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A NOTE ON THE SUBSET SELECTION FOR SIMULATION OPTIMIZATION

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ABSTRACT

In this paper, we consider the problem of selecting an optimal subset from a finite set of simulated designs. Using the optimal computing budget allocation (OCBA) framework, we formulate the problem as that of maximizing the probability of correctly selecting the top m designs subject to a constraint on the total number of samples available. For an approximation of the probability of correct selection, we derive an asymptotically optimal subset selection procedure that is easy to implement. More importantly, we provide some useful insights on characterizing an efficient subset selection rule and how it can be achieved by adjusting the budgets allocated to the optimal and non-optimal subsets.

1 INTRODUCTION

The problem we consider is selecting the top m ($m > 1$) designs from a finite set of k design alternatives, where the performance of each design is estimated with noise (uncertainty). The primary context is simulation, where the goal is to determine the best allocation of simulation replications among the various designs in order to maximize the probability of correct selection (PCS). This problem setting falls in the well-established branch of statistics known as ranking and selection (R&S) or multiple comparison procedures. For a comprehensive review of this field, see Branke et al. (2007), Kim and Nelson (2007).

Most existing R&S research has focused on selecting the best design. The indifference-zone (IZ) approach aims to provide a guaranteed lower bound for *PCS*, assuming that the mean performance of the best design is at least δ^* better than each alternative, where δ^* is the minimum difference worth detecting (Dudewicz and Dalal 1975, Rinott 1978, Kim and Nelson 2001, Nelson et al. 2001). The optimal computing budget allocation (OCBA) method allocates the samples sequentially in order to maximize *PCS* under a simulation budget constraint (Chen et al. 2000, Chen et al. 2008, Chen and Lee 2011). The expected value of information (EVI) procedure allocates samples to maximize the EVI obtained from sampling in two stages or sequentially using predictive distributions of further samples (Chick and Inoue 2001b, Chick and Inoue 2001a).

The problem of selecting the top m designs is motivated by recent developments in global simulation optimization algorithms, which require the selection of an elite subset of good candidate solutions in each iteration of the algorithm (Chambers 1995, Rubinstein and Kroese 2004, Hu et al. 2007, Hu et al. 2008). The information from the elite set is used to guide the search in subsequent iterations for the global optimum. Since the performance of these algorithms depends heavily on the quality of the selected solutions, how to efficiently select an optimal subset then becomes a critical problem for implementation of these algorithms.

The optimal subset selection problem has been considered in Koenig and Law (1985). A two-stage procedure was established to provide a *PCS* guarantee. However, the number of additional simulation replications for the second stage is computed based on a least favorable configuration and causes the computational cost to be much higher than actually needed. A sequential subset selection procedure was developed in Chen et al. (2008), which maximizes *PCS* using the OCBA method. The optimal subset selection problem with the expected opportunity cost (EOC), a common quality measure other than PCS, was considered in Gao and Chen (2015).

In this paper, we characterize a new and efficient simulation budget allocation rule, called $OCBA_{ss}$, for solving the optimal subset selection problem from a finite set of simulated designs. $OCBA_{ss}$ is developed using the PCS measure and the OCBA framework, and when $m = 1$, i.e., selecting the single best design, $OCBA_{ss}$ degrades to the well-known OCBA allocation rule in Chen et al. (2000). It can be demonstrated in numerical testing that $OCBA_{ss}$ has better performance than the existing allocation methods in the literature. More importantly, we provide some useful insights for the subset selection problem. They reveal properties of an efficient allocation and how it can be achieved by adjusting the proportions of the total simulation budget allocated to the designs in the optimal and non-optimal subsets.

The rest of the paper is organized as follows. In Section 2, we formulate the simulation budget allocation problem for selecting the top m designs. In Section 3, we develop a new and efficient budget allocation strategy and provide some insights on it. The performance of the proposed method is illustrated with numerical examples in Section 4. Section 5 concludes the paper.

2 PROBLEM FORMULATION

In this research, the best design is defined as the design with the smallest mean performance (the largest mean performance could be handled similarly). We introduce the following notation:

T: total number of simulation replications (budget);
k: total number of designs;
$L_{i,l}$: output of the l-th simulation replication for design i;
J_i: mean of $L_{i,l}$, i.e., $J_i = E[L_{i,l}]$;
σ_i^2: variance of $L_{i,l}$, i.e., $\sigma_i^2 = Var[L_{i,l}]$;
N_i: number of simulation replications for design i;
α_i: proportion of the total simulation budget to design i, i.e., $\alpha_i = N_i/T$;
$\bar{J}_i$: sample mean of design i, i.e., $\bar{J}_i = \frac{1}{N_i}\sum_{l=1}^{N_i} L_{i,l}$;
S_o: set of the true top m designs (optimal subset);
S_n: set of the designs that are not in S_o (non-optimal subset);
$\delta_{i,j} = J_i - J_j$;
$\sigma_{i,j}^2 = \sigma_i^2/N_i + \sigma_j^2/N_j$.

In this study, we assume no ties in means among the k designs for selection. The simulation output samples are assumed to be normally distributed and independent from replication to replication, as well as independent across different designs.

A correct selection occurs when the optimal subset is S_o selected, and the probability of making a correct selection is:

$$PCS = P\left(\bigcap_{i\in S_o}\bigcap_{j\in S_n}(\bar{J}_i < \bar{J}_j)\right). \tag{1}$$

The goal is to find a simulation budget allocation that maximizes the *PCS* given in (1). However, in general, the maximization of *PCS* is analytically intractable due to the lack of convenient expression for *PCS*. To address this difficulty, we develop an approximation of *PCS* using a lower bound.

Using the Bonferroni inequality,

$$PCS \geq 1 - \sum_{i\in S_o}\sum_{j\in S_n} P(\bar{J}_j < \bar{J}_i) \equiv APCS. \tag{2}$$

We refer to this lower bound of *PCS* as the approximated probability of correct selection (APCS). Then, in this study, we consider the following selection problem instead:

$$\begin{aligned} \max \quad & APCS \\ s.t. \quad & \sum_{i=1}^{k} N_i = T. \end{aligned} \tag{3}$$

This formulation falls in the OCBA framework. It implicitly assumes that the computational cost of each replication is constant across designs; however, it can be generalized to other settings by changing the budget constraint to $\sum_{i=1}^{k} c_i N_i = T$ where c_i reflects the (relative) cost of a replication for design i, and T reflects a more general computing budget rather than simply the total number of simulation replications.

3 EFFICIENT SIMULATION BUDGET ALLOCATION

In this section, we derive the asymptotic (as the budget $T \to \infty$) optimality conditions for problem (3) and provide some useful insights for them. A sequential selection procedure is then designed for implementation.

3.1 Asymptotic Optimality Conditions

To solve (3), we first prove the following lemma.

Lemma 1 Consider $u_j, v_j, w_j, z_j \in \mathbb{R}$ with $u_j, w_j > 0$ and $v_j, z_j < 0$, $j = 1, 2, \ldots, m$. If for $x \in \mathbb{R}$,

$$\sum_{j=1}^{m} u_j \exp(v_j x) = \sum_{j=1}^{m} w_j \exp(z_j x) \tag{4}$$

as $x \to +\infty$, then, $\max_{j \in \{1,\ldots,m\}} v_j = \max_{j \in \{1,\ldots,m\}} z_j$.

Proof. Let $j_v = \arg\max_{j \in \{1,\ldots,m\}} v_j$ and $j_z = \arg\max_{j \in \{1,\ldots,m\}} z_j$. Note that as $x \to +\infty$,

$$\begin{aligned} \frac{u_j \exp(v_j x)}{u_{j_v} \exp(v_{j_v} x)} =& o(1) \quad \text{for } j \neq j_v, \\ \frac{w_j \exp(z_j x)}{w_{j_z} \exp(z_{j_z} x)} =& o(1) \quad \text{for } j \neq j_z, \end{aligned}$$

where for functions $G(x)$ and $H(x)$, $G(x) = o(H(x))$ means that $H(x)$ is higher-order infinitesimal than $G(x)$ as $x \to +\infty$. From (4),

$$u_{j_v} \exp(v_{j_v} x)(1 + o(1)) = w_{j_z} \exp(z_{j_z} x)(1 + o(1)). \tag{5}$$

Take natural log on both sides of (5),

$$\log(u_{j_v}) + v_{j_v} x + \log(1 + o(1)) = \log(w_{j_z}) + z_{j_z} x + \log(1 + o(1)). \tag{6}$$

Divide both sides of (6) by x. As $x \to +\infty$, $v_{j_v} = z_{j_z}$. □

According to Gao and Shi (2015b), $P(\bar{J}_j < \bar{J}_i)$ is asymptotically convex for designs $i \in S_o$ and $j \in S_n$. *APCS* is then an asymptotically concave function and (3) is an asymptotically convex function. Therefore, to solve (3), we can find the Karush-Kuhn-Tucker (KKT) conditions (Boyd and Vandenberghe 2004) of it.

Theorem 2 Denote $I_{i,j}=\frac{\delta_{i,j}^2}{\sigma_i^2/\alpha_i+\sigma_j^2/\alpha_j}$ for $i\in S_o$ and $j\in S_n$, $j_i=\arg\min_{j\in S_n} I_{i,j}$ for $i\in S_o$ and $i_j=\arg\min_{i\in S_o} I_{i,j}$ for $j\in S_n$. Problem (3) is asymptotically optimized if

$$\sum_{i\in S_o}\frac{N_i^2}{\sigma_i^2}=\sum_{j\in S_n}\frac{N_j^2}{\sigma_j^2}, \tag{7}$$

$$I_{i,j_i}=I_{i',j_{i'}},\quad i,i'\in S_o \text{ and } i\neq i', \tag{8}$$

$$I_{i_j,j}=I_{i_{j'},j'},\quad j,j'\in S_n \text{ and } j\neq j'. \tag{9}$$

Proof. Let $\mathscr{F}$ be the Lagrangian relaxation of (3) with Lagrange multiplier $\lambda>0$, i.e., $\mathscr{F}=APCS-\lambda(\sum_{i=1}^k N_i-T)$. The KKT conditions of (3) are:

$$\frac{\partial\mathscr{F}}{\partial N_i}=-\sum_{j\in S_n}\frac{1}{2\sqrt{2\pi}}\exp\left\{-\frac{\delta_{i,j}^2}{2\sigma_{i,j}^2}\right\}\frac{\delta_{i,j}\sigma_i^2}{\sigma_{i,j}^3N_i^2}-\lambda=0,\quad i\in S_o; \tag{10}$$

$$\frac{\partial\mathscr{F}}{\partial N_j}=-\sum_{i\in S_o}\frac{1}{2\sqrt{2\pi}}\exp\left\{-\frac{\delta_{i,j}^2}{2\sigma_{i,j}^2}\right\}\frac{\delta_{i,j}\sigma_j^2}{\sigma_{i,j}^3N_j^2}-\lambda=0,\quad j\in S_n. \tag{11}$$

Apply (10) for all $i\in S_o$ and (11) for all $j\in S_n$:

$$-\sum_{i\in S_o}\sum_{j\in S_n}\frac{1}{2\sqrt{2\pi}}\exp\left\{-\frac{\delta_{i,j}^2}{2\sigma_{i,j}^2}\right\}\frac{\delta_{i,j}}{\sigma_{i,j}^3}=\sum_{i\in S_o}\lambda\frac{N_i^2}{\sigma_i^2}=\sum_{j\in S_n}\lambda\frac{N_j^2}{\sigma_j^2}.$$

That is,

$$\sum_{i\in S_o}\frac{N_i^2}{\sigma_i^2}=\sum_{j\in S_n}\frac{N_j^2}{\sigma_j^2}. \tag{12}$$

To investigate the relationship between the budgets allocated to the designs in S_o, pick $i,i'\in S_o$ with $i\neq i'$. From (10),

$$\sum_{j\in S_n}\frac{1}{2\sqrt{2\pi}}\exp\left\{-\frac{1}{2}I_{i,j}T\right\}\frac{\delta_{j,i}\sigma_i^2}{\sigma_{i,j}^3N_i^2}=\sum_{j\in S_n}\frac{1}{2\sqrt{2\pi}}\exp\left\{-\frac{1}{2}I_{i',j}T\right\}\frac{\delta_{j,i'}\sigma_{i'}^2}{\sigma_{i',j}^3N_{i'}^2}. \tag{13}$$

Apply Lemma 1 to (13). Asymptotically as the budget $T\to\infty$,

$$I_{i,j_i}=I_{i',j_{i'}},\quad i,i'\in S_o \text{ and } i\neq i'. \tag{14}$$

We can similarly obtain the relationship between the budgets allocated to the designs $j,j'\in S_n$ with $j\neq j'$. Asymptotically from (11),

$$I_{i_j,j}=I_{i_{j'},j'},\quad j,j'\in S_n \text{ and } j\neq j'. \tag{15}$$

□

3.2 Analysis of the Optimality Conditions

We provide some insights of the optimality conditions (7), (8) and (9) derived.

For (7), it indicates the number of simulation budget that should be spent on the optimal subset S_o and the non-optimal subset S_n. It serves to provide a general balance for the simulation efforts devoted to the two subsets so that neither of the subsets is over-sampled. In determining this general balance, just the variance information of the designs in the two subsets is employed. Such information represents the hardness of the designs in a subset for being distinguished from the other subset. The larger the variances are, the harder it is to distinguish a subset, and the more simulation budget this subset receives. The other dimension of the hardness for distinguishing the two subsets involves the difference in means between the designs in these two subsets. However, such hardness is mutual for the two subsets and can be thought of as "canceled" when determining the budgets devoted to them.

In particular, for the special case of $|S_o| = 1$ and $|S_n| = k-1$, (7) degrades to the well-known OCBA allocation rule for the best single design selection (Chen and Lee 2011):

$$\frac{N_t^2}{\sigma_t^2} = \sum_{j=1, j\neq t}^{k} \frac{N_j^2}{\sigma_j^2},$$

where design t is the true best design among the k competing alternatives.

To interpret (8) and (9), we first consider $I_{i,j}$ defined in Theorem 2. It has been shown in Gao and Shi (2015a) that a good approximation and upper bound for $P(\bar{J}_j < \bar{J}_i)$ for $i \in S_o$ and $j \in S_n$ is given by

$$P(\bar{J}_j < \bar{J}_i) \approx \exp\left\{-\frac{1}{2} I_{i,j} T\right\}.$$

Note that the event $\bar{J}_j < \bar{J}_i$ corresponds to a wrong selection. Then, $P(\bar{J}_j < \bar{J}_i)$ denotes the probability of making a wrong selection when making a pair-wise comparison between designs $i \in S_o$ and $j \in S_n$. As the total budget T increases, this probability goes to 0, and its exponential converging rate is characterized by $\frac{1}{2} I_{i,j}$. The larger $\frac{1}{2} I_{i,j}$ is, the higher the converging rate is, and the less likely we make a wrong selection in the pair-wise comparison of designs i and j.

In (8), for an $i \in S_o$, j_i is taken as $\arg\min_{j\in S_n} I_{i,j}$. That is, j_i is the design in S_n that is most likely to lead to a wrong selection when design i is pair-wisely compared with all the designs in S_n. The hardness of comparing i and j_i is used to represent the hardness of correctly observing i in the simulation budget allocation. This is not surprising because if designs i and j_i are correctly compared, designs i and j for $j \in S_n$ and $j \neq j_i$ are likely to be correctly compared, and correctly comparing designs i and j for all $j \in S_n$ means that design i is correctly observed. In the optimal budget allocation status, the simulation budget is allocated to the designs in S_o such that the hardness of correctly observing these designs remains the same. We can perform similar analysis to (9) and reach the conclusion that the optimal budget allocation requires the hardness of correctly observing the designs in S_n remains the same too.

In summary, optimality condition (7) provides a general balance between the simulation budgets devoted to the optimal and non-optimal subsets. Optimality conditions (8) and (9) attempt to enforce appropriate proportions of the simulation budget for each design in the optimal subset and non-optimal subset respectively.

Still, for the special case of $|S_o| = 1$ and $|S_n| = k-1$, let t be the true best design. (8) vanishes, and (9) degrades to

$$\frac{\delta_{t,j}^2}{\frac{\sigma_t^2}{N_t} + \frac{\sigma_j^2}{N_j}} = \frac{\delta_{t,j'}^2}{\frac{\sigma_t^2}{N_t} + \frac{\sigma_{j'}^2}{N_j}} \quad j \neq j'.$$

If we further assumes $N_t \gg N_j$ for all $j \neq t$, then,

$$\frac{N_j}{N_{j'}} = \left(\frac{\sigma_j/\delta_{t,j}}{\sigma_{j'}/\delta_{t,j'}}\right)^2 \quad j \neq j',$$

which is also identical to the OCBA result.

3.3 Sequential Budget Allocation Procedure

Based on the discussion above, we propose a sequential budget allocation procedure to satisfy the optimality conditions (7), (8) and (9). At each iteration, we provide an incremental budget Δ and calculate $\mathscr{U}_o = \sum_{i\in S_o} \frac{N_i^2}{\sigma_i^2}$ and $\mathscr{U}_n = \sum_{j\in S_n} \frac{N_j^2}{\sigma_j^2}$. If $\mathscr{U}_o < \mathscr{U}_n$, Δ is allocated to the design $i^* \in S_o$ with $i^* = \arg\min I_{i^*,j_{i^*}}$; otherwise, Δ is allocated to the design $j^* \in S_n$ with $j^* = \arg\min I_{i_{j^*},j^*}$. This is because designs i^* and j^* correspond to the largest violations of (8) and (9) respectively, and allocating additional replications to these designs can alleviate or eliminate these violations. This process is iterated until the given budget T is consumed. Since this procedure is developed within the OCBA framework, we call it $OCBA_{ss}$, the OCBA allocation for subset selection.

$OCBA_{ss}$ Allocation Procedure

1. For a set of k simulated designs, specify the size of the optimal set m, total simulation budget T, the initial simulation replication number n_0 and the incremental budget Δ_0. Iteration counter $r \leftarrow 0$. Perform n_0 simulation replications to all designs. $N_i^r = n_0$ for $i = 1,2,...,k$.
2. For all designs $i = 1,2,...,k$, calculate sample mean $\bar{J}_i$ and sample variance s_i^2.
3. If $\sum_{i=1}^k N_i^r = T$, stop. Otherwise,
   a. Calculate the estimates $\hat{\mathscr{U}}_o$, $\hat{\mathscr{U}}_n$, $\hat{i}^*$ and $\hat{j}^*$ for $\mathscr{U}_o$, $\mathscr{U}_n$, i^* and j^* using $\bar{J}_i$ and s_i^2, $i = 1,2,...,k$.
   b. Provide an incremental simulation budget $\Delta = \min\{\Delta_0, T - \sum_{i=1}^k N_i^r\}$. If $\hat{\mathscr{U}}_o < \hat{\mathscr{U}}_n$, allocate Δ to design $\hat{i}^*$, $N_{\hat{i}^*}^{r+1} = N_{\hat{i}^*}^r + \Delta$; otherwise, allocate Δ to design $\hat{j}^*$, $N_{\hat{j}^*}^{r+1} = N_{\hat{j}^*}^r + \Delta$.
   c. Update the sample mean and sample variance of the design receiving additional replications.
   d. $r \leftarrow r+1$.

4 NUMERICAL EXPERIMENTS

In this section, we test the proposed $OCBA_{ss}$ procedure by comparing it with different simulation budget allocation methods on several typical selection problems.

We use the following two budget allocation approaches for comparison.

- *Equal Allocation*: This is the simplest way to conduct simulation experiments and has been widely applied. The total simulation budget is equally allocated to each design, so that all the designs are simulated equally often. The performance of equal allocation serves as a benchmark for comparison.
- *OCBA-m Allocation*: *OCBA-m* is a sequential budget allocation procedure developed to select the top m designs using the *PCS* criterion (Chen et al. 2008). In each iteration, it provides an incremental budget and allocates it to the candidate designs according to

$$\frac{N_i}{N_j} = \left(\frac{\sigma_i/\delta_i}{\sigma_j/\delta_j}\right)^2, i,j \in \{1,2,...,k\} \text{ and } i \neq j,$$

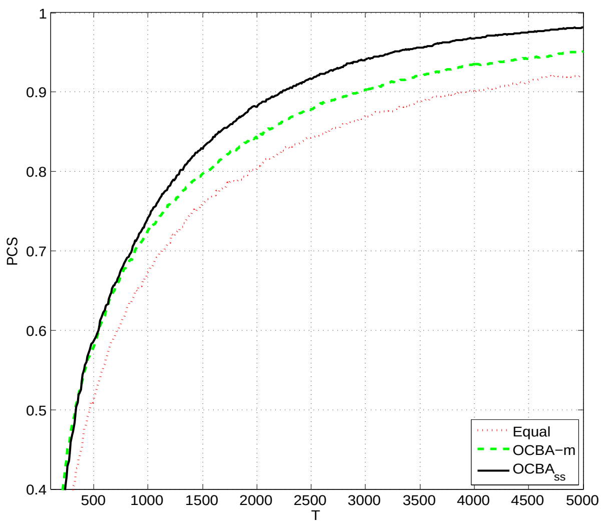
  where $\delta_i = J_i - c$ and c is a pre-specified parameter. Although *OCBA-m* is also developed within the OCBA framework, it is different from the proposed $OCBA_{ss}$ allocation rule.

In order to compare the performance of these allocation approaches, we test them empirically on three typical selection examples.

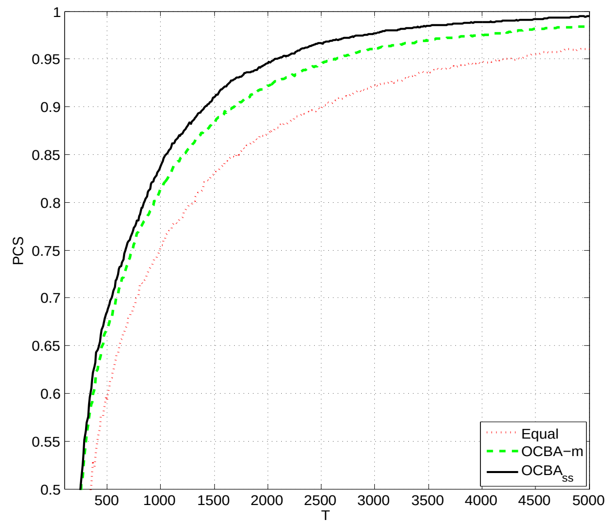
- *Example 1*: Monotone means and constant variances.
  It has 10 designs and $|S_o| = 3$. Design i has a distribution of $N(i, 10^2)$, $i = 1,2,...,10$.
- *Example 2*: Monotone means and increasing variances.
  It has 10 designs and $|S_o| = 3$. Design i has a distribution of $N(i, 20i)$, $i = 1,2,...,10$.

- *Example 3*: Monotone means and decreasing variances.
  It has 10 designs and $|S_o| = 3$. Design i has a distribution of $N(i, 20(11-i))$, $i = 1, 2, ..., 10$.

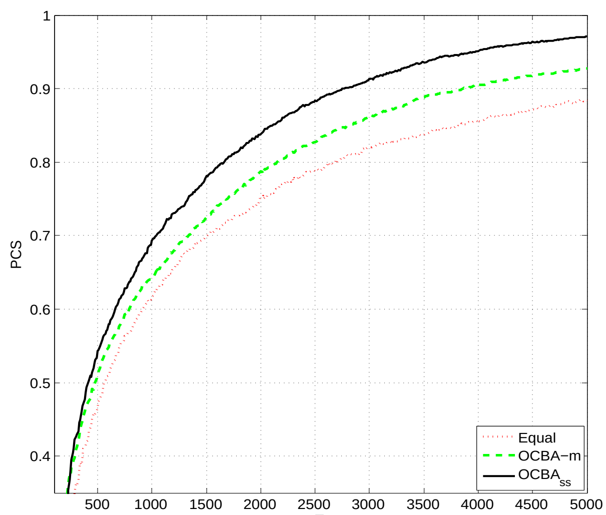
For *OCBA-m* and $OCBA_{ss}$, we perform 10 initial replications for each design and the incremental budget is 10. The estimate of *PCS* is based on the average of 8000 independent replications of each procedure to the problem. The comparison of the three approaches is reported in Figure 1.



(a) Example 1



(b) Example 2



(c) Example 3

Figure 1: Comparison results of the three methods.

From the results, it is observed that the proposed $OCBA_{ss}$ works the best. It reaches higher *PCS* with different budgets on all the tested examples, except that $OCBA_{ss}$ performs slightly worse than *OCBA-m* on example 1 when the simulation budget is small.

The performance of *OCBA-m* is second. There are two possible reasons for *OCBA-m* being less efficient than $OCBA_{ss}$. The first is that, in the special case of $m = 1$, $OCBA_{ss}$ degrades to the OCBA allocation rule while *OCBA-m* does not, which suggests that $OCBA_{ss}$ might offer better approximation to the optimal allocation strategy. The other possible reason lies in the parameter c introduced by *OCBA-m*. Theoretically c can be any real numbers between $\max_{i\in S_o} J_i$ and $\min_{j\in S_n} J_j$ to validate the *OCBA-m* allocation rule, but how the value of c is determined has a great influence to the efficiency of *OCBA-m*. In Chen et al. (2008), c is suggested to take the average of $\max_{i\in S_o} J_i$ and $\min_{j\in S_n} J_j$. However, intuitively, the optimal c value should depend on the problem structure and should be different from case to case. These two reasons might explain why *OCBA-m* is not so efficient as $OCBA_{ss}$.

The equal allocation performs the worst. This is not surprising because the equal allocation cannot adapt to the structure of each design and involve the information of sample mean and sample variance to guide the allocation as the other two procedures do.

5 Conclusions

In this study, an efficient simulation budget allocation procedure is presented for selecting the top m designs from a finite set of design alternatives. The objective is to maximize the probability of correct selection within a given computing budget. We develop an approximation for the correct selection probability, and then derive an asymptotically optimal selecting procedure for this approximate measure. When $m = 1$, the new procedure degrades to the OCBA allocation rule. Numerical testing indicates that the proposed approach is more efficient than other methods in the literature. We also perform some analysis on the budget allocation method derived. It provides some useful insights for determining an efficient subset selection and how it can be achieved by adjusting the budgets allocated to the optimal and non-optimal subsets.

In this research, we have attacked the subset selection problem within the OCBA framework. A possible alternative is the knowledge gradient (KG), which is another common approach for R&S problems (Frazier et al. 2008). KG is typically based on Bayesian framework and dynamic programming formulation, and its efficiency has been demonstrated via a variety of numerical examples (Frazier et al. 2008, Frazier et al. 2009). It indicates a promising line of future research along which the subset selection problem might be efficiently solved.

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