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# EFFICIENT MULTI-FIDELITY SIMULATION OPTIMIZATION

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## ABSTRACT

Simulation models of different fidelity levels are often available for a complex system. High-fidelity simulations are accurate but time-consuming. Therefore, they can only be applied to a small number of solutions. Low-fidelity simulations are faster and can evaluate a large number of solutions. But their results may contain significant bias and variability. We propose an Multi-fidelity Optimization with Ordinal Transformation and Optimal Sampling (MO$^2$TOS) framework to exploit the benefits of high- and low-fidelity simulations to efficiently identify a (near) optimal solution. MO2TOS uses low-fidelity simulations for all solutions and then assigns a fixed budget of high-fidelity simulations to solutions based on low-fidelity simulation results. We show the benefits of MO$^2$TOS via theoretical analysis and numerical experiments with deterministic simulations and stochastic simulations where noise is negligible with sufficient replications. We compare MO$^2$TOS to Equal Allocation (EA) and Optimal Computing Budget Allocation (OCBA). MO$^2$TOS consistently outperforms both EA and OCBA.

## 1 INTRODUCTION

Simulation models have been increasingly used to find optimal or near optimal solutions for complex systems that are intractable to traditional analytical methods. Examples include finding the optimal production schedule in a manufacturing system via running a simulation model to estimate the performance (e.g., throughput) of alternative production plans (Hsieh, Chen, and Chang 2007; Li and Yu 2007; Rausch and Liao 2010; Schwartz, Wang, and Rivera 2006; Subulan and Cakmakci 2012; Villarreal et al. 2013). Such method is often referred to as simulation-based optimization or simply simulation optimization (Chen and Lee 2011; Lee et al. 2010). There are often multiple simulation models with different fidelity levels for the same system under study. High-fidelity simulation models can accurately predict the performance of a solution. But the simulation has high computation cost and can be very time-consuming. As a result, only a small number of candidate solutions can be evaluated via high-fidelity simulations in the simulation optimization process. Low-fidelity simulation models are much faster, but

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simulation results are much less reliable, possibly with significant bias and variability. In this paper, we propose a novel framework MO$^2$TOS (Multi-fidelity Optimization with Ordinal Transformation & Optimal Sampling) to effectively exploit the benefits of high- and low-fidelity simulations and improve the efficiency of simulation optimization.

While the actual *values* of low-fidelity simulations can be very different from the “true” values, i.e., significant biases may exist, “good” low-fidelity models can often correctly determine the relative order among solutions in terms of their performance. This is because many low-fidelity simulation models are built by some reasonable abstractions and simplifications of the underlying physical processes. The MO$^2$TOS framework builds on this property and employ an Ordinal Transformation (OT) approach to use low-fidelity simulations to estimate the relative orders of all solutions. Then the original decision space is transformed into a new one-dimensional space. To see the benefit of such a transformation, recall that the original solution space can be high-dimensional, have multiple locally optimal solutions spread far apart, and include a mix of continuous, discrete, and categorical variables. After OT, the new solution space is one-dimensional, display some trend (depending on how the transformation is done), and greatly simplifies further optimization using just a small number of high-fidelity simulations.

In this paper, we propose to partition solutions in the transformed space into groups based on their ranks in the transformed space. Compared to other ways of partitioning the original solution space, our approach can place solutions with similar performance into one group, which might be far apart from each other in the original solution space. As a result, the variability of solution quality within a group, which we refer to as *group variance* in the rest of the paper, can be reduced significantly. Furthermore, these groups are also more separable, i.e., the differences in quality between solutions in different groups tend to be larger than other partitioning schemes in the original solution space. We will measure this difference using the average performance of solutions in a group and refer to it as *group distance* in the following.

The MO$^2$TOS framework employs an Optimal Sampling (OS) approach to select solutions in the transformed one-dimensional space for evaluations using the high-fidelity model. The OS step is critical to the actual performance of MO$^2$TOS. This is because the bias in low-fidelity models is unknown and can be quite large. As a result, it is important to sample both broadly and efficiently. In this paper, we propose a sampling approach that works with the groups of solutions formed after the OT step. As we shall demonstrate later, because OT forms groups that have *smaller group variance* and *larger group distances*, the OS approach can work more efficiently than in the original solution space without OT.

There has been related work on the optimization of complex systems with multi-fidelity simulations. The Multi-Fidelity Sequential Kriging Optimization (MFSKO) procedure constructs kriging models to approximate the difference in simulation output between models of consecutive fidelity levels (Huang et al. 2006). MFSKO then sequentially determines the next solution to simulate and the level of fidelity for that simulation with an objective to maximize the expected improvement. The Value-based Global Optimization (VGO) procedure has a similar spirit, although there are some significant technical differences in how kriging models are used in determining the next solution to simulate and the fidelity level (Moore 2012). March and Willcox (2012) used a radial basis function (RBF) interpolation to create a surrogate model of the high-fidelity simulation model in the neighborhood of a trust region.

All these methods essentially create a surrogate model using an interpolation method (kriging, RBF, or polynomial) to correct the bias of the low-fidelity model and perform the optimization using the “corrected” low-fidelity model. While they have been shown to work reasonably well on a number of engineering design problems, the performance of these methods depends critically on the quality and applicability of the interpolation method. It is well known that interpolation methods such as kriging and RBF would require a large number of design points to perform well when the underlying response surface is highly nonlinear and multimodal, and/or the dimension of the solution space is high. In many complex system design problems, there are a mix of continuous, discrete, and categorical decision variables. This would present additional challenges to these interpolation methods.

In comparison, MO$^2$TOS is a very general and flexible framework and has the following important advantages: 1) MO$^2$TOS handle a mix of continuous (through discretization), discrete, and categorical decision variables in a high-dimensional solution space; 2) MO$^2$TOS is a general framework and is not restricted to any specific interpolation technique such as kriging; and 3) MO$^2$TOS is amenable to different implementations that offer useful tradeoffs between performance and ease-of-use.

The rest of the paper is organized as follows. In Section 2, we illustrate the principles and benefits of MO$^2$TOS using a machine application example in the context of semiconductor manufacturing. In Section 3, we present a mathematical model and analysis to show the benefits of OT and derive a specific OS strategy. We also present a simulation optimization algorithm under the general MO$^2$TOS framework in Section 3. Section 4 presents preliminary numerical results. We conclude the paper and point out future research directions in Section 5.

## 2 AN ILLUSTRATIVE EXAMPLE

We use a flexible semiconductor manufacturing system as an example to illustrate the basic principles and potential benefits of MO$^2$TOS. There are two types of products and five work stations. Each product type has a processing sequence and needs to re-enter some work stations multiple times. Each station has multiple machines. Inter-arrival and service times are all independent, identical, and normally distributed (truncated between zero and infinity). Figure 1 shows the flow of jobs through this manufacturing system. When more than one type of products are waiting for the same machine, product 1 has higher priority over product 2. The machine can perform serial batches with two same products to save the setup time. The re-entrant process flow and the non-exponential inter-arrival and service times make simulation necessary. We need to determine the number of machines in each machine group. The objective is to minimize the average production time. The total number of machines in the system is 37 and the number of machines in each work station must be between 5 and 10. So the optimization problem has five integer decision variables and a total of 780 feasible solutions.

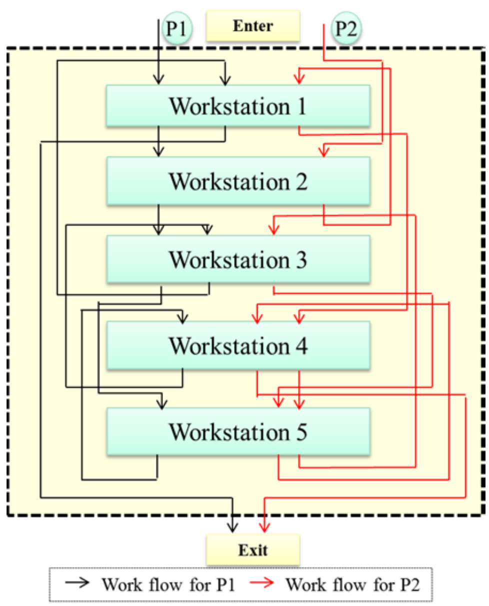


Figure 1: A reentrant semiconductor manufacturing system with two product types.

A high-fidelity model is a discrete-event simulation model that fully captures the reentrant and batching aspects of the system. One possible low-fidelity simulation model can be obtained by assuming that all inter-arrival and service times are exponentially distributed and estimating the average production time using M/M/c equations. Obviously, computing these closed-form equations are faster. But the simplification may lead to significant bias in final results. We use the M/M/c queuing equations as the low-fidelity model to estimate the production time for all 780 alternative solutions. We run a large number of simulations to obtain very reliable estimates of the performance of a solution according to the high-fidelity model.

In Figure 2(a), we plot high-fidelity model results. Because this is a 5-dimensional problem, we cannot draw the results in the original 5-dimensional space. Instead, we indexed solutions based on their positions in the original space and then placed them on one axis using the indices. This represents *one* possible way to partition the original solution space. We then show in Figure 2(b) both the low- fidelity (the blue curve above) and the high-fidelity (the red curve below) simulation estimates of all 780 solutions after OT. The horizontal axis gives the rank of a solution as determined by the low-fidelity model. The left side represents solutions that are ranked to be better.

From Figure 2, it is quite remarkable that despite the big bias in low-fidelity results, the relative order among solutions is actually quite accurate, which is shown by the roughly monotonic trend in the high-fidelity model result curve. Figure 2 also compares the drastically different groups that could be formed. It is quite obvious that we can partition solutions in Figure 2(b) into three groups, as shown in the figure. Solutions within the left and the middle groups have quite similar performance and thus these two groups have quite small group variance. While the right group shows substantial variability, it is less a problem because these three groups have large group distances and we can safely sample within the left and middle groups to search for the optimal solution. In comparison, the partition in Figure 2(a) would only lead to groups with high group variance and very small group distances. Therefore,  a sampling strategy would have to keep sampling from all three groups.

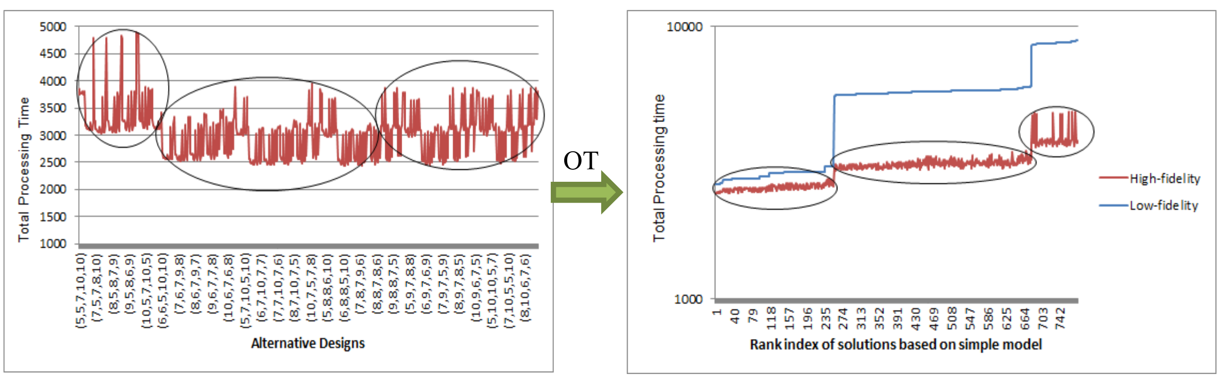


Figure 2: (a) left: High-fidelity simulation results plotted in the original solution space;  and (b) right: Low- and high-fidelity simulation results after OT.

For this particular example, the low-fidelity model results agree very well with the high-fidelity results in terms of ordinal ranking and thus the partition based on the low-fidelity results turns out to be a very good one. Based on this partition, one may be tempted to conclude that the middle and right groups can be thrown away and sampling should only focus on the left group. In general, we would not know *a priori* whether the partition based on low-fidelity model results alone is good or not. Therefore, it is important to design an OS strategy that focuses on more promising groups and at the same time also sample other groups to avoid being misled by the unknown bias in the low-fidelity model.

We summarize the key observations in this illustrative example below:

- OT allows us to partition solutions into groups with small group variances and large group distances, which is very difficult to achieve with any partitioning scheme in the original solution space;
- The small group variances and large group distances allow an OS strategy to efficiently search for the optimal solution.

## 3 MATHEMATICAL MODEL, ANALYSIS, AND ALGORITHM

In this section, we use a mathematical model to analyze MO$^2$TOS and show its benefits in terms of reduced group variances and enlarged group distances in a rigorous manner. We also propose a practical two-stage algorithm as a specific implementation of MO$^2$TOS.

### 3.1 Ordinal Transformation

Without loss of generality, we work on a minimization problem. We first introduce our notations below

- $X$: an alternative solution;
- $N$: the total number of feasible solutions;
- $g(X)$ / $f(X)$: the result of the low-fidelity/high-fidelity simulation model evaluated at solution $X$. In this paper, we restrict our attention to deterministic cases and will study stochastic simulation models in our future work
- $\delta(X)$: the bias of the low-fidelity model at solution $X$

We thus have the following equation:

$$f(X) = g(X) + \delta(X) \tag{1}$$

The quality of the low-fidelity model has a major impact on the performance of MO$^2$TOS. We propose to measure the quality of a low-fidelity model by $\rho$, the correlation between $g(X)$ and $f(X)$. We make the following assumptions on $g(X)$, $f(X)$, and $\delta(X)$.

**Assumption 1** *$f(X_i)$'s, $i=1,2,\ldots,N$, are N i.i.d realizations of a random variable with finite variance $c^2$; $g(X_i)$'s, $i=1,2,\ldots,N$, are N i.i.d realizations of a uniformly distributed random variable; for each solution $X_i$, $g(X_i)$ and $\delta(X_i)$ are independent.*

Notice that the independence of $g(X_i)$ and $\delta(X_i)$ means that the bias in the low-fidelity model is independent of solution $X_i$. For simplicity, we consider equal group size in this paper and assume we form $k$ groups each containing $n$ solutions (for simplicity, we assume $N$ is divisible by $k$). So the total number of solutions is $N=kn$. As a benchmark, we form equal-size groups in the original solution space by random sampling. In comparison, with the OT procedure in the MO$^2$TOS framework, we rank all solutions using the low-fidelity model. The solution deemed to be the best by the low-fidelity model receives a rank of 1 and the worst receives a rank of $N$. We then partition solutions into equal size groups based on their ranks. For example, if $n$=100, then the first group includes solutions with ranks 1 to 100, and the second group includes solutions with ranks 101 to 200, etc. We want to point out this is an *equal-quantile* (of $g(X)$) partitioning strategy. We use $\bar{f}_j$ to denote the group mean of group $j$

$$\bar{f}_j = \frac{1}{n}\sum_{i=(j-1)n+1}^{jn} f(X_i).$$

We then define the group variance of group $j$ as

$$\sigma_j^2 = E\left[\frac{1}{n-1}\sum_{i=(j-1)n+1}^{jn}\left(f(X_i) - \bar{f}_j\right)^2\right]. \tag{2}$$

When the group is formed by i.i.d. sampling $n$ solutions from the original space, group variance is simply the variance of $f(X)$, which we will denote as $\mathrm{Var}(f(X)) = c^2$. Under Assumption 1, we have Theorem 1 on the reduction of group variance described in (2) after OT.

**Theorem 1**: *Under equal-size grouping, the group variances after OT are smaller than that of random sampling from the original solution space when k⩾3 and n⩾3.*

*Proof*: Due to space constraint, please see Xu et al. (2014).

We next examine the benefit of OT in terms of increased group distance $\delta_{j_1,j_2}$ between two neighboring groups after OT. We first formally define group distance as the difference between the expected value of the group mean performance

$$\delta_{j_1,j_2} = \left| E\left[\frac{1}{n}\sum_{i=(j_1-1)n+1}^{j_1 n} f(X_i)\right] - E\left[\frac{1}{n}\sum_{i=(j_2-1)n+1}^{j_2 n} f(X_i)\right]\right|. \tag{3}$$

We have Theorem 2 on the increased group distance between any two groups after OT.

**Theorem 2**: *Under equal-size grouping, the magnitude of group distance after OT is larger than that of random sampling from the original solution space.*

*Proof*: Due to space constraint, please see Xu et al. (2014).

We plot the percentage of group variance reduction and the increase in group distance after OT as a function of $\rho$ for $n$=5, $k$=5 in Figure 3. The parameter $c$ is set to 1.

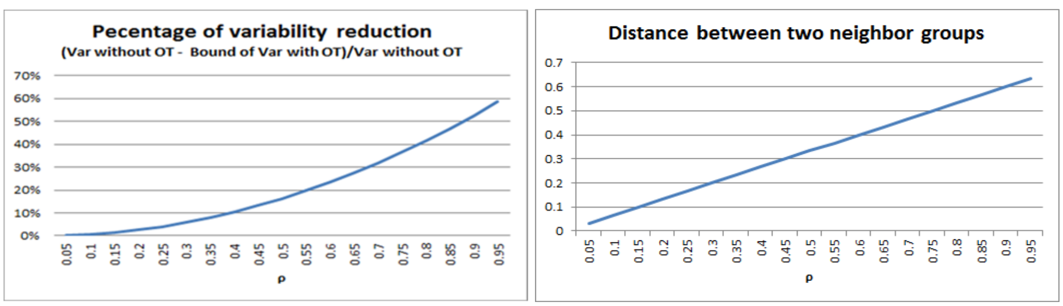


Figure 3: (a) left: Percentage of group variance reduction through OT; (b) right: Group distance between two neighboring groups.

## 3.2 Optimal Sampling

It is not advisable to only use high-fidelity models to evaluate "top" solutions, or the "best" group according to the low-fidelity model after OT. The reason is the unknown and potentially significant bias in low-fidelity model. Therefore, it is important to balance using high-fidelity models to closely examine groups of solutions that appear to be good according to the low-fidelity model, and to broadly explore groups of solutions that appear to be not as attractive. The partitioning of solutions into groups after OT has the benefits of reducing group variance and increasing group distances. These two benefits make it possible to design an efficient OS strategy that intelligently maintains such balance and improves the efficiency of $MO^2TOS$.

We have the following theorem on the OS to select the best group (i.e., with the best average group performance). We assume that the distribution of $f(X)$ within a group can be approximated by a normal distribution with an unknown but constant group mean and variance. The goal is to design an OS strategy that optimally allocates the sampling efforts using the high-fidelity model among the groups to maximize the probability of correctly selecting the best group, i.e, the group with the largest group mean.

In this paper, we propose to use an OS strategy based on the Optimal Computing Budget Allocation (OCBA) (Chen et al. 2000; Chen et al. 2014; Yan, Zhou, and Chen 2012). We state the result in Theorem 3. The proof of this theorem can be easily adapted from the theorem.

**Theorem 3**: *Assume f(X)*'s are *independent and normally distributed for all X in a group. Let b be the index for the group of solution with the best group mean thus far. Let $N_j$ be the number of high-fidelity evaluations allocated to group j, j=1,2,…,k. An approximation of the probability of correctly selecting the best group, i.e., the group distance is asymptotically maximized when*

$$\frac{N_l}{N_j} = \left( \frac{\delta_{b,j} / \sigma_j}{\delta_{b,l} / \sigma_l} \right)^2 \text{, where } j \neq l \neq b \text{, and } N_b = \sigma_b \sqrt{\sum_{l=1, l \neq b}^{k} \frac{N_l^2}{\sigma_l^2}} \text{ .} \tag{6}$$

From Theorem 3, we see that the larger the group distance between group $l$ and the current observed best group $b$, the smaller the number of high-fidelity evaluations allocated to group $l$. This is reasonable as such a group is unlikely to contain better solutions. However, if the group variance $\sigma_l^2$ is larger, group $j$ should also receive more high-fidelity evaluations because there is more uncertainty about the performance of the solution in this group.

Equation (6) also illustrates the benefit of the OT step. Compared to using the same OS prior to OT, OT typically reduces group variances $\sigma_j^2$ and increases group distances $\delta_{b,i}$. As a result, more computing budget would be spent on exploring more promising groups rather than reducing uncertainty in each group. It is reasonable to expect that the OS strategy will be able to work more efficiently and lead to even more savings in computing budget.

### 3.3 The MO$^2$TOS Algorithm

We present a specific implementation of the MO$^2$TOS framework in this section. The total budget for high-fidelity simulation is fixed and given *a priori*. Because we do not know $\sigma_j^2$ and $\delta_{b,i}$ in practice, we propose to equally allocate $n_0$ high-fidelity evaluations to all groups at the end of the OT step to obtain initial estimates of $\sigma_j^2$ and $\delta_{b,j}$ in the OS step. Then for the remaining computing budget, we plug in the estimates of $\sigma_j^2$ and $\delta_{b,j}$ into (9) to determine the number of high-fidelity samples for each group. We then randomly sample without replacement from each group for high-fidelity simulations.

Because the initial estimates based on $n_0$ high-fidelity evaluations can be quite unreliable, this process can be refined into an iterative process. Each iteration only assigns a fixed number of high-fidelity evaluations, denoted as $\Delta T$, based on the allocation rule in (6) and the estimates of $\sigma_j^2$ and $\delta_{b,i}$ at that iteration. The algorithm iterates until all computing budget has been used. The flowchart of the algorithm is given in Figure 4.

## 4 NUMERICAL EXPERIMENTS

We present preliminary experiments of the MO$^2$TOS Algorithm in this section. In the following experiments, the initial sample size for both OCBA and MO$^2$TOS is set to $n_0$=2. All experiment results are based on 10,000 IID replications and the average results are plotted. In each replication, we follow the same steps but when we randomly sample solutions from a group for high-fidelity evaluations, we use independent random number streams.

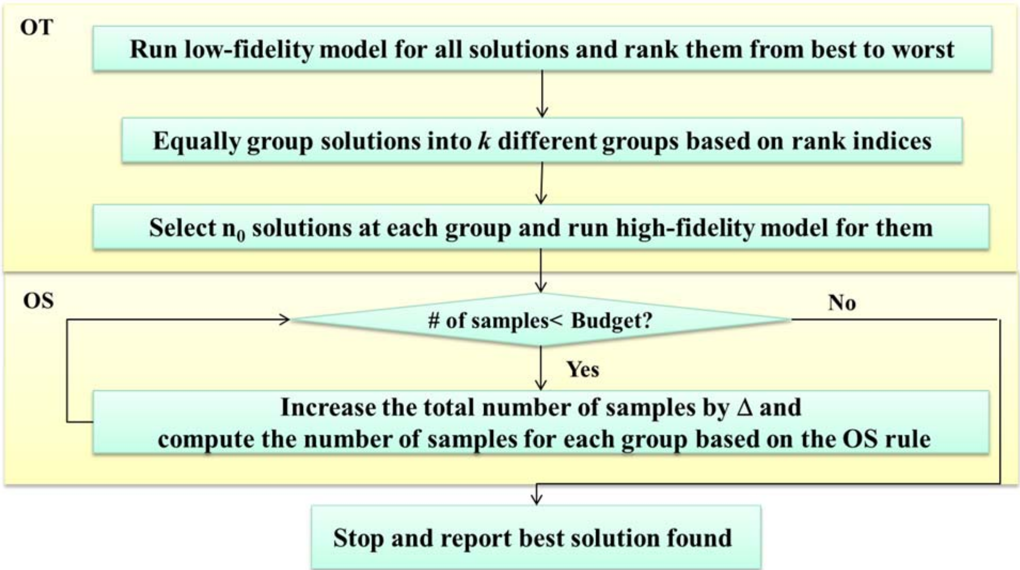


Figure 4: Flowchart of the MO$^2$TOS algorithm.

The first example is the machine allocation problem described in Section 2. We consider three different approaches to find the best solution in this simulation optimization problem. This problem requires running stochastic simulations on a solution when high-fidelity evaluation is needed. As explained in Section 2, we do not study how to optimally determine the number of stochastic simulation replications in this paper. Instead, we assume that each high-fidelity evaluation involves a sufficiently large number of simulation replications to deliver a very accurate result. Sampling within each group is random sampling without replacement. In all of experiments, we only examine the performance of the algorithms for a relatively small total computing budget. So we never exhaustively sample a group with the high-fidelity model. This represents the realistic situation where high-fidelity models are extremely time-consuming to run and thus only a small fraction of solutions can be evaluated.

We compare three procedures in the experiment. The first procedure is equal allocation. We first partition solutions into equal-sized groups based on the positions of these solutions in the original 5-dimensional space. We then equally allocate high-fidelity samples to all groups. While different partitions would lead to different results, we would not know *a priori* which partitioning would give the best result. So our experiment represents one typical run of such an equal allocation procedure on the original solution space. The second procedure is using OCBA procedure on the groups of solutions formed on the original solution space. The partitioning is the same as in the equal allocation case. We will see the benefit of using an OS strategy by comparing results of this procedure to the equal allocation case. Finally, we report MO$^2$TOS results, which show the benefit of using an OS strategy after OT.

Figure 5 plots the performance of the best solution found by these three procedures as a function of total computing budge. We partition the 780 solutions into 10 groups with 78 solutions in each group. We notice that OCBA achieves significant savings compared to equal allocation. The experiment confirms that MO$^2$TOS achieves further savings in computing budget on the machine allocation problem. For example, in order to find a solution with a production time of 2450, OCBA needed about 75 high-fidelity simulations. In comparison, MO$^2$TOS only used about 65 high-fidelity simulations, representing a 13% savings in computing budget. This benefit comes from using OT with the low-fidelity model to partition solutions into groups that have lower group variances and larger group distances.

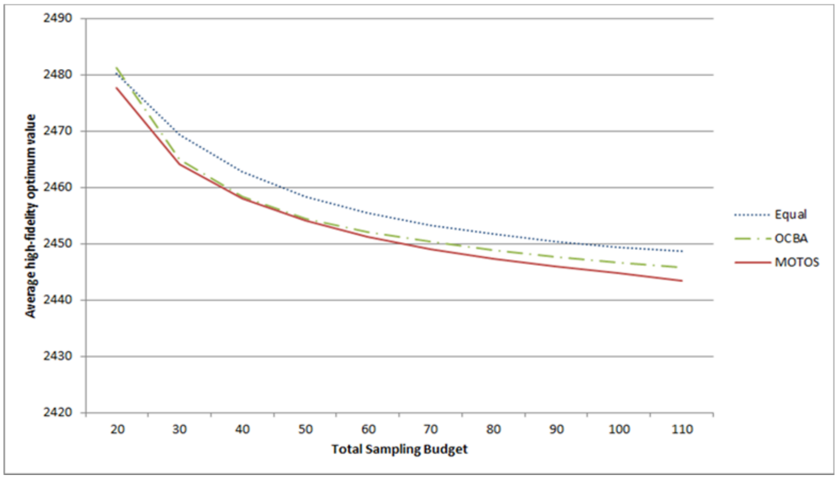


Figure 5: Results of the machine allocation optimization problem.

We test MO²TOS on another test problem, which is a maximization of a one-dimensional multimodal function given by

$$f(x)=\frac{\sin^6(0.09\pi x)}{2^{2\left(\frac{x-10}{80}\right)^2}}+0.1\cos(0.5\pi x)+0.5\left(\frac{x-40}{60}\right)^2+0.4\sin\left(\frac{x-25}{100}\pi\right).$$

We use a low-fidelity function

$$g(x)=\frac{\sin^6(0.09\pi(x-1.2))}{2^{2\left(\frac{x-10}{80}\right)^2}}.$$

Note that the low-fidelity function is adapted from a test function in simulation optimization literature (Xu et al. 2013). The maximum value of this function is 1.4277. We discretize the solution space by a grid of 0.1resulting in 1000 solutions. We form 10 groups, each with 100 solutions. We plot the high-

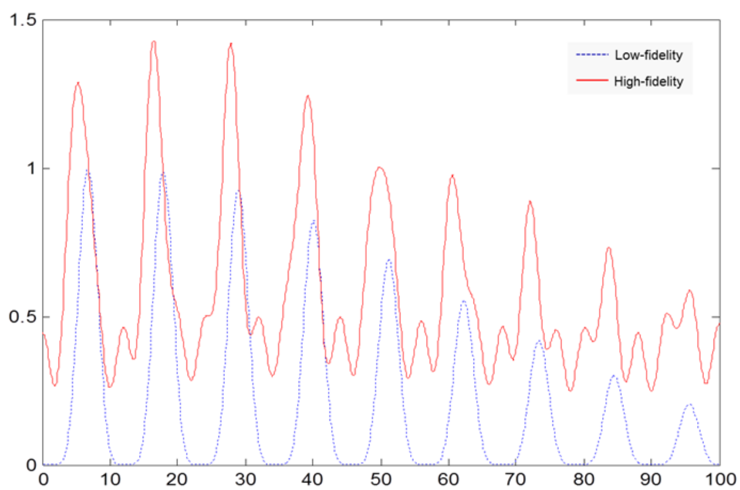


Figure 6: The high-fidelity and low-fidelity functions of the multi-modal test problem.

fidelity and low-fidelity function in Figure 6, which shows that the low-fidelity function only provides a fair approximation to the high-fidelity function, and has significant bias in the entire solution. Specially, the location of global and local optimal solutions are quite different. But as we see from Figure 7, $MO^2TOS$ was still able to achieve quite substantial savings in computing budget compared to OCBA.

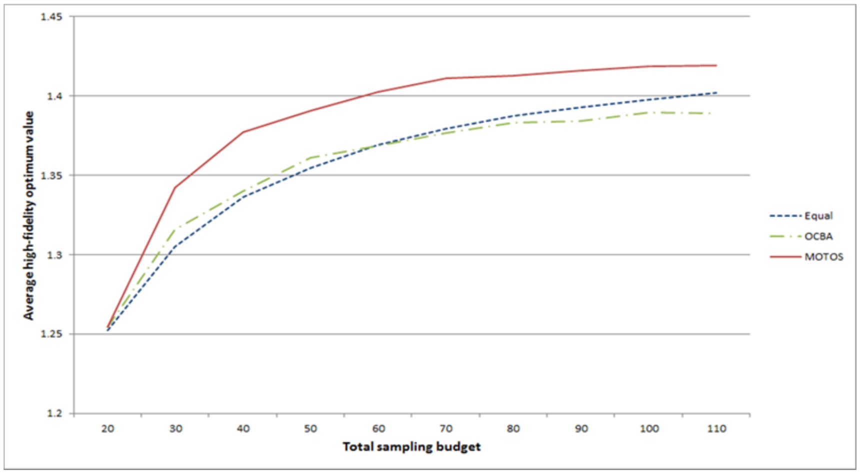


Figure 7: Results of the multi-modal test function.

## 5 CONCLUSIONS AND FUTURE RESEARCH

In this paper, we report a novel framework for multi-fidelity optimization. The new $MO^2TOS$ framework provides a flexible, effective, and easy to implement approach to exploit simulation models of different fidelity levels. Instead of directly modeling the bias as most existing approaches do, the proposed $MO^2TOS$ framework takes on a drastically different approach and instead uses the lower-fidelity model to find information on the relative orders of feasible solutions. That ordinal information is then used to transform the original solution space, which may be high-dimensional and highly nonlinear and multimodal, into a one-dimensional and much better behaved solution space. We show through a rigorous theoretical analysis how groups formed after OT have reduced group variances and enlarged group distances. These features facilitate the adoption of an OS strategy and enhanced its efficiency. We conduct numerical experiments comparing $MO^2TOS$ to equal allocation and OCBA on a multi-model function (deterministic) and a realistic machine allocation problem (stochastic but noise reduced to negligible levels with a large number of replications). Results demonstrate how $MO^2TOS$ can be applied in practice.

The proposed $MO^2TOS$ framework is very general and flexible and opens up a new research avenue. While this study is preliminary, it points out to many future research directions that may provide a solid theoretical and algorithmic foundation for successful $MO^2TOS$-based optimization algorithms. We highlight the following key questions that need to be further explored:

1. When there are multiple lower-fidelity models, how should we measure the quality of these models and choose which model(s) to use and how to combine their predictions when performing OT?
2. When lower-fidelity models' computing cost is not negligible, how should we optimally allocate computing budget among different models?
3. When stochastic simulation noise is present (i.e., reducing noise to negligible levels for all solutions is not possible due to limit on simulation budget), how should we optimally allocate computing budget among different models and design points?

## ACKNOWLEDGMENTS

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