OPTIMAL COMPUTING BUDGET ALLOCATION WITH INPUT UNCERTAINTY

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ABSTRACT

In this study, we consider ranking and selection problems where the simulation model is subject to input uncertainty. Under the input uncertainty, we compare system designs based on their worst-case performance, and seek to maximize the probability of selecting the design with the best performance under the worst-case scenario. By approximating the probability of correct selection (PCS), we develop an asymptotically (as the simulation budget goes to infinity) optimal solution of the resulting problem. An efficient selection procedure is designed within the optimal computing budget allocation (OCBA) framework. Numerical tests show the high efficiency of the proposed method.

1 INTRODUCTION

We consider the problem of selecting the best system design among a finite number of choices, where the performance of each design is evaluated via stochastic simulation. The goal is to determine the best allocation of simulation replications in order to maximize the probability of correct selection (PCS) for the best design. 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 Kim and Nelson (2007), Xu et al. (2015).

There are three common approaches for solving R&S problems. The indifference-zone (IZ) approach seeks 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 expected value of information procedure (VIP) procedure describes the evidence for correct selection with Bayesian posterior distributions and allocates the simulation budget to maximize the expected value of information in the simulation samples (Chick and Inoue 2001b, Chick and Inoue 2001a, Chick and Frazier 2012, Xie et al. 2016). The optimal computing budget allocation (OCBA) method allocates the samples sequentially to maximize PCS under a simulation budget constraint (Chen et al. 2000, Chen et al. 2008, Gao and Chen

2015, Gao and Chen 2016a, Gao and Chen 2016b). The high efficiency of the OCBA approach has been demonstrated in various numerical experiments (Branke et al. 2007, Chen et al. 2014).

Most of the abovementioned R&S procedures implicitly assume that the input distributions and their parameters can be specified accurately for the simulation model. However, in real applications, the input distributions and their parameters are typically unknown and have to be estimated from limited historical data. As a result, there often exists profound input uncertainty for the simulation model, which might (severely) affect the selection for the best design. To address this issue, Corlu and Biller (2013) developed a subset selection procedure that accounts for the input uncertainty. Fan et al. (2013) presented a robust IZ-based R&S formulation that selects the best design with respect to the worst-case performance among a finite collection of possible input models, called *robust selection of the best* (RSB). Song et al. (2015) explored the impact of model risk due to input uncertainty on R&S procedures. This issue is also related to two streams of literature. The first is input uncertainty quantification, which quantifies the impact of input uncertainty on the simulation output (Chick 2006, Barton 2012, Barton et al. 2014). The other is robust optimization (RO) (Delage and Ye 2010, Goh and Sim 2010, Ben-Tal et al. 2013). Different from simulation-based optimization in which targeted problems do not have nice structures to be exploited, RO often requires that the optimization problems are available explicitly in closed form.

To approach R&S problems with input uncertainty, in this study, we assume that each design has a finite number of scenarios, each corresponding to an input distribution. An OCBA-based procedure, called $OCBA_R$, is proposed to maximize the probability of correctly selecting the design with the best performance under the worst-case scenario. Since making decisions based on the worst-case scenario can prevent potential high risk, this setting is preferred by conservative decision makers. According to $OCBA_R$, we only need to concentrate our simulation budget on a small fraction of all the scenarios under consideration to improve efficiency. For the special case that each design has only one scenario, $OCBA_R$ reduces to the original OCBA allocation rule derived previously in Chen et al. (2000).

The rest of the paper is organized as follows. Section 2 formulates the R&S problem with input uncertainty. Section 3 derives the asymptotic optimal solution for the problem formulated. Numerical experiments are provided in Section 4, followed by conclusions in Section 5.

2 PROBLEM SETTING

We consider the problem of selecting the best design from a given set of k designs. For all the k designs, we assume that the set of possible input distributions U is identical and contains a finite number m of scenarios. We call U the *uncertainty set*, which incorporates the uncertainty from both the input distributions and their associated parameters. Note that this assumption is not restrictive for practical purposes. From historical data, we can first identify a number of appropriate input distributions for the simulation model and then discretize the possible ranges of the associated parameters to establish U.

Let $J_{i,j}$, $\sigma_{i,j}^2$ and $\bar{J}_{i,j}$ be the mean, variance and sample mean for the simulation output of the scenario j of design i, i = 1, 2, ..., k and j = 1, 2, ..., m. T is the total simulation budget and $\alpha_{i,j}$ is the proportion of T allocated to scenario j of design i. The performance of design i is represented by the performance of its worstcase scenario, i.e., $\max_{j \in \{1,2,...,m\}} J_{i,j}$, and the true best design is $t = \arg \min_{i \in \{1,2,...,k\}} \max_{j \in \{1,2,...,m\}} J_{i,j}$. We assume that for each design $i \in \{1, 2, ..., k\}$, there exists scenario j_i such that $J_{i,j_i} > J_{i,j}$ for all $j \in \{1, 2, ..., m\}$ and $j \neq j_i$, and there exists design $i \in \{1, 2, ..., k\}$ such that $J_{i,j_i} < J_{i',j_{i'}}$ for all $i' \in \{1, 2, ..., k\}$ and $i' \neq i$. This assumption ensures that the worst-case scenario of each design and the true best design are uniquely defined. In order to make the derivation more tractable, we further assume that the simulation output samples for each scenario are normally distributed for all the designs and are independent from replication to replication and across different designs and scenarios.

Design *t* is correctly selected when for any design $l \in \{1, 2, ..., k\}$ and $l \neq t$, there exists some scenario *r* of design *l* such that for any scenario *j* of design *t*, $J_{\bar{t},j} \leq J_{\bar{l},r}$. Thus,

$$PCS = P\left\{\bigcap_{l=1, l \neq t}^{k} \bigcup_{r=1}^{m} \bigcap_{j=1}^{m} (\bar{J}_{l,j} \leq \bar{J}_{l,r})\right\}.$$
(1)

In general, PCS in (1) is analytically intractable when both $k \ge 2$ and $m \ge 2$. In this study, we develop a surrogate for the problem of maximizing PCS by approximating PCS using a lower bound.

Theorem 1 Denote the worst-case scenario $r_l = \arg \max_{r \in \{1,2,...,m\}} J_{l,r}$ for design $l \in \{1,2,...,k\}$ and $l \neq t$. Then,

$$PCS \ge 1 - \sum_{l=1, l \neq t}^{k} \sum_{j=1}^{m} P\{\bar{J}_{l,j} > \bar{J}_{l,r_l}\} \equiv APCS.$$

Theorem 1 can be proved using the Bonferroni inequality. Detailed proof of it is in Gao et al. (2016). We refer to this lower bound of PCS as the *approximated probability of correct selection* (APCS). In this research, we consider the following optimization problem,

$$\max_{\alpha_{i,j}} APCS
s.t. \sum_{i=1}^{k} \sum_{j=1}^{m} \alpha_{i,j} = 1,
\alpha_{i,j} \ge 0, \ i = 1, ..., k, \ j = 1, ..., m.$$
(2)

Compared to PCS, APCS can be computed easily and quickly. More importantly, by making the approximation, we derive a selection rule which is easy to compute and implement and can help provide important insights about the selection problem under consideration.

3 ASYMPTOTIC OPTIMAL SOLUTION

Denote $\delta_{ij,uv} = J_{i,j} - J_{u,v}$ for any $i, u \in \{1, 2, ..., k\}$ and $j, v \in \{1, 2, ..., m\}$. $I_{tj,lr} = \frac{\delta_{l,j/r}^2}{2(\sigma_{l,j}^2/\alpha_{l,j} + \sigma_{l,r}^2/\alpha_{l,r})}$ for any $l \in \{1, 2, ..., k\}$ and $l \neq t$ and $j, r \in \{1, 2, ..., m\}$. Define design l_j and scenario j_l such that

$$I_{tj,l_jr_{l_j}} = \min_{l \in \{1,2,\dots,k\}, l \neq t} I_{tj,lr_l}, \quad j \in \{1,2,\dots,m\},$$
$$I_{tj_l,lr_l} = \min_{j \in \{1,2,\dots,m\}} I_{tj,lr_l}, \quad l \in \{1,2,\dots,k\}, l \neq t.$$

In order to solve optimization problem (2), we can investigate the Karush-Kuhn-Tucker (KKT) conditions (Boyd and Vandenberghe 2004) of it. This result is referred as *robust optimal computing budget allocation* ($OCBA_R$). The detailed derivation and the sequential procedure for implementing the allocation rule can also be found in Gao et al. (2016).

Theorem 2 Problem (2) is asymptotically (as $T \rightarrow \infty$) optimized if

$$\sum_{j=1}^{m} \frac{\alpha_{t,j}^2}{\sigma_{t,j}^2} = \sum_{l=1,l\neq t}^{k} \frac{\alpha_{l,r_l}^2}{\sigma_{l,r_l}^2},$$
(3)

$$I_{tj,l_jr_{l_j}} = I_{tj',l_{j'}r_{l_{j'}}}, \quad j,j' \in \{1,2,...,m\}, j \neq j',$$
(4)

$$I_{tj_l, lr_l} = I_{tj_{l'}, l'r_{l'}}, \quad l, l' \in \{1, 2, \dots, k\}, l \neq l' \neq t.$$
(5)

According to Theorem 2, it is not necessary to correctly compare all the km scenarios. Let $S_1 = \{\text{scenario } j \text{ of design } t : j \in \{1, 2, ..., m\}\}$ and $S_2 = \{\text{scenario } r_l \text{ of design } l : l \in \{1, 2, ..., k\}$ and $l \neq t\}$. We only need to correctly distinguish scenarios in S_1 and S_2 , i.e., the m scenarios of the best design and the worst-case scenario of all the k-1 non-best designs. This is sufficient to lead to a correct selection. Since there are only k+m-1 scenarios in S_1 and S_2 , by focusing the simulation budget on these two sets of scenarios, the scale of the problem is reduced and the efficiency of the selection procedure might be considerably improved.

In the special case that each design has only one scenario, i.e., there is no input uncertainty and the input distributions are accurately specified, the optimality condition (3) reduces to

$$\frac{\alpha_{t,1}^2}{\sigma_{t,1}^2} = \sum_{l=1, l \neq t}^k \frac{\alpha_{l,1}^2}{\sigma_{l,1}^2}.$$
(6)

Equation (4) becomes invalid and (5) reduces to

$$\frac{\delta_{t1,l1}^2}{\sigma_{t,1}^2/\alpha_{t,1} + \sigma_{l,1}^2/\alpha_{l,1}} = \frac{\delta_{t1,l'1}^2}{\sigma_{t,1}^2/\alpha_{t,1} + \sigma_{l',1}^2/\alpha_{l',1}}, \quad l,l' \in \{1,2,...,k\}, l \neq l' \neq t.$$
(7)

If we further assume that $\alpha_{t,1} \gg \alpha_{l,1}$ for all $l \neq t$, (7) becomes,

$$\frac{\alpha_{l,1}}{\alpha_{l',1}} = \left(\frac{\sigma_{l,1}/\delta_{l1,l1}}{\sigma_{l',1}/\delta_{l1,l'1}}\right)^2.$$
(8)

Note that (6) and (8) are identical to the original OCBA allocation rule (Chen et al. 2000) for selecting the best design without input uncertainty.

4 NUMERICAL EXPERIMENTS

In this section, we implement numerical experiments to investigate the performance of the proposed $OCBA_R$ algorithm. We test three selection examples, which are described as follows.

- *Example 1*: Constant-variance configuration. $J_{i,j} = i + j 1$ and $\sigma_{i,j}^2 = 25$ for i = 1, 2, ..., k and j = 1, 2, ..., m. The best design t = 1.
- *Example 2*: Increasing-variance configuration. $J_{i,j} = i + j 1$ and $\sigma_{i,j}^2 = 20 + j$ for i = 1, 2, ..., k and j = 1, 2, ..., m. The best design t = 1.
- *Example 3*: Decreasing-variance configuration. $J_{i,j} = i + j 1$ and $\sigma_{i,j}^2 = 31 j$ for i = 1, 2, ..., k and j = 1, 2, ..., m. The best design t = 1.

In the numerical experiments, we employ two different selection methods for comparison.

- *Equal Allocation (EA)*: This is the simplest way to conduct simulation experiments and has been widely applied. The total simulation budget is equally allocated to all the *km* scenarios under consideration. The equal allocation is easy to implement in practice. Although equal allocation does not appear to have any efficient mechanism for R&S with input uncertainty, it supplies a good benchmark against which improvement may be measured.
- Robust Selection of the Best (RSB): This is an IZ-based procedure that selects the design with the best worst-case performance for R&S problems with input uncertainty (Fan et al. 2013). RSB has two layers. The first layer conducts an IZ-based R&S procedure to select for design *i* a scenario which deviates at most δ_1 from the worst-case scenario of this design with at least a specified probability level, i = 1, 2, ..., k. The second layer conducts an IZ-based R&S procedure to select a

scenario which deviates at most δ_2 from the best one among the scenarios selected in layer 1 with at least a specified probability level. In this test, we will use the KN procedure (Kim and Nelson 2001) to satisfy the IZ criteria.

Among the three methods for comparison, RSB must be implemented differently. It keeps increasing the sample size until PCS is guaranteed at a pre-specified level, while $OCBA_R$ and EA should be performed with a fixed sample size. In order to compare the three methods, we first run RSB for 3000 replications and calculate the averaged total sample size and PCS. Next, we run $OCBA_R$ and EA for 3000 replications with the total sample size being the averaged total sample size of RSB. The PCS of $OCBA_R$ and EA is estimated and compared with that of RSB. When implementing RSB, the target probability level for PCS is set at 95%. The IZ parameters $\delta_1 = \delta_2 = 1$ and the initial number of simulation replications for each scenario is 20. For $OCBA_R$, the initial number of simulation replications for each scenario is 20 and the incremental simulation budget in each iteration is 20. Table 1 reports the PCS of $OCBA_R$, RSB and EA with different values of k and m for the three tested examples. The sample sizes of the three methods are also reported in the table.

			OCBA _R	RSB	EA	Sample Size
Example 1	<i>k</i> = 5	m = 3	0.996	0.986	0.9556	2.26×10^{3}
		m = 5	0.9983	0.9843	0.944	3.23×10^{3}
		m = 10	1	0.9873	0.9496	5.08×10^{3}
	k = 10	m = 3	1	0.988	0.9716	4.51×10^{3}
		m = 5	1	0.9913	0.9726	6.27×10^{3}
		m = 10	1	0.9897	0.9603	9.39×10^{3}
Example 2	<i>k</i> = 5	m = 3	0.9946	0.981	0.9486	2.60×10^{3}
		m = 5	0.9963	0.9823	0.9487	3.71×10^{3}
		m = 10	1	0.9833	0.966	5.74×10^{3}
	<i>k</i> = 10	<i>m</i> = 3	1	0.9853	0.971	4.93×10^{3}
		m = 5	1	0.9896	0.9733	7.04×10^{3}
		m = 10	1	0.988	0.9636	1.04×10^{4}
Example 3	<i>k</i> = 5	<i>m</i> = 3	0.9966	0.9893	0.9646	1.96×10^{3}
		m = 5	0.998	0.9913	0.9496	2.78×10^{3}
		m = 10	1	0.9906	0.919	4.06×10^{3}
	k = 10	m = 3	1	0.9936	0.956	3.60×10^{3}
		m = 5	0.9996	0.99	0.9266	5.12×10^{3}
		m = 10	1	0.9906	0.8763	7.66×10^{3}

Table 1: PCS comparison of $OCBA_R$, RSB and EA.

It is observed that the proposed $OCBA_R$ procedure performs the best among the three selection methods in all the cases tested. The advantage of $OCBA_R$ in performance tends to increase with the scale of the problem. This is because $OCBA_R$ concentrates the simulation budget on the k + m - 1 scenarios in sets S_1 and S_2 in order to improve efficiency. This effect becomes more significant with larger k and m. The performance of RSB is second to $OCBA_R$. RSB is not so efficient as $OCBA_R$ probably due to the

conservativeness in budget allocation that was observed for IZ-based procedures (Branke et al. 2007). EA has the worst performance. This is not surprising because EA does not appear to have any efficient mechanism for selecting the best design with input uncertainty.

5 CONCLUSIONS

The optimal solutions of R&S problems may depend heavily on the specification of the input distributions and their associated parameters. However, due to limited data or information, it is often difficult to specify or estimate them precisely. If the input uncertainty is not properly managed, the optimal solution obtained for these problems may turn out to be rather suboptimal. Our work aims to account for the input uncertainty by selecting the design with the best performance under the worst-case scenario. Although an exact solution appears to be intractable for the general case, we are able to propose an asymptotic optimal solution that captures the important features of an efficient allocation rule. Numerical results indicate the higher efficiency of the proposed procedure than the compared methods.

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