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OPTIMAL COMPUTING BUDGET ALLOCATION FOR MULTI-OBJECTIVE RANKING AND SELECTION UNDER BERNOULLI DISTRIBUTION

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ABSTRACT

This paper studies a multi-objective ranking and selection (MORS) issue with observations following Bernoulli distribution. The Pareto-optimal set is aimed to be selected with each design and performance measure pair being evaluated separately. Our contribution is twofold. (i) We provide a frequentist work under Bernoulli assumption in MORS where a robust asymptotic optimal sampling strategy is derived based on large deviation principle (LDP). (ii) From the optimal sampling strategy, we propose a sequential selection procedure, named MOCBA-B. Numerical results based on averaged probability of correct selection (PCS) show that MOCBA-B is significantly superior to equal allocation (EA) and is comparable to the theoretically optimal allocation strategy.

1 INTRODUCTION

Due to the complexity of real-world problems and continuous development of computing technology, optimization via simulation (OvS) has been regarded as a vital and popular technique to optimize the performances of complicated systems (see Long-Fei and Le-Yuan 2013; Amaran et al. 2016 for a quick review). As considering the decision variables merely taking discrete values, discrete optimization via simulation (DOvS) has extensive applications such as choosing the most effective medicine or selecting the best routing algorithm (Hong and Nelson 2009), etc.

A well-studied problem for DOvS is ranking and selection (R&S) (see Fu and Henderson 2017; Hong et al. 2021 for a review) where finite designs are simulated with multiple times in stochastic environments. R&S can be characterized into two types: fixed-precision R&S and fixed-budget R&S. For the former problem, indifference zone (IZ) procedures (Fan et al. 2016; Elkadry and McDonald 2018), most frequently used, preset a parameter to tell the smallest distance between pairwise alternatives that is statistically significant and seek to correctly select the best alternative whenever the best alternative is sufficiently separated from others. Then for the latter problem, an effective method is knowledge-gradient (KG) policy (Frazier and Powell 2008; Frazier et al. 2008; Frazier et al. 2009), which can be viewed as a single-step Bayesian look-ahead policy. It allocates one budget to the measurement whose single-period expected increase in value is the largest. Another method is optimal computing budget allocation (OCBA), which maximizes the probability of correct selection (PCS) asymptotically. OCBA samples alternatives

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sequentially with budget constraints and in each iteration the budget allocation ratio is adaptive to the sampling information updated (Chen et al. 2000; Xiao et al. 2013; Zhang et al. 2016).

In some real and complicated cases, the alternatives are required to be measured by no less than two criteria or objectives which drives researchers to turn their attention from single-objective ranking and selection (SORS) to multi-objective ranking and selection (MORS) (see Yoon and Bekker 2017; Hunter et al. 2019 for a review). The general target of such problem is to obtain the Pareto-optimal set which contains alternatives with different trade-offs.

We characterize MORS into two categories: Bayesian and frequentist. From a Bayesian perspective, Branke and Zhang (2015) propose myopic multi-Objective budget allocation (M-MOBA) procedure which allocates a single budget to the alternative changing the observed Pareto set with the largest probability in each iteration and best designs are selected when budget exhaust. Later M-MOBA is applied with various performance criteria in bi-objective problems (Branke et al. 2016; Branke and Zhang 2019). The current numerical experiments can only prove the effectiveness of M-MOBA in problems with two objectives.

From a frequentist perspective, large deviation principle (LDP), firstly introduced in SORS by Glynn and Juneja (2004), is adopted as a theoretical device to determine the optimal budget ratio vector $\boldsymbol{\alpha}^*$ that maximizes the rate function of probability of false selection (PFS). Sampling criteria for optimization using rate estimators (SCORE) (Feldman and Hunter 2018) introduce the concept of phantom Pareto and let the number of non-Pareto systems tends to infinity so that the exact rate function of PFS becomes available for a bi-objective R&S problem. Applegate et al. (2020) apply SCORE into the multi-objective scheme with an approximated PFS decay rate.

The niche we focus on is multi-objective optimal computing budget allocation (MOCBA) adopting LDP to select the Pareto set. It discards the regime of SCORE that non-Pareto systems are sent to infinity and considers a more general case where the designs and objectives are finite. In this case, however, PFS decay rate does not have the explicit form and the bounds of rate function are considered instead. To the best of our knowledge, only two works are found in this niche. Liu et al. (2017) provide asymptotic allocation strategy which derives precise allocation ratio of each performance through maximizing the upper bound of PFS decay rate. The limitation is that the maximization of PFS decay rate is less valid by optimizing its upper bound. The formulation proposed by Li et al. (2017) maximizes the lower bound of the decay rate instead. However their work merely assigns budget to designs but not to each performance measure. Note that both works above have not proposed a practical selection procedure in the case that true parameters are covered.

Studies on Bernoulli distribution in SORS are already mature (Glynn and Juneja 2004; Malone 2004; Szechtman and Yucesan 2008; Peng et al. 2018). However relevant research on MORS is far underdeveloped with merely a small numerical experiment conducted to compare the optimal allocation between Gaussian distribution and Bernoulli distribution (Li et al. 2017). We assist in filling this blank with a MOCBA procedure.

This work aims at correctly identifying the Pareto set from the design space through observations on each performance measure, which follows Bernoulli distribution, for all designs with given total budget. Related practical problems can be found in drug discovery (Beck et al. 2022) where multiple one-off experiments are carried to identify the specific small molecules which can effectively bind to their biological targets. Two contributions are made. (i) For frequentist works of MORS, we provide an explicit asymptotic optimal allocation rule with Bernoulli assumption to maximize the lower bound of PCS. (ii) For MOCBA adopting LDP to select the Pareto set, we propose an easy-to-use sequential algorithm to select the Pareto set.

The rest of the paper is organized as follows. Section 2 formulates the typical MORS problem we study and provides necessary notations along with assumptions. Section 3 derives explicit asymptotic optimal allocation rule with Bernoulli assumption. Section 4 proposes a sequential selection procedure. Numerical experiments are conducted in Section 5 and this research is concluded in Section 6.

2 PROBLEM STATEMENT

This study considers a MORS problem where h alternatives from a finite design space $S := \{1,2,\cdots,h\}$ are available to be selected. Each design i, $i \in S$, is evaluated by v binary performance measures subject to random noise and $\mathcal{V} := \{1,2,\cdots,v\}$ is the set containing all performance measures. This research targets at identifying a subset of the best designs from the design space S through sample means given fixed budget number.

The basic notations in this study are listed as below:

- X_{ij}: the random variable of performance measure j for design i where $i \in S$ and $j \in \mathcal{V}$;
- q_{ij}: the mean of X_{ij}, i.e., $q_{ij} = E[X_{ij}]$, and let $\boldsymbol{q}_i = (q_{i1}, q_{i2}, \cdots, q_{iv})$ be the mean vector for design i where $i \in S$;
- N: the total budget number;
- α_{ij}: the ratio of budget allocated to the performance measure j of design i, for $i \in S$ and $j \in \mathcal{V}$;
- X_{ij}^r: the observed output of X_{ij} in r^{th} replication for $i \in S$, $j \in \mathcal{V}$ and $r \leq N\alpha_{ij}$;
- $\bar{X}_{ij}$: the sample mean of X_{ij}, i.e., $\bar{X}_{ij} = \frac{1}{N\alpha_{ij}} \sum_{r=1}^{N\alpha_{ij}} X_{ij}^r$, for $i \in S$ and $j \in \mathcal{V}$ and let $\bar{\boldsymbol{X}}_i = (\bar{X}_{i1}, \bar{X}_{i2}, \cdots, \bar{X}_{iv})$ be the sample mean vector for design i where $i \in S$;
- S_p, $\overline{S}_p$: the true Pareto set, i.e., $S_p = \{i | i \in S \text{ and } l \not\prec i, \forall l \in S, l \neq i\}$, of which the cardinality is represented as $|S_p|$ and the true non-Pareto set, i.e., $\overline{S}_p = S \backslash S_p$, of which the cardinality is represented as $|\overline{S}_p|$;
- $\hat{S}_p$, $\hat{\overline{S}}_p$: the observed Pareto set, i.e., $\hat{S}_p = \{i | i \in S \text{ and } l \hat{\not\prec} i, \forall l \in S, l \neq i\}$ and the the observed non-Pareto set, i.e., $\hat{\overline{S}}_p = S \backslash \hat{S}_p$.

Additionally, let $\Lambda^{X_{ij}}(\lambda_{ij})$ be the logarithmic moment generating function of random variable X_{ij}, for $i \in S$ and $j \in \mathcal{V}$, with effective domain $\mathcal{D}_{\Lambda^{X_{ij}}} = \{\lambda_{ij} \in \mathbb{R} : \Lambda^{X_{ij}}(\lambda_{ij}) < \infty\}$. Meanwhile, $\Lambda^{\bar{\boldsymbol{X}}_i}(\boldsymbol{\lambda}_i)$ is the logarithmic moment generating function of sample mean vector $\bar{\boldsymbol{X}}_i$, for $i \in S$ and its effective domain is $\mathcal{D}_{\Lambda^{\bar{\boldsymbol{X}}_i}} = \{\boldsymbol{\lambda}_i \in \mathbb{R}^v : \Lambda^{\bar{\boldsymbol{X}}_i}(\boldsymbol{\lambda}_i) < \infty\}$. Subsequently let $I_{ij}(x_{ij})$ be the Fenchel-Legendre transform of $\Lambda^{X_{ij}}(\lambda_{ij})$, i,e., $I_{ij}(x_{ij}) = \sup_{\lambda_{ij} \in \mathbb{R}} (\lambda_{ij} x_{ij} - \Lambda^{X_{ij}}(\lambda_{ij}))$, for $i \in S$ and $j \in \mathcal{V}$.

In this study, we adopt Pareto optimality for best designs selection and subsequently provide the mathematical definition of dominance relationship as the preliminary to introduce Pareto set:

Definition 1 (Dominance): Design l is said to be dominated by design i, denoted as $i \prec l$, when design i is not worse than design l for all the performance measures, and there exists at least one performance measure that design i is better than design l. Such relationship can be further defined that $i \prec l$ holds, if and only if $\forall j \in \mathcal{V}$, $q_{ij} \leqslant q_{lj}$ and $\exists j \in \mathcal{V}$, $q_{ij} < q_{lj}$. When the conditions fail to hold, then design l is not dominated by design i, denoted as $i \not\prec l$. Additionally, notation $\hat{\prec}$ is utilized to express the estimated dominance relationship based on sample averages.

With the definition of dominance relationship, the Pareto set S_p can be easily constructed accommodating all the non-dominated designs in the design space S. It is often the case that the observed Pareto set failed to be equivalent to the true one. Accordingly we can achieve the aim of identifying the true Pareto set by minimizing the *probability of false selection* (PFS):

$$\min PFS := Pr(\hat{S}_p \neq S_p)$$

Assumptions utilized in the rest of the paper have been made as follows.

Assumption 1 For each design i, $i \in S$, its performance measures are independent and identically distributed (i.i.d.) following Bernoulli distribution.

Assumption 2 Any two mean vectors $\boldsymbol{q}_i$ and $\boldsymbol{q}_l$, for $i \in S$, $l \in S$, $l \neq i$, are not equivalent.

Remark 1 Assumption one is guaranteed when each trial is simulated independently. The second assumption prevents that all the budget is allocated to differentiate designs which share identical performance measures.

3 ASYMPTOTIC OPTIMAL BUDGET ALLOCATION STRATEGY

3.1 Bounds for Probability of False Selection

We try to minimize PFS in order to solve the multi-objective ranking and selection problem. False selection is related to two types of errors, i.e., *Type I error* (E_1) and *Type II error* (E_2) and either E_1 or E_2 happens triggering the best designs being falsely selected. Therefore we show the general expression of PFS:

$$PFS = Pr(E_1 \bigcup E_2) \tag{1}$$

and provide the descriptions of these two types of errors:

1. *Type I error* (E_1): It happens when design i, essentially belonging to the Pareto set, is assigned to the observed non-Pareto set because it is dominated by other design(s).
2. *Type II error* (E_2): It occurs when design k, essentially belonging to the non-Pareto set, is assigned to the observed Pareto set because it can not be dominated by any other designs.

Based on the descriptions, the probability of Type I error $Pr(E_1)$ and Type II error $Pr(E_2)$ can be shown as:

$$Pr(E_1) = Pr(\bigcup_{i \in S_p} \bigcup_{l \in S, l \neq i} l \hat{\prec} i) \tag{2}$$

$$Pr(E_2) = Pr(\bigcup_{k \in \overline{S}_p} \bigcap_{l \in S, l \neq k} l \hat{\nprec} k) \tag{3}$$

and the explicit expression of PFS can be derived by combining (1), (2) and (3):

$$PFS = Pr(\bigcup_{i \in S_p} \bigcup_{l \in S, l \neq i} l \hat{\prec} i \cup \bigcup_{k \in \overline{S}_p} \bigcap_{l \in S, l \neq k} l \hat{\nprec} k) \tag{4}$$

Because PFS (4) is analytically intractable, we provide the following proposition to give valid upper and lower bounds for it.

Proposition 1 The upper and lower bounds of PFS are both demonstrated as below,

$$PFS \leq (h + h|S_p| - 2|S_p|) \max\{\max_{i \in S_p} \max_{l \in S, l \neq i} Pr(l \hat{\prec} i), \max_{k \in \overline{S}_p} \min_{l \in S, l \neq k} Pr(l \hat{\nprec} k)\}$$

$$PFS \geq \max\{\max_{i \in S_p} \max_{l \in S, l \neq i} Pr(l \hat{\prec} i), \max_{k \in \overline{S}_p} \prod_{l=1, l \neq k}^{h} Pr(l \hat{\nprec} k)\}$$

Proof. The bounds based on Bonferroni inequality for (2) and (3) are:

$$\max_{i \in S_p} \max_{l \in S, l \neq i} Pr(l \hat{\prec} i) \leq Pr(E_1) \leq (h|S_p| - |S_p|) \max_{i \in S_p} \max_{l \in S, l \neq i} Pr(l \hat{\prec} i) \tag{5}$$

$$\max_{k \in \overline{S}_p} \prod_{l=1, l \neq k}^{h} Pr(l \hat{\nprec} k) \leq Pr(E_2) \leq (h - |S_p|) \max_{k \in \overline{S}_p} \min_{l \in S, l \neq k} Pr(l \hat{\nprec} k) \tag{6}$$

where the lower bound of $Pr(E_2)$ is available based on Lee et al. (2010) and (1) indicates that

$$PFS \leq Pr(E_1) + Pr(E_2) \tag{7}$$

$$PFS \geq \max\{Pr(E_1), Pr(E_2)\} \tag{8}$$

The result is available by plugging (5) and (6) into (7) and (8). □

In the following subsections, the bounds for PFS in proposition 1 are transformed into the bounds for the rate function of PFS with LDP to acquire an explicit asymptotic optimal budget allocation strategy for identifying the true Pareto set under Bernoulli assumption.

3.2 Rate Function of the Probability of False Selection

In this subsection we derive the rate function of PFS by introducing LDP. And the prerequisite for such purpose is to obtain the rate functions of $Pr(l\hat{\preceq}i)$ and $Pr(l\hat{\not\preceq}k)$ in the first place.

Proposition 2 The rate functions of $Pr(l\hat{\preceq}i)$ and $Pr(l\hat{\not\preceq}k)$ are given as below,

$$\lim_{n\to\infty} -\frac{1}{n}\log Pr(l\hat{\preceq}i) = \sum_{j=1}^{v} G_{ij,lj}, \forall i \in S_p, l \in S, l \neq i \tag{9}$$

$$\lim_{n\to\infty} -\frac{1}{n}\log Pr(l\hat{\not\preceq}k) = \min_{j\in\mathcal{V}} G^{non}_{kj,lj}, \forall k \in \overline{S}_p, l \in S, l \neq k \tag{10}$$

where

$$G_{ij,lj} = \inf_{x_{lj}\leq x_{ij}} (\alpha_{ij}I_{ij}(x_{ij}) + \alpha_{lj}I_{lj}(x_{lj}))$$
$$G^{non}_{kj,lj} = \inf_{x_{kj}\leq x_{lj}} (\alpha_{kj}I_{kj}(x_{kj}) + \alpha_{lj}I_{lj}(x_{lj}))$$

Proof. With (9), it is easy to get $\lim_{n\to\infty} -\frac{1}{n}\log Pr(l\hat{\preceq}i) = \lim_{n\to\infty} -\frac{1}{n}\log Pr(\bar{\boldsymbol{X}}_l \preceq \bar{\boldsymbol{X}}_i)$ where n is the budget number. Then let $Z = (\bar{\boldsymbol{X}}_i, \bar{\boldsymbol{X}}_l) \in \mathbb{R}^{2v}$ and $\langle\cdot,\cdot\rangle$ be the scalar inner product, thus the logarithmic moment generating function of Z can be derived by definition, i.e., $\Lambda^Z_n(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_l) = \log E[e^{\langle(\boldsymbol{\lambda}_i,\boldsymbol{\lambda}_l),(\bar{\boldsymbol{X}}_i,\bar{\boldsymbol{X}}_l)\rangle}]$. Furthermore due to the independence assumption declared before and the fact that X^r_{ij} shares the same probability space with X_{ij}, for $i \in S_p$, $l \in S$, $l \neq i$ and $r \leq n\alpha_{ij}$, we can have $\Lambda^Z_n(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_l) = \lim_{n\to\infty}\frac{1}{n}\Lambda^Z_n(n\boldsymbol{\lambda}_i, n\boldsymbol{\lambda}_l) = \sum_{j=1}^{v} \alpha_{ij}\Lambda^{X_{ij}}(\frac{\lambda_{ij}}{\alpha_{ij}}) + \alpha_{lj}\Lambda^{X_{lj}}(\frac{\lambda_{lj}}{\alpha_{lj}})$. Then by Gartner-Ellis Theorem, $I(\boldsymbol{x}_i, \boldsymbol{x}_l) = \sup_{\boldsymbol{\lambda}_i,\boldsymbol{\lambda}_l\in\mathbb{R}^v} (\langle(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_l), (\boldsymbol{x}_i, \boldsymbol{x}_l)\rangle - \Lambda^Z_n(\boldsymbol{\lambda}_i, \boldsymbol{\lambda}_l)) = \sum_{j=1}^{v} \alpha_{ij}I_{ij}(x_{ij}) + \alpha_{lj}I_{lj}(x_{lj})$. Accordingly the rate function of $Pr(l\hat{\preceq}i)$ is available. The rate function of $Pr(l\hat{\not\preceq}k)$, i.e., (10), can be transformed into $\min_{j\in\mathcal{V}}\lim_{n\to\infty} -\frac{1}{n}\log Pr(\bar{X}_{kj} \leq \bar{X}_{lj})$ and the rest of proof follows similar procedures. □

Proposition 3 The bounds for the rate function of PFS are shown as below,

$$\lim_{n\to\infty} -\frac{1}{n}\log PFS \geq \min\{\min_{i\in S_p}\min_{l\in S, l\neq i}\sum_{j=1}^{v} G_{ij,lj}, \min_{k\in\overline{S}_p}\max_{l\in S, l\neq k}\min_{j\in\mathcal{V}} G^{non}_{kj,lj}\} \tag{11}$$

$$\lim_{n\to\infty} -\frac{1}{n}\log PFS \leq \min\{\min_{i\in S_p}\min_{l\in S, l\neq i}\sum_{j=1}^{v} G_{ij,lj}, \min_{k\in\overline{S}_p}\sum_{l=1,l\neq k}^{h}\min_{j\in\mathcal{V}} G^{non}_{kj,lj}\} \tag{12}$$

Rationale behind proposition 3 is that the rate function of PFS can not be explicitly expressed which can be attributed to the entangled information of multi-dimensional performance measures among non-Pareto designs by comparing (11) and (12). Hence the bounds of PFS decay rate are considered instead. A robust way is to maximize the lower bound of the rate function, which is considered to be equivalent to minimize the upper bound of PFS. Furthermore by looking into expression (11), the limitation of the rate function can be down to two situations. (i) There exists a pair of designs where design i is most unlikely to dominate design l. (ii) There exists a pair of designs where design l dominates design k with the least difficulty comprehensively. However, on the j^{th} performance measure, design l surpasses design k with the least amount.

Lastly we provide the explicit expressions of $G_{ij,lj}$ and $G^{non}_{kj,lj}$. With Bernoulli assumption, it is well-known that $I_{ij}(x_{ij}) = x_{ij}\log\frac{x_{ij}}{q_{ij}} + (1-x_{ij})\log\frac{1-x_{ij}}{1-q_{ij}}$, for $i \in S$ and $j \in \mathcal{V}$, then we get the following equations by plugging it into $G_{ij,lj}$ and $G^{non}_{kj,lj}$:

$$G_{ij,lj} = \inf_{x_{lj}\le x_{ij}} (\alpha_{ij}(x_{ij}\log\frac{x_{ij}}{q_{ij}} + (1-x_{ij})\log\frac{1-x_{ij}}{1-q_{ij}}) + \alpha_{lj}(x_{lj}\log\frac{x_{lj}}{q_{lj}} + (1-x_{lj})\log\frac{1-x_{lj}}{1-q_{lj}})) \tag{13}$$

$$G^{non}_{kj,lj} = \inf_{x_{kj}\le x_{lj}} (\alpha_{kj}(x_{kj}\log\frac{x_{kj}}{q_{kj}} + (1-x_{kj})\log\frac{1-x_{kj}}{1-q_{kj}}) + \alpha_{lj}(x_{lj}\log\frac{x_{lj}}{q_{lj}} + (1-x_{lj})\log\frac{1-x_{lj}}{1-q_{lj}})) \tag{14}$$

The expressions above are strictly concave and can be easily solved by adopting Lagrange functions with corresponding Karush-Kuhn-Tucker (KKT) conditions.

Lemma 1 The explicit forms of $G_{ij,lj}$ and $G^{non}_{kj,lj}$ are shown as below,

$$G_{ij,lj} = \mathbf{1}_{q_{ij}<q_{lj}}\{-(\alpha_{ij}+\alpha_{lj})\log[q_{ij}^{\frac{\alpha_{ij}}{\alpha_{ij}+\alpha_{lj}}} q_{lj}^{\frac{\alpha_{lj}}{\alpha_{ij}+\alpha_{lj}}} + (1-q_{ij})^{\frac{\alpha_{ij}}{\alpha_{ij}+\alpha_{lj}}}(1-q_{lj})^{\frac{\alpha_{lj}}{\alpha_{ij}+\alpha_{lj}}}]\} \tag{15}$$

$$G^{non}_{kj,lj} = \mathbf{1}_{q_{kj}>q_{lj}}\{-(\alpha_{kj}+\alpha_{lj})\log[q_{kj}^{\frac{\alpha_{kj}}{\alpha_{kj}+\alpha_{lj}}} q_{lj}^{\frac{\alpha_{lj}}{\alpha_{kj}+\alpha_{lj}}} + (1-q_{kj})^{\frac{\alpha_{kj}}{\alpha_{kj}+\alpha_{lj}}}(1-q_{lj})^{\frac{\alpha_{lj}}{\alpha_{kj}+\alpha_{lj}}}]\} \tag{16}$$

Proof. For (15), the Lagrange function obtained from (13) is

$$L(x_{ij},x_{lj},\nu) = \alpha_{ij}(x_{ij}\log\frac{x_{ij}}{q_{ij}} + (1-x_{ij})\log\frac{1-x_{ij}}{1-q_{ij}}) + \alpha_{lj}(x_{lj}\log\frac{x_{lj}}{q_{lj}} + (1-x_{lj})\log\frac{1-x_{lj}}{1-q_{lj}}) + \nu(x_{lj}-x_{ij})$$

and it can be solved when these two conditions hold, i.e., $-\frac{\partial_{x_{ij}}G_{ij,lj}}{\partial_{x_{lj}}G_{ij,lj}} = 1$ and $x_{ij} = x_{lj}$. Also note that $\mathbf{1}_{q_{ij}<q_{lj}}$ is an indicator function characterized by $q_{ij} < q_{lj}$. The derivation of (16) from (14) follows the exact same steps.

□

3.3 Asymptotic Optimal Budget Allocation Problem

Due to the existence of a gap between the bounds of PFS rate function based on LDP, a robust strategy has been adopted that the lower bound of PFS rate function, i,e., right hand of (11) is to be maximized, which is equivalent to minimizing the upper bound of PFS, thus letting PFS converge to zero asymptotically. The optimization problem $\boldsymbol{P}$ is shown as below.

$$\begin{array}{llll} \textit{Problem } \boldsymbol{P}: & \max & z & \\ & s.t. & z \le \sum_{j=1}^{v} G_{ij,lj}, & \forall i \in S_p, l \in S, l \ne i, \\ & & z \le \max_{l\in S, l\ne k}\min_{j\in\mathcal{V}} G^{non}_{kj,lj}, & \forall k \in \overline{S}_p, \\ & & \sum_{i=1}^{h}\sum_{j=1}^{v}\alpha_{ij} = 1, & \alpha_{ij} \ge 0, \forall i \in S, j \in \mathcal{V}. \end{array}$$

Because $G_{ij,lj}$ and $G^{non}_{kj,lj}$ are both strictly concave functions as stated above, the problem $\boldsymbol{P}$ is a convex optimization problem and an unique optimal solution $\boldsymbol{\alpha}^*$ exists as well. Meanwhile corresponding KKT conditions are necessary and sufficient for the optimality of this problem (Boyd and Vandenberghe 2004). To show the essence of problem $\boldsymbol{P}$, we employ the definition of *reference designs* introduced by Li et al. (2017).

Definition 2 (Reference Design): For $\forall i \in S$, the reference design r_i of design i is

$$r_i = \arg\min_{l \in S, l \neq i} \lim_{n \to \infty} -\frac{1}{n} \log Pr(l \precsim i), \forall i \in S \tag{17}$$

Definition 2 argues that for each design i, $i \in S$, there exists a reference design r_i which dominates design i with the largest probability and reference designs belong to Pareto set or *phantom* Pareto set (refer to Feldman and Hunter 2018). Furthermore an equivalent problem $\boldsymbol{T}$ is given by putting (17) into the problem $\boldsymbol{P}$:

$$\begin{array}{llll} Problem\ \boldsymbol{T}: & \max & z & \\ & s.t. & z \leq \sum_{j=1}^{v} G_{ij,r_ij}, & \forall i \in S_p, \\ & & z \leq\ G^{non}_{kj,r_kj}, & \forall k \in \overline{S}_p, j \in \mathcal{V}, \\ & & \sum_{i=1}^{h} \sum_{j=1}^{v} \alpha_{ij} = 1, & \alpha_{ij} \geq 0, \forall i \in S, j \in \mathcal{V}. \end{array}$$

Noteworthily the inequality constraints for design k, $k \in \overline{S}_p$ in problems $\boldsymbol{P}$ and $\boldsymbol{T}$ are equivalent in that they conform to the interpretation of proposition 3 that the limitation of PFS rate function can be partially attributed to a pair of designs k and r_k where on the j^{th} performance measure, design r_k surpasses design k with the least amount.

Theorem 1 If the optimal solution $\boldsymbol{\alpha}^*$ asymptotically minimizes the probability of false selection, then the following equilibrium holds:

$$\frac{w_i \Delta G^*_{ij,r_ij}}{u_{kj} \Delta G^{non^*}_{kj,r_kj}} = 1, \quad \forall i \in S_p, k \in \overline{S}_p, j \in \mathcal{V},$$

where $\Delta G^*_{ij,r_ij}$ is the total increment of G_{ij,r_ij} at optimal point $(\alpha^*_{ij}, \alpha^*_{r_ij})$ and $\Delta G^{non^*}_{kj,r_kj}$ is the total increment of G^{non}_{kj,r_kj} at optimal point $(\alpha^*_{kj}, \alpha^*_{r_kj})$. Additionally the relationship $\sum_{i=1}^{|S_p|} w_i + \sum_{k=1}^{|\overline{S}_p|} \sum_{j=1}^{v} u_{kj} = 1$ holds.

Proof. The optimality of problem $\boldsymbol{T}$ can be reached by solving the corresponding KKT conditions:

$$\sum_{i=1}^{|S_p|} w_i + \sum_{k=1}^{|\overline{S}_p|} \sum_{j=1}^{v} u_{kj} = 1,$$

$$\sum_{i=1}^{|S_p|} w_i \sum_{j=1}^{v} (\partial_{\alpha_{ij}} G^*_{ij,r_ij} + \partial_{\alpha_{r_ij}} G^*_{ij,r_ij}) = \sum_{i=1}^{|S_p|} \sum_{j=1}^{v} \nu,$$

$$\sum_{k=1}^{|\overline{S}_p|} \sum_{j=1}^{v} u_{kj} (\partial_{\alpha_{kj}} G^{non^*}_{kj,r_kj} + \partial_{\alpha_{r_kj}} G^{non^*}_{kj,r_kj}) = \sum_{k=1}^{|\overline{S}_p|} \sum_{j=1}^{v} \nu.$$

□

Theorem 1 indicates that the optimality is met on the condition that a certain equilibrium holds where the weighted total increment of G_{ij,r_ij} equals to the weighted total increment of G^{non}_{kj,r_kj} for $i \in S_p$, $k \in \overline{S}_p$, $j \in \mathcal{V}$.

4 SEQUENTIAL SELECTION PROCEDURE

In this section, we propose a three-staged heuristic sequential selection procedure named multi-objective optimal computing budget allocation with Bernoulli distribution (MOCBA-B) which approaches the optimal allocation with small steps. The primary work in three stages is briefly explained below:

- **Stage One**: Allocate equal budget for all performance measures.
- **Stage Two**: Allocate a single budget to each performance measure of design a^* and b^* whose rate function value is the lowest in the current iteration. Note that b^* is equivalent to r_{a^*}.
- **Stage Three**: Identify design a^* and b^* firstly. If $a^* \in \hat{S}_p$, allocate a single budget to each performance measure of design a^* and b^*; If $a^* \in \hat{\hat{S}}_p$, allocate a single budget to performance measure j^* of design a^* and b^* because the lowest rate function value only concerns with the performance measure j^*.

Remark 2 Stage one provides us with basic information. Stage two samples designs following the information given by rate functions. In the final stage, a single budget is allocated precisely to performance measures conforming to (11) because noise is far less misleading after stage two.

Several new notations are supplemented before showing the specific algorithm. Let N_t be the replication number required in the t^{th} stage, i.e., $N = \sum_{t=1}^{3} N_t$ and c be the iteration counter. Furthermore we denote n_{ij}^c as the accumulative budget received until the c^{th} iteration, $\bar{X}_{ij}^c$ as the sample mean in the c^{th} iteration and α_{ij}^c as the budget ratio in the c^{th} iteration, i.e., $\alpha_{ij}^c = \frac{n_{ij}^c}{\sum_{i=1}^{h}\sum_{j=1}^{v} n_{ij}^c}$, for $i \in S,\ j \in \mathcal{V}$. All the $\hat{G}_{ij,lj}$ and $\hat{G}_{kj,lj}^{non}$ are available with corresponding sample means and budget ratio in each iteration. Lastly let $\hat{R}_{a^*b^*}^{lb}$ be the lower bound decay rate value of PFS in each iteration, i.e., $\hat{R}_{a^*b^*}^{lb} = \min\{\min_{i \in \hat{S}_p} \min_{l \in S, l \neq i} \sum_{j=1}^{v} \hat{G}_{ij,lj}, \min_{k \in \hat{\hat{S}}_p} \max_{l \in S, l \neq k} \min_{j \in \mathcal{V}} \hat{G}_{kj,lj}^{non}\}$. More specifically, if $a^* \in \hat{S}_p$, then $\hat{R}_{a^*b^*}^{lb} = \sum_{j=1}^{v} \hat{G}_{a^*j,b^*j}$; if $a^* \in \hat{\hat{S}}_p$, then $\hat{R}_{a^*b^*}^{lb} = \min_{j \in \mathcal{V}} \hat{G}_{a^*j,b^*j}^{non} = \hat{G}_{a^*j^*,b^*j^*}^{non}$. MOCBA-B is demonstrated as follows:

Algorithm 1 MOCBA-B procedure

Input N_1, N_2, N_3: budget required for the first, second and third stage

Initialization: $c \leftarrow 1$, $n_{ij}^c \leftarrow \frac{N_1}{hv}$ (supposed to be an integer), for $i \in S,\ j \in \mathcal{V}$
while $N_2 + N_3 > 0$ **do**
    Update: $\bar{X}_{ij}^c$, α_{ij}^c, for $i \in S,\ j \in \mathcal{V}$
    Update: $\hat{S}_p$, $\hat{\hat{S}}_p$
    Update: $\hat{G}_{ij,lj}$, for $i \in \hat{S}_p,\ l \in S,\ l \neq i,\ j \in \mathcal{V}$ and $\hat{G}_{kj,lj}^{non}$, for $k \in \hat{\hat{S}}_p,\ l \in S,\ l \neq k,\ j \in \mathcal{V}$
    Identify $\hat{R}_{a^*b^*}^{lb}$ and obtain indexes a^* and b^*
    if $N_2 > 0$ **then**
        $c \leftarrow c+1$, $n_{a^*j}^c \leftarrow n_{a^*j}^{(c-1)} + 1$, $n_{b^*j}^c \leftarrow n_{b^*j}^{(c-1)} + 1$, for $j \in \mathcal{V}$
        $N_2 \leftarrow N_2 - 2v$
    else $N_3 > 0$
        if $a^* \in \hat{S}_p$ **then**
            $c \leftarrow c+1$, $n_{a^*j}^c \leftarrow n_{a^*j}^{(c-1)} + 1$, $n_{b^*j}^c \leftarrow n_{b^*j}^{(c-1)} + 1$, for $j \in \mathcal{V}$
            $N_3 \leftarrow N_3 - 2v$
        else $a^* \in \hat{\hat{S}}_p$
            Identify the performance measure j^*
            $c \leftarrow c+1$, $n_{a^*j^*}^c \leftarrow n_{a^*j^*}^{(c-1)} + 1$, $n_{b^*j^*}^c \leftarrow n_{b^*j^*}^{(c-1)} + 1$
            $N_3 \leftarrow N_3 - 2$
        end if
    end if
end while

Output $\hat{S}_p$

5 NUMERICAL EXPERIMENTS

This section tests the effectiveness of MOCBA-B by comparing it with other two algorithms introduced as follows. And it is worth noting that the **scipy.optimize** module from SciPy library is used as a convenient and swift way to solve convex problems in this study.

- **Equal Allocation (EA)**: Simulation replications are identical for all the performance measures, i.e., $\alpha_{ij}^* = \frac{1}{hv}$, $i \in \mathcal{S}$, $j \in \mathcal{V}$.
- **MOCBA-B***: It assumes all parameters are known so that the theoretically optimal allocation ratio $\boldsymbol{\alpha}^*$ is acquired through solving the corresponding convex optimization problem $\boldsymbol{P}$.

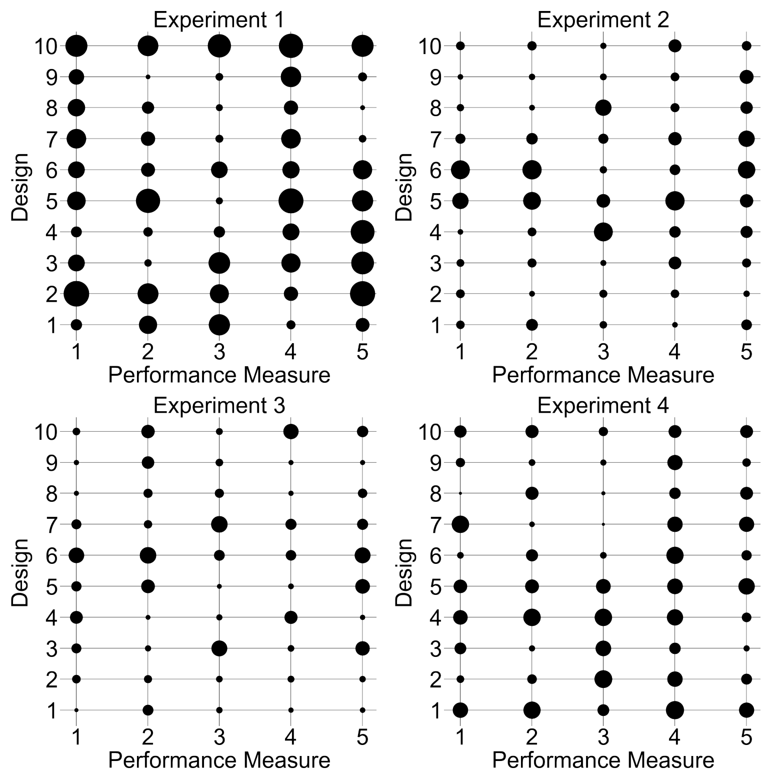

Figure 1: 10×5 Mean Matrices Demonstration.

In order to obtain concrete results, we specify four typical experimental problems shown in Figure 1 and set $h = 10$ designs, $v = 5$ performance measures and $|S_p| = 5$ designs in each of those experiments. For additional notification, the bigger dot in Figure 1 indicates a lower mean value as such designs in the Pareto set can be identified by intuitively comparing the size of dots in the diagrams.

- **Experiment 1 (Best of the Mass)**: The mean matrix is randomly generated with a continuous uniform distribution $U(0,1)$ and the designs in this experiment show no distinct features.
- **Experiment 2 (Best of the Best)**: The mean matrix is randomly generated with a continuous uniform distribution $U(0,0.5)$ where the designs are all considered to be competitive.
- **Experiment 3 (Best of the Mediocre)**: The mean matrix is randomly generated with a continuous uniform distribution $U(0.25,0.75)$ where the performances of designs are all mediocre.
- **Experiment 4 (Best of the Worst)**: The mean matrix is randomly generated with a continuous uniform distribution $U(0.5,1)$ where the performances of designs are far from satisfactory.

The three algorithms are compared with averaged *probability of correct selection* (PCS) values. The total budget N is 15000 and we set $N_1 = 1000$, $N_2 = 10000$, $N_3 = 4000$. The whole simulation process is repeated for 10000 times. The averaged PCS values are recorded at the checkpoint every 1000 budget.

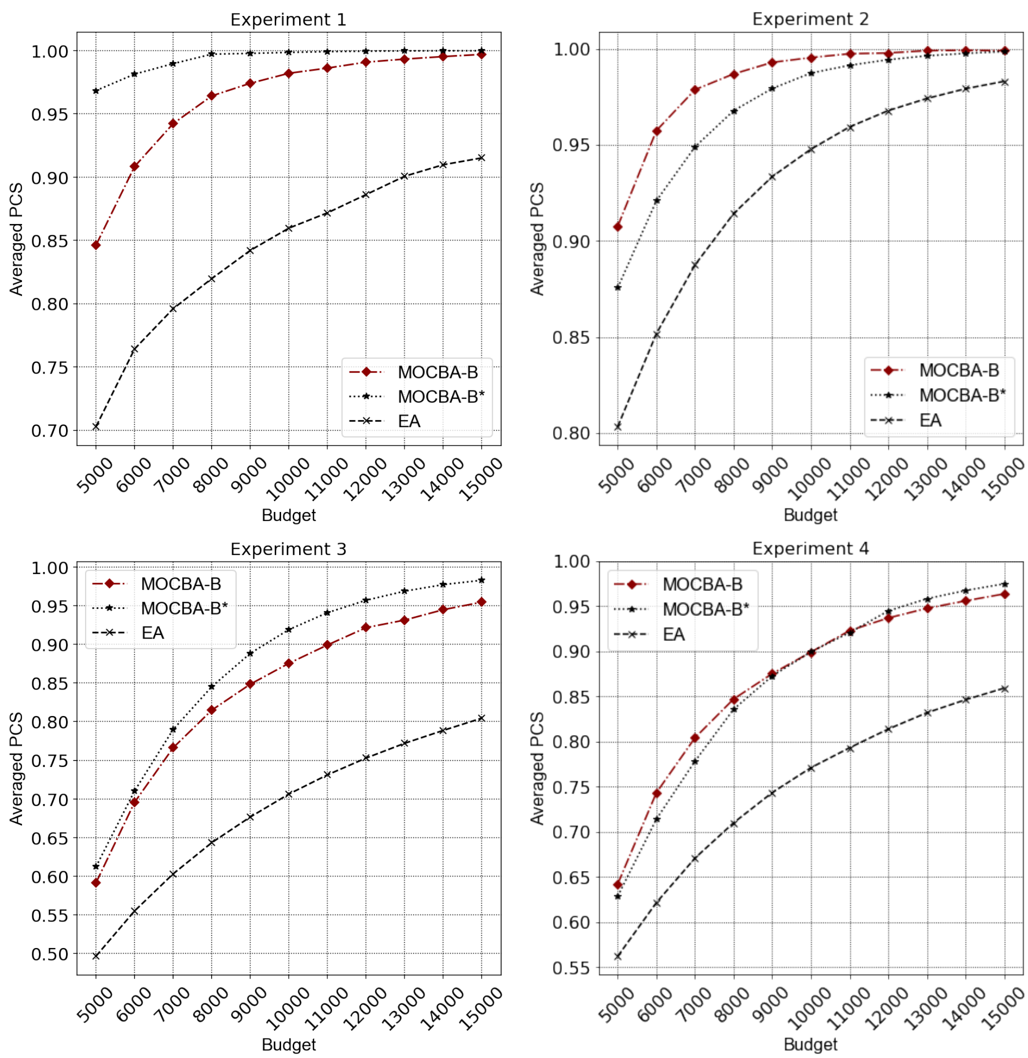

Figure 2: Averaged PCS of Three Algorithms.

Figure 2 displays the averaged PCS values of three algorithms in four experiments with budget range [5000,15000]. It is quite straightforward that more computing budget contributes to higher PCS for all the methods. More importantly, MOCBA-B and MOCBA-B* are significantly superior to EA due to their effective mechanisms making them capable of allocating more budget to critical designs or performance measures. Furthermore performances between MOCBA-B and MOCBA-B* are quite close and MOCBA-B even surpasses MOCBA-B* through the whole simulation process in experiment 2. An explanation for the figure of experiment 2 is provided that MOCBA-B, which is less greedier than MOCBA-B*, prevents more dominated designs from being assigned to the observed Pareto set given that nondominated designs are identified with less difficulty in this experiment. The numerical results prove MOCBA-B to be promising.

6 CONCLUSION

In this paper, we consider a multi-objective ranking and selection problem where the Pareto set is aimed to be selected correctly based on observations following Bernoulli distribution. Our study contributes to filling two research blanks. (i) We develop a frequentist framework to study Bernoulli distribution in MORS and our asymptotic optimal allocation strategy drawn from the framework samples flexibly in different performance measures. (ii) For MOCBA adopting LDP to select the Pareto set, we propose a simple sequential selection procedure, i.e., MOCBA-B, and numerical results prove it to be promising.

Some elements remain to be studied further. MOCBA-B uses sample means to estimate the lower bound of PFS decay rate. However, this may not lead to the most efficient budget allocation and the optimal statistics should be found in the future. Additionally, the consistency and the convergence rate of MOCBA-B remain to be developed further.

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