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FIXED BUDGET RANKING AND SELECTION WITH STREAMING INPUT DATA

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ABSTRACT

We consider a fixed budget ranking and selection problem with input uncertainty, where unknown input distributions can be estimated using input data arriving in batches of varying sizes over time. Each time a batch arrives, the input distribution is updated and additional simulations can be run with a given simulation budget. Within each time stage, we apply the large deviations theory to compute the rate function of the probability of false selection (PFS) with input distribution and formulate an optimization problem to maximize the decay rate of PFS. With the derived optimality condition, we design a dynamic optimal budget allocation procedure with sequentially updated input distributions under streaming input data. We prove the consistency and asymptotic optimality of the procedure, and numerically show the high efficiency of our procedure compared to the equal allocation rule and a simple extension of the Optimal Computing Budget Allocation (OCBA) algorithm.

1 INTRODUCTION

Ranking and Selection (R&S) studies the problem of identifying the best among a finite number of designs, whose performance are unknown and need to be estimated through statistical simulation. In this paper, we restrict the performance measure to the mean performance. Two most common settings of R&S are fixed budget and fixed confidence. In the fixed budget setting, the goal is to achieve a probability of correct selection (PCS) as high as possible with a given simulation budget; whereas in the fixed confidence setting, the goal is to achieve a pre-specified PCS using the least possible amount of simulation effort.

For the fixed budget setting, one of the well-known methods, called optimal computing budget allocation (OCBA), was first developed in Chen et al. (2000) under the assumption of normal simulation uncertainty (SU). Later Glynn and Juneja (2004) applied the large deviations technique to maximize the convergence rate of the probability of false selection (PFS) for general distributions beyond normal. Moreover, various extensions of OCBA have been studied in the past years. For example, Chen et al. (2008) and Gao and Chen (2015) extended OCBA framework to optimal subset selection; Gao et al. (2019), Jin et al. (2019) and Cakmak et al. (2022) extended the OCBA to study R&S with covariates. Other well-known fixed budget R&S procedures include the expected value of information (EVI) approach proposed by Chick and Inoue (2001) and the knowledge-gradient (KG) approach proposed by Frazier et al. (2009), where EVI is derived by asympototically minimizing a bound of the expected loss and KG determines the optimal sampling allocation policy by maximizing the acquisition function. For the fixed confidence setting, the indifference-zone (IZ) framework aims to select a design within δ difference from the best design with a pre-specified confidence level. The Rinott's Procedure proposed by Rinott (1978), the NSGS procedure proposed by Nelson et al. (2001), and the KN procedure proposed by Kim and Nelson (2001) fall into the

IZ framework. More recently, Fan et al. (2016) proposed an IZ-free procedure for fixed confidence R&S. For a more comprehensive overview of R&S works, we refer the interested reader to Hong et al. (2021).

In the aforementioned R&S works, design performance is estimated via simulation with a fixed known input distribution. However, the input distribution is seldom known in practice and often estimated from data. The uncertainty of the estimated input distribution is often referred to as the "input uncertainty (IU)". There is a sophisticated literature on quantifying the impact of IU on simulation output, and we refer the reader to Corlu et al. (2020) for a recent review. Despite the extensive study on IU quantification, R&S with input uncertainty has only been studied in recent years. For example, Corlu and Biller (2013), Corlu and Biller (2015) develop procedures which return a subset of superior designs with desired confidence, where the size of the subset depends on the simulation budget as well as the impact of IU; Gao et al. (2017) considers a robust approach to deal with IU, where the authors assume a finite number of parametrized input distributions and select one design with the best worst-case performance; Kim et al. (2021) also takes a robust approach but with a different robust optimality criteria called the most probable best, which selects the design with the largest posterior probability of being the best given the real-world data; Song and Nelson (2019) derives asymptotically valid concentration bounds to account for both IU and SU with the assumption that simulation budget goes to infinity as the number of input data goes to infinity. Wu and Zhou (2017) and Xu et al. (2020) take a different perspective and formulates the R&S with input uncertainty as an budget allocation problem, which allocates the computing budget to balance input distribution estimation and performance estimation.

In many real applications, input data come sequentially over time and hence are referred to as streaming input data. They create a unique opportunity as well as challenges for simulation: the input distribution estimate can be updated with the new coming input data over time to improve the estimation accuracy, but the simulation outputs are generated under different input distributions and become correlated over time. Regardless of the challenges, Zhou and Liu (2018) and Liu and Zhou (2019) studied IU quantification in this setting of streaming input data, and Song and Shanbhag (2019), Liu et al. (2021), and Liu et al. (2022) studied continuous simulation optimization with streaming input data. In the area of R&S, Wu and Zhou (2019) and Wu et al. (2022) are the first to consider streaming input data in the fixed confidence setting and design a data-driven approach that aggregates simulation outputs under past input distributions with a moving average over time.

In this paper, we also consider streaming input data in R&S, but instead focus on the fixed budget setting. Specifically, we extend the result in Glynn and Juneja (2004) to apply large deviations theory to compute the rate function of a performance estimator with input distribution. There is a large body of work extending this large deviations approach. For example, Chen and Ryzhov (2019) designed a fully sequential R&S algorithm for general distributions using the optimality conditions as in Glynn and Juneja (2004); Pasupathy et al. (2014) applied large deviations theory to constrained R&S; Gao et al. (2019) extended the large deviations approach to contextual R&S. We formulate the optimization problem of allocating the simulation budget to all design-input pairs to maximize the decay rate of PFS and derive the necessary and sufficient optimality condition for this optimization problem. Based on the optimality condition, we design a data-driven and fully sequential computing budget allocation procedure, named OCBA-SID, that aims to satisfy the optimality condition asymptotically. We prove the consistency and asymptotic optimality of OCBA-SID and carry out numerical experiments to show the efficiency of the procedure by comparing with the equal allocation rule and a simple extension of OCBA for the streaming data setting.

2 PROBLEM STATEMENT

We consider the fixed budget R&S problem, where the input distribution is estimated through streaming data that arrive sequentially over time. Suppose we have a set of finite number of designs $\mathscr{I} = \{1, 2, \cdots, K\}$. Denote by ζ the input random variable, which is common for all designs. Let $X_i(\zeta)$ denote the simulation outcome of design i conditioned on ζ. We assume X_i has the following form:

$$X_i(\zeta) = \mu_i(\zeta) + \varepsilon_i(\zeta),$$

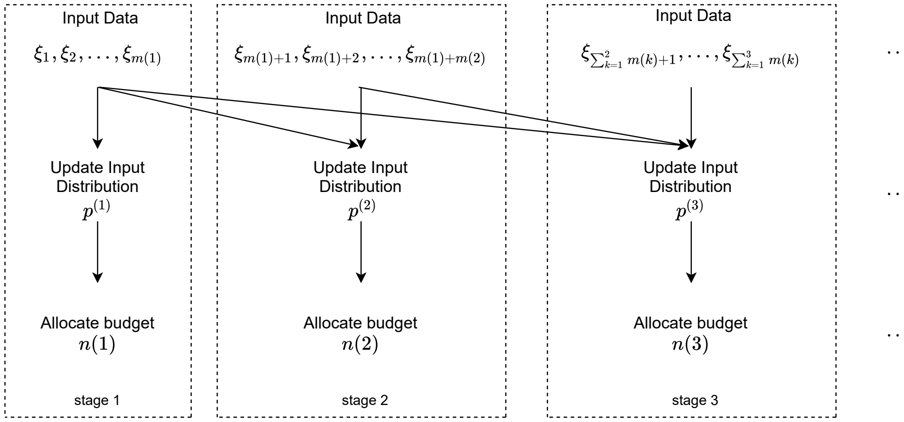


Figure 1: Illustration of budget allocation with streaming input data.

where μ_i is the expected performance of design i conditioned on ζ, and $\varepsilon_i(\zeta)$ is the simulation error. Denote by $\bar{\mu}_i = \mathbf{E}[\mathbf{E}[X_i(\zeta)]] = \mathbf{E}[\mu_i(\zeta)]$, the expected performance of design i. Our goal is to select the design with largest expected performance. Specifically, we want to find design b (for best) such that

$$b = \arg\max_{1 \leq i \leq K} \bar{\mu}_i.$$

The underlying input distribution is estimated via given data from the real world and such input data come in a streaming fashion. Specifically, when beginning the simulation experiment, we may only have a rough estimation of the input distribution. At time stage t, new input data of batch size $m(t)$ can be obtained and used to update the estimate of the input distribution. In particular, the input distribution can be estimated by the empirical distribution consisting of the observed data. Then we allocate simulation budget $n(t)$ to design-input pairs to maximize the PCS with respect to the current estimated input distribution. We assume both $n(t)$ and $m(t)$ are given. This process is illustrated in Figure 1. We make the following assumptions on the input distribution and simulation output.

Assumption 1

1. The true (unknown) input distribution F_ζ has a finite support $\{\zeta_1, \zeta_2, \cdots, \zeta_B\}$, with probability mass function (pmf) $\mathbf{P}(\zeta = \zeta_j) = p_j, \ j = 1, \ldots, B$.
2. The simulation error $\varepsilon_{i,j} = \varepsilon_i(\zeta_j)$ follows a normal distribution $\mathbf{N}(0, \sigma_{i,j}^2)$ where the variance is known.
3. The optimal expected performance $\bar{\mu}_b$ is unique.
4. Denote by $X_{i,j} = X_i(\zeta_j)$ and $X_{i,j}^{(l)}$ the lth replication for $X_{i,j}$. The simulation output $\{X_{i,j}^{(l)}\}$ are independent for all i, j and l.

Assumption 1.1 can be viewed as a discretized approximation of a general input distribution. The latter three assumptions are common in R&S literature. Denote by $\mu_{i,j} = \mu_i(\zeta_j)$. Furthermore, we make the following assumption on the input data.

Assumption 2 $\{\xi_s\}_{s=1}^{\infty}$ are identically and independently distributed.

With Assumption 1.1 and 2, at each stage t the input distribution can be estimated by updating the empirical pmf, denoted by $\{p_j^{(t)}\}_{j=1}^B$, where $p_j^{(t)} = \frac{\sum_{s=1}^{M(t)} \mathbb{1}\{\xi_s = \zeta_j\}}{M(t)}$ and $M(t) = \sum_{\tau=1}^t m(\tau)$. We then allocate the simulation budget of the current stage, $n(t)$, to design-input pairs. It is worth noting that one can choose a specific input realization to run simulation in finding the best design, while for implementation the input distribution is given to the decision maker. To find the budget allocation rule for each stage, we apply the large deviations theory to formulate an optimization problem under the current estimated input distribution and characterize its optimality condition to derive the optimal budget allocation rule. These will be presented in Section 3 and 4 below. Based on the stage-wise budget allocation rule, the desired data-driven procedure under streaming input data will be presented in Section 5, and its convergence properties will be analyzed in Section 6.

3 STAGE-WISE OPTIMAL BUDGET ALLOCATION PROBLEM

We first formulate and solve a static optimal budget allocation problem for each stage under the current estimated input distribution. Let $n_{i,j}$ denote the simulation budget allocated to design i under input realization ζ_j. Denote by $\hat{\bar{\mu}}_i(n_i) = \sum_{j=1}^{B} p_j^{(t)} \hat{\mu}_{i,j}(n_{i,j})$ the estimated performance, where $n_i = (n_{i,1}, \ldots, n_{i,B})^\intercal$ and $\hat{\mu}_{i,j}(n_{i,j}) = \frac{1}{n_{i,j}} \sum_{s=1}^{n_{i,j}} X_{i,j}^{(s)}$. Let $i_b = \arg\max_{1\le i\le K} \hat{\bar{\mu}}_i(n_i)$ be the selected best design under policy $\{n_{i,j}\}$. Then we are interested in the following optimization problem.

$$
\begin{aligned}
\max_{n_{i,j}, 1\le i\le K, 1\le j\le B} \quad & PCS = \mathbf{P}(i_b = b) \\
s.t. \quad & \sum_{i=1}^{K}\sum_{j=1}^{B} n_{i,j} = n. \\
& n_{i,j} \ge 0 \quad \forall i, j.
\end{aligned}
\tag{1}
$$

When IU is not considered (i.e., $n_{i,j}$ is simplified as n_i, and $i_b = \arg\max_i 1/n_i \sum_{s=1}^{n_i} X_i^{(s)}$), Glynn and Juneja (2004) applied the large deviations theory to study the optimization problem (1) by replacing the objective function with the large deviations rate (LDR) of PFS. We extend this approach to the IU setting by computing the LDR of the aggregated sample mean $\hat{\bar{\mu}}_i(n_i)$.

3.1 Large Deviations Rate Formulation

Recall that $\bar{\mu}_i$ is the true expected performance that we want to estimate. Without loss of generality, assume that $\bar{\mu}_1 > \bar{\mu}_2 \ge \cdots \ge \bar{\mu}_K$. Hence, the true best design $b = 1$. Consider an allocation policy that allocates $\alpha_{i,j}$ proportion of the total simulation budget n to the design i under input realization ζ_j, where $\alpha_{i,j} > 0$, $1 \le i \le K, 1 \le j \le B$ and $\sum_{i=1}^{K}\sum_{j=1}^{B} \alpha_{i,j} = 1$. For derivation of the procedure, here we ignore the minor issue that $\alpha_{i,j}n$ is not an integer. Let $\alpha_i = (\alpha_{i1}, \alpha_{i2}, \cdots, \alpha_{iB})^\intercal$. Denote by $\hat{\bar{\mu}}_i(\alpha_i, n) = \sum_{j=1}^{B} p_j \hat{\mu}_i(\alpha_{i,j}n)$ the estimate of $\bar{\mu}_i$, where $\hat{\mu}_i(\alpha_{i,j}n)$ is the sample mean of $X_i(\zeta_j)$ with sample size $\alpha_{i,j}n$. Notice here we use the true input distribution p_j rather than $p_j^{(t)}$ for derivation purpose, and hence the randomness in $\hat{\bar{\mu}}_i(\alpha_{i,j}n)$ only comes from simulation output.

According to (Glynn and Juneja 2004), define the rate function of event

$$
\mathbf{G}_i(\alpha_1, \alpha_i) = -\lim_{n\to\infty} \frac{1}{n} \log \mathbf{P}\left(\hat{\bar{\mu}}_1(\alpha_1, n) \le \hat{\bar{\mu}}_i(\alpha_i, n)\right)
$$

for all $i \ge 2$. $\min_{2\le i\le K} \mathbf{G}_i(\alpha_1, \alpha_i)$ is the asymptotically exponential decay rate of PFS when given the allocation rule $\alpha = (\alpha_{i,j})_{1\le i\le K, 1\le j\le B}$. Replacing the objective of PCS with this rate function, the optimization problem (1) becomes

$$
\begin{aligned}
\max_{\alpha_{i,j}, 1\le i\le K, 1\le j\le B} \quad & z \\
s.t. \quad & \mathbf{G}_i(\alpha_1, \alpha_i) - z \ge 0 \qquad 2 \le i \le K \\
& \sum_{i=1}^{K}\sum_{j=1}^{B} \alpha_{i,j} = 1 \\
& \alpha_{i,j} \ge 0 \qquad\qquad 1 \le i \le K, 1 \le j \le B.
\end{aligned}
\tag{2}
$$

To solve the optimization problem (2), we need to compute the rate function $\mathbf{G}_i(\alpha_1,\alpha_i)$. Without input uncertainty, this is well studied in Glynn and Juneja (2004). Here, with input uncertainty we have a more complicated structure that each G_i has $2*B$ variables rather than 2 as in Glynn and Juneja (2004). Although we cannot directly apply their result here, with the normal assumption of the simulation error, we can compute the rate function in a similar way using the Gartner-Ellis Theorem (see Dembo et al. (1994)).

3.2 Calculation of the Rate Function

Let's calculate $\mathbf{G}_i(\alpha_1,\alpha_i)$ explicitly. For a fixed i, denote by $\Lambda_{i,j}(\cdot)$ the log-moment generating function of $X_{i,j}$ and $\Lambda_n(\cdot,\cdot)$ the log-moment generating function of $Z_n=(\hat{\bar{\mu}}_1(\alpha_1,n),\hat{\bar{\mu}}_i(\alpha_i,n))$. Then

$$\frac{1}{n}\Lambda_n(n\lambda_1,n\lambda_i)=\sum_{j=1}^{B}\alpha_{1,j}\Lambda_{1,j}\left(\frac{\lambda_1 p_j}{\alpha_{1,j}}\right)+\sum_{j=1}^{B}\alpha_{i,j}\Lambda_{i,j}\left(\frac{\lambda_i p_j}{\alpha_{i,j}}\right).$$

Let $I(x_1,x_i)$ be the Fenchel-Legendre transform of Λ_n. Then,

$$\begin{aligned}
I(x_1,x_i)&=\sup_{\lambda_1,\lambda_i}\left\{\lambda_1x_1+\lambda_ix_i-\sum_{j=1}^{B}\alpha_{1,j}\Lambda_{1,j}\left(\frac{\lambda_1 p_j}{\alpha_{1,j}}\right)-\sum_{j=1}^{B}\alpha_{i,j}\Lambda_{i,j}\left(\frac{\lambda_i p_j}{\alpha_{i,j}}\right)\right\}\\
&=\sup_{\lambda_1}\left\{\lambda_1x_1-\sum_{j=1}^{B}\alpha_{1,j}\Lambda_{1,j}\left(\frac{\lambda_1 p_j}{\alpha_{1,j}}\right)\right\}+\sup_{\lambda_i}\left\{\lambda_ix_i-\sum_{j=1}^{B}\alpha_{i,j}\Lambda_{i,j}\left(\frac{\lambda_i p_j}{\alpha_{i,j}}\right)\right\}\\
&=\sup_{\lambda_1}\left\{\lambda_1x_1-\sum_{j=1}^{B}\left(\lambda_1p_j\mu_{1,j}+\frac{1}{2}\frac{\sigma_{1,j}^2\lambda_1^2p_j^2}{\alpha_{1,j}}\right)\right\}+\sup_{\lambda_i}\left\{\lambda_ix_i-\sum_{j=1}^{B}\left(\lambda_ip_j\mu_{i,j}+\frac{1}{2}\frac{\sigma_{i,j}^2\lambda_i^2p_j^2}{\alpha_{i,j}}\right)\right\}\\
&=\underbrace{\frac{1}{2}\frac{(x_1-\bar{\mu}_1)^2}{\sum_{j=1}^{B}\frac{\sigma_{1,j}^2p_j^2}{\alpha_{1,j}}}}_{I_1}+\underbrace{\frac{1}{2}\frac{(x_i-\bar{\mu}_i)^2}{\sum_{j=1}^{B}\frac{\sigma_{i,j}^2p_j^2}{\alpha_{i,j}}}}_{I_2}.
\end{aligned}$$

By the Gartner-Ellis Theorem, $\mathbf{G}_i(\alpha_1,\alpha_i)=\inf_{x_1\le x_i}I(x_1,x_i)$. It is easily seen that I_1 is decreasing for $x_1\le\bar{\mu}_1$ and increasing for $x_1\ge\bar{\mu}_1$, while I_2 is decreasing for $x_i\le\bar{\mu}_i$ and increasing for $x_i\ge\bar{\mu}_i$. Since $\bar{\mu}_1>\bar{\mu}_i$, we must have

$$\mathbf{G}_i(\alpha_1,\alpha_i)=\inf_{\bar{\mu}_i\le x\le\bar{\mu}_1}I(x,x)=\frac{(\bar{\mu}_1-\bar{\mu}_i)^2}{2\left(\sum_{j=1}^{B}\frac{\sigma_{1,j}^2p_j^2}{\alpha_{1,j}}+\sum_{j=1}^{B}\frac{\sigma_{i,j}^2p_j^2}{\alpha_{i,j}}\right)}. \tag{3}$$

To ensure the optimization problem (2) is well-posed, we need the following lemma which summarizes some important properties of $\mathbf{G}_i(\alpha_1,\alpha_i)$.

Lemma 1 Suppose Assumption 1 holds. Then,

1. $\mathbf{G}_i(\alpha_1,\alpha_i)$ is strictly increasing in $\alpha_{1,j}$ and $\alpha_{i,j}$ for $(\alpha_{1,j},\alpha_{i,j})>0$ if $p_j>0$. Moreover, $\mathbf{G}_i(\alpha_1,\alpha_i)=0$ if there exists j_0 with $p_{j_0}>0$ and $\min(\alpha_{1,j_0},\alpha_{i,j_0})=0$.
2. $\mathbf{G}_i(\alpha_1,\alpha_i)$ is concave in (α_1,α_i) for $(\alpha_1,\alpha_i)>0$.

Proof. Lemma 1.1 is easily seen from (3). To prove Lemma 1.2, it suffices to show the concavity of the function for $x>0$ with form $f(x)=1/(\sum_{i=1}^{n}\frac{a_i}{x_i})$, where $a_i>0$ for $i=1,2,\ldots,n$. We prove the concavity of the multivariate function by proving the concavity along all lines. For any $y\in\mathbb{R}^n$, let $g(t)=f(x+ty)$ where $t\in\mathbb{R}$ such that $x+ty>0$. We have

$$g''(t)=\frac{2}{(\sum_{i=1}^{n}\frac{a_i}{x_i+ty_i})^3}\left\{\left[\sum_{i=1}^{n}\frac{a_iy_i}{(x_i+ty_i)^2}\right]^2-\sum_{i=1}^{n}\frac{a_iy_i^2}{(x_i+ty_i)^3}\sum_{i=1}^{n}\frac{a_i}{x_i+ty_i}\right\}\le 0,$$

where the inequality uses the Cauchy inequality. Hence, f is concave in $x > 0$. $\square$

Lemma 1.1 implies that any "effective" design-input pair (i.e., (i, j) with $p_j > 0$) must be allocated with a positive ratio of the simulation budget; otherwise, the rate will be zero. Lemma 1.2 claims the concavity of $\mathbf{G}_i$, which guarantees the optimality condition for the optimization problem (2) in the following section.

4 OPTIMAL ALLOCATION POLICY

In this section we characterize the optimal allocation policy, which is the optimal solution to (2).

Theorem 1 Suppose Assumption 1 holds. Let $\alpha \geq 0$ be a feasible allocation policy. Then α is the optimal solution to (2) if and only if $p_j = 0 \Rightarrow \alpha_{i,j} = 0$ and the following three conditions hold:

1. $$\frac{\partial \mathbf{G}_i(\alpha_1, \alpha_i)}{\partial \alpha_{i,j}} = \frac{\partial \mathbf{G}_i(\alpha_1, \alpha_i)}{\partial \alpha_{i,j'}} \quad 2 \leq i \leq K \text{ and } 1 \leq j < j' \leq B, \quad \text{if } p_j, p_{j'} > 0; \tag{4}$$
2. $$\sum_{i=2}^{K} \frac{\partial \mathbf{G}_i(\alpha_1, \alpha_i)/\partial \alpha_{1,j}}{\partial \mathbf{G}_i(\alpha_1, \alpha_i)/\partial \alpha_{i,j}} = 1 \quad 1 \leq j \leq B, \quad \text{if } p_j > 0; \tag{5}$$
3. $$\mathbf{G}_i(\alpha_1, \alpha_i) = \mathbf{G}_{i'}(\alpha_1, \alpha_{i'}) \quad 2 \leq i < i' \leq K. \tag{6}$$

Or equivalently in the explicit form:

1. $$\frac{\alpha_{i,j}}{\sigma_{i,j} p_j} = \frac{\alpha_{i,j'}}{\sigma_{i,j'} p_{j'}} \quad 2 \leq i \leq K,\ 1 \leq j \leq B, \tag{7}$$
2. $$\left(\frac{\alpha_{1,j}}{\sigma_{1,j}}\right)^2 = \sum_{i=2}^{K} \left(\frac{\alpha_{i,j}}{\sigma_{i,j}}\right)^2 \quad 1 \leq j \leq B, \tag{8}$$
3. $$\frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\sum_{j=1}^{B} \frac{\sigma_{1,j}^2 p_j^2}{\alpha_{1,j}} + \sum_{j=1}^{B} \frac{\sigma_{i,j}^2 p_j^2}{\alpha_{i,j}}} = \frac{(\bar{\mu}_1 - \bar{\mu}_{i'})^2}{\sum_{j=1}^{B} \frac{\sigma_{1,j}^2 p_j^2}{\alpha_{1,j}} + \sum_{j=1}^{B} \frac{\sigma_{i',j}^2 p_j^2}{\alpha_{i',j}}} \quad 2 \leq i < i' \leq K. \tag{9}$$

Furthermore, the optimal solution α^* to (2) is unique.

Proof. We first show the existence of α and prove that $\alpha_{i,j} = 0$ if $p_j = 0$. The existence follows from the continuity of G_i with respect to $\alpha \in \Delta^{KB-1}$, where Δ^n denotes the n-dimensional simplex. By Lemma 1.1, G_i is strictly increasing in $\alpha_{1,j'}$ and $\alpha_{i,j'}$ for those j' with $p_{j'} > 0$ and is independent of $\alpha_{1,j}$ and $\alpha_{i,j}$ if $p_j = 0$. Hence, we must have $\alpha_{i,j} = 0$ for $i = 1, 2, \cdots, K$ if $p_j = 0$. Therefore, without loss of generality, to prove the theorem, we can assume all $p_j > 0$. Then by Lemma 1.1, the optimal solution α must satisfy $\alpha_{i,j} > 0$ for all i, j.

Now we show the necessity of the three optimality conditions. By Lemma 1.2, the optimization problem (2) is a concave maximization problem, and therefore the Karush–Kuhn–Tucker(KKT) conditions are both sufficient and necessary for the optimality. With α strictly positive, the KKT conditions can be written as

$$1 - \sum_{i=1}^{K} \lambda_i = 0, \tag{10}$$

$$\lambda_i \frac{\partial G_i}{\partial \alpha_{i,j}}(\alpha_1, \alpha_i) = \gamma \quad 2 \leq i \leq K,\ 1 \leq j \leq B, \tag{11}$$

$$\sum_{i=2}^{K} \lambda_i \frac{\partial G_i}{\partial \alpha_{1,j}}(\alpha_1, \alpha_i) = \gamma \quad 1 \leq j \leq B, \tag{12}$$

$$\lambda_i (G_i(\alpha_1, \alpha_i) - z) = 0 \quad 2 \leq i \leq K, \tag{13}$$

for some γ and $\lambda_i \geq 0,\ 2 \leq i \leq K$. By (10) there exists at least one i_0 such that $\lambda_{i_0} > 0$. Then since G_i is increasing in $\alpha_{i,j}$, we have $\frac{\partial G_{i_0}}{\partial \alpha_{i_0,j}}(\alpha_1, \alpha_{i_0}) > 0$. This implies $\gamma > 0$ by (11). Hence, we must have $\lambda_i > 0$ for all $2 \leq i \leq K$. Then we have $\frac{\partial \mathbf{G}_i(\alpha_1,\alpha_i)}{\partial \alpha_{i,j}} = \frac{\gamma}{\lambda_i},\ 1 \leq j \leq B,\ 2 \leq i \leq K$, which proves (4). Since $\lambda_i > 0$, $G_i(\alpha_1, \alpha_i) = z,\ 2 \leq i \leq K$ by (13). Hence, (6) holds. To see why (5) holds, solving for $\lambda_i = \frac{\gamma}{\frac{\partial G_i}{\partial \alpha_{i,j}}(\alpha_1,\alpha_i)}$ in (11) and substituting λ_i in (12), we get the desired result.

For sufficiency, first let $\lambda_i = \frac{1}{\partial G_i(\alpha_1,\alpha_i)/\partial \alpha_{i,j}} / (\sum_{k=2}^{K} \frac{1}{\partial G_k(\alpha_1,\alpha_k)/\partial \alpha_{k,j}})$ for $i \geq 2$. Notice that $\lambda_i > 0$ and does not depend on the choice of j by (4). Moreover, $\{\lambda_i\}_{i \geq 2}$ satisfy condition (10). Further let $\gamma = (\sum_{k=2}^{K} \frac{1}{\partial G_k(\alpha_1,\alpha_k)/\partial \alpha_{kj}})^{-1}$, which is also independent of j. We can easily verify that both (11) and (12) hold. (10) also holds by setting $z = G_i(\alpha_1, \alpha_i)$, which is independent of i by (6).

Now we are only left to show the uniqueness of α. First notice that from (7) and (8), we have

$$\frac{\alpha_{1,j}}{\sigma_{1,j} p_j} = \sqrt{\sum_{i=2}^{B} (\frac{\alpha_{i,j}}{\sigma_{i,j} p_j})^2} = \sqrt{\sum_{i=2}^{B} (\frac{\alpha_{i,j'}}{\sigma_{i,j'} p_{j'}})^2} = \frac{\alpha_{1,j'}}{\sigma_{1,j'} p_{j'}} \quad 1 \leq j < j' \leq B.$$

Letting $\beta_i = \frac{\alpha_{i,j}}{\sigma_{i,j} p_j}$, we can write $\alpha_{i,j} = p_j \sigma_{i,j} \beta_i$ for all $i = 1, 2, \cdots, K$. Since α and $\beta = (\beta_1, \cdots, \beta_K)$ are bijective, it is sufficient to show the uniqueness of β. Plugging $\alpha_{i,j}$ into (9) and (8), we have

$$\frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\frac{\sum_{j=1}^{B} \sigma_{1,j} p_j}{\beta_1} + \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j}{\beta_i}} = \frac{(\bar{\mu}_1 - \bar{\mu}_{i'})^2}{\frac{\sum_{j=1}^{B} \sigma_{1,j} p_j}{\beta_1} + \frac{\sum_{j=1}^{B} \sigma_{i',j} p_j}{\beta_{i'}}} \quad 2 \leq i < i' \leq K$$

with $\beta_1^2 = \sum_{i=2}^{K} \beta_i^2$. Let $\eta = \frac{\beta}{\beta_1}$. Then η satisfies

$$\frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j}{\eta_i}} = \frac{(\bar{\mu}_1 - \bar{\mu}_{i'})^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{i',j} p_j}{\eta_{i'}}} \quad 2 \leq i < i' \leq K \tag{14}$$

with $1 = \sum_{i=2}^{K} \eta_i^2$. If there exists $\eta' \neq \eta$ satisfying these two conditions, then there must be $i \neq k \neq 1$ such that $\eta_i < \eta'_i$ and $\eta_k > \eta'_k$. Then, we have

$$\frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j}{\eta_i}} < \frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j}{\eta'_i}} = \frac{(\bar{\mu}_1 - \bar{\mu}_k)^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{k,j} p_j}{\eta'_k}} < \frac{(\bar{\mu}_1 - \bar{\mu}_k)^2}{\sum_{j=1}^{B} \sigma_{1,j} p_j + \frac{\sum_{j=1}^{B} \sigma_{k,j} p_j}{\eta_k}},$$

which contradicts (14). Hence, η is unique, which implies $\beta = C * \eta$ for some constant C. Then if there exists $\beta' \neq \beta$ and both are optimal, we have $\beta > (<) \beta'$. This implies the corresponding $\alpha > (<) \alpha'$, which contradicts $\sum_{i,j} \alpha_{i,j} = \sum_{i,j} \alpha'_{i,j} = 1$. □

Compared with the optimality condition in Glynn and Juneja (2004), here we have the additional optimality condition (4), the local balance condition for the derivative. It states that within the allocation for a certain design i, the partial derivative of the rate function $\mathbf{G}_i$ taken with respect to $\alpha_{i,j}$ is the same if $p_j > 0$. That is, simulation for each fixed input realization should provide same improvement to identify that design 1 is better than i. Furthermore, with normally distributed simulation error, from (7) we see for a fixed design i the optimal allocation ratio $\alpha_{i,j}$ should be proportional to the input probability mass p_j and its variance $\sigma_{i,j}$, which quantitatively characterizes how input uncertainty affects the optimal allocation policy. Also notice for fixed i, (7) only contains information from design i, which means the relative allocation ratios among different input realizations for a certain design do not depend on other designs. On the other hand, however, from (9) it can be seen that the relative allocation ratios among designs under the same input realization j are affected by all p_j, which means directly applying OCBA to designs with a fixed j may perform poorly since it does not take information from other design-input pairs into consideration. In addition, if $B=1$, which means there is no input uncertainty, the optimality condition coincides with that in Glynn and Juneja (2004), showing our result is an extension to account for input uncertainty. Moreover, notice that the three optimality conditions (4)-(6) not only hold for Gaussian simulation noise but also hold as long as the rate function G_i has the properties shown in Lemma 1.

5 SEQUENTIAL PROCEDURE WITH STREAMING INPUT DATA

In this section, we give a fully sequential procedure, named as OCBA-SID, for simulation budget allocation with streaming input data using the optimality conditions in Theorem 1. By optimality equation (7), we can write $\alpha_{i,j} = p_j \sigma_{i,j} \beta_i$ for some $\beta_i,\ 1 \le i \le K$. Plugging $\alpha_{i,j}$ into (9), we have

$$\frac{(\bar{\mu}_1 - \bar{\mu}_i)^2}{\frac{\sum_{j=1}^{B} \sigma_{1,j} p_j}{\beta_1} + \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j}{\beta_i}} = \frac{(\bar{\mu}_1 - \bar{\mu}_{i'})^2}{\frac{\sum_{j=1}^{B} \sigma_{1,j} p_j}{\beta_1} + \frac{\sum_{j=1}^{B} \sigma_{i',j} p_j}{\beta_{i'}}}, \quad 2 \le i < i' \le K.$$

Assume $\beta_1 \gg \beta_i,\ \forall i \ne 1$. Then we have $\frac{\beta_i}{\beta_{i'}} \approx \frac{\sum_{j=1}^{B} \sigma_{i,j} p_j / (\bar{\mu}_1 - \bar{\mu}_i)^2}{\sum_{j=1}^{B} \sigma_{i',j} p_j / (\bar{\mu}_1 - \bar{\mu}_{i'})^2}$. Replacing p_j with its estimate $p_j^{(t)}$ and plugging $\beta_i = \frac{\alpha_{i,j}}{p_j^{(t)} \sigma_{i,j}}$ into the equation above, we have

$$\frac{\alpha_{i,j}}{\alpha_{i',j'}} = \frac{p_j^{(t)} \sigma_{i,j} \sum_{k=1}^{B} \sigma_{i,k} p_k^{(t)} / (\bar{\mu}_1 - \bar{\mu}_i)^2}{p_{j'}^{(t)} \sigma_{i',j'} \sum_{k=1}^{B} \sigma_{i',k} p_k^{(t)} / (\bar{\mu}_1 - \bar{\mu}_{i'})^2}, \quad i, i' \ne 1. \tag{15}$$

Furthermore, with (8) and $\sum_{i=1}^{K} \sum_{j=1}^{K} \alpha_{i,j} = 1$, we can calculate $\alpha_{i,j}$ explicitly. Specifically, the procedure OCBA-SID is shown as follows:

OCBA-SID (Optimal Computing Budget Allocation with Streaming Input Data)

1. **Input.** Number of designs K, input distribution support $\{\zeta_1, \zeta_2, \cdots, \zeta_B\}$, initial sample size n_0, total simulation budget n, input data batch size $\{m(t)\}_{t=1}^{\infty}$ and stage-wise simulation budget $\{n(t)\}_{t=1}^{\infty}$.
2. **Initialization.** Time stage counter $t \leftarrow 0$, replication counter $l \leftarrow 0$, total input data $M(t) \leftarrow 0$. Collect n_0 initial samples for each design-input pair (i, ζ_j). Set $N_{i,j}^{(l)} = n_0$. Compute the initial sample mean $\hat{\mu}_{i,j}^{(l)}$ and $\hat{\bar{\mu}}_i^{(l)}$.
3. **WHILE** $\sum_{i=1}^{K} \sum_{j=1}^{B} N_{i,j}^{(l)} < n$ **DO**
4. $t \leftarrow t+1$, given input data of batch size $m(t)$, let $M(t) = \sum_{\tau=1}^{t} m(\tau)$ and update $p_j^{(t)} = \frac{\sum_{s=1}^{M(t)} \mathbb{1}\{\xi_s = \zeta_j\}}{M(t)}$ for $j = 1, 2, \cdots, B$.
5. **FOR** num = 1:n(t) **DO**
6. $l \leftarrow l+1$. $\hat{b}^{(l)} \leftarrow \arg\max_i \hat{\bar{\mu}}_i^{(l)}$.
7. Update $\hat{\alpha}_{i,j}^{(l)}$ using (15) and (8). Calculate $\hat{N}_{i,j}^{(l)} = \hat{\alpha}_{i,j}^{(l)} \left(1 + \sum_{i=1}^{K} \sum_{j=1}^{B} N_{i,j}^{(l)}\right), \quad \forall 1 \le i \le K,\ 1 \le j \le B$.
8. Find the design-input pair index $(I, J) = \arg\max_{i,j} \left(\hat{N}_{i,j}^{(l)} - N_{i,j}^{(l)}\right)$. Simulate the pair (I, J) once. Update $\hat{\mu}_{I,J}^{(l)}$ and $\hat{\bar{\mu}}_I^{(l)}$ using the new simulation output, and set $\hat{\mu}_{ij}^{(l)} = \hat{\mu}_{ij}^{(l-1)}$ and $\hat{\bar{\mu}}_i^{(l)} = \hat{\bar{\mu}}_i^{(l-1)}$ for $i \ne I, j \ne J$. Let $N_{I,J}^{(l)} = N_{I,J}^{(l-1)} + 1$ and $N_{i,j}^{(l)} = N_{i,j}^{(l-1)}$ for all $i \ne I, j \ne J$.

9. **END FOR**
10. **END WHILE**
11. **Output:** Output $i_b = \arg\max_i \hat{\bar{\mu}}_i^{(l)}$ as the best design.

We make the Assumption $\beta_1 \gg \beta_i$ in OCBA-SID for computational efficiency. A more general approach by extending Chen and Ryzhov (2019) to this setting with input distribution is of interest as future work.

6 CONSISTENCY AND ASYMPTOTIC OPTIMALITY

In this section we show consistency and asymptotic optimality of OCBA-SID. In classical R&S consistency is usually guaranteed by the Strong Law of Large Number (SLLN) as long as we simulate each design infinitely many times. However, here we also need the convergence of input distribution estimate $\{p^{(t)}\}$ to ensure we have the correct estimate of the true expected performance. For this purpose, we make the following assumption about the input data batch size and simulation budget in each stage.

Assumption 3 At stage t, the input data batch size $m(t)$ and simulation budget $n(t)$ satisfy

$$\lim_{T\to\infty}\sum_{t=1}^{T} n(t) = \infty, \quad \lim_{T\to\infty}\sum_{t=1}^{T} m(t) = \infty.$$

Assumption 3 ensures that both the input data batch size and total simulation replications go to infinity as time stage t goes to infinity, which helps guarantee the consistency of both the input estimate and the performance estimate. The following theorem shows the statistical validity of OCBA-SID.

Theorem 2 Suppose Assumption 1, 2 and 3 hold and the total simulation budget $n = \infty$. Then,

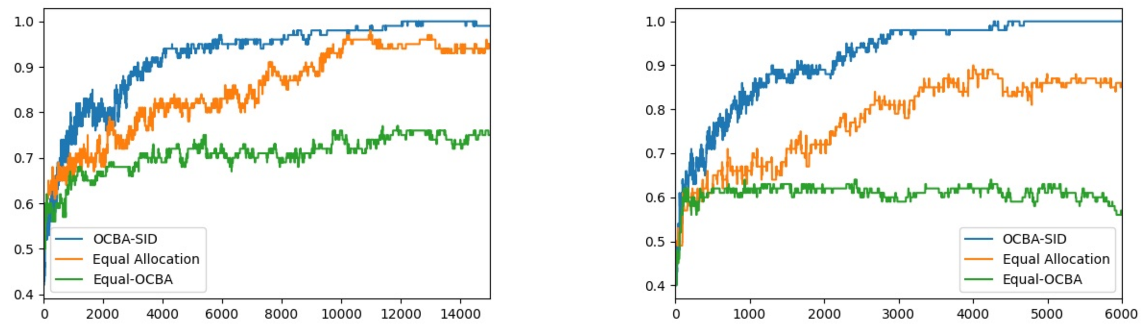
1. (Consistency) OCBA-SID selects the optimal design almost surely (a.s.) as $t \to \infty$.
2. (Asymptotic optimality) $\lim_{l\to\infty} \frac{N_{i,j}^{(l)}}{N^{(l)}} = \alpha_{i,j}^*$ *a.s.*, $1 \le i \le K, 1 \le j \le B$, where $\alpha_{i,j}^*$ satisfies the optimality condition (15) and (8).

Proof. Since $\sum_{s=1}^{t} n(s) \to \infty$ as $t \to \infty$, we know the empirical distribution $p_j^{(t)} \to p_j$ *a.s.* by Glivenko-Cantelli Theorem. Hence, if we can show $N_{i,j}^{(l)} \to \infty$ *a.s.* for j with $p_j > 0$, we then have $\hat{\bar{\mu}}_i^{(l)} \to \bar{\mu}_i$ *a.s.* by the SLLN and the fact that $p_j^{(t)} \to p_j$ *a.s.*. Hence, to prove 1 and 2, it suffices to show $N_{i,j}^{(l)} \to \infty$ *a.s.* for $p_j > 0$. Denote by $A = \{(i,j)|N_{i,j}^{(l)} \to \infty\} \neq \emptyset$ and $J_a = \{1 \le j \le B | p_j > 0\}$ the valid input support set.

Proof of 1. Denote by ω any sequence of sample outputs. We fix a sample path ω in the following proof. Prove by contradiction. Suppose there exists $(i_0, j_0) \notin A$ and $j_0 \in J_a$. Since $\hat{\mu}_{i,j}^{(l)}$ will always converge, no matter whether $N_{i,j}^{(l)}$ will tend to infinity, $\hat{\mu}_{i,j}^{(l)}$ will also converge. Denote by $N^{(l)} = \sum_{i,j} N_{i,j}^{(l)}$. Then there exists an allocation policy $\{\tilde{\alpha}_{i,j}\}$ satisfying $\lim_{l\to\infty} \frac{\hat{N}_{i,j}^{(l)}}{N^{(l)}} = \tilde{\alpha}_{i,j}$. Since (i_0, j_0) can be sampled for at most finitely many times, it must hold for l large enough, $\hat{N}_{i_0,j_0}^{(l)} - N_{i_0,j_0}^{(l)} \le \hat{N}_{i,j}^{(l)} - N_{i,j}^{(l)}$ for any $(i,j) \in A$. Then we have

$$\liminf_{l\to\infty} \frac{\hat{N}_{i_0,j_0}^{(l)} - N_{i_0,j_0}^{(l)}}{N^{(l)}} \le \liminf_{l\to\infty} \frac{\hat{N}_{i,j}^{(l)} - N_{i,j}^{(l)}}{N^{(l)}}. \tag{16}$$

The left hand side (LHS) of (16) = $\lim_{l\to\infty} \frac{\hat{N}_{i_0,j_0}^{(l)}}{N^{(l)}}$ = $\tilde{\alpha}_{i_0,j_0} > 0$, where positiveness comes from the fact that $\alpha_{i,j} > 0$ if $p_j > 0$ by proof of Theorem 1, where we replace the true $\bar{\mu}$ with the limit of $\hat{\bar{\mu}}^{(l)}$. On the other hand, the right hand side (RHS) of (16) $= \lim_{l\to\infty} \frac{\hat{N}_{i,j}^{(l)}}{N^{(l)}} - \limsup_{l\to\infty} \frac{N_{i,j}^{(l)}}{N^{(l)}} = \tilde{\alpha}_{i,j} - \limsup \frac{N_{i,j}^{(l)}}{N^{(l)}}$. Hence, we



(a) constant batch size. (b) random batch size.

Figure 2: Performance comparison with constant and random batch sizes.

have $\limsup_{l\to\infty} \frac{N_{i,j}^{(l)}}{N^{(l)}} \leq \tilde{\alpha}_{i,j} - \tilde{\alpha}_{i_0,j_0} < \tilde{\alpha}_{i,j}$. Since this holds for all $(i,j) \in A$, we have

$$1 = \sum_{i,j} \frac{N_{i,j}^{(l)}}{N^{(l)}} = \limsup_{l\to\infty} \sum_{i,j} \frac{N_{i,j}^{(l)}}{N^{(l)}} \leq \sum_{i,j} \limsup_{l\to\infty} \frac{N_{i,j}^{(l)}}{N^{(l)}} = \sum_{(i,j)\in A} \limsup_{l\to\infty} \frac{N_{i,j}^{(l)}}{N^{(l)}} < \sum_{(i,j)\in A} \tilde{\alpha}_{i,j} \leq 1 - \tilde{\alpha}_{i_0,j_0} < 1,$$

a contradiction.

Proof of 2. Due to the limited space, the proof of 2 is omitted. □

7 NUMERICAL EXPERIMENT

We carry out numerical experiments to test the performance of OCBA-SID with (i) equal allocation of simulation budget to all design-input pairs, denoted by Equal Allocation; and (ii) equal allocation to input realizations while OCBA for allocating simulation budget among designs under the same input realization, denoted by Equal-OCBA.

7.1 Test Problem

We use a quadratic problem to test the procedures. The problem is to minimize the expected value of a quadratic function $X_i = (i-\zeta)^2 + \varepsilon_i(\zeta)$, where ζ takes value in $\{0,1,\cdots,5\}$ with probability p_j, $j = 0,1,\ldots,5$, and $\varepsilon_i(\zeta)|\zeta$ follows the normal distribution with mean 0 and stand deviation $\sigma_i(\zeta)$. $\{p_j\}$ is uniformly randomly chosen before running the procedures, and $\sigma_i(\zeta)$ is also randomly chosen from a uniform distribution on $[1,2]$. The candidate designs are $\mathscr{I} = \{2+0.5\cdot i : i \in [-5,5] \cap \mathbf{Z}\}$. The true best design is $b = \arg\min_{i\in\mathscr{I}} \sum_{j=0}^{5} (i-j)^2 p_j$.

7.2 Experiment Results

To run the procedures, we set the initial simulation budget for each design-input pair $n_0 = 10$. Let the initial batch size of input data $m_0 = 10$. We carry out experiments for two scenarios: (i) constant input data batch size ($m(t) = 30$) and simulation budget ($n(t) = 50$) and (ii) varying input data batch size and simulation budget. For the second scenario, we set $m(t)$ and $n(t)$ uniformly chosen from $\{\bar{d}, 2\bar{d}, \cdots, 5\bar{d}\}$ and $\bar{d} = 20$. Figure 2a and 2b present the empirical PCS based on 100 replications of each procedure with respect to the total simulation budget. The observations from Figure 2 can be summarized as follows:

1. In both scenarios, OCBA-SID achieves a higher PCS with same simulation budget than Equal Allocation and Equal-OCBA, showing high efficiency for solving R&S with input uncertainty.

2. Using OCBA blindly without considering the input uncertainty is no better or even worse than the naive equal allocation procedure. The reason is that for different realizations of the input parameter, the conditional performance of designs can be ranked quite differently from the true (unconditional) expected performance. Equal-OCBA over allocates simulation budget to the design-input pair (i, j) where i is optimal under realization ζ_j but suboptimal overall. These simulations are useless for Equal-OCBA to find the true optimal design, making the procedure worse than equal allocation since it cannot allocate sufficient simulation budget to (b, j) under the same input realization ζ_j.

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