_a(\gamma) - (\frac{1}{2}\log I_b(\gamma) - \frac{1}{2}\log(np_b) - np_bI_b(\gamma)))\\
&= \lim_{n\to\infty}(\frac{1}{2}\log I_a(\gamma) - \frac{1}{2}\log(np_a^*(1+\frac{c_a}{n+T/2})) - np_a^*(1+\frac{c_a}{n+T/2})I_a(\gamma)\\
&- (\frac{1}{2}\log I_b(\gamma) - \frac{1}{2}\log(np_b^*(1+\frac{c_b}{n+T/2})) - np_b^*(1+\frac{c_b}{n+T/2})I_b(\gamma)))\\
&= \lim_{n\to\infty}(\log I_a(\gamma) - \frac{1}{2}\log(1+\frac{c_a}{n+T/2}) - \frac{n}{T}(1+\frac{c_a}{n+T/2}) - (\log I_b(\gamma)\\
&- \frac{1}{2}\log(1+\frac{c_b}{n+T/2}) - \frac{n}{T}(1+\frac{c_b}{n+T/2})))\\
&= \lim_{n\to\infty}(\log I_a(\gamma) - \frac{1}{2}\log(1+\frac{c_a}{n+T/2}) - \frac{n}{n+T/2}\log I_a(\gamma) - (\log I_b(\gamma)\\
&- \frac{1}{2}\log(1+\frac{c_b}{n+T/2}) - \frac{n}{n+T/2}\log I_b(\gamma)))\\
&= 0
\end{aligned}
$$

Which is a contradiction. Therefore $\lim_{n\to\infty}(N_i^*(n) - np_i) = 0$, $i = 1, ..., r$. ■

3.3.3 FLD Allocation Rule and its Superiority

Suppose the design outputs are normally distributed. Since in previous subsection we have observed that budgets allocated by $\boldsymbol{p}$ converge to optimal values, we expect that when the total budget n is sufficient large $\boldsymbol{p}$ should perform better than ALD/OCBA rule. Let $n_g = \frac{2c_1}{1-\sqrt{5}} - \frac{T}{2}$, we now prove the following lemma,

Lemma 3.1 *When $n \geq n_g$, allocation rule $\boldsymbol{p}$ performs no worse than $\boldsymbol{p^*}$. Furthermore, if $I_i(\gamma)$'s are not all equal, $\boldsymbol{p}$ always performs better than $\boldsymbol{p^*}$.*

Proof: If $I_1(\gamma) = I_2(\gamma) = ... = I_r(\gamma)$, $c_1 = c_2 = ... = c_r = 0$, allocation rule $\boldsymbol{p}$ is the same as $\boldsymbol{p^*}$. $\boldsymbol{p}$ and $\boldsymbol{p^*}$ have the same performance.

If $I_i(\gamma)$'s are not all equal, let $f_2(x) = \sum_{i=1}^r \int_{-\infty}^{\sqrt{\frac{2n}{T}(1+xc_i)}} e^{-\frac{t^2}{2}} dt$. $f_2(0) = g_n(p_1^*, ..., p_r^*)$, $f_2(\frac{1}{n+T/2}) = g_n(p_1, ..., p_r)$. Since $f_2'(x) = \sum_{i=1}^r e^{-\frac{n}{T}(1+xc_i)} (\frac{2n}{T}(1+xc_i))^{-\frac{1}{2}} \frac{n}{T} c_i$, $g_n(p_1, ..., p_r) - g_n(p_1^*, ..., p_r^*) = \int_0^{\frac{1}{n+T/2}} f_2{}'(x)dx = (\frac{n}{2T})^{\frac{1}{2}} e^{-\frac{n}{T}} \int_0^{\frac{1}{n+T/2}} \sum_{i=1}^r e^{-\frac{n}{T}xc_i} (1 + xc_i)^{-\frac{1}{2}} c_i dx$.

When $x \in [0, \frac{1}{n+T/2}]$, if $c_i \geq 0$, $e^{-\frac{n}{T}xc_i} \geq e^{-\frac{n}{T}\frac{1}{n+T/2}c_i}$, if $c_i < 0$, $e^{-\frac{n}{T}xc_i} \leq e^{-\frac{n}{T}\frac{1}{n+T/2}c_i}$. Therefore,

$$\begin{aligned}
\int_0^{\frac{1}{n+T/2}} \sum_{i=1}^r e^{-\frac{n}{T}xc_i} (1 + xc_i)^{-\frac{1}{2}} c_i &\geq \sum_{i=1}^r e^{-\frac{n}{T}\frac{1}{n+T/2}c_i} \int_0^{\frac{1}{n+T/2}} (1 + xc_i)^{-\frac{1}{2}} c_i \\
&= 2\sum_{i=1}^r e^{-\frac{n}{T}\frac{1}{n+T/2}c_i} ((1 + \frac{1}{n+T/2}c_i)^{\frac{1}{2}} - 1) \\
&= \frac{2}{n+T/2} \sum_{i=1}^r e^{-\frac{n}{T}\frac{1}{n+T/2}c_i} \frac{c_i}{(1 + \frac{1}{n+T/2}c_i)^{\frac{1}{2}} + 1} \\
&= \frac{2}{n+T/2} \sum_{i=1}^r c_i e^{-\frac{c_i}{T}} e^{\frac{c_i}{2}\frac{1}{n+T/2}} \frac{1}{(1 + \frac{1}{n+T/2}c_i)^{\frac{1}{2}} + 1}
\end{aligned}$$

Let function $h(y) = \frac{e^{\frac{y}{2}}}{(1+y)^{\frac{1}{2}}+1}$, $h'(y) = \frac{e^{\frac{y}{2}}(1+y)^{-\frac{1}{2}}(y+(1+y)^{-\frac{1}{2}})}{2((1+y)^{\frac{1}{2}}+1)^2}$. When $y \geq \frac{1-\sqrt{5}}{2}$, $h'(y) \geq 0$, the equality holds only when $y = \frac{1-\sqrt{5}}{2}$. $h(y)$ is a strict increasing function in $[\frac{1-\sqrt{5}}{2}, \infty)$. Let $y_i = \frac{c_i}{n+T/2}$, we have $n \geq \frac{2c_1}{1-\sqrt{5}} - \frac{T}{2}$, $y_i \geq \frac{c_1}{n+T/2} \geq \frac{1-\sqrt{5}}{2}$. Hence there exists a positive constant K, when $c_i \geq 0$, $h(y_i) > K$, when $c_i < 0$, $h(y_i) < K$. Therefore,

$$\int_0^{\frac{1}{n+T/2}} \sum_{i=1}^r e^{-\frac{n}{T}xc_i} (1 + xc_i)^{-\frac{1}{2}} c_i dx > \frac{2K}{n+T/2} \sum_{i=1}^r c_i e^{-\frac{c_i}{T}}$$

Since $\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = 0$, $\sum_{i=1}^r c_i e^{-\frac{c_i}{T}} = e^{\frac{1}{T}\sum_{i=1}^r \frac{\log I_i(\gamma)}{I_i(\gamma)}} \sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = 0$. We have $\int_0^{\frac{1}{n+T/2}} \sum_{i=1}^r e^{-\frac{n}{T}xc_i}(1+xc_i)^{-\frac{1}{2}} c_i dx > 0$. Hence $g_n(p_1, ..., p_r) - g_n(p_1^*, ..., p_r^*) > 0$, allocation rule $\boldsymbol{p}$ performs better than $\boldsymbol{p}^*$. ■

We now consider the coefficient $\frac{1}{n+T/2}$ in the formula of $\boldsymbol{p}$, $p_i = p_i^*(1 + \frac{1}{n+T/2}c_i)$. Observe $p_i^*(1 + xc_i)$, where x is some coefficient. If $I_1(\gamma) = ... = I_r(\gamma)$, $c_1 = ... = c_r = 0$, no matter what the coefficient is, $p_i = p_i^*$. Suppose the scenario is nontrivial, not all $I_i(\gamma)$'s are equal. In the proof of lemma 1, we have denoted $f_2(x) = \sum_{i=1}^r \int_{-\infty}^{\sqrt{\frac{2n}{T}(1+xc_i)}} e^{-\frac{t^2}{2}} dt$. Note that $f_2(0) = g_n(p_1^*, ..., p_r^*)$, $f_2(\frac{1}{n+T/2}) = g_n(p_1, ..., p_r)$. Taking derivative, $f_2'(x) = \sum_{i=1}^r e^{-\frac{n}{T}(1+xc_i)}(\frac{2n}{T}(1+xc_i))^{-\frac{1}{2}}\frac{n}{T}c_i$, $f_2'(0) = e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r c_i$. The second derivative $f_2''(x) = -e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r e^{-\frac{n}{T}xc_i}(1+xc_i)^{-\frac{1}{2}}c_i^2(\frac{n}{T}+\frac{1}{2}(1+xc_i)^{-1}) < 0$.

Let k be the index of the first nonnegative c_i, that means $c_{k-1} < 0, c_k \geq 0$. Since $\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = 0$, $\sum_{i=1}^r c_i = \sum_{i=1}^r c_i I_i(\gamma)/I_i(\gamma) > \sum_{i=1}^r c_i I_k(\gamma)/I_i(\gamma) = I_k(\gamma)\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = 0$. Thus $f_2'(0) > 0$. It implies that $f_2'(x) > 0$ when x is positive and small enough, which means we could benefit from the modification from p_i^* to $p_i^*(1+xc_i)$ if positive x is small enough.

The best choice of x should be the value making $f_2'(x) = 0$. Note that $f_2'(\frac{1}{n}) = e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r c_i e^{-\frac{c_i}{T}}(1+\frac{c_i}{n})^{-\frac{1}{2}} < e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r c_i e^{-\frac{c_i}{T}} = 0$. The best choice of x should be in the interval $(0, \frac{1}{n})$. Since x is in the neighborhood of 0, we make the approximation $1 + xc_i = e^{xc_i}$, $f_2'(\frac{1}{n+T/2}) = e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r e^{-\frac{n}{T}\frac{1}{n+T/2}c_i}e^{-\frac{1}{2}\frac{1}{n+T/2}c_i}c_i = e^{-\frac{n}{T}}(\frac{n}{2T})^{\frac{1}{2}}\sum_{i=1}^r e^{-\frac{c_i}{T}}c_i = 0$. $\frac{1}{n+T/2}$ is a good approximation of the solution to equation $f_2'(x) = 0$.

When the total simulation budget n is large, $\frac{1}{n+T/2}$ is small, the approximation is relatively accurate. Lemma 1 guarantees if $n \geq n_g$, the modification from p_i^* to $p_i^*(1+\frac{1}{n+T/2}c_i)$ is always beneficial. However, if n is very limited, $\frac{1}{n+T/2}$ may be too large to be a good coefficient. In the scenario $n < n_g$, we want the coefficient x in the formula $p_i^*(1+xc_i)$ is relatively small compared to $\frac{1}{n+T/2}$ and is continuous with the scenario $n \geq n_g$. The most direct and easy to implement way is to fix x to be $\frac{1}{n_g+T/2}$ when $n < n_g$, which results in our FLD allocation rule in normal environment:

FLD allocation rule: If $n \leq n_g$, the ratio of budget allocated to design i is $p_i = p_i^*(1+\frac{1}{n_g+T/2}c_i)$, $i = 1, 2, ..., r$. If $n > n_g$, $p_i = p_i^*(1+\frac{1}{n+T/2}c_i)$, $i = 1, 2, ..., r$.

We now illustrate that this setting is reasonable.

Theorem 3.1 *FLD allocation rule performs no worse than ALD/OCBA rule. Furthermore, if $I_i(\gamma)$'s are not all equal, FLD allocation rule always performs better than ALD/OCBA rule.*

Proof: If $I_1(\gamma) = ... = I_r(\gamma)$, $c_1 = ... = c_r = 0$, FLD rule is identical with ALD/OCBA rule.

Suppose $I_i(\gamma)$'s are not all equal. Remember $f_2(x) = \sum_{i=1}^r \int_{-\infty}^{\sqrt{\frac{2n}{T}(1+xc_i)}} e^{-\frac{t^2}{2}} dt$, $f_2'(x) = \sum_{i=1}^r e^{-\frac{n}{T}(1+xc_i)}(\frac{2n}{T}(1+xc_i))^{-\frac{1}{2}}\frac{n}{T}c_i$. If $n \geq n_g$, lemma 1 has proved that FLD's performance is always better than ALD/OCBA. If $n < n_g$, when $c_i \geq 0$, $e^{-\frac{n}{T}xc_i} \geq e^{-\frac{n_g}{T}xc_i}$, when $c_i < 0$, $e^{-\frac{n}{T}xc_i} < e^{-\frac{n_g}{T}xc_i}$. Therefore,

$$
\begin{aligned}
g_n(p_1, ..., p_r) - g_n(p_1^*, ..., p_r^*) &= f_2(\frac{1}{n_g + T/2}) - f_2(0) \\
&= (\frac{n}{2T})^{\frac{1}{2}} e^{-\frac{n}{T}} \int_0^{\frac{1}{n_g+T/2}} \sum_{i=1}^r e^{-\frac{n}{T}xc_i}(1 + xc_i)^{-\frac{1}{2}} c_i dx \\
&> (\frac{n}{2T})^{\frac{1}{2}} e^{-\frac{n}{T}} \int_0^{\frac{1}{n_g+T/2}} \sum_{i=1}^r e^{-\frac{n_g}{T}xc_i}(1 + xc_i)^{-\frac{1}{2}} c_i dx
\end{aligned}
$$

From lemma 1, we know when $n = n_g$, $g_{n_g}(q_1, ..., q_r) > g_{n_g}(p_1, ..., p_r)$. Hence

$$
\begin{aligned}
g_{n_g}(p_1, ..., p_r) - g_{n_g}(p_1^*, ..., p_r^*) = (\frac{n_g}{2T})^{\frac{1}{2}} e^{-\frac{n_g}{T}} \int_0^{\frac{1}{n_g+T/2}} \sum_{i=1}^r e^{-\frac{n_g}{T}xc_i}(1 + xc_i)^{-\frac{1}{2}} c_i \\
> 0
\end{aligned}
$$

Therefore $\int_0^{\frac{1}{n_g+T/2}} \sum_{i=1}^r e^{-\frac{n_g}{T}xc_i}(1 + xc_i)^{-\frac{1}{2}} c_i > 0$, $g_n(p_1, ..., p_r) > g_n(p_1^*, ..., p_r^*)$. FLD allocation rule performs better than ALD/OCBA when $n < n_g$. ■

3.3.4 FLD Allocation Rule in General Distribution Scenarios

In this subsection, we no longer require that the output distribution is normal. Remember that g_n is represented as

$$g_n(\alpha_1, ..., \alpha_r) = \sum_{i \in \mathcal{S}_Y} P(\bar{X}_i(n\alpha_i) < \gamma) + \sum_{i \in \mathcal{S}_N} P(\bar{X}_i(n\alpha_i) > \gamma)$$

A major difficulty in solving feasibility determination problem in general distribution situation is that g_n does not have closed form expression as in normal distribution case. To facilitate the development of optimal allocation rules, we derive an closed form approximation of g_n.

Let $\Lambda_i(\theta) = \log E[\exp(\theta X_{i,j})]$ be the cumulant generating function of $X_{i,j}$, for $i = 1, ..., r$. Let $I_i(\cdot)$ be the large deviations rate function for design i

$$I_i(x) = \sup_{\theta \in \mathbb{R}} (\theta x - \Lambda_i(\theta))$$

Since $\theta = 0$ always leads to $\theta x - \Lambda_i(\theta) = 0$, $I_i(x) \geq 0$. In assumption 2 we set $\mu_i \neq \gamma$, hence $I_i(\gamma) > 0$, for $i = 1, ..., r$. Remember WLOG, we assume $I_1(\gamma) \leq I_2(\gamma) \leq ... \leq I_r(\gamma)$. In the following, we consider $i \in \mathcal{S}_Y$ and $i \in \mathcal{S}_N$ individually. First let us consider the case $i \in \mathcal{S}_Y$, which means the design is actually feasible, $\mu_i < \gamma$. To bound the term $P(\bar{X}_i(n\alpha_i) < \gamma)$, we observe for $\theta \geq 0$

$$
\begin{aligned}
P(\bar{X}_i(n\alpha_i) < \gamma) &= 1 - P(\bar{X}_i(n\alpha_i) \geq \gamma) \\
&= 1 - E[\mathcal{I}_{\bar{X}_i(n\alpha_i)-\gamma\geq 0}] \\
&\geq 1 - E[\exp(n\alpha_i\theta(\bar{X}_i(n\alpha_i) - \gamma))] \\
&= 1 - e^{-n\alpha_i\theta\gamma} \prod_{j=1}^{n\alpha_i} E[e^{\theta X_{i,j}}] \\
&= 1 - e^{-n\alpha_i(\theta\gamma - \Lambda_i(\theta))} \qquad (3.7)
\end{aligned}
$$

where $\mathcal{I}$ is the indicator function.

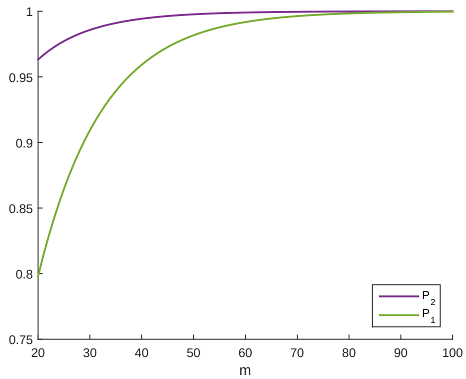
It was shown in (Dembo and Zeitouni [26]) that for random variable X, if $x > E[X]$, we have

$$I(x) = \sup_{\theta\geq 0}(\theta x - \Lambda(\theta))$$

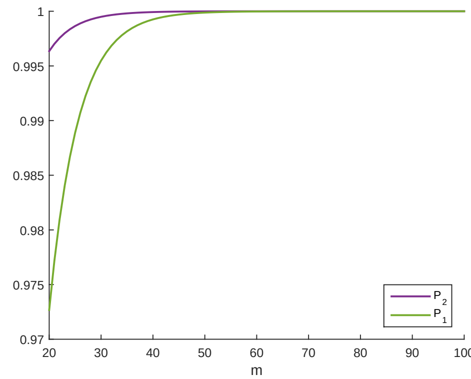
Since $\gamma > \mu_i$, from equation (7) we can derive

$$P(\bar{X}_i(n\alpha_i) < \gamma) \geq 1 - e^{-n\alpha_i I_i(\gamma)}$$

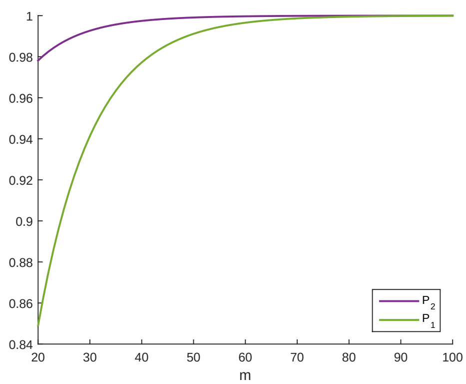
Although the bound may not be tight for a small n, $\lim_{n\to\infty}(1 - e^{-n\alpha_i I_i(\gamma)}) = 1$. It can serve as a good approximation for $P(\bar{X}_i(n\alpha_i) < \gamma)$ when n is large. To verify this, we conduct numerical experiments to compare $P_1 = 1 - e^{-mI(\gamma)}$ with $P_2 = P(\bar{Y}(m) < \gamma)$ under different m values. Here $\bar{Y}(m) = \sum_{i=1}^{m} Y_i$ is the sample mean of m replicates of Y. The comparison is conducted in three distributions, $Y \sim N(0,1)$, $Y \sim Exponential(1)$, and $Y \sim Bernoulli(0.4)$. For each distribution we test two γ values. The results are illustrated in Figure 3.5, from the figure we can see that P_1 converges to P_2 quite fast with m.



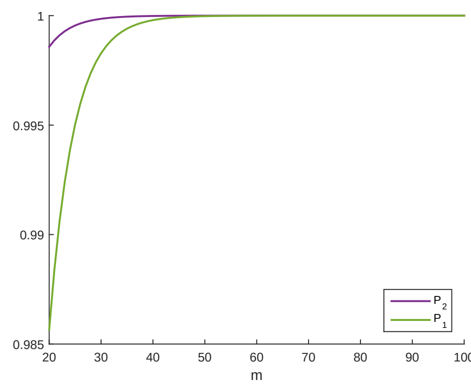
(a) $Y \sim N(0,1)$, $\gamma = 0.4$



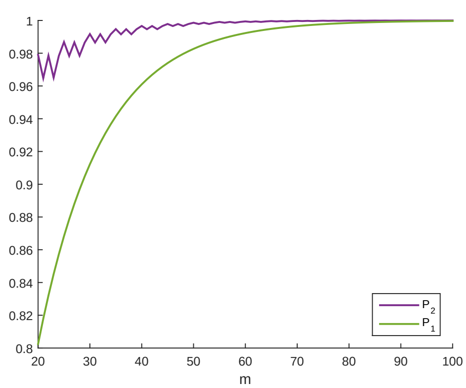
(b) $Y \sim N(0,1)$, $\gamma = 0.6$



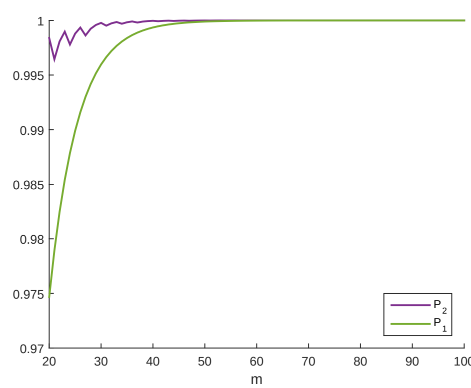
(c) $Y \sim Exponential(1)$, $\gamma = 1.5$



(d) $Y \sim Exponential(1)$, $\gamma = 1.8$



(e) $Y \sim Bernoulli(0.4)$, $\gamma = 0.6$



(f) $Y \sim Bernoulli(0.4)$, $\gamma = 0.7$

Figure 3.3: Convergence of $P_1 = 1 - e^{-mI(\gamma)}$ to $P_2 = P(\bar{Y}(m) < \gamma)$ with m.

Similarly for $i \in \mathcal{S}_N$, we can deduce

$$P(\bar{X}_{ij}(n\alpha_i) > \gamma) \geq 1 - e^{-n\alpha_i I_i(\gamma)}$$

We use the lower bound $1-e^{-n\alpha_i I_i(\gamma)}$ to approximate $P(\bar{X}_{ij}(n\alpha_i) > \gamma)$. Now we have a closed form expression to approximate g_n, $g_n(\alpha_1, ..., \alpha_r) = \sum_{i=1}^{r}(1 - e^{-n\alpha_i I_i(\gamma)})$. The original budget allocation problem $\mathcal{P}$ can be transformed to

$$\begin{aligned} Problem\ \mathcal{P}2 : \min_{\alpha_1,\ldots,\alpha_r} & \sum_{i=1}^{r} e^{-n\alpha_i I_i(\gamma)} \\ s.t. & \sum_{i=1}^{r} \alpha_i = 1 \\ & \alpha_i \geq 0, i = 1, ..., r \end{aligned}$$

As in the previous subsection, let $c_i = \log(I_i(\gamma)) \sum_i \frac{1}{I_i(\gamma)} - \sum_i \frac{\log(I_i(\gamma))}{I_i(\gamma)}$, for $i = 1, 2, ..., r$. Observe that $\sum_{i=1}^{r} \frac{c_i}{I_i(\gamma)} = 0$ still holds. Hence same as in the previous subsection, $\sum_{i=1}^{r} c_i \geq 0$, the equality holds only when $I_1(\gamma) = ... = I_r(\gamma)$. Let $T = \sum_{i=1}^{r} I_i(\gamma)^{-1}$.

Proposition 3.4 *When $n \geq -c_1$, problem $\mathcal{P}2$ is solved by $\alpha_i = p_i^*(1 + \frac{\alpha_i}{n})$, $i = 1, ..., r$.*

Proof: First we prove that problem $\mathcal{P}2$ is a convex optimization problem. $e^{-n\alpha_i I_i(\gamma)}$ is a convex function of α_i since it is twice differentiable and its second order derivative $n^2 I_i(\gamma)^2 e^{-n\alpha_i I_i(\gamma)}$ is positive. $\sum_{i=1}^{r} e^{-n\alpha_i I_i(\gamma)}$ is sum of convex functions, thus it is a convex function. Since all the constraints of problem $\mathcal{P}2$ are linear, we can conclude that it is a convex optimization problem.

We now omit the constraint $\alpha_i \geq 0$. Consider the problem $\widetilde{\mathcal{P}2}: \min_{\alpha_1,\ldots,\alpha_r} \sum_{i=1}^r e^{-n\alpha_i I_i(\gamma)}$ $s.t. \sum_{i=1}^r \alpha_i = 1$. This is still a convex optimization problem, the solution satisfying KKT conditions is the optimal solution to the problem (Boyd and Vandenberghe [12]). We use λ to denote a constant, the KKT conditions are stated as follows:

$$nI_i(\gamma)e^{-n\alpha_i I_i(\gamma)} = \lambda, i = 1, ..., r \tag{3.8}$$

$$\sum_{i=1}^r \alpha_i = 1 \tag{3.9}$$

Taking log function of both sides of condition (3.8), the condition is equivalent with

$$\log I_i(\gamma) - nI_i(\gamma)\alpha_i = \lambda, i = 1, ..., r$$

We plug in $\alpha_i = p_i^*(1 + \frac{c_i}{n})$,

$$\begin{aligned}\log I_i(\gamma) - nI_i(\gamma)\alpha_i &= \log I_i(\gamma) - \frac{n}{T}(1 + \frac{c_i}{n}) \\ &= \log I_i(\gamma) - \frac{n}{T} - \frac{c_i}{T} \\ &= \frac{1}{T}\sum_{i=1}^r \frac{\log I_i(\gamma)}{I_i(\gamma)} - \frac{n}{T}\end{aligned}$$

which is independent of special i. Therefore $\alpha_i = p_i^*(1 + \frac{c_i}{n})$ satisfies condition (3.8). $\sum_{i=1}^r p_i^*(1 + \frac{c_i}{n}) = \sum_{i=1}^r p_i^* + \frac{1}{nT}\sum_{i=1}^r \frac{c_i}{I_i(\gamma)} = \sum_{i=1}^r p_i^* = 1$. $\alpha_i = p_i^*(1 + \frac{c_i}{n})$ satisfies condition (3.9). Hence $\alpha_i = p_i^*(1 + \frac{c_i}{n})$ is the solution to problem $\widetilde{\mathcal{P}2}$. When $n \geq -c_1$, $p_i^*(1 + \frac{c_i}{n}) \geq p_i^*(1 + \frac{c_1}{n}) \geq p_i^*(1 - \frac{c_1}{c_1}) = 0$. $\alpha_i = p_i^*(1 + \frac{c_i}{n})$ satisfies constraint $\alpha_i \geq 0$. $\alpha_i = p_i^*(1 + \frac{c_i}{n})$ solves problem $\mathcal{P}2$. ■

Same as in normal distribution case, the optimal allocation rule has the form $p_i^*(1+$

xc_i), where $x = O(\frac{1}{n})$. If $I_1(\gamma) = ... = I_r(\gamma)$, $c_1 = ... = c_r = 0$. The optimal allocation rule degenerates to rule $\boldsymbol{p^*}$. Suppose not all $I_i(\gamma)$'s are equal. Let $f_3(x) = \sum_{i=1}^{r} e^{-nI_i(\gamma)p_i^*(1+xc_i)}$. $f_3'(x) = -\frac{n}{T}e^{-\frac{n}{T}}\sum_{i=1}^{r} e^{-\frac{n}{T}xc_i}c_i$, $f_3''(x) = \frac{n^2}{T^2}e^{-\frac{n}{T}}\sum_{i=1}^{r} e^{-\frac{n}{T}xc_i}c_i^2 > 0$. Note that $f_3'(0) = -\frac{n}{T}e^{-\frac{n}{T}}\sum_{i=1}^{r} c_i < 0$. If x is positive and small, the allocation based on ratio $p_i^*(1 + xc_i)$ should perform better than based on ratio p_i^*.

When we use $\sum_{i=1}^{r}(1 - e^{-n\alpha_i I_i(\gamma)})$ to approximate g_n, we derive the value of x as $\frac{1}{n}$. However in previous subsection, when we use exact closed form expression for g_n in normal case, we figured out that $\frac{1}{n}$ is slightly larger than the optimal choice of x and we set x to be $\frac{1}{n+T/2}$. Since small x guarantees superiority here we choose to use the more conservative $x = \frac{1}{n+T/2}$ instead of $x = \frac{1}{n}$. The allocation rule will be $p_i^*(1 + \frac{c_i}{n+T/2})$. Note that the approximation of g_n is more accurate when n is large, in which case the difference of $\frac{1}{n}$ and $\frac{1}{n+T/2}$ is negligible.

The approximation of g_n works quite well when n is large. However, when n is small, the approximation could be not so accurate. Hence similar with the normal case, we want to set a threshold n_g. When $n \leq n_g$, the allocation ratio is fixed to be $p_i^*(1+\frac{c_i}{n_g+T/2})$, for $i = 1, ..., r$. In normal case, n_g is selected so that $1 + \frac{c_1}{n_g+T/2} = \frac{3-\sqrt{5}}{2}$. In general distribution case, we can set a parameter ϵ, $0 < \epsilon < 1$. $n_g = \frac{c_1}{\epsilon-1} - \frac{T}{2}$. By this setting $1 + \frac{c_1}{n_g+T/2} = \epsilon$.

In summary, the FLD allocation rule could be generalized to general distribution scenarios. The only change is the setting of threshold n_g. In general distribution case, $n_g = \frac{c_1}{\epsilon-1} - \frac{T}{2}$, $0 < \epsilon < 1$. ϵ could be selected based on concrete examples and practical experiences. The superior performance of FLD allocation rule in general distribution case is also verified by the numerical experiments.

3.3.5 FLD Allocation Procedure

In this subsection, we present our budget allocation algorithm for FD problem. Initially the LD rate function of each design is unknown, so must be estimated via simulation. Therefore we propose a heuristic sequential allocation algorithm. First we warm-up each design with n_0 replicates and estimate the LD rate function of each design. At each step, these estimates are used to estimate the optimal allocation rule. Based on the optimal rule we allocate additional Δ replicates. Combining the outputs of new replicates we update our estimate of the LD rate function. We iterate this procedure until the total budget is exhausted. The algorithm is stated as follows:

$\boldsymbol{Finite\ simulation\ budget\ LD-based\ (FLD)\ Algorithm}$

1 For a set of r designs, specify the total simulation budget n, the initial simulation budget for each design n_0, the incremental budget Δ and the parameter ϵ, $0 < \epsilon < 1$.

2 Iteration counter $t \leftarrow 0$. Perform n_0 simulation replications to each design, $N_1^t = N_2^t = ... = N_r^t = n_0$.

3 If $N^t = \sum_{i=1}^r N_i^t \geq n$, stop. Otherwise,

  a update LD rate function $I_i(\gamma)$ for each design

  b compute p_i^* and c_i for $i = 1, ..., r$, compute $T = \sum_{i=1}^r I_i(\gamma)^{-1}$

  c compute $d = \max\{\frac{c_1}{\epsilon-1} - \frac{T}{2} - N^t, 0\}$

  d compute allocation ratio $\alpha_i = p_i^*(1 + \frac{c_i}{N^t+d+T/2}), i = 1, ..., r$

  e perform $\Delta_i = \max\{0, \alpha_i(N^t+\Delta)-N_i^t\}$ simulation replications to design $i, i = 1, ..., r$

  f $N_i^{t+1} = N_i^t + \Delta_i, t \leftarrow t + 1$

4 Determine the feasibility of each design based on sample means of the performance measure.

One important step in the preceding algorithm is the estimate of LD rate function $I_i(\gamma)$. Denote the empirical cumulant generating function of design i as $\Lambda_i^{(m)}(\theta) = \log(\frac{1}{m}\sum_{j=1}^{m} e^{\theta X_{i,j}})$, here m is the number of samples. The LD rate function of design i is

$$\begin{aligned} I_i^{(m)}(\gamma) &= \sup_{\theta\in\mathbb{R}}(\theta\gamma - \Lambda_i^{(m)}(\theta)) \\ &= \theta_i^*\gamma - \Lambda_i^{(m)}(\theta_i^*) \end{aligned}$$

where θ_i^* solves the root problem

$$\gamma = \frac{\sum_{j=1}^{m} X_{i,j} e^{\theta_i^* X_{i,j}}}{\sum_{j=1}^{m} e^{\theta_i^* X_{i,j}}}$$

If the distribution of the observations of each design is known or assumed, the estimate of LD rate function can be significantly simplified. For example, if $X_{i,j}$ is normally distributed as $N(\mu_i, \sigma_i^2)$, LD rate function $I_i(\gamma) = \frac{(\gamma-\mu_i)^2}{2\sigma_i^2}$. Therefore after we perform a certain number of simulation replications of design i, we estimate the sample mean and sample variance. The estimate of LD rate function can then be easily derived by plugging the sample mean and sample variance into the previous formula. Similarly, if $X_{i,j}$ follows Bernoulli distribution with success probability μ_i, LD rate function $I_i(\gamma) = \gamma \log\frac{\gamma}{\mu_i} + (1-\gamma)\log\frac{1-\gamma}{1-\mu_i}$. Thus we can estimate μ_i first and then using the formula to obtain the estimate of $I_i(\gamma)$.

Remark 3.1 *It was shown in (Glynn and Juneja [44]) that the estimate of LD rate function is consistent. Therefore as more and more budget is allocated, the estimated* *optimal allocation rule will converge to the exact optimal rule. The allocation procedure is asymptotically valid.*

3.4 Numerical Experiments

In this section, we test the proposed simulation budget allocation procedure for FD problem by comparing it with following allocation procedures.

- *Equal Allocation (EA)*: The total simulation budget is allocated equally to each design. This is the simplest allocation rule and has been widely applied.
- *Asymptotic LD-based Allocation (ALD)*: ALD method allocates simulation budget to each design based on the asymptotically optimal rule that maximizes the exponential rate of decay for the expected number of incorrect determinations. The rule is derived using the LD techniques and allows the systems have a general lighted tail distribution. (Szechtman and Yücesan [83]) discussed ALD method in detail.
- *OCBA*: OCBA is a class of sequential simulation budget allocation procedures for normally distributed designs, initially proposed by (Chen [17]). Based on the approach described in (Lee et al. [58]), we derive a variation for FD problem. In this variation, at each iteration, we allocate an incremental budget to the designs according to $\alpha_i = \frac{\sigma_i^2/(\mu_i-\gamma)^2}{\sum_{j=1}^{r}\sigma_j^2/(\mu_j-\gamma)^2}$, where μ_i and σ_i are mean and variance of design i.

We first explore the relative performance of these algorithms and our FLD algorithm on three illustrative examples with normal or non-normal distribution and on one toy application in facility-sizing determination. We then present an emergency department setup application, which is adapted from Ahmed and Alkhamis [1].

3.4.1 Illustrative Example Problems

The relative effectiveness of the algorithms is measured by the expected number of the correct determinations g_n, where n is the total simulation budget. To make the comparisons convenient, in this subsection we rescale the g_n. Assume we have r systems, we use $\frac{g_n}{r}$, the expected ratio of correct determinations (ERCD) as our performance measure. We introduce the following illustrative examples.

- *Example 1*: Ten designs with $X_{i,j} \sim N(i, \sigma^2)$, $i = 1, 2, ..., 10$, $\sigma = 10$. The threshold $\gamma = 6.4$. Designs $1, 2, 3, 4, 5, 6$ are feasible.

- *Example 2*: Twenty designs with $X_{i,j} \sim \mathit{Exponential}(\lambda_i)$, rate $\lambda_i = 10.2 - 0.2i$, $i = 1, 2, ..., 20$. That means the mean μ_i of system i is $\frac{1}{10.2-0.2i}$. The threshold $\gamma = 0.126$. Designs $1, 2, .., 11$ are feasible.

- *Example 3*: Five designs with $X_{i,j} \sim \mathit{Bernoulli}(\mu_i)$, success probability $\mu_i = 0.45 + 0.05i$, $i = 1, 2, ..., 5$. The threshold $\gamma = 0.61$. Designs $1, 2, 3$ are feasible.

- *Example 4*: It is a facility-sizing problem which is adapted from (Rengarajan and Morton [74]). Suppose there are 20 facilities at which nonnegative capacities $x_i, i = 1, ..., 20$ are to be installed, $\boldsymbol{x} = [x_1, ..., x_{20}]^{\mathrm{T}}$. The random demand at facility i is denoted ξ_i, and the joint distribution of the random vector $\xi = [\xi_1, ..., \xi_{20}]^{\mathrm{T}}$ follows a 20 dimensional truncated multivariate normal distribution. The distribution has mean 10 and variance 1 for each component, and correlation coefficient $\rho_{i,j} = 0.8, i \neq j$. ξ is truncated so that $\xi \geq 0$.

A realization of the demand $\xi = [\xi_1, ..., \xi_{20}]^{\mathrm{T}}$ is said to be satisfied if $x_i \geq \xi_i$, for all $i = 1, ..., 20$. Thus the risk of failing to satisfy demand is $p(\boldsymbol{x}) = \mathbb{P}(\xi \nleq \boldsymbol{x})$, where $\xi \nleq \boldsymbol{x}$ means there exists at least one facility i such that $\xi_i > x_i$. We set a risk parameter 0.1. A proposed $\boldsymbol{x}$ is defined to be feasible if $\mathbb{P}(\xi \nleq \boldsymbol{x}) \leq 0.1$. The per unit cost of installing capacity for each capacity is 1. We now have 5 alternative designs of $\boldsymbol{x}$, which are summarized in Table 3.1. In the table (i, j, k) means we have i facilities with capacity 13, j facilities with capacity 12, k facilities with capacity 11, thus the cost should be $13 * i + 12 * j + 11 * k$. For example, design 5 is $(8, 10, 2)$, which means that we have 8 facilities with capacity 13, 10 facilities with capacity 12 and 2 facilities with capacity 11. The total cost is $13*8+12*10+11*2 = 246$. Our goal is to select the $\boldsymbol{x}$ with lowest installation cost from among the feasible designs. Since the total cost of each design is deterministic, we need only to use simulation to detect the feasibility of each $\boldsymbol{x}$. From the table we can see design 2 is the optimal one.

Table 3.1: The five designs for the facility-sizing problem.

Design	1	2	3	4	5
x setting	$(0, 20, 0)$	$(10, 10, 0)$	$(20, 0, 0)$	$(16, 0, 4)$	$(8, 10, 2)$
risk $p(x)$	0.1045	0.0796	0.0096	0.2862	0.2255
feasible or not	N	Y	Y	N	N
cost	240	250	260	252	246

Y means feasible, N means infeasible.

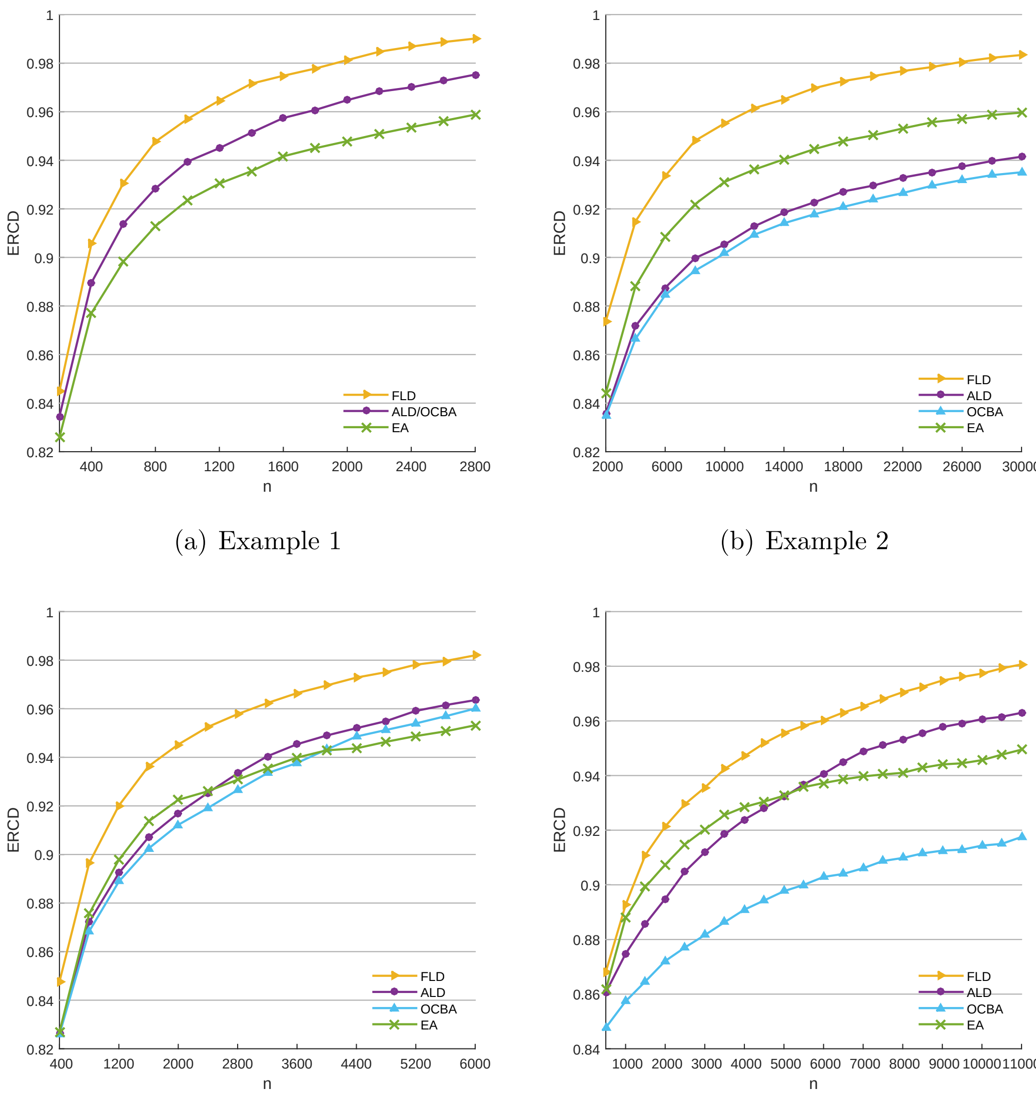
In comparing the procedures, the measure ERCD is estimated based on 5000 independent experiments of each algorithm. In FLD, we set the initial budget per design, the incremental budget per iteration and the maximum budget as Table 3.2. Sequential procedures ALD and OCBA follow the same parameter settings. FLD has an additional parameter ϵ. We use the ϵ value in normal case, that is, $\frac{3-\sqrt{5}}{2} \doteq 0.38$, in all four examples.

Table 3.2: Parameter settings of FLD for different examples.

	Initial budget	Incremental budget	Maximum budget
Ex.1	10	50	2800
Ex.2	10	50	30000
Ex.3	10	50	6000
Ex.4	10	50	11000

The performance of the four procedures with different budgets and simulation budget needed to reach ERCD level 0.97 are illustrated in Figure 3.4 and Table 3.3. If the observations of designs have normal distribution, ALD and OCBA have the same allocation rule. Hence in example 1, the performances of ALD and OCBA are illustrated simultaneously by one curve. We can see that in all four problem settings FLD outperforms other procedures. It is significantly more efficient than EA, which is most commonly used in practice. Thus practitioners can substantially enhance efficiency by using FLD procedure instead.

The unstable performance of ALD and OCBA seems surprising. In example 1 ALD performs better than EA while in example 2, EA performs better than ALD. In example 3 and 4, ALD performs worse than EA when the total simulation budget is small. When the total simulation budget is above some threshold, the performance of ALD surpasses that of EA. This phenomenon of unstable performance of ALD is due to the effect of



(a) Example 1 (b) Example 2

(c) Example 3 (d) Example 4

Figure 3.4: ERCD comparison in different examples.

Table 3.3: Simulation budget needed to reach ERCD level 0.97.

	FLD	ALD	OCBA	EA
Ex.1	1400	2400	2400	4600
Ex.2	16300	88900	>100000	51200
Ex.3	4100	7100	7800	12900
Ex.4	8000	13900	53700	30000

initial budget setting.

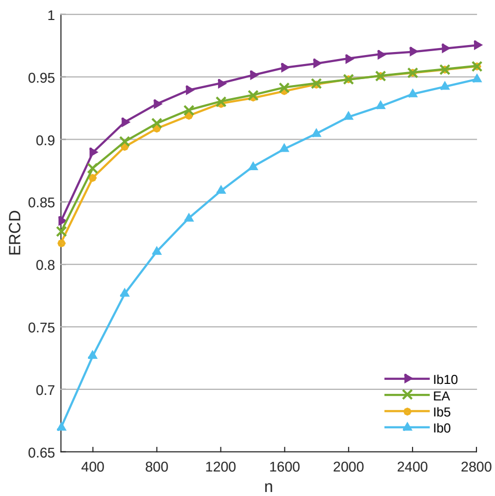
To illustrate this phenomenon we use a two design example. Suppose the two designs are distributed as $N(2, 2^2), N(4, 2^2)$ respectively. Assume the threshold value is 3.9. According to ALD allocation rule, the idealized optimal budget allocation fraction is $(0.0028, 0.9972)$, the second design will consume 99.72% of the total budget. Hence we can see that when the total simulation budget is limited the fraction of budget allocated to the first design is too few, which impedes simulationist from obtaining the optimal ERCD level. Assume we have total budget 400, according to the ALD rule, we should simulate the first design once and the second design 399 times. This allocation yields ERCD 0.83, which is not so satisfying compared to the 0.88 ERCD level the equal allocation yields.

However, in practice we have to assign an initial budget n_0 to each design to estimate the parameters. This forces us to allocate at least n_0 budget to each relatively easy design, even this allocation breaks the theoretical ALD rule. In this two design example if we set $n_0 = 5$, the ALD allocation is changed to be $(5, 395)$, which yields ERCD 0.91. Now ALD exhibits a better performance than the equal allocation. We test the relationship between the performance of ALD and the initial budget setting in numerical example 1, 2 and 3, the results are demonstrated in Figure 3.5.

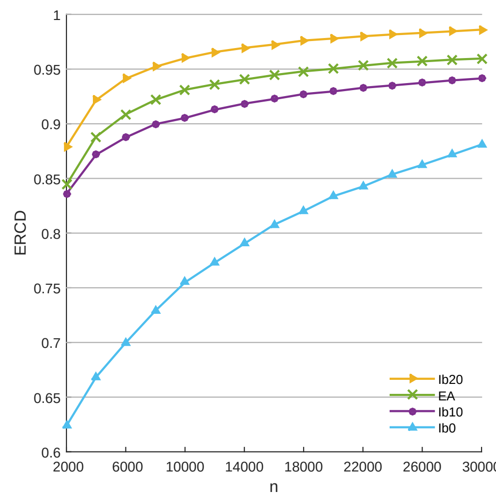
In Figure 3.5, Ib0 means we use exact values of parameters when deriving ALD rule so we do not need initial budget to estimate them, thus the initial budget is set to be 0. Ib5, Ib10 and Ib20 means that we set the initial budget to be 5, 10 and 20 respectively. From the figure we can see the idealized implementation of ALD (Ib0) performs significantly worse than EA in all three examples. The existence of initial budget could improve the performance of ALD. Different settings of initial budget make ALD exhibit different performance compared to EA, which is in accordance with our observation in Figure 3.4.

The increase of the initial budget seems to be a good method to improve the ALD performance. However, it is not suffice to solve the drawback of ALD. On the one hand, we do not know the optimal initial budget setting in advance. A high initial budget could make some designs obtain unnecessarily high budget, which prohibits the algorithm from obtaining optimal performance. On the other hand, there is no guarantee that there exists an initial budget which could make ALD perform better than EA. For instance, in the two design example, if the total budget is 10, the optimal allocation should be $(6, 4)$. In this case, since the ALD allocation is $(0.0028, 0.9972)$, no matter what the initial budget is the budget allocated to the first design is always less than that allocated to the second one. The performance of ALD could not be better than EA for any initial budget setting. The increase of the initial budget could not solve the drawback of ALD, which motivate us to seek more intelligent allocations. Our FLD is a possible candidate.

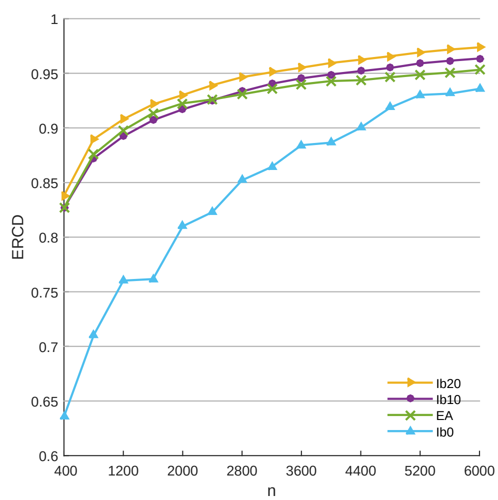
The situation of OCBA is similar with ALD. However, OCBA is designed in normal environment. It suffers from the skewness of the design output distribution. Hence in example 2, 3 and 4, OCBA behaves even worse than ALD. Especially in example 4, the



(a) Example 1



(b) Example 2



(c) Example 3

Figure 3.5: The effect of different initial budget settings in ALD procedure.

high skewness of output distribution affect the performance of OCBA heavily.

In order to achieve ERCD level 0.97, FLD can reduce the simulation budget by 41.7%, 68.2%, 42.3% and 42.4% on the four examples respectively compared to the second best method and save much more budget compared to the other 3 methods.

3.4.2 Emergency Department Setup

To demonstrate the effectiveness of our FLD method in a more realistic application setting, we use an emergency department setup example, which is introduced by Ahmed and Alkhamis [1]. Here we use the version provided by Gutierrez [48] in the Simulation Optimization Library.

Assume we want to set up an emergency department. The department receives both walk-in patients and ambulance patients. Walk-in patients go through the receptionist and then wait for availability of an examination room, while ambulance patients enter the examination queue directly. In the examination room, a doctor will decide if the patient needs further tests. If so, the patient leaves the examination room and enters a test queue until a lab technician is available. After the test, the patient re-enters the examination queue.

If no extra tests are necessary, the doctor will assess the status of the patients and decide if they need treatment. Patients who do not require treatment are provided their medication and released immediately. Patients who need treatment are classified into two categories, critical or non-critical. Non-critical patients are routed into the treatment room and wait for a minor treatment, which is performed by a treatment room nurse. Critical patients are routed into the emergency room, where an emergency room nurse provides complete treatment and close observation to the patient. After the treatment, the patients leave the system. The whole process is depicted in figure 3.6.

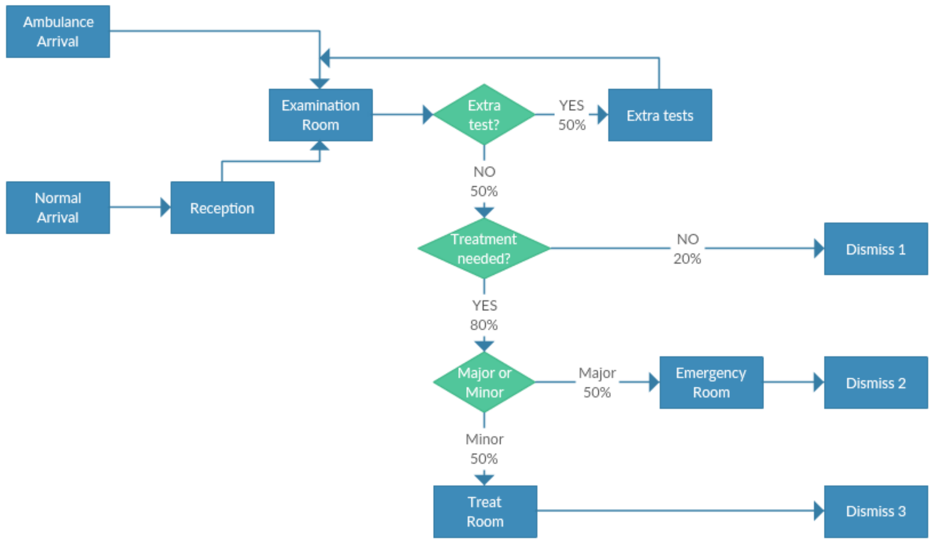


Figure 3.6: Emergency department process view

The hospital wants the total waiting time for the critical patients must not exceed 2 hours. Assume the salary of receptionists, doctors, lab technicians, and nurses are $\$40,000$, $\$120,000$, $\$50,000$, and $\$35,000$ respectively. The goal is to find the configuration of the employees that has the lowest total salary while satisfying the aforementioned waiting time constraint. We now have five proposals of employee configuration. Each configuration has the form (i, j, k, l), where i represents the number of receptionists, j represents the number of doctors, k is the number of lab technicians, and l is the number of nurses in emergency room. The number of nurses in treat room does not affect the waiting time of the critical patients, hence we do not take this number into account. The critical patients waiting time, the feasibility, and the total salary of each configuration are summarized in table 3.4. From the table we can see configuration 2 is the best choice.

In our numerical experiment, in each simulation run we use a 4 day warm-up period

Table 3.4: The five configurations of the emergency department employee.

configuration	1	2	3	4	5
employee setting	$(1,3,2,7)$	$(1,3,2,8)$	$(1,3,3,6)$	$(1,3,3,7)$	$(1,4,2,5)$
waiting time	2.03	1.86	2.49	1.95	12.02
feasible or not	N	Y	N	Y	N
total salary	745,000	780,000	760,000	795,000	795,000

Y means feasible, N means infeasible.

and run for 100 more days. The obtained critical patient waiting time of each run is the average waiting time of the critical patients during the 100 days. Therefore we can assume this waiting time is approximately normally distributed among different runs. The total simulation budget is 40. In ALD/OCBA and FLD setting, the initial budget is 4 for each configuration and the incremental budget is 5. The parameter ϵ for FLD algorithm is still set to be 0.38.

The performances of each algorithm are reported in table 3.5. The expected number of correct determinations g_n is estimated based on 400 independent experiments of each algorithm. The standard errors are in the column *std err*. From the table we can see, our FLD algorithm is superior to other algorithms.

Table 3.5: The performances of different algorithms in emergency department setup problem.

algorithm	g_n	*std err*
EA	4.48	3.04e−2
ALD/OCBA	4.61	2.75e−2
FLD	4.72	2.30e−2

Chapter 4

Feasibility Determination via Stochastic Control

The feasibility determination (FD) budget allocation process can also be modeled as a stochastic control problem (SCP). In this chapter, we first compare the SCP approach with the previous frequentist approach to demonstrate the necessity of considering FD in SCP framework. We then formulate the FD as a SCP, and propose a one-step lookahead policy. The dynamic implementation of FLD method is also discussed. Numerical examples are provided to illustrate the performance of our approaches.

4.1 The Necessity of Stochastic Control Approach

In the previous chapter, we formulate the FD budget allocation problem as a static optimization problem. That is, let $g_n(\alpha_1, ..., \alpha_r)$ denote the expected number of correct determinations under total budget n. We solve

$$
\begin{aligned}
Problem\ \mathcal{P} : &\max_{\alpha_1,...,\alpha_r} g_n(\alpha_1, ..., \alpha_r) \\
s.t. &\sum_{i=1}^{r} \alpha_i = 1 \\
&\alpha_i \geq 0, i = 1, ..., r
\end{aligned}
$$

The solution of the problem $\mathcal{P}$ is deemed as the optimal allocation ratio. However, in Figure 3.5, we note that the performance of allocation procedure with true parameters is worse than the heuristic sampling procedure in which the parameters are unknown and need to be estimated. To see this more clearly, we design an experiment with 10 identical alternatives follow normal distribution $N(1, 10^2)$. The threshold is set as $\gamma = 0$. By symmetry, we know equal allocation (EA) is the optimal solution of the static optimization problem $\mathcal{P}$.

We allocate the budget by EA and ALD to decide the feasibility of each design. In ALD, 10 initial replications are allocated to each alternative to estimate the unknown parameters at the first stage, and 20 incremental budget is added sequentially until total budget 600. ERCD is estimated by 10000 Macro simulations. In Figure 4.1, we can see that the ALD procedure denoted as Heuristic has even better performance than EA/OPT that follows the optimal solution of the static optimization problem $\mathcal{P}$.

This example demonstrates that the static optimization approach is inadequate for the FD budget allocation problem. It is possible that a design that is theoretically easy to identify its feasibility (due to the large difference between its mean and the threshold, or the small variance of the simulation noise, or both) may exhibit performance close to the threshold during the simulation. In this case, it needs much more simulation

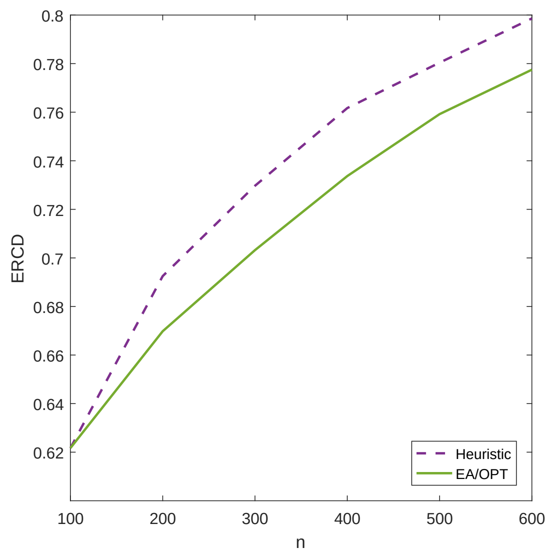


Figure 4.1: Comparison of Optimal EA and Heuristic ALD.

budget than the theoretically optimal value. On the contrary, it is possible that a design with actual performance close to the threshold has simulation results far from the threshold, hence there is no need to consume so much budget as expected. In summary, we should decide the budget allocation based on the dynamic simulation results, not based on a predetermined theoretical optimal ratio. The SCP framework is a more realistic description of the FD budget allocation problem. Next we formulate the problem as a SCP.

4.2 SCP Formulation

In this section, we propose a rigorous dynamic sampling allocation framework for FD, where the dynamic sampling decision is a SCP. Suppose we have r alternative designs, the performance of each design μ_i, $i = 1, 2, ..., r$ is unknown and we can only estimate them by sampling, $\boldsymbol{\mu} = \{\mu_1, ..., \mu_r\}'$. The threshold is γ and a design is defined as feasible if $\mu_i \leq \gamma$. $\mathcal{S}_Y$ is the set consists of all feasible designs. In this chapter, for simplicity we use $\mathcal{S}$ instead of $\mathcal{S}_Y$. Given a total simulation budget, we want to determine the feasible set $\mathcal{S} = \{i : \mu_i \leq \gamma\}$.

For each design $i = 1, 2, ..., r$, let $q(\cdot|\theta_i)$ be the probability density function or probability mass function for samples from design i, where θ_i comprises all unknown parameters residing in a parameter space Θ. $\boldsymbol{\theta} = \{\theta_1, ..., \theta_r\}'$. Generally, the mean $\mu_i \in \theta_i$, $i = 1, 2, ..., r$. In Bayesian setting, we place a prior probability distribution on each unknown θ_i. The prior distribution expresses our subject beliefs about the parameter. It could come from historical knowledge, expert opinion, or personal experience. If we know little or no information about the parameter, we can use some uninformative prior. To facilitate computation, we adopt conjugate prior, $\theta_i \sim f(\cdot|\zeta_i^{(0)})$, $\zeta_i^{(0)}$ contains all hyper-parameters for the prior distribution of θ_i and resides in state space Λ. Denote by $\boldsymbol{\zeta}^{(0)}$ the vector composed of $\zeta_i^{(0)}$ with i ranging from 1 to r. It is generally tractable to find conjugate priors for distributions coming from exponential family (DeGroot [25]).

Time is indexed by $t = 1, 2, ..., n$. Since the prior is conjugate, at each time t the posterior distribution of θ_i is $f(\cdot|\zeta_i^{(t)})$, where $\zeta_i^{(t)}$ is the updated parameter. We denote the vector composed of $\zeta_1^{(t)}, ..., \zeta_r^{(t)}$ as $\boldsymbol{\zeta}^{(\boldsymbol{t})}$. At each time $t \geq 1$, we select a design A_t, $A_t \in \{1, 2, ..., r\}$. We then simulate design A_t once, and observe the corresponding sample $y_t \sim f(\cdot|\theta_{A_t})$. We define an information set $\mathcal{E}_t$, which is the sigma-algebra generated by $\boldsymbol{\zeta}^{(\mathbf{0})}, A_1, y_1, ..., A_t, y_t$. Since the selection decision A_{t+1} can be made only by information through time t, we have $A_{t+1} \in \mathcal{E}_t$.

Let $\mu_i^{(t)}$ denote the posterior mean of design i after t simulation replications have been allocated. At each time t, we can approximate the feasible set $\mathcal{S}$ by $\mathcal{S}_t = \{i : \mu_i^{(t)} \leq \gamma\}$. There is no reward at each selection, and the final reward is set as $h(\mathcal{S}_n, \boldsymbol{\mu}, \gamma) \doteq$

$\sum_{i\in\mathcal{S}_n}\mathbf{1}\{\mathbf{i}\in\mathcal{S}\}+\sum_{\mathbf{i}\notin\mathcal{S}_\mathbf{n}}\mathbf{1}\{\mathbf{i}\notin\mathcal{S}\}$, where $\mathbf{1}\{\cdot\}$ is an indicator function that is one if the event in the bracket is true and is zero otherwise.

An allocation policy is a sequence of selection decisions $\mathcal{A}=(A_1,...,A_n)$. Our goal is to find a policy that maximizes the expected final reward, i.e, to solve the problem

$$\sup_{\mathcal{A}} E^{\mathcal{A}}[h(\mathcal{S}_n,\boldsymbol{\mu},\gamma)] \tag{4.1}$$

4.3 Sampling Allocation Policy

In this section, we derive solutions for problem (4.1). Suppose r alternatives follow independent normal distribution $N(\mu_i,\sigma_i^2)$, $i=1,2,...,r$, with unknown means and known variances. The conjugate prior distribution of μ_i is a normal distribution and we set the prior mean and variance are $\mu_i^{(0)}$ and $(\sigma_i^0)^2$. In the case where the variances are unknown, we use their sample estimates as plug-in for the true values.

Suppose $X_{i,j}$ is the jth replication of design i, t_i is the total number of replications assigned to design i up to time t. The posterior distribution of μ_i is $N(\mu_i^{(t)},(\sigma_i^{(t)})^2)$, where

$$\begin{aligned} m_i^{(t)} &\doteq \frac{\sum_{j=1}^{t_i} X_{i,j}}{t_i} \qquad (4.2)\\ \mu_i^{(t)} &= (\sigma_i^{(t)})^2\left(\frac{\mu_i^{(0)}}{(\sigma_i^{(0)})^2}+\frac{t_i m_i^{(t)}}{\sigma_i^2}\right)\\ (\sigma_i^{(t)})^2 &= \left(\frac{1}{(\sigma_i^{(0)})^2}+\frac{t_i}{\sigma_i^2}\right)^{-1} \end{aligned}$$

If $\sigma_i^{(0)}\to\infty$, $\mu_i^{(t)}=m_i^t$ and $(\sigma_i^t)^2=\sigma_i^2/t_i$, which is called a noninformative prior. In the following, we first construct an myopic one-step lookahead policy, and then we construct a policy based on the FLD rule.

4.3.1 One-step Lookahead Policy

In principle, the finite horizon optimal control problem can be solved by backward induction, however, the computational complexity is typically exponential. We address the computational difficulty by using an approximate dynamic programming (ADP) paradigm that is not guaranteed to achieve the optimal policy, but can overcome the "curse of dimensionality" through value function approximation (VFA) (Powell [72]). The ADP approach relies on VFA to make sampling allocation decision rather than the true value function obtained by backward induction, and keeps learning VFA with more information collected from allocated replications.

Since we seek one-step lookahead policy, we do not consider the total time horizon n and suppose any step t could be the last step. At step t, the value function for correct feasibility determination is

$$\begin{aligned}\mathbb{E}[h(\mathcal{S}_t, \boldsymbol{\mu}, \gamma|\mathcal{E}_t] &= \sum_{i\in\mathcal{S}_t} P(\mu_i \leq \gamma|\mathcal{E}_t) + \sum_{i\notin\mathcal{S}_t} P(\mu_i > \gamma|\mathcal{E}_t)\\ &= \sum_{i\in\mathcal{S}_t} P(Z_i \leq (\gamma - \mu_i^{(t)})/\sigma_i^{(t)}|\mathcal{E}_t) + \sum_{i\notin\mathcal{S}_t} P(Z_i > (\gamma - \mu_i^{(t)})/\sigma_i^{(t)}|\mathcal{E}_t),\end{aligned}$$

where Z_i, $i = 1, \ldots, r$, are independent standard normal random variables. Let $d_i^{(t)} \doteq \left|\left(\mu_i^{(t)} - \gamma\right)/\sigma_i^{(t)}\right|, \quad i = 1, \ldots, r$. A popular bound and approximation of cumulative distribution function of standard normal distribution is $P(Z_i \leq d_i^{(t)}) \geq 1 - \frac{1}{d_i^{(t)}} \exp(-\frac{(d_i^{(t)})^2}{2})$ (Durrett [31]). Use this approximation, we have our VFA as,

$$\widetilde{V}_t(\mathcal{E}_t) = r - \sum_i \frac{1}{d_i^{(t)}} e^{-\frac{(d_i^{(t)})^2}{2}}$$

If the $(t+1)$th replication is the last one, a VFA looking one step ahead at step t by allocating the ith design can be given as follows:

$$\widetilde{V}_t(\mathcal{E}_t; i) = \mathbb{E}\left[\widetilde{V}_{t+1}(\mathcal{E}_t, X_{i,t_i+1})\middle| \mathcal{E}_t\right] \ .$$

Since above expectation is difficult to calculate, we use the following certainty equivalence (Bertsekas [8]) as an approximation:

$$\begin{aligned}\widehat{V}_t(\mathcal{E}_t; i) &\doteq \widetilde{V}_{t+1}\left(\mathcal{E}_t, \mathbb{E}\left[X_{i,t_i+1}\middle| \mathcal{E}_t\right]\right)\\ &= r - \sum_{j\neq i} \frac{1}{d_j^{(t)}} e^{-\frac{(d_j^{(t)})^2}{2}} - |\mu_i^{(t)} - \gamma|^{-1}\left(\frac{1}{(\sigma_i^{(0)})^2} + \frac{t_i+1}{\sigma_i^2}\right)^{-\frac{1}{2}} e^{-\frac{(\mu_i^{(t)}-\gamma)^2}{2}\left(\frac{1}{(\sigma_i^{(0)})^2}+\frac{t_i+1}{\sigma_i^2}\right)}\end{aligned}$$

An approximately optimal allocation policy is given by

$$\widehat{A}_{t+1}(\mathcal{E}_t) = \arg\max_{i=1,\ldots,r} \widehat{V}_t(\mathcal{E}_t; i)$$

To make $\widehat{V}_t(\mathcal{E}_t; i)$ the largest, it is equivalent to make $\widehat{V}_t(\mathcal{E}_t; i) - \widetilde{V}_t(\mathcal{E}_t)$ the largest. This difference is equivalent to

$$\frac{1}{d_i^{(t)}} e^{-\frac{(d_i^{(t)})^2}{2}} \left(1 - \left(\frac{\sigma_i^2 + t_i(\sigma_i^{(0)})^2}{\sigma_i^2 + (t_i+1)(\sigma_i^{(0)})^2}\right)^{\frac{1}{2}} e^{-\frac{(\mu_i^{(t)}-\gamma)^2}{2\sigma_i^2}}\right)$$

Note that when t_i tends to infinity, $d_i^{(t)}$ tends to infinity, and the rightmost bracket part converges to a constant. We use Δ_i to represent this constant. Hence when t_i is sufficient large, $\frac{1}{d_i^{(t)}} e^{-\frac{(d_i^{(t)})^2}{2}}$ is the dominant part of the difference. To see this more clearly, we can observe the log of the approximate difference, $\log \Delta_i - \log d_i^{(t)} - \frac{(d_i^{(t)})^2}{2}$. When t_i is sufficient large, $\log \Delta_i$ is neglible. Hence to make this difference the largest, we need to select design i with the smallest $d_i^{(t)}$. We obtain our approximate optimal policy

$$\widehat{A}_{t+1}(\mathcal{E}_t) = \arg\min_{i=1,\ldots,r} d_i^{(t)} \ . \tag{4.3}$$

This policy is same with the approximately optimal allocation policy (AOAP) presented by Peng [70]. Remember that the large deviation rate function of design i is $I_i(x) = \frac{1}{2}(\frac{\mu_i - x}{\sigma_i})^2$, and the asymptotical optimal allocation ratio $p_i^* = \frac{1/I_i(\gamma)}{\sum_{i=1}^r 1/I_i(\gamma)}, i = 1, 2, ..., r$. From a theoretical perspective, Peng [70] proved that this policy possesses the following desirable asymptotic properties.

Theorem 4.1 *Suppose the sampling distribution for alternative i is $N(\mu_i, \sigma_i^2)$ with unknown mean and known variance, and μ_i follows the conjugate prior, $i = 1, \ldots, r$. AOAP is consistent, i.e.*

$$\lim_{t\to\infty} \mathcal{S}_t = \mathcal{S} \quad a.s.$$

In addition, the sampling ratio of each alternative asymptotically achieves the optimal large deviations ratio p_i^*, i.e.,

$$\lim_{t\to\infty} p_i^{(t)} = p_i^*, \quad a.s. \quad i = 1, .., r,$$

where $p_i^{(t)} \doteq t_i/t$.

4.3.2 The Stochastic Control Approach of FLD

In this subsection, we focus on the stochastic control implementation of FLD rule. To be accordant with the FLD derivation, we adopt the terminal payoff as $h(\mathcal{S}_n, \boldsymbol{\mu}, \gamma) \doteq \sum_{i\in\mathcal{S}_n} \mathbf{1}\{\mathbf{i} \in \mathcal{S}\} + \sum_{\mathbf{i}\notin\mathcal{S}_\mathbf{n}} \mathbf{1}\{\mathbf{i} \notin \mathcal{S}\}$. To ease the computation, we use the noninformative prior.

At step t, suppose a budget $n > t$ is allocated according to a sampling allocation ratio $\boldsymbol{w} = (w_1, ..., w_r)$. We try to optimize the following posterior performance:

$$\begin{aligned} Problem\ \mathcal{P}3 : & \max_{\boldsymbol{w}} V_n(\boldsymbol{w}; \mathcal{E}_t) \\ s.t. & \sum_{i=1}^{r} w_i = 1 \\ & w_i \geq 0, i = 1, ..., r \end{aligned}$$

where

$$V_n(\boldsymbol{w}; \mathcal{E}_t) \doteq E[h(\mathcal{S}_n, \boldsymbol{\mu}, \gamma)|\mathcal{E}_t] \ .$$

The object value of problem $\mathcal{P}3$ is the largest expected final reward we can receive given the information set $\mathcal{E}_t$, hence can be adopted as the value function. We have

$$\begin{aligned} V_n(\boldsymbol{w}; \mathcal{E}_t) &= E\left[\sum_{i \in \mathcal{S}_n} P\left(\mu_i \leq \gamma | \, \mathcal{E}_n\right) + \sum_{i \notin \mathcal{S}_n} P\left(\mu_i > \gamma | \, \mathcal{E}_n\right) \middle| \, \mathcal{E}_t\right] \\ &= E\left[\sum_{i \in \mathcal{S}_n} P\left(Z \leq (\gamma - \mu_i^{(n)})/\sigma_i^{(n)} \middle| \, \mathcal{E}_n\right) + \sum_{i \notin \mathcal{S}_n} P\left(Z > -(\mu_j^{(n)} - \gamma)/\sigma_i^{(n)} \middle| \, \mathcal{E}_n\right) \middle| \, \mathcal{E}_t\right] \\ &= E\left[\sum_{i=1,..,r} \Phi\left(\sqrt{w_i n} |\mu_i^{(n)} - \gamma|/\sigma_i\right) \middle| \, \mathcal{E}_t\right], \end{aligned}$$

where Z is a standard normally distributed random variable and $\Phi(\cdot)$ is its distribution function. By a certainty equivalence (Bertsekas [8]) , we approximate $V_n(\boldsymbol{w}; \mathcal{E}_t)$ by

$$\begin{aligned} g_n^{(t)}(\boldsymbol{w}) &= \sum_{i=1,..,r} \Phi\left(\sqrt{w_i n} |E[\mu_i^{(n)}|\mathcal{E}_t] - \gamma|/\sigma_i\right) \\ &= \sum_{i=1,..,r} \Phi\left(\sqrt{2 w_i n I_i^{(t)}(\gamma)}\right) \ . \end{aligned}$$

where

$$I_i^{(t)}(\gamma) \doteq \frac{1}{2}\left(\frac{\mu_i^{(t)} - \gamma}{\sigma_i}\right)^2, \quad i = 1, \ldots, r.$$

We then consider the following optimization problem:

$$\begin{aligned} \textit{Problem } \mathcal{P}4: \ & \max_{w} g_n^{(t)}(\boldsymbol{w}) \\ & s.t. \sum_{i=1}^{k} w_i = 1, \quad w_i \geq 0, \quad i = 1, \ldots, r. \end{aligned}$$

Similar with Chapter 3, we can show $\Phi(\sqrt{2w_i n I_i^{(t)}(\gamma)})$ is a concave function of w_i. The objective function of problem $\mathcal{P}4$ is sum of concave functions, thus it is also a concave function. Since all the constraints are linear, we can conclude that problem $\mathcal{P}4$ is a convex optimization problem. Thus the solution satisfying the KKT conditions is the optimal solution.

Problem $\mathcal{P}4$ can be approximated solved by FLD allocation rule. Let $T^{(t)} \doteq \sum_{i=1}^{r} 1/I_i^{(t)}(\gamma)$, $w_i^{(t)} \doteq \frac{1/I_i^{(t)}(\gamma)}{T^{(t)}}$, $c_i^{(t)} \doteq \log I_i^{(t)}(\gamma) T^{(t)} - \sum_{j=1}^{r} \log I_j^{(t)}(\gamma)/I_j^{(t)}(\gamma)$. Let $c_{\langle 1 \rangle}^{(t)}$ is the smallest value among all $c_i^{(t)}$, and set $n_0^{(t)} \doteq \frac{-2c_{\langle 1 \rangle}^{(t)}}{\sqrt{5}-1} - \frac{T^{(t)}}{2}$. The FLD allocation rule $\widetilde{w}_i^{(t)}(n)$ is

$$\widetilde{w}_i^{(t)}(n) \doteq \begin{cases} w_i^{(t)}\left(1 + \dfrac{c_i^{(t)}}{n + T^{(t)}/2}\right) & n > n_0^{(t)}, \\ w_i^{(t)}\left(1 + \dfrac{c_i^{(t)}}{n_0^{(t)} + T^{(t)}/2}\right) & n \leq n_0^{(t)}, \end{cases}$$

Based on the property of FLD, we can have some insights about $\widetilde{w}_i^{(t)}(n)$. For example, based on Theorem (3.1), we can see for any n, we have $g_n^{(t)}(\widetilde{\boldsymbol{w}}^{(t)}(n)) \geq g_n^{(t)}(\boldsymbol{w}^{(t)})$. That is, allocation rule $\widetilde{\boldsymbol{w}}^{(t)}(n)$ always has a better approximate value function than the asymptotical allocation rule $\boldsymbol{w}^{(t)}$.

In the stochastic control setting, for any step t and simulation budget $n > t$, the remaining $n - t$ replications can be allocated according to the sampling ratio $\widetilde{\boldsymbol{w}}^{(t)}(n)$.

Particularly, let $n = t+1$ and the “most starving” technique in Chen and Lee [18] can be used to obtain a fully sequential allocation policy as follows:

$$A_{t+1}(\mathcal{E}_t) = \arg\max_{i=1,\dots,r} \left\{ (t+1)\widetilde{w}_i^{(t)}(t+1) - t_i \right\} \ .$$

We use FLD-D to denote this policy, which means dynamic FLD. At any step t, this sequential sampling procedure allocates the next replication to the alternative that has the largest difference between the number of replications suggested by optimizing a posterior performance subject to $t+1$ budget constraint and the actual number replications allocated to that alternative so far.

4.4 Numerical Experiments

In this part, we focus on compare the performances of dynamic approach methods and static approach methods. Analogous with FLD-D, by stochastic control setting and “most starving” technique, we develop a dynamic ALD method (ALD-D). We will test the performance of FLD and ALD with true parameter values, and compare them with FLD-D and ALD-D to demonstrate the effectiveness of stochastic control approach. We also test the performance of the new proposed AOAP approach and the benchmark EA method.

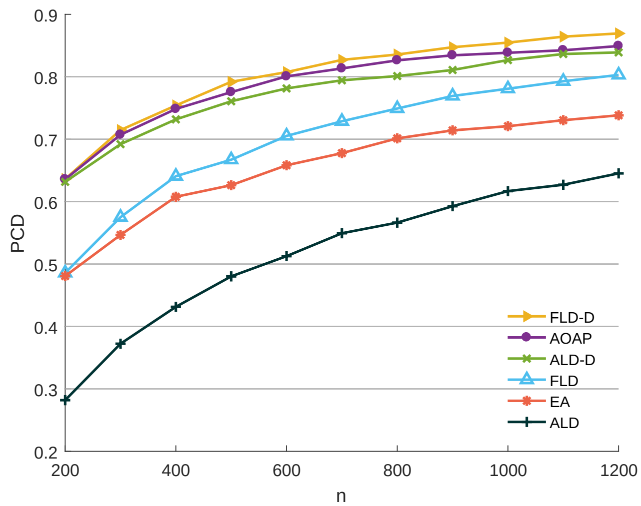
The performance of different procedure is measured by the probability of correct determination (PCD), $P(\mathcal{S}_n = \mathcal{S})$, which is measured by 10000 Macro simulations. The two numerical examples are stated as follows:

- *Example 1*: There are 10 alternatives following $N(\mu_i, \sigma_i^2)$ with $\mu_i \sim N(\mu_i^{(0)}, (\sigma_i^{(0)})^2)$, where $\mu_i^{(0)} = 0$ and $\sigma_i^{(0)} = \sigma_i = 1$, $i = 1, \dots, 10$. The threshold is set by $\gamma = 0$.

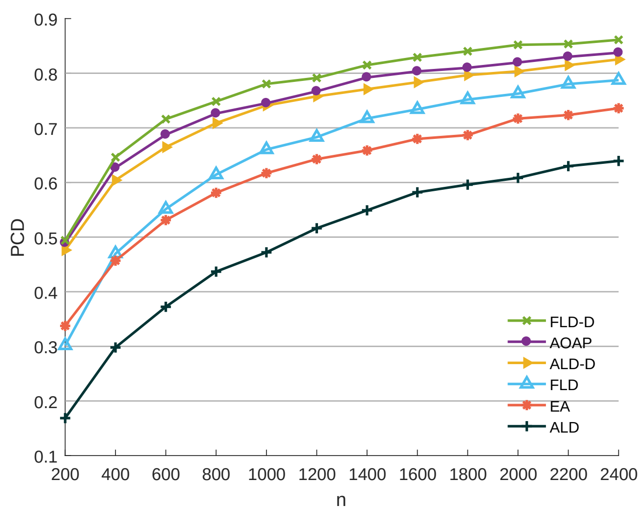
- *Example 2*: There are 10 alternatives following $N(\mu_i, \sigma_i^2)$ with $\mu_i \sim N(\mu_i^{(0)}, (\sigma_i^{(0)})^2)$, where $\mu_i^{(0)} = 0.1 * i$, $\sigma_i^{(0)} = 1$, and $\sigma_i = 2$, $i = 1, ..., 10$. The threshold is set by $\gamma = 0.5$.

For the dynamic methods FLD-D, AOAP, and ALD-D, 10 initial replications are allocated to each alternative for estimating sample mean and variance. For static methods FLD and ALD, we use the true values for the needed parameters. In example 1 we use noninformative prior, while in example 2 we incorporate the prior information in dynamic approaches.

The performance of each procedure is shown in Figure 4.2. From the figure we can see that all the dynamic approaches have better performance than the static approaches, which justifies the importance of addressing the FD problem from stochastic control perspective. Note that the figure also exhibits the importance of finite budget perspective, as asymptotical method ALD has unsatisfying performance.



(a) Example 1



(b) Example 2

Figure 4.2: PCD comparison in different examples.

Chapter 5

Optimal Budget Allocation with Kriging

Traditional allocation procedures for FD problem do not consider the relationships between different designs. The only source from which they draw information about the design performance is the simulation results of the design itself. In practice, however, the designs with close parameters often have similar performances. The performance of the nearby designs could be a useful information source when we evaluate the performance of a design. Integrating the information from both sources when evaluating design performance has the potential to enhance simulation efficiency.

In this chapter, we use the kriging model to extract information about the design performance from the simulation results of its nearby design points. Based on the Bayesian framework, we then incorporate this information with the simulation results of the design itself to evaluate its performance. We develop a new budget allocation procedure in the context of this new performance evaluation method. Numerical experiments are conducted to demonstrate the effectiveness of our procedure.

5.1 Problem Formulation

5.1.1 Problem Statement

Suppose we have a fixed number r of alternative design points, $\mathbf{x}_1, ..., \mathbf{x}_r$, where $\mathbf{x}_i \in \mathbb{R}^k$. Each design point has a performance measure $y(\mathbf{x}_i) = E[f(\mathbf{x}_i)]$. $y(\mathbf{x}_i)$ is unknown and can only be estimated via simulation with noise. The simulated performance at design point $\mathbf{x}_i$ is denoted as $f(\mathbf{x}_i)$. We use $\epsilon(\mathbf{x}_i)$ to represent the simulation noise at design point $\mathbf{x}_i$. $\epsilon(\mathbf{x}_i)$ is normally distributed with mean 0 and variance $\sigma^2(\mathbf{x}_i)$, hence it can handle the heteroscedasticity of simulation outputs at different design points. We assume the noise is independent from replication to replication as well as independent across different design points. For ease of notation, we use σ_i^2 to represent $\sigma^2(\mathbf{x}_i)$. The simulation output $f(\mathbf{x}_i)$ can then be represented by the following expression:

$$f(\mathbf{x}_i) = y(\mathbf{x}_i) + \epsilon(\mathbf{x}_i);\ i = 1, ..., r, \epsilon(\mathbf{x}_i) \sim N(0, \sigma_i^2)$$

Given a constant $\gamma \in \mathbb{R}$, a design point $\mathbf{x}_i$ is defined to be feasible if $y(\mathbf{x}_i) < \gamma$ and infeasible if $y(\mathbf{x}_i) > \gamma$. Here we assume that there is no design point has the performance measure that lies exactly at the boundary, that is, $y(\mathbf{x}_i) \neq \gamma$, for $i = 1, ..., r$. Our objective is to use limited total simulation budget to determine for each design point $\mathbf{x}_i$ whether it is feasible or not effectively.

The total simulation budget n is allocated to each design point in order to maximize the expected number of correct determinations. Let α_i represent the proportion of simulation budget that is allocated to sampling at design point $\mathbf{x}_i$, $\alpha = (\alpha_1, ..., \alpha_r)^{\mathrm{T}}$. In this research we ignore the minor technicalities associated with $n\alpha_i$ not being an integer.

Let g_n denote the expected number of correct determinations under total budget n. The budget allocation problem in feasibility determination is to

$$
\begin{aligned}
Problem\ \mathcal{P}: \max_{\alpha_1,...,\alpha_r} & \ g_n(\alpha_1, ..., \alpha_r) \\
s.t. \sum_{i=1}^{r} \alpha_i &= 1 \\
\alpha_i &\geq 0, i = 1, ..., r
\end{aligned}
$$

In the following subsections, we will try to figure out an analytic form expression for $g_n(\alpha_1, ..., \alpha_r)$.

5.1.2 A Kriging Metamodel

It is not uncommon in reality that nearby design points have similar performance measures. That means, if $\mathbf{x}_i$ is close to $\mathbf{x}_j$, $y(\mathbf{x}_i)$ should not deviate too far from $y(\mathbf{x}_j)$. In this context, knowing the performance measure of nearby design points of $\mathbf{x}_i$ could help us infer $y(\mathbf{x}_i)$. Hence there is potential to enhance simulation efficiency if we can extract information about $y(\mathbf{x}_i)$ from simulation results at nearby design points and integrate it with our information obtained by simulating at $\mathbf{x}_i$ directly.

In this thesis, we apply kriging methodology to provide information about $y(\mathbf{x}_i)$ based on simulation results at other design points. The traditional kriging method models the simulation output at a design point $\mathbf{x}$ as

$$f(\mathbf{x}) = M(\mathbf{x}) + \epsilon(\mathbf{x}) \tag{5.1}$$

where $M(\mathbf{x})$ is a stationary Gaussian process with mean 0 and covariance function $\sigma^2\rho(\cdot, \cdot)$, and $\epsilon(\mathbf{x})$ is a normal random variable with mean 0 and variance $\sigma^2(\mathbf{x})$ (Sun et al. [82]).

In Equation (4.1), the stationary Gaussian process $M(\mathbf{x})$ models the unknown performance measure $y(\mathbf{x})$. $M(\mathbf{x})$ exhibits space correlation, which means the values $M(\mathbf{x}_i)$ and $M(\mathbf{x}_j)$ are close to each other if $\mathbf{x}_i$ and $\mathbf{x}_j$ are close to each other. This space correlation is exploited to capture the similarity between performance measures of close design points. Using $M(\mathbf{x})$ to model $y(\mathbf{x})$ embeds a deterministic problem into a probabilistic framework so that statistical inference about $y(\mathbf{x})$ at values of $\mathbf{x}$ not simulated (not just an estimate of value $y(\mathbf{x})$) can be obtained, which is important in incorporating information of $y(\mathbf{x})$ from nearby design points and from simulating at $\mathbf{x}$ directly.

The correlation function $\rho(\mathbf{x}_i, \mathbf{x}_j) = Corr(M(\mathbf{x}_i), M(\mathbf{x}_j))$ is typically a function of $\mathbf{x}_i - \mathbf{x}_j$, which we denote as $R(\mathbf{x}_i - \mathbf{x}_j)$. It is the crucial ingredient in a Gaussian process predictor, as it defines space correlation of $M(\mathbf{x})$. We require that $R(\mathbf{x}_i - \mathbf{x}_j) \to 0$ as the distance between $\mathbf{x}_i$ and $\mathbf{x}_j$ goes to infinity, and $R(0) = 1$. Several functional forms are often used as correlation function. For instance, the squared exponential correlation function $R(t) = \exp(-at^2)$ with parameter $a > 0$, the exponential correlation function $R(t) = \exp(-at)$ with parameter $a > 0$, and the Matérn correlation function $R(t) = \frac{1}{\Gamma(\nu)2^{\nu-1}}(\sqrt{2\nu}\frac{t}{l})^\nu K_\nu(\sqrt{2\nu}\frac{t}{l})$ with non-negative parameters ν and l, where Γ is the gamma function and K_ν is the modified Bessel function of the second kind.

The error term $\epsilon(\mathbf{x})$ captures the noise in the simulation output. It is common in kirging model to assume $\epsilon(\mathbf{x})$ is independent with $M(\mathbf{x})$ since they capture completely different sources of randomness. In accordance with our assumption that the noise is independent from different design points, we assume that $Cov(\epsilon(\mathbf{x}_i), \epsilon(\mathbf{x}_j)) = 0$ for any $\mathbf{x}_i \neq \mathbf{x}_j$.

Suppose we have run simulation at m design points $\mathbf{x}_1, ..., \mathbf{x}_m$, and in each design point $\mathbf{x}_i$ we have taken N_i simulation replications. Let the output obtained from the jth simulation replication at $\mathbf{x}_i$ be

$$f_j(\mathbf{x}_i) = M(\mathbf{x}_i) + \epsilon_j(\mathbf{x}_i)$$

Let sample mean $\bar{f}(\mathbf{x}_i) = \frac{1}{N_i}\sum_{j=1}^{N_i} f_j(\mathbf{x}_i)$ and let $\bar{\mathbf{f}} = (\bar{f}(\mathbf{x}_1), ..., \bar{f}(\mathbf{x}_m))^{\mathrm{T}}$. Now we want to estimate the performance measure at $\mathbf{x}_0$ conditioned on the observed data. Let Σ_M be the $m \times m$ covariance matrix whose (i,j)th element is $Cov[M(\mathbf{x}_i), M(\mathbf{x}_j)]$, and let $\Sigma_M(\mathbf{x}_0, \cdot)$ be the $m \times 1$ vector $(Cov[M(\mathbf{x}_0), M(\mathbf{x}_1)], ..., Cov[M(\mathbf{x}_0), M(\mathbf{x}_m)])^{\mathrm{T}}$. Let Σ_ϵ be the $m \times m$ covariance matrix of noises whose (i,i)th element is $\sigma^2(\mathbf{x}_i)/N_i$ whereas all other elements are 0. The kriging model predicts that $y(\mathbf{x}_0)$ is normally distributed with mean

$$\widehat{y}(\mathbf{x}_0) = \Sigma_M(\mathbf{x}_0, \cdot)^{\mathrm{T}}(\Sigma_M + \Sigma_\epsilon)^{-1}\bar{\mathbf{f}} \tag{5.2}$$

and variance

$$V(\mathbf{x}_0) = \sigma^2 - \Sigma_M(\mathbf{x}_0, \cdot)^{\mathrm{T}}(\Sigma_M + \Sigma_\epsilon)^{-1}\Sigma_M(\mathbf{x}_0, \cdot) \tag{5.3}$$

Remark 5.1 *Ankenman et al. [4] show that for any $\mathbf{x}_0$, $\widehat{y}(\mathbf{x}_0)$ is the MSE-optimal linear predictor of $y(\mathbf{x}_0)$. The corresponding optimal MSE is exactly given by $V(\mathbf{x}_0)$.*

The kriging metamodel provides us knowledge about $y(\mathbf{x}_0)$ based on observed simulation results at other design points. Our next goal is to incorporate this knowledge with information obtained by simulating at $\mathbf{x}_0$ directly, which is the task of next subsection.

5.1.3 A Bayesian Framework for Combining Information

Suppose we have run simulation at all r design points, and for each design point $\mathbf{x}_i$ we have N_i simulation replications. Now we want to draw information about $y(\mathbf{x}_i), 1 \leq i \leq r$

from observed simulation outputs to determine the feasibility of each design point. For any design point $\mathbf{x}_i$, there are two data sources we can draw information from. The first one is directly simulation results at $\mathbf{x}_i$, $f_1(\mathbf{x}_i), ..., f_{N_i}(\mathbf{x}_i)$. The second one is simulation results at other design points, from which we can use stochastic kriging metamodel to gain information about $y(\mathbf{x}_i)$. In this thesis we turn to a bayesian framework to combine information from these two data sources.

Let $\Sigma_M^{(i)}$ be the $(r-1)\times(r-1)$ covariance matrix across $M(\mathbf{x}_1), ..., M(\mathbf{x}_{i-1}), M(\mathbf{x}_{i+1}), ..., M(\mathbf{x}_r)$, and let $\Sigma_M(\mathbf{x}_i, \cdot)$ be the $(r-1)\times 1$ vector $(Cov[M(\mathbf{x}_i), M(\mathbf{x}_1)], ..., Cov[M(\mathbf{x}_i), M(\mathbf{x}_{i-1})], Cov[M(\mathbf{x}_i), M(\mathbf{x}_{i+1})], ..., Cov[M(\mathbf{x}_i), M(\mathbf{x}_r)])^{\mathrm{T}}$. Let $\Sigma_\epsilon^{(i)}$ be the matrix whose diagonal elements are $\{\sigma^2(\mathbf{x}_1)/N_1, ..., \sigma^2(\mathbf{x}_{i-1})/N_{i-1}, \sigma^2(\mathbf{x}_{i+1})/N_{i+1}, ..., \sigma^2(\mathbf{x}_r)/N_r\}$ whereas all other elements are 0. Let $\bar{\mathbf{f}}^{(i)} = (\bar{f}(\mathbf{x}_1), ..., \bar{f}(\mathbf{x}_{i-1}), \bar{f}(\mathbf{x}_{i+1}), ..., \bar{f}(\mathbf{x}_r))^{\mathrm{T}}$. Using equation (4.2) and (4.3), based on simulation outputs at other design points than $\mathbf{x}_i$ we predict that $y(\mathbf{x}_i)$ is normally distributed with mean

$$\widehat{y}(\mathbf{x}_i) = \Sigma_M(\mathbf{x}_i, \cdot)^{\mathrm{T}}(\Sigma_M^{(i)} + \Sigma_\epsilon^{(i)})^{-1}\bar{\mathbf{f}}^{(i)} \tag{5.4}$$

and variance

$$V(\mathbf{x}_i) = \sigma^2 - \Sigma_M(\mathbf{x}_i, \cdot)^{\mathrm{T}}(\Sigma_M^{(i)} + \Sigma_\epsilon^{(i)})^{-1}\Sigma_M(\mathbf{x}_i, \cdot) \tag{5.5}$$

We can see this normal distribution as a prior distribution for $y(\mathbf{x}_i)$. We have N_i measurements of $y(\mathbf{x}_i)$, $f_1(\mathbf{x}_i), ..., f_{N_i}(\mathbf{x}_i)$. Hence the posterior distribution for $y(\mathbf{x}_i)$ is an updated normal distribution (Murphy [63]) with mean

$$\widetilde{y}(\mathbf{x}_i) = \frac{V(\mathbf{x}_i)}{\frac{\sigma_i^2}{N_i} + V(\mathbf{x}_i)}\bar{f}(\mathbf{x}_i) + \frac{\frac{\sigma_i^2}{N_i}}{\frac{\sigma_i^2}{N_i} + V(\mathbf{x}_i)}\widehat{y}(\mathbf{x}_i) \tag{5.6}$$

and variance

$$\widetilde{V}(\mathbf{x}_i) = (\frac{1}{V(\mathbf{x}_i)} + \frac{N_i}{\sigma_i^2})^{-1} \tag{5.7}$$

Remark 5.2 *When $N_i \to \infty$, $\bar{f}(\mathbf{x}_i)$ converges a.s. to $y(\mathbf{x}_i)$. Hence when $N_i \to \infty$, $\widetilde{y}(\mathbf{x}_i)$ converges a.s. to $y(\mathbf{x}_i)$, $\widetilde{y}(\mathbf{x}_i)$ is consistent. When $N_i \to \infty$, $N_i\widetilde{V}(\mathbf{x}_i)$ converges to σ_i^2.*

After combining information from two data sources, we derive that $N(\widetilde{y}(\mathbf{x}_i), \widetilde{V}(\mathbf{x}_i))$ could be used to infer $y(\mathbf{x}_i)$. Naturally, if $\widetilde{y}(\mathbf{x}_i) < \gamma$, we see design point $\mathbf{x}_i$ as feasible since in this case $P(y(\mathbf{x}_i) < \gamma) > P(y(\mathbf{x}_i) \geq \gamma)$. The probability that we made an incorrect determination is

$$P(y(\mathbf{x}_i) \geq \gamma) = \int_{\frac{\gamma - \widetilde{y}(\mathbf{x}_i)}{\sqrt{\widetilde{V}(\mathbf{x}_i)}}}^{\infty} e^{-\frac{t^2}{2}} dt$$

Similarly, if $\widetilde{y}(\mathbf{x}_i) \geq \gamma$, we see the design point $\mathbf{x}_i$ as infeasible and the incorrect determination probability is

$$P(y(\mathbf{x}_i) < \gamma) = \int_{-\infty}^{\frac{\gamma - \widetilde{y}(\mathbf{x}_i)}{\sqrt{\widetilde{V}(\mathbf{x}_i)}}} e^{-\frac{t^2}{2}} dt$$

Let $\widetilde{I}(\mathbf{x}_i) = \frac{(\gamma - \widetilde{y}(\mathbf{x}_i))^2}{2\widetilde{V}(\mathbf{x}_i)N_i}$, $i = 1, ..., r$. When $N_i \to \infty$, $\widetilde{y}(\mathbf{x}_i)$ converges a.s. to $y(\mathbf{x}_i)$ and $\widetilde{V}(\mathbf{x}_i)N_i$ converges to σ_i^2. Therefore $\widetilde{I}(\mathbf{x}_i)$ converges a.s. to $I_{\mathbf{x}_i}(\gamma) = \frac{(\gamma - y(\mathbf{x}_i))^2}{2\sigma_i^2}$, where $I_{\mathbf{x}_i}(\cdot)$ is large deviation rate function of $f(\mathbf{x}_i)$.We can then derive an analytic form expression for $g_n(\alpha_1, ..., \alpha_r)$,

$$g_n(\alpha_1, ..., \alpha_r) = r - \sum_{i=1}^{r} \int_{\sqrt{2N_i\widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$$

Since n is allocated to each design point $\mathbf{x}_i$, when n is exhausted we have $n\alpha_i = N_i$. α_i is implicitly included in the above equation. The original problem $\mathcal{P}$ can be transformed to

$$\begin{aligned} Problem\ \mathcal{P}5: & \min_{\alpha_1,...,\alpha_r} \sum_{i=1}^{r} \int_{\sqrt{2N_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt \\ s.t. & \sum_{i=1}^{r} \alpha_i = 1 \\ & \alpha_i \geq 0, i = 1, ..., r \end{aligned}$$

5.2 Analysis of Optimal Simulation Budget Allocation with Kriging

5.2.1 Derivation of OAK Allocation Rule

In this subsection, we derive OAK rule based on problem $\mathcal{P}5$. To facilitate the derivations, we adopt the same strategy with (Chen et al. [19]), (Glynn and Juneja [44]) and (Szechtman and Yücesan [83]), which is finding an asymptotically optimal allocation rule. Namely, we consider the case that $n \to \infty$. In our budget allocation with kriging setting, the asymptotically optimal allocation rule improves efficiency significantly compared to other existing methods.

Let $\Sigma^{(i)} = \Sigma_M^{(i)} + \Sigma_\epsilon^{(i)}$. Note that $\Sigma_\epsilon^{(i)} = Diag\{\frac{\sigma^2(\mathbf{x}_1)}{n\alpha_1}, ..., \frac{\sigma^2(\mathbf{x}_{i-1})}{n\alpha_{i-1}}, \frac{\sigma^2(\mathbf{x}_{i+1})}{n\alpha_{i+1}}, ..., \frac{\sigma^2(\mathbf{x}_r)}{n\alpha_r}\}$ has no relationship with α_i. Based on equation (4) and (5), we can derive that $\frac{\partial \bar{y}(\mathbf{x}_i)}{\alpha_i} = 0$ and $\frac{\partial V(\mathbf{x}_i)}{\alpha_i} = 0$. When the simulation budget n tends to infinity, $\Sigma_\epsilon^{(i)}$ tends to a zero matrix. In our derivation n is large enough, $\Sigma^{(i)} \approx \Sigma_M^{(i)}$, the stochastic kriging model degenerates to a deterministic kriging model (Stein [81]). In this case $\frac{\partial \bar{y}(\mathbf{x}_i)}{\alpha_j} = 0$ and $\frac{\partial V(\mathbf{x}_i)}{\alpha_j} = 0$, where $j \neq i$.

Consider $\widetilde{I}(\mathbf{x}_i) = \frac{(\gamma-\widetilde{y}(\mathbf{x}_i))^2}{2\widetilde{V}(\mathbf{x}_i)n\alpha_i}$, $i = 1, ..., r$. The first order derivatives of $\widetilde{I}(\mathbf{x}_i)$ with respect to α are,

$$
\begin{aligned}
\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} &= \frac{\partial((\gamma - \frac{V(\mathbf{x}_i)}{\frac{\sigma_i^2}{n\alpha_i}+V(\mathbf{x}_i)}\bar{f}(\mathbf{x}_i) - \frac{\frac{\sigma_i^2}{n\alpha_i}}{\frac{\sigma_i^2}{n\alpha_i}+V(\mathbf{x}_i)}\widehat{y}(\mathbf{x}_i))^2(\frac{1}{2V(\mathbf{x}_i)n\alpha_i}+\frac{1}{2\sigma_i^2}))}{\partial \alpha_i} \\
&= (\gamma - \widetilde{y}(\mathbf{x}_i))\frac{\sigma_i^2 V(\mathbf{x}_i)}{n\alpha_i^2}(\frac{\sigma_i^2}{n\alpha_i}+V(\mathbf{x}_i))^{-2}(\hat{y}(\mathbf{x}_i) \\
&- \bar{f}(\mathbf{x}_i))(\frac{1}{V(\mathbf{x}_i)n\alpha_i}+\frac{1}{\sigma_i^2}) - (\gamma - \widetilde{y}(\mathbf{x}_i))^2\frac{1}{2V(\mathbf{x}_i)n\alpha_i^2}
\end{aligned}
\tag{5.8}
$$

and for $j \neq i$ we have

$$
\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_j} = 0 \tag{5.9}
$$

Note that when $n \to \infty$, $\widetilde{y}(\mathbf{x}_i)$ and $\bar{f}(\mathbf{x}_i)$ converge a.s. to $y(\mathbf{x}_i)$. Meanwhile, $\hat{y}(\mathbf{x}_i)$ converges to a finite value and $V(\mathbf{x}_i)$ converges to a nonzero constant. Therefore $\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} \propto \frac{1}{n}$ and converges to 0 as n tends to infinity. We now prove

Lemma 5.1 $\mathcal{P}5$ *is an asymptotically convex optimization problem.*

Proof: The first order derivatives of $\widetilde{I}(\mathbf{x}_i)$ with respect to α are shown in (4.8) and (4.9). We now derive the second order derivatives. Obviously, $\frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_j \partial \alpha_i} = 0$ and $\frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_j} = 0$, where $j \neq i$. Rearrange equation (4.8), we have

$$
\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} = \frac{\gamma - \widetilde{y}(\mathbf{x}_i)}{n\alpha_i^2}(\sigma_i^2 V(\mathbf{x}_i)(\frac{\sigma_i^2}{n\alpha_i}+V(\mathbf{x}_i))^{-2}(\hat{y}(\mathbf{x}_i)-\bar{f}(\mathbf{x}_i))(\frac{1}{V(\mathbf{x}_i)n\alpha_i}+\frac{1}{\sigma_i^2})-\frac{\gamma-\widetilde{y}(\mathbf{x}_i)}{2V(\mathbf{x}_i)})
$$

Let $A = \frac{\gamma-\widetilde{y}(\mathbf{x}_i)}{n\alpha_i^2}$, $B = \sigma_i^2 V(\mathbf{x}_i)(\frac{\sigma_i^2}{n\alpha_i} + V(\mathbf{x}_i))^{-2}(\hat{y}(\mathbf{x}_i) - \bar{f}(\mathbf{x}_i))(\frac{1}{V(\mathbf{x}_i)n\alpha_i} + \frac{1}{\sigma_i^2})$ and $C = \frac{\gamma-\widetilde{y}(\mathbf{x}_i)}{2V(\mathbf{x}_i)}$. Note that $A \propto \frac{1}{n}$. When n goes to infinity, A tends to 0. Meanwhile, B

and C converges to some finite values. $\frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_i} = \frac{\partial A}{\partial \alpha_i}(B - C) + A(\frac{\partial B}{\partial \alpha_i} - \frac{\partial C}{\partial \alpha_i})$. We now consider $\frac{\partial A}{\partial \alpha_i}$, $\frac{\partial B}{\partial \alpha_i}$ and $\frac{\partial C}{\partial \alpha_i}$ respectively.

$$
\begin{aligned}
\frac{\partial A}{\partial \alpha_i} &= \frac{(\frac{\sigma_i^2}{n\alpha_i} + V(\mathbf{x}_i))^{-2}\sigma_i^2 V(\mathbf{x}_i)(\hat{y}(\mathbf{x}_i) - \bar{f}(\mathbf{x}_i)) - 2(\gamma - \widetilde{y}(\mathbf{x}_i))n\alpha_i}{n^2\alpha_i^4} \\
\frac{\partial B}{\partial \alpha_i} &= \sigma_i^2 V(\mathbf{x}_i)(\hat{y}(\mathbf{x}_i) - \bar{f}(\mathbf{x}_i))(2(\frac{\sigma_i^2}{n\alpha_i} + V(\mathbf{x}_i))^{-3}\frac{\sigma_i^2}{n\alpha_i^2}(\frac{1}{V(\mathbf{x}_i)n\alpha_i} + \frac{1}{\sigma_i^2}) \\
&\quad - (\frac{\sigma_i^2}{n\alpha_i} + V(\mathbf{x}_i))^{-2}\frac{1}{V(\mathbf{x}_i)n\alpha_i^2}) \\
\frac{\partial C}{\partial \alpha_i} &= \frac{\sigma_i^2}{2n\alpha_i^2}(\frac{\sigma_i^2}{n\alpha_i} + V(\mathbf{x}_i))^{-2}(\hat{y}(\mathbf{x}_i) - \bar{f}(\mathbf{x}_i))
\end{aligned}
$$

We can observe that $\frac{\partial A}{\partial \alpha_i}$, $\frac{\partial B}{\partial \alpha_i}$ and $\frac{\partial C}{\partial \alpha_i}$ all $\propto \frac{1}{n}$. Therefore $\frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_i} \propto \frac{1}{n}$ and vanishes when n goes to infinity. We then consider the second order derivatives of $\int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$. We can easily check that $\frac{\partial^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt}{\partial \alpha_j \partial \alpha_i} = 0$ and $\frac{\partial^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt}{\partial^2 \alpha_j} = 0$, where $j \neq i$. The first order derivative of $\int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$ with respect to α_i is

$$
\frac{\partial \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt}{\partial \alpha_i} = -e^{-n\alpha_i \widetilde{I}(\mathbf{x}_i)}(2n\alpha_i \widetilde{I}(\mathbf{x}_i))^{-\frac{1}{2}}(n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i})
$$

The second order derivative is

$$
\begin{aligned}
\frac{\partial^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt}{\partial^2 \alpha_i} =& e^{-n\alpha_i \widetilde{I}(\mathbf{x}_i)}(2n\alpha_i \widetilde{I}(\mathbf{x}_i))^{-\frac{1}{2}}[(n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i})^2 - (2n\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} + n\alpha_i \frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_i})] \\
&+ \frac{1}{2}e^{-n\alpha_i \widetilde{I}(\mathbf{x}_i)}(2n\alpha_i \widetilde{I}(\mathbf{x}_i))^{-\frac{3}{2}}(n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i})^2
\end{aligned}
$$

Since $\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} \propto \frac{1}{n}$ and $\frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_i} \propto \frac{1}{n}$, when n is sufficient large $[(n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i})^2 - (2n\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} + n\alpha_i \frac{\partial^2 \widetilde{I}(\mathbf{x}_i)}{\partial^2 \alpha_i})]$ would be nonnegative. Therefore, when n is sufficient large, $\frac{\partial^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt}{\partial^2 \alpha_i}$ would be nonnegative. The second order derivatives of $\int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$

with respect to α, $\nabla^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$ is a diagonal matrix with nonnegative diagonal elements. Hence when n is sufficient large, $\nabla^2 \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$ is a positive semi-definite matrix, which means $\int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$ is a convex function. The objective function of problem $\mathcal{P}5$ is the sum of convex functions, hence itself is a convex function. The constraints of $\mathcal{P}5$ are linear, thus problem $\mathcal{P}5$ is an asymptotically convex optimization problem. ■

We now omit the constraint $\alpha_i \geq 0$ in problem $\mathcal{P}5$ and consider problem $\widetilde{\mathcal{P}5}$,

$$Problem\ \widetilde{\mathcal{P}5} : \min_{\alpha_1,\ldots,\alpha_r} \sum_{i=1}^{r} \int_{\sqrt{2n\alpha_i \widetilde{I}(\mathbf{x}_i)}}^{\infty} e^{-\frac{t^2}{2}} dt$$

$$s.t. \sum_{i=1}^{r} \alpha_i = 1$$

This is still an asymptotically convex optimization problem. Let λ be the Lagrange multiplier. The Karush-Kuhn-Tucker (KKT) conditions of problem $\widetilde{\mathcal{P}5}$ are stated as follows:

$$e^{-n\alpha_i \widetilde{I}(\mathbf{x}_i)} (2n\alpha_i \widetilde{I}(\mathbf{x}_i))^{-\frac{1}{2}} (n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i}) = \lambda, i = 1, ..., r \tag{5.10}$$

$$\sum_{i=1}^{r} \alpha_i = 1 \tag{5.11}$$

Observing term $n\widetilde{I}(\mathbf{x}_i) + n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i}$ in equation (4.10), since $\frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i} \propto \frac{1}{n}$, when n tends to infinity $n\alpha_i \frac{\partial \widetilde{I}(\mathbf{x}_i)}{\partial \alpha_i}$ become much smaller than the other term and is negligible. This implies the condition (4.10) could be approximated by

$$e^{-n\alpha_i \widetilde{I}(\mathbf{x}_i)} (2n\alpha_i \widetilde{I}(\mathbf{x}_i))^{-\frac{1}{2}} n\widetilde{I}(\mathbf{x}_i) = \lambda, i = 1, ..., r$$

Taking the natural log on both sides, we have

$$-n\alpha_i\widetilde{I}(\mathbf{x}_i) - \frac{1}{2}\log(2\alpha_i) + \frac{1}{2}\log(n\widetilde{I}(\mathbf{x}_i) = \log(\lambda), i = 1, ..., r$$

When $n \to \infty$, all the log terms become negligible. This yields

$$-n\alpha_i\widetilde{I}(\mathbf{x}_i) = \log(\lambda), i = 1, ..., r \tag{5.12}$$

Solving equations (4.11) and (4.12), we obtain $\alpha_i = \frac{1/\widetilde{I}(\mathbf{x}_i)}{\sum_{i=1}^{r} 1/\widetilde{I}(\mathbf{x}_i)}$, $i = 1, ..., r$. With the convexity, the solution satisfying the KKT conditions is the optimal solution to problem $\widetilde{\mathcal{P}5}$. We can check that $\frac{1/\widetilde{I}(\mathbf{x}_i)}{\sum_{i=1}^{r} 1/\widetilde{I}(\mathbf{x}_i)} \geq 0, i = 1, ..., r$. The solution satisfies constraint $\alpha_i \geq 0$ in problem $\mathcal{P}5$, hence it is also the optimal solution to problem $\mathcal{P}5$. $\alpha_i = \frac{1/\widetilde{I}(\mathbf{x}_i)}{\sum_{i=1}^{r} 1/\widetilde{I}(\mathbf{x}_i)}$, $i = 1, ..., r$ is our OAK allocation rule and we have the following result:

Theorem 5.1 *Problem $\mathcal{P}5$ can be asymptotically minimized with the following allocation rule:*

$$\alpha_i = \frac{1/\widetilde{I}(\mathbf{x}_i)}{\sum_{i=1}^{r} 1/\widetilde{I}(\mathbf{x}_i)}, i = 1, ..., r$$

Initially $\widetilde{I}(\mathbf{x}_i)$ is unknown, therefore we must warm-up each design point with N_i replicates. The parameters involved in the kriging model can be estimated using several methods (Santner et al. [77], Fang et al. [32]) and the most well known method is maximum likelihood estimation (MLE). After $\widetilde{y}(\mathbf{x}_i)$ and $\widetilde{V}(\mathbf{x}_i)$ are calculated based on the Bayesian framework, $\widetilde{I}(\mathbf{x}_i)$ can then be obtained based on $\widetilde{I}(\mathbf{x}_i) = \frac{(\gamma - \widetilde{y}(\mathbf{x}_i))^2}{2\widetilde{V}(\mathbf{x}_i)N_i}$, $i = 1, ..., r$.

5.2.2 OAK Allocation Procedure

In this subsection, we present our budget allocation algorithm based on OAK allocation rule. The allocation rule can only be determined after we know the mean and variance of each design point and the parameters for the kriging model. However, these pieces of information are unknown before simulation experiments are conducted. Therefore, we suggest a sequential simulation budget allocation algorithm that uses simulation results to estimate OAK allocation rule step by step. The algorithm is stated as follows:

Optimal simulation budget Allocation with Kriging (OAK) Algorithm

1 For a set of r design points, specify the total simulation budget n, the initial simulation budget for each design point n_0, the incremental budget Δ. Select appropriate variance function in kriging model.

2 Iteration counter $t \leftarrow 0$. Perform n_0 simulation replications to each design point, $N_1^t = N_2^t = ... = N_r^t = n_0$.

3 If $N^t = \sum_{i=1}^r N_i^t \geq n$, stop. Otherwise,

a update the mean and variance of each design point

b estimate the parameters in variance function of kriging model

c for each design point, compute the kriging mean and variance based on equation (4.4) and (4.5)

d for each design point, compute the posterior mean and posterior variance based on equation (4.6) and (4.7)

e for each design point, compute $\widetilde{I}(\mathbf{x}_i)$

f compute allocation ratio $\alpha_i = \frac{1/\widetilde{I}(\mathbf{x}_i)}{\sum_{i=1}^r 1/\widetilde{I}(\mathbf{x}_i)}, i = 1, ..., r$

g perform $\Delta_i = \max\{0, \alpha_i(N^t + \Delta) - N_i^t\}$ simulation replications to design point $\mathbf{x}_i, i = 1, ..., r$

h $N_i^{t+1} = N_i^t + \Delta_i, t \leftarrow t + 1$

4 Determine the feasibility of each design point based on the posterior mean of performance measure.

Remark 5.3 *In step 3(c) of the above procedure, when computing the kriging mean and variance of one design point we include observations from all other design points. This may not be necessary when some design points are not within the spatial correlation range of this design point. We can add a k nearest neighbor search or some similar operation to screen out a subset of design points for kriging.*

5.3 Numerical Experiments

The OAK procedure applies kriging metamodel to capture the inter-design relationships, and incorporates this information into ALD procedure. Analogous with Chapter 3, we can also consider this methodology from finite budget perspective. We combine kriging with FLD and derive OAK$^+$ procedure. In this section, we test the effectiveness of OAK and OAK$^+$ by comparing them with procedures without inter-design relationships consideration. The test is conducted on two numerical examples, one with one-dimensional design points and the other with two-dimensional design points:

- *Example 1*: A function taken from (Torn and Zilinskas [85]), $f(x) = \sin(x) + \sin(10x/3) + \ln(x) - 0.84x + 3 + N(0, 6^2)$, $3 \le x \le 8$. Threshold $\gamma = 0$.

- *Example 2*: Six-hump camel function taken from (Molga and Smutnicki [62]), $f(\mathbf{x}) = (4 - 2.1x_1^2 + x_1^4/3)x_1^2 + x_1x_2 + (-4 + 4x_2^2)x_2^2 + N(0, 6^2)$, $-2 \le x_1 \le 2, -1 \le x_2 \le 1$. Threshold $\gamma = 2$.

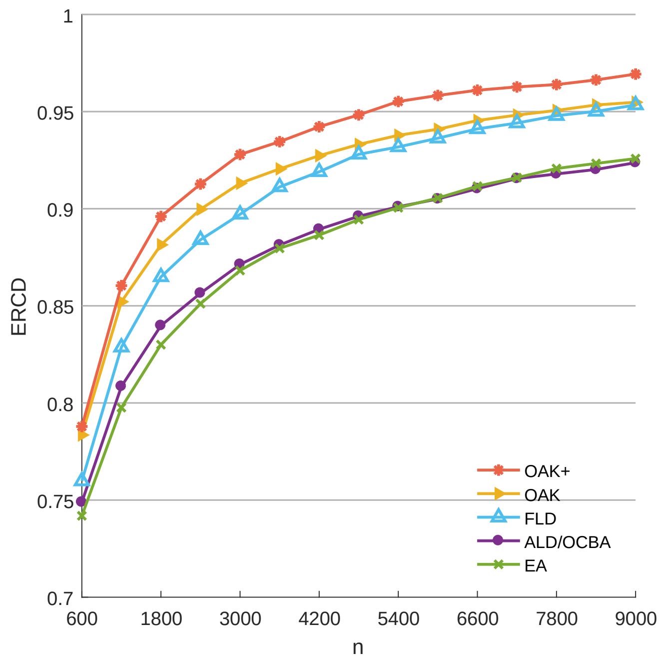
In comparing the procedures, the measure ERCD is estimated based on 5000 independent experiments of each algorithm. Since the position of the design points have great effect on the kriging model, in each experiment we randomly pick $r = 15$ design points from available domain so that the test results are independent of the special design points position selection. In OAK and OAK$^+$, we set the initial budget per design point, the incremental budget per iteration and the maximum budget as Table 5.1. Sequential procedures ALD/OCBA and FLD follow the same parameter settings. In OAK and OAK$^+$ we have to specify the functional form of the correlation function in the kriging model. Here we use the squared exponential correlation function, $Cov(M(\mathbf{x}_i), M(\mathbf{x}_j)) = \sigma^2 \exp(-a\|\mathbf{x}_i - \mathbf{x}_j\|^2)$, where parameters σ and a are estimated using MLE method.

Table 5.1: Parameter settings of OAK for different examples.

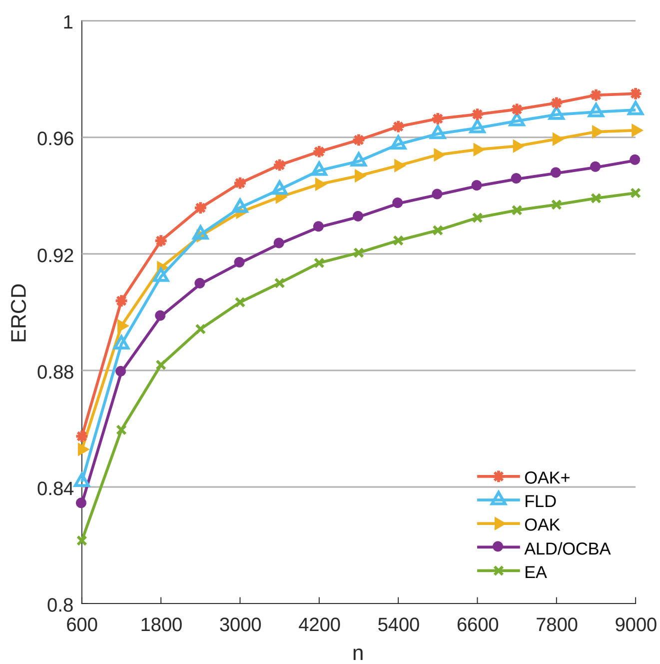
	Initial budget	Incremental budget	Maximum budget
Ex.1	20	100	9000
Ex.2	20	100	9000

Remember that ALD and OCBA have the same allocation rule in the normal environment, hence the performance of ALD and OCBA are illustrated simultaneously by one curve. The performance of the five procedures with different budgets and simulation budget needed to reach ERCD level 0.95 are illustrated in Figure 5.1 and Table 5.2. We can see that in both problem settings, OAK$^+$ outperforms FLD and OAK outperforms ALD/OCBA. These imply that taking the relationships between different design points into consideration could enhance the simulation efficiency.

In order to achieve ERCD level 0.95, incorporating kriging metamodel in ALD/OCBA can reduce simulation budget by 55.0% and 36.7% on the two examples respectively, and incorporating kriging metamodel in FLD can reduce simulation budget by 41.7%



(a) Example 1



(b) Example 2

Figure 5.1: Comparison of OAK with other methods

Table 5.2: Simulation budget needed to reach ERCD level 0.95.

	OAK^+	OAK	FLD	ALD/OCBA	EA
Ex.1	4900	7700	8400	19000	17100
Ex.2	3500	5400	4600	8500	12000

and 23.9%.

Chapter 6

Future Research

In this thesis, we seek various methods to address the FD budget allocation problem in small budget environment. The FD problem arises in a variety applications. One such application is to use FD to select appropriate manufacturing schedules. In the future, I will utilize the FD allocation procedure in a Kimberly-Clark (K-C) paper production scheduling project.

In previous methods, we determined the feasibility of each design based on its expected performance, which is risk neutral. However, there are indeed situations in which the decision makers are risk averse. For example, in financial risk management, instead of expected return, value at risk is often used to assess the risk of the portfolios. In engineering design problems, the physical properties of a system can often be estimated by numerical simulation. When implemented in the real world, we often require the physical properties of the system satisfy some hard constraints, meaning that even a small violation of the constraints cannot be tolerated. In this case, the expected performance of the system is not suitable for feasibility determination. We have to develop FD methods that improve the robustness of decision quality.

We introduce risk averse feasibility determination by applying robust optimization techniques (Bertsimas et al. [9]). The philosophy of robust optimization is to represent model uncertainty by deterministic set based values, and then seek optimal solutions in worst-case scenarios. In future research, we incorporate robust implementation decisions into a Bayesian framework to address the risk averse FD problems.

6.1 Manufacturing Application of FD Methodology

The K-C has constructed a new paper mill in Oklahoma. The mill consists of 2 tissue machines, 1 off-line-unit, and 12 converting lines. Currently the schedules of the mill is generated manually. The mill has several mid-term schedulers and for every asset there is a person in charge of its schedule. The company hope we can develop a tool to aid them generating schedules.

There are multiple criterions to judge if a schedule is good or not. The most important one is to finish customer orders on time. Other considerations include stocking level, machine utilization, production line balance rate and so on. It is hard or even impossible to combine these criterions together to form a single standard. Hence we often provide multiple schedules with different emphasis to the decision-maker. When a schedule is generated, the company usually simulates it in their PLC simulation platform to predict the aforementioned performances.

There is fluctuations in the K-C production line. The major concern is the randomness in production rates, whose distribution is unknown. We address this randomness through robust optimization. We set an uncertainty set for the production rate, and generate the schedules in the worst scenario. To avoid over conservativeness, we have to use some parameters to control the size of the uncertainty set. The different conservativeness level results in different schedules. In addition, the different setting of the objective function leads to different schedules too. Usually, we can generate a bunch of schedules, which need to be tested in the simulation platform. We want to select some promising schedules for the decision-maker through feasibility determination.

The simulation time for the schedule simulation is quite limited. Sometimes there is major breakdown or other emergent incidents. The refreshing schedules need to be generated in a very limited time. Thus, the simulation efficiency is very important. Another issue is that several thresholds need to be set for different performance measures simultaneously. Thus multiple performance FD is considered in our future work.

6.2 The Robust Feasibility Determination

We state a formal model for the Bayesian FD problem, and then formulate it as a dynamic program.

Suppose we have k alternative designs. For each $x \in \{1, ..., k\}$, the underlying performance of design x is θ_x. Assume the threshold is d, a design is defined to be feasible if $\theta_x \leq d$. Hence we want to determine the set $\mathbb{B} = \{x : \theta_x \leq d\}$.

Let $\theta = (\theta_1, ..., \theta_k)^T$. We take a Bayesian approach, placing a normal prior probability distribution on each unknown θ_x. Suppose we can have exactly N measurements, and time is indexed by $n = 0, 1, ..., N-1$. At each time n, we select a design x^n to measure. Assume the measurement has an error ϵ^{n+1}, which is normally distributed with mean 0 and finite known variance σ_ϵ^2. Assume the measurement errors are independent of each other and independent with θ. The observed value would be $y^{n+1} = \theta_{x^n} + \epsilon^{n+1}$.

We define a filtration $(\mathcal{F}^n)_{n=0}^N$, where $\mathcal{F}^n$ is the sigma-algebra generated by $x^0, y^1, ..., x^{n-1}, y^n$. Let $E_n[\cdot]$ denote the conditional expectation taken with respect to $\mathcal{F}^n$, so $E_n[\cdot] = E[\cdot|\mathcal{F}^n]$. The measurement decision is made only based on the information from measurements observed and decisions made in the past. That is, x^n is $\mathcal{F}^n$ measurable.

Let $N(\mu_x^0, (\sigma_x^0)^2)$ be the prior predictive distribution of θ_x, for each $x \in \{1, ..., k\}$. Let $\mu_x^n = E_n[\theta_x]$ be the mean of the predictive distribution after n measurements have been observed. Similarly let $(\sigma_x^n)^2 = Cov[\theta_x|\mathcal{F}^n]$ be the covariance of the predictive distribution given $\mathcal{F}^n$. The measurement process is at time n, our knowledge of θ_x is $N(\mu_x^n, (\sigma_x^n)^2)$. We then select a design x^n to measure and the observation value is y^{n+1}. Based on this new information we update our knowledge of θ_x, which is represented by a updated normal distribution $N(\mu_x^{n+1}, (\sigma_x^{n+1})^2)$.

At time N, we determine the set of feasible designs B based on the measurements recorded. Define a terminal payoff function r:

$$r(B;\theta,d) = \sum_{x \notin B} \mathbf{1}_{x \notin \mathbb{B}} + \sum_{x \in B} \mathbf{1}_{x \in \mathbb{B}}$$

$B^* \subseteq \{1, ..., k\}$ is chosen to maximize the expected terminal payoff after N measurements.

$$B^* = \arg\max_{B} E_N[r(B;\theta,d)]$$

Our goal is to find a optimal measurement policy $(x^0, ..., x^{N-1})$ that maximized the expected total reward. Let Π be the set consisting of all measurement strategies $\pi = (x^0, ..., x^{N-1})$. The objective function of our problem is

$$\sup_{\pi \in \Pi} E^{\pi}[r(B^*;\theta,d)]$$

In reality, decision makers are possibly risk averse when determining feasibility of the designs. We propose an alternative definition of feasibility which is adapted to this situation. After all measurements are finished, we have certain knowledge about θ_x. Define a design x is feasible if $P(\theta_x \leq d) \geq 1 - \alpha$, where α is some risk tolerance parameter. Now we want to determine the set $\mathbb{B}' = \{x : P(\theta_x \leq d) \geq 1 - \alpha\}$.

In this new setting, we still use B to denote the set of feasible designs that we determine based on the measurements recorded. The terminal payoff function is changed to be:

$$r^{'}(B;\theta,d) = \sum_{x\notin B} \mathbf{1}_{x\notin \mathbb{B}'} + \sum_{x\in B} \mathbf{1}_{x\in \mathbb{B}'}$$

$B^{'} \subseteq \{1, ..., k\}$ is chosen to maximize the expected terminal payoff after N measurements.

$$B^{'} = \arg\max_{B} E_N[r^{'}(B;\theta,d)]$$

Our goal is to find a optimal measurement policy $(x^0, ..., x^{N-1})$ that maximized the new expected total reward. Hence the new objective function is

$$\sup_{\pi\in\Pi} E^{\pi}[r^{'}(B^{'};\theta,d)]$$

Bibliography

[1] M. A. Ahmed and T. M. Alkhamis. Simulation optimization for an emergency department healthcare unit in kuwait. *European journal of operational research*, 198(3):936–942, 2009.

[2] S. Andradóttir and S.-H. Kim. Fully sequential procedures for comparing constrained systems via simulation. *Naval Research Logistics (NRL)*, 57(5):403–421, 2010.

[3] S. Andradóttir, D. Goldsman, and S.-H. Kim. Finding the best in the presence of a stochastic constraint. In *Proceedings of the 37th conference on Winter simulation*, pages 732–738. Winter Simulation Conference, 2005.

[4] B. Ankenman, B. L. Nelson, and J. Staum. Stochastic kriging for simulation metamodeling. *Operations research*, 58(2):371–382, 2010.

[5] R. R. Barton and M. Meckesheimer. Metamodel-based simulation optimization. *Handbooks in operations research and management science*, 13:535–574, 2006.

[6] D. Batur and F. Choobineh. A quantile-based approach to system selection. *European Journal of Operational Research*, 202(3):764–772, 2010.

[7] D. Batur and S.-H. Kim. Finding feasible systems in the presence of constraints on multiple performance measures. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 20(3):13, 2010.

[8] D. P. Bertsekas. Dynamic programming and suboptimal control: A survey from adp to mpc. *European Journal of Control*, 11(4-5):310–334, 2005.

[9] D. Bertsimas, D. B. Brown, and C. Caramanis. Theory and applications of robust optimization. *SIAM review*, 53(3):464–501, 2011.

[10] E. Bofinger and G. J. Lewis. Two-stage procedures for multiple comparisons with a control. *American Journal of Mathematical and Management Sciences*, 12(4): 253–275, 1992.

[11] G. E. Box. The exploration and exploitation of response surfaces: some general considerations and examples. *Biometrics*, 10(1):16–60, 1954.

[12] S. Boyd and L. Vandenberghe. *Convex optimization*. Cambridge university press, 2004.

[13] J. Branke, S. E. Chick, and C. Schmidt. Selecting a selection procedure. *Management Science*, 53(12):1916–1932, 2007.

[14] M. W. Brantley, L. H. Lee, C.-H. Chen, and A. Chen. Efficient simulation budget allocation with regression. *IIE Transactions*, 45(3):291–308, 2013.

[15] M. W. Brantley, L. H. Lee, C.-H. Chen, and J. Xu. An efficient simulation budget allocation method incorporating regression for partitioned domains. *Automatica*, 50(5):1391–1400, 2014.

[16] J. Butler, D. J. Morrice, and P. W. Mullarkey. A multiple attribute utility theory approach to ranking and selection. *Management Science*, 47(6):800–816, 2001.

[17] C.-H. Chen. A lower bound for the correct subset-selection probability and its application to discrete-event system simulations. *IEEE transactions on automatic control*, 41(8):1227–1231, 1996.

[18] C.-h. Chen and L. H. Lee. *Stochastic simulation optimization: an optimal computing budget allocation*, volume 1. World scientific, 2011.

[19] C.-H. Chen, J. Lin, E. Yücesan, and S. E. Chick. Simulation budget allocation for further enhancing the efficiency of ordinal optimization. *Discrete Event Dynamic Systems*, 10(3):251–270, 2000.

[20] C.-H. Chen, D. He, M. Fu, and L. H. Lee. Efficient simulation budget allocation for selecting an optimal subset. *INFORMS Journal on Computing*, 20(4):579–595, 2008.

[21] H.-C. Chen, C.-H. Chen, and E. Yucesan. Computing efforts allocation for ordinal optimization and discrete event simulation. *IEEE Transactions on Automatic Control*, 45(5):960–964, 2000.

[22] S. E. Chick and K. Inoue. New two-stage and sequential procedures for selecting the best simulated system. *Operations Research*, 49(5):732–743, 2001.

[23] M. Chih. A more accurate second-order polynomial metamodel using a pseudo-random number assignment strategy. *Journal of the Operational Research Society*, 64(2):198–207, 2013.

[24] H. Damerdji and M. K. Nakayama. Two-stage procedures for multiple comparisons with a control in steady-state simulations. In *Proceedings of the 28th conference on Winter simulation*, pages 372–375. IEEE Computer Society, 1996.

[25] M. H. DeGroot. *Optimal statistical decisions*, volume 82. John Wiley & Sons, 2005.

[26] A. Dembo and O. Zeitouni. *Large Deviations Techniques and Applications*. Springer, 2nd edition, 1998.

[27] E. Dudewicz and J. Ramberg. Multiple comparisons with a control: Unknown variances. In *The Annual Technical Conference Transactions of the American Society of Quality Control*, volume 26, pages 483–488, 1972.

[28] E. J. Dudewicz and S. R. Dalal. Allocation of observations in ranking and selection with unequal variances. *Sankhyā: The Indian Journal of Statistics, Series B*, pages 28–78, 1975.

[29] E. J. Dudewicz and S. R. Dalal. Multiple-comparisons with a control when variances are unknown and unequal. *American Journal of Mathematical and Management Sciences*, 3(4):275–295, 1983.

[30] C. W. Dunnett. A multiple comparison procedure for comparing several treatments with a control. *Journal of the American Statistical Association*, 50(272):1096–1121, 1955.

[31] R. Durrett. *Probability: theory and examples*. Cambridge university press, 2010.

[32] K.-T. Fang, R. Li, and A. Sudjianto. *Design and modeling for computer experiments*. CRC Press, 2005.

[33] R. Franke. Scattered data interpolation: tests of some methods. *Mathematics of computation*, 38(157):181–200, 1982.

[34] P. I. Frazier, W. B. Powell, and S. Dayanik. A knowledge-gradient policy for sequential information collection. *SIAM Journal on Control and Optimization*, 47(5): 2410–2439, 2008.

[35] J. H. Friedman. Multivariate adaptive regression splines. *The annals of statistics*, pages 1–67, 1991.

[36] M. C. Fu. Optimization via simulation: A review. *Annals of Operations Research*, 53(1):199–247, 1994.

[37] M. C. Fu, F. W. Glover, and J. April. Simulation optimization: a review, new developments, and applications. In *Simulation conference, 2005 proceedings of the winter*, pages 13–pp. IEEE, 2005.

[38] S. Gao and W. Chen. Efficient subset selection for the expected opportunity cost. *Automatica*, 59:19–26, 2015.

[39] S. Gao and W. Chen. A new budget allocation framework for selecting top simulated designs. *IIE Transactions*, 48(9):855–863, 2016.

[40] S. Gao and W. Chen. Efficient feasibility determination with multiple performance measure constraints. *IEEE Transactions on Automatic Control*, 62(1):113–122, 2017.

[41] S. Gao and L. Shi. Selecting the best simulated design with the expected opportunity cost bound. *IEEE Transactions on Automatic Control*, 60(10):2785–2790, 2015.

[42] S. Gao, W. Chen, and L. Shi. A new budget allocation framework for the expected opportunity cost. *Operations Research*, 2017.

[43] J. Gittins. A dynamic allocation index for the sequential design of experiments. *Progress in statistics*, pages 241–266, 1974.

[44] P. Glynn and S. Juneja. A large deviations perspective on ordinal optimization. In *Simulation Conference, 2004. Proceedings of the 2004 Winter*, volume 1. IEEE, 2004.

[45] D. Goldsman and B. L. Nelson. Ranking, selection and multiple comparisons in computer simulation. In *Simulation Conference Proceedings, 1994. Winter*, pages 192–199. IEEE, 1994.

[46] D. Goldsman, S.-H. Kim, and B. Nelson. Statistical selection of the best system. In *Simulation Conference, 2005 Proceedings of the Winter*, pages 10–pp. IEEE, 2005.

[47] S. S. Gupta and K. J. Miescke. Bayesian look ahead one-stage sampling allocations for selection of the best population. *Journal of statistical planning and inference*, 54(2):229–244, 1996.

[48] G. Gutierrez. Emergency department health care, 2009.

[49] C. Healey, S. Andradóttir, and S.-H. Kim. Selection procedures for simulations with multiple constraints under independent and correlated sampling. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 24(3):14, 2014.

[50] Y. Hochberg and A. C. Tamhane. *Multiple comparison procedures.* Wiley, 1987.

[51] J. Hsu. *Multiple comparisons: theory and methods.* CRC Press, 1996.

[52] S. R. Hunter and R. Pasupathy. Optimal sampling laws for stochastically constrained simulation optimization on finite sets. *INFORMS Journal on Computing*, 25(3):527–542, 2013.

[53] S.-H. Kim and B. L. Nelson. A fully sequential procedure for indifference-zone selection in simulation. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 11(3):251–273, 2001.

[54] S.-H. Kim and B. L. Nelson. On the asymptotic validity of fully sequential selection procedures for steady-state simulation. *Operations Research*, 54(3):475–488, 2006.

[55] S.-H. Kim and B. L. Nelson. Recent advances in ranking and selection. In *Simulation Conference, 2007 Winter*, pages 162–172. IEEE, 2007.

[56] L. W. Koenig and A. M. Law. A procedure for selecting a subset of size m containing the l best of k independent normal populations, with applications to simulation. *Communications in Statistics-Simulation and Computation*, 14(3):719–734, 1985.

[57] A. M. Law and W. D. Kelton. *Simulation Modeling and Analysis.* McGraw-Hill, 3rd edition, 2000.

[58] L. H. Lee, N. A. Pujowidianto, L.-W. Li, C. Chen, and C. M. Yap. Approximate simulation budget allocation for selecting the best design in the presence of stochastic constraints. *IEEE Transactions on Automatic Control*, 57(11):2940–2945, 2012.

[59] Y. Li, S. H. Ng, M. Xie, and T. Goh. A systematic comparison of metamodeling techniques for simulation optimization in decision support systems. *Applied Soft Computing*, 10(4):1257–1273, 2010.

[60] A. Mahajan and D. Teneketzis. Multi-armed bandit problems. *Foundations and Applications of Sensor Management*, pages 121–151, 2008.

[61] E. Masson and Y.-J. Wang. Introduction to computation and learning in artificial neural networks. *European Journal of Operational Research*, 47(1):1–28, 1990.

[62] M. Molga and C. Smutnicki. Test functions for optimization needs. *Test functions for optimization needs*, page 101, 2005.

[63] K. P. Murphy. Conjugate bayesian analysis of the gaussian distribution. *def*, 1 ($2\sigma2$):16, 2007.

[64] R. H. Myers, D. C. Montgomery, and C. M. Anderson-Cook. *Response surface methodology: process and product optimization using designed experiments*. John Wiley & Sons, 2016.

[65] B. L. Nelson and D. Goldsman. Comparisons with a standard in simulation experiments. *Management Science*, 47(3):449–463, 2001.

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

[67] G. Palermo, C. Silvano, and V. Zaccaria. An efficient design space exploration methodology for on-chip multiprocessors subject to application-specific constraints. In *Application Specific Processors, 2008. SASP 2008. Symposium on*, pages 75–82. IEEE, 2008.

[68] R. Pasupathy, S. R. Hunter, N. A. Pujowidianto, L. H. Lee, and C.-H. Chen. Stochastically constrained ranking and selection via score. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 25(1):1, 2015.

[69] E. Paulson. On the comparison of several experimental categories with a control. *The Annals of Mathematical Statistics*, pages 239–246, 1952.

[70] Y. Peng. Dynamic sampling allocation for efficient feasibility determination. *Technical Report*, 2017.

[71] Y. Peng, C.-H. Chen, M. C. Fu, and J.-Q. Hu. Dynamic sampling allocation and design selection. *INFORMS Journal on Computing*, 28(2):195–208, 2016.

[72] W. B. Powell. *Approximate Dynamic Programming: Solving the curses of dimensionality*, volume 703. John Wiley & Sons, 2007.

[73] N. Quan, J. Yin, S. H. Ng, and L. H. Lee. Simulation optimization via kriging: a sequential search using expected improvement with computing budget constraints. *Iie Transactions*, 45(7):763–780, 2013.

[74] T. Rengarajan and D. P. Morton. Estimating the efficient frontier of a probabilistic bicriteria model. In *Simulation Conference (WSC), Proceedings of the 2009 Winter*, pages 494–504. IEEE, 2009.

[75] Y. Rinott. On two-stage selection procedures and related probability-inequalities. *Communications in Statistics-Theory and methods*, 7(8):799–811, 1978.

[76] I. Sabuncuoglu and S. Touhami. Simulation metamodelling with neural networks: an experimental investigation. *International Journal of Production Research*, 40 (11):2483–2505, 2002.

[77] T. J. Santner, B. J. Williams, and W. I. Notz. *The design and analysis of computer experiments*. Springer Science & Business Media, 2013.

[78] D. Shin, M. Broadie, and A. Zeevi. Tractable sampling strategies for quantile-based ordinal optimization. In *Winter Simulation Conference (WSC), 2016*, pages 847–858. IEEE, 2016.

[79] M. Shin, R. G. Sargent, and A. L. Goel. Optimization and response surfaces: Gaussian radial basis functions for simulation metamodeling. In *Proceedings of the 34th conference on Winter simulation: exploring new frontiers*, pages 483–488. Winter Simulation Conference, 2002.

[80] T. W. Simpson, J. Poplinski, P. N. Koch, and J. K. Allen. Metamodels for computer-based engineering design: survey and recommendations. *Engineering with computers*, 17(2):129–150, 2001.

[81] M. L. Stein. *Interpolation of spatial data: some theory for kriging*. Springer Science & Business Media, 2012.

[82] L. Sun, L. J. Hong, and Z. Hu. Balancing exploitation and exploration in discrete optimization via simulation through a gaussian process-based search. *Operations Research*, 62(6):1416–1438, 2014.

[83] R. Szechtman and E. Yücesan. A new perspective on feasibility determination. In *Proceedings of the 40th Conference on Winter Simulation*, pages 273–280. Winter Simulation Conference, 2008.

[84] R. Szechtman and E. Yücesan. A bayesian approach to feasibility determination. In *Winter Simulation Conference (WSC), 2016*, pages 782–790. IEEE, 2016.

[85] A. Torn and A. Zilinskas. Global optimization: Lecture notes in computer science. *New York springerverlag*, 350, 1989.

[86] H. Xiao, L. H. Lee, and C.-H. Chen. Optimal budget allocation rule for simulation optimization using quadratic regression in partitioned domains. *IEEE Transactions on Systems, Man, and Cybernetics: Systems*, 45(7):1047–1062, 2015.

[87] J. Xie and P. I. Frazier. Sequential bayes-optimal policies for multiple comparisons with a known standard. *Operations Research*, 61(5):1174–1189, 2013.

[88] S. Yan, E. Zhou, and C.-H. Chen. Efficient selection of a set of good enough designs with complexity preference. *IEEE Transactions on Automation Science and Engineering*, 9(3):596–606, 2012.

[89] S. Zhang, L. H. Lee, E. P. Chew, J. Xu, and C.-H. Chen. A simulation budget allocation procedure for enhancing the efficiency of optimal subset selection. *IEEE Transactions on Automatic Control*, 61(1):62–75, 2016.