V-SHAPED SAMPLING BASED ON KENDALL-DISTANCE TO ENHANCE OPTIMIZATION WITH RANKS

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ABSTRACT

In the area of discrete optimization via simulation (DOvS), optimization over rank values has been of concern in computer science and, more recently, in multi-fidelity simulation optimization. Specifically, Chen et al. (2015) proposes the concept of Ordinal Transformation to translate multi-dimensional discrete optimization problems into single-dimensional problems which are simpler, and the transformed solution space is referred as *ordinal space*. In this paper, we build on the idea of ordinal transformation and its properties in order to derive an efficient sampling algorithm for identifying the solution with the best rank in the setting of multi-fidelity optimization. We refer to this algorithm as V-shaped and we use the concept of Kendall distance adopted in the machine learning theory, in order to characterize solutions in the OT space. The algorithm is presented for the first time and preliminary performance results are provided comparing the algorithm with the sampling proposed in Chen et al. (2015).

1 INTRODUCTION

Recently, multi-fidelity simulation and simulation-optimization have become a primary research area in industrial engineering and they encompass several engineering domains. In this setting, we want to identify the best solution for a discrete deterministic optimization problem where a high fidelity simulation model is available to measure the exact deterministic response. However, we can only run few high fidelity simulations whereas a low fidelity simulator can be run for *every* solution in the feasible space. We want to use high fidelity to guide the search for the optimal solution when each candidate solution is characterized by its low fidelity value.

The basic motivation behind this problem statement is that there often are multiple simulation models with different accuracy levels (referred to as fidelity). All the simulation models serve to represent the same system, but they differ in the accuracy of the estimated response as well as the computational effort

required to run them. In fact, it can be argued that the larger the accuracy the more expensive will be the simulator in terms of time taken to simulate a single replication. On the contrary, low fidelity models may be as simple as returning a function value, but may have associated a large bias.

Chen et al. (2015) developed for the first time a framework for simulation optimization of this nature, namely, Ordinal Transformation (OT). In this framework, the low-fidelity model is used to rank the solutions. Once the ranking has been performed, the original design space is replaced by the rank and referred to as the *ordinal space* (from which the OT terms). Compared to the original design space, which can be highly nonlinear, high-dimensional, and includes a mix of discrete and categorical decision variables, the ordinal space is one-dimensional and often exhibits a global trend. Such a structural property significantly increases the efficiency of subsequent optimization processes.

In the OT perspective adopted by this paper, a general discrete event optimization problem is transformed into a rank–based optimization, where a complete rank is provided by the low fidelity model, even if subject to bias, while the high fidelity simulation returns an exact, but partial rank. In learning and computer science, this problem has been intensively studied in the scope of the realization of recommendation systems (Sun et al. 2012). Nevertheless, recommendation systems target to learn the rank based on features provided by the user and there is no issue concerned with the identification of the rank-1 solution. The well-developed theory in this field can be adopted to formalize the concept of likelihood of a certain low fidelity rank when high fidelity information is available.

This paper makes use of the OT framework and uses concepts from ranking in recommendation systems in order to assign a different score to each solution to be sampled. Such score is used to perform an approximation of the function (high fidelity vs. low fidelity) building upon the fact that such a function has a unique minimum (only one rank–1 solution exists). Similarly in spirit to a quadratic approximation in the continuous space, we propose a V-shape approximation in the ordinal space and we do it with the purpose to associate each candidate sampled point a score which is subsequently used for sampling purposes.

The remainder of the paper is structured as follows: Section 2 summarizes the key literature at the foundation of this manuscript. The methodology is presented in Section 3. Preliminary results are presented in Section 4. Section 5 closes the paper.

2 LITERATURE REVIEW

The basic idea of OT is to order designs using a fast low fidelity model and transform the decision space into a one-dimensional ordinal space with better structural properties.

In Xu et al. (2014b), Xu et al. (2014a), OT was applied to a resource allocation problem in a flexible manufacturing system with an objective to maximize system resilience as measured by steady-state cycle time (smaller is better) under demand disruptions and machine failures. There are two types of products and five workstations. Each product type has a processing sequence and needs to re-enter some workstations multiple times. Each station has multiple machines. Inter-arrival and service times are all independent, identical, and normally distributed (truncated between zero and infinity).

In the example used by the authors, the machine can perform serial batches with two same products to save the setup time. The re-entrant process flow and the nonexponential 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 workstation must be between 5 and 10. So the optimization problem has five integer decision variables and a total of 780 feasible solutions.

The original decision space is 5-dimensional with multiple local optima and thus is difficult to search directly. In Xu et al. (2014b), Xu et al. (2014a), the authors propose the use of a low-fidelity model based on Jackson network analysis to estimate cycle times. Once the low fidelity evaluation has been performed, the candidate solutions can be ordered by their rankings according to the low-fidelity model. Each solution is now associated with a positional value, its low fidelity rank.

Now, we can look at the low fidelity rank as a complete rank characterized by uncertainty, whereas the high fidelity evaluations provide an exact, although partial rank. In light of this, we can see the OT framework as the attempt to translate the traditional discrete optimization problem of finding the solution associated with the best value of the objective function to the problem of searching the most likely rank–1 solution, where the likelihood needs to be rigorously defined in the OT space. In order to do so, we propose the use of rank-based distance, in particular, we proposed a modified Kendall-*tau* measure (Sun et al. 2012).

The estimation of distances and density functions over ranks has received an important attention in the field of *recommendation systems* (Breese et al. 1998; Pennock et al. 2000; Heckerman et al. 2001; Sarwar et al. 2001; Marlin 2003; Hofmann (2004)). Data in recommendation systems are collections of incomplete tied preferences across n items that are associated with m different users. Given an incomplete tied preference associated with an additional m + 1-th user, the system recommends unobserved items to that user on the basis of the preference relations of the m + 1 users. Currently deployed recommendation systems include book recommendations at amazon.com, movie recommendation systems (that recommend to users items that are truly preferred over other items) is important for assisting users as well as increasing business profitability. It is an important topic of on-going research in machine learning and data mining. In the concern of this paper, the literature on recommendation systems provide a very rigorous way to define the *distance* among ranks and, consequently, the probability associated with a particular rank.

In this paper, we have to solve a slightly simpler problem with respect to the traditional recommendation system in that we want to provide the best solution and not the entire rank. Nevertheless, the proposed approach uses definitions from recommendation systems in order to guide the sampling in the OT framework. The next section will show the methodology with more detail.

3 METHODOLOGY

As stated in the introduction, we want to solve a discrete deterministic optimization problem. In this context, let Θ indicate the set of all candidate solutions. A low fidelity model is available which can generate in a very low computational time the response for each $\mathbf{x} \in \Theta$. The low fidelity estimate is biased and noisy. We can know the exact function value for each candidate point, $\mathbf{g}(\mathbf{x})$, running the high-fidelity simulation that, however, is computationally expensive and, therefore, cannot be performed for all the solutions. Whereas, a low fidelity value $\tilde{\mathbf{g}}(\mathbf{x})$ can be computed with a bias $\delta_{\mathbf{x}}$, i.e.,

$$\tilde{\mathbf{g}}(\mathbf{x}) = \mathbf{g}(\mathbf{x}) + \delta_{\mathbf{x}}.$$
(1)

The OT framework (Xu, Zhang, Huang, Chen, Lee, and Celik 2014a) suggests that $\tilde{\mathbf{g}}(\mathbf{x})$ are evaluated for all \mathbf{x} . Such low fidelity estimation is used to sample \mathbf{x} in the search procedure aiming at optimizing $\mathbf{g}(\mathbf{x})$. In this paper, we use $S_k \subseteq \Theta$ to represent the set of all sampled solutions at iteration k, and

$$l(\mathbf{x}), h(\mathbf{x}) \in \{1, \dots, |\Theta|\}, \forall \mathbf{x} \in \Theta$$
(2)

to denote the ranks associated to each candidate solution according to the low and high-fidelity simulation, respectively. Note that, the true value of $h(\mathbf{x})$ is unknown until $S_k = \Theta$, i.e., all the solutions have been sampled. Therefore, at the generic iteration k, we will only have a partial, but exact, rank being generated by the high fidelity evaluations, namely:

$$\hat{h}(\mathbf{x}) \in \{1, \dots, |S_k|\}, \forall \mathbf{x} \in S_k$$
(3)

that indicates the partial ranking among the sampled solutions according to the high-fidelity values.

Regardless of the nature of underlying optimization problems, e.g., single or multiple objectives, minimization or maximization, as long as the objective values at both fidelity models, i.e., \mathbf{g} and $\tilde{\mathbf{g}}$, can be

ranked in sequence, we can map our discrete optimization problem into a ranking problem, where we are interested in finding the solution associated with the lowest high fidelity rank, namely:

$$\mathbf{x}^* \in \operatorname*{arg\,min}_{\mathbf{x} \in \Theta} h\left(\mathbf{x}\right) \tag{4}$$

In this paper, we provide a sampling algorithm which efficiently addresses this problem by making use of the complete low fidelity rank $l(\mathbf{x}), \forall \mathbf{x} \in \Theta$ and the partial rank generated by the high fidelity simulations at the generic iteration k, i.e., $\hat{h}(\mathbf{x}), \forall \mathbf{x} \in S_k$.

The essentials of the OT framework is to transform a general multi-dimensional solution space into ordinal, so that difficulties induced by the original solution space, e.g., high-dimensional categorized decisions, bumpy response surface, can be avoided. However, in the transformed ordinal space, different optimal sampling schemes can be applied to identify the optimal solution in an efficient way.

In MO²TOS (Xu et al. 2014a; Huang et al. 2015; Chen et al. 2015) and MO-MO²TOS (Li et al. 2015), the solutions in the ordinal space is categorized into groups, and a group is sampled followed by an individual solution within the sampled group. It is believed that,

- after the ordinal transformation, the variation of high-fidelity values within group decreases and the difference between groups increases;
- however, it is not guaranteed that the best high-fidelity values occur with the best or the worst low-fidelity values. In fact, quite often, the optimal solution could occur in the middle of the ordinal space.

These ideas constitute the backbone within the OT framework. And we use them in order to propose our V-Shaped approximation of the high fidelity in the OT space in order to derive a likelihood of being rank–1 solution for all the un-sampled points.

Indeed, the proposed algorithm makes use of the OT framework and assumes that arranging all solutions according to their low-fidelity ranks, the plot of their high-fidelity ranks has a V-shape. Figure 1 represents an example where the dashed function is the assumed high fidelity rank conditional on the next sampling point x_{k+1} in the ordinal space of the low fidelity rank before any simulation is performed at that point. Using the results in (Xu et al. 2014a), we assume that this rank sequence in monotonically increasing due to the fact that close solutions in the low-fidelity space are supposed to be close in the high-fidelity space as well. Therefore, assuming that x_{k+1} will be the best solution, the right-hand side and left-hand side ranks will be a non-decreasing sequence of values.

In Figure 1, we report the V-shape generated corresponding to a generic point x_{k+1} in the low fidelity space, which has not been sampled yet. As suggested by the figure, the idea behind the V-shape approximation in the ordinal space is really simple: assuming that the point to sample is the true optimum, i.e., it has rank-1, then the high-fidelity ranks will form a monotonically increasing function on both sides.

In other words, the V-shape is a result of the conjecture that, if we assign high-fidelity rank $h(\mathbf{x}^*) = 1$ to the solution \mathbf{x}^* , then $h(\mathbf{x})$ will be monotonically increasing in the low fidelity rank on both left and right-hand side of the candidate solution.

It is apparent how the V-shape can be obtained only in case the low fidelity rank and the high fidelity correspond. Nevertheless, event when \mathbf{x}^* is unknown, and the high fidelity rank does not correspond to the low fidelity, we can still adopt the *V-Shape* concept to associate a score measure to each candidate solution, which we use to associate a sampling probability to each point.

In particular, this score is constructed using the Kendall- τ rank correlation coefficient, which quantifies the difference between two sequences (Sun et al. 2012). Specifically, the following holds:

Definition 1 If A and B are the two sequences of the same set of n elements $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, $a(\mathbf{x})$ is the index of \mathbf{x} in sequence A, and $b(\mathbf{x})$ is the index of \mathbf{x} in sequence B, the coefficient τ is defined as

$$\tau(A,B) = \frac{\sum_{i,j\in\{1,\dots,n\}, i\neq j} \left(\mathbbm{1}_{a(\mathbf{x}_i) < a(\mathbf{x}_j)} \cdot \mathbbm{1}_{b(\mathbf{x}_i) < b(\mathbf{x}_j)} - \mathbbm{1}_{a(\mathbf{x}_i) < a(\mathbf{x}_j)} \cdot \mathbbm{1}_{b(\mathbf{x}_i) > b(\mathbf{x}_j)}\right)}{n(n-1)/2}.$$
(5)

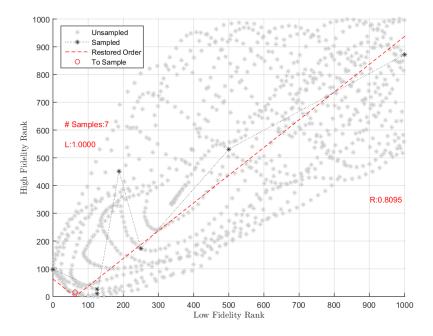


Figure 1: V-shape concept.

Note that, $\tau(A,B) \in [-1,1]$, in which $\tau(A,B) = 1$ implies *A*, *B* have exactly the same sequence, and $\tau(A,B) = -1$ implies that the sequences are completely reversed. Whereas, when $\tau(A,B) = 0$, we are in the most undecidable situation: in this case 50% of the components are in a consistent ordering and 50% are not. Differently, positive values of the distance reflect an agreement between the two sequences, whereas negative values reflect a predominant contradiction between the two sequences.

In the following, we use the Kendall- τ to measure the similarity between the order "predicted" by the slope 1 V-shape and the high fidelity ordering. In particular, due to the V-shape we compare two sequences (L,R), i.e., the sequence of V-shape ranks and high fidelity ranks on the left-hand side of the candidate solution, and the same sequence, but computed on the right-hand side of the candidate solution. In particular, the following definition applies:

Definition 2 For each candidate solution $\hat{\mathbf{x}}$ and the corresponding low fidelity rank \hat{l} , a V-shape having its vertex in $\hat{\mathbf{x}}$ and slope equal to 1 will automatically generate a left sequence, which we refer to as L and a right sequence, which we refer to as R. In particular, let l represent the low fidelity rank. Then a(l(x)) represents the rank constructed according to the V-shape. We can then create the two following rank sequences:

$$L_{A} = \{a(l(x))\} : \{\mathbf{x} \in S_{k} \mid l(x) < \hat{l}(x)\},$$
(6)

$$R_{A} = \{a(l(x))\} : \{\mathbf{x} \in S_{k} \mid l(x) > \hat{l}(x)\}.$$
(7)

Here, the set L_A is defined by all the *sampled* solutions having a low fidelity rank lower than the candidate sequenced in ascending order, while R_A is the set of solutions having rank larger than the candidate. We can define the two paired sequences in the high fidelity space by simply assigning to L_A and R_A the rank according to the high fidelity evaluation, i.e., assigning the index $h(l) \leftarrow \hat{h}(x) = q(l(x))$. Then

rank according to the high fidelity evaluation, i.e., assigning the index $b(l) \leftarrow \hat{h}(x) : l(x) = a(l(x))$. Then the following holds:

$$L_B = \left\{ b(l(x)) = \hat{h}(x) : l(x) = a(l(x)), a(l(x)) \in L_A \right\},$$
(8)

$$R_B = \left\{ b(l(x)) = \hat{h}(x) : l(x) = a(l(x)), a(l(x)) \in R_A \right\}.$$
(9)

We then construct the *two-sided* Kendall- τ indicator summing the L and R coefficient:

$$f_k(\hat{\mathbf{x}}) \leftarrow [\tau(R_A, R_B) - \tau(L_A, L_B)].$$
(10)

In the following, we make a numerical example to clarify the provided definitions. **Example** Let us define the following hold:

$$\mathbf{l} = [1, 2, 3, 4, 5, 6], \text{ with } \hat{l} = 4,$$

$$S_k = [1, 2, 3, 5, 6],$$

$$\mathbf{h} = [5, 3, 2, 1, 4].$$
(11)

Then we obtain the following sets:

$$L_A = [3, 2, 1],$$

 $R_A = [5, 6],$
 $L_B = [2, 3, 5],$
 $R_B = [1, 4].$

(12)

Figure 2 gives an example of the value of the distance over the OT space.

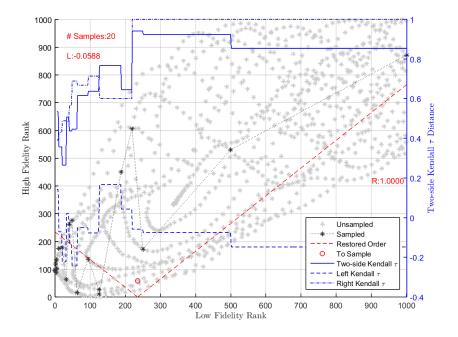


Figure 2: Example of V-shape and Kendall-Distance over the OT space.

3.1 The Algorithm

Firstly, we apply the Kendall Coefficient τ to measure the fitness of the *V*-Shape given any $\hat{\mathbf{x}} \in \Theta \setminus S_k$ as $f_k(\hat{\mathbf{x}})$, in iteration k. The procedure is described in Algorithm 1.

Algorithm 1: Measure Fitness of V-Shape, $f_k(\hat{\mathbf{x}})$
1 Construct L_A, L_B and R_A, R_B using definition 2;
2 Compute the Value of fitness function for the candidate $\hat{\mathbf{x}}$:
3 $f_k(\hat{\mathbf{x}}) \leftarrow [au(R_A,R_B) - au(L_A,L_B)]$

Algorithm 2: V-Shape Ordinal Restoration

1 $S_1 \leftarrow \{ \arg\min_{\mathbf{x}\in\Theta} l(\mathbf{x}), \arg\max_{\mathbf{x}\in\Theta} l(\mathbf{x}) \}, \text{ and } k \leftarrow 1;$ 2 while not stopped do 3 $C_k \leftarrow \{ \mathbf{x}\in\Theta\setminus S_k \mid f_k(\mathbf{x}) = \max_{\mathbf{x}'\in\Theta\setminus S_k} f_k(\mathbf{x}') \}, \text{ and sort } C_k \text{ according to } l(\mathbf{x});$ 4 $\hat{\mathbf{x}}_k \leftarrow C_k \left(\left\lceil \frac{|C_k|}{2} \right\rceil \right), S_{k+1} \leftarrow S_k \cup \{ \hat{\mathbf{x}}_k \}, \text{ and } k \leftarrow k+1;$ 5 end

The V-Shape approximation procedure is described in Algorithm 2. Note that, in the algorithm, C_k is the set of candidate solutions that have equally good fitness, $\hat{\mathbf{x}}_k$ is the solution sampled at iteration k.

An example of the historical sequence of the proposed algorithm is shown in Figure 3. In particular, the stars represent the sampled set, whereas the circle is the candidate with the maximum fitness value (equation (10)). As shown in the algorithm, this point minimizes the Kendall- τ distance between the ideal V-shape (represented by the dashed lines in the figure) and the partial rank defined by the high fidelity evaluations (black sampled points).

4 NUMERICAL EXPERIMENTS

In this section, we compare the developed algorithm with MO^2TOS using the benchmark problem proposed in Xu et al. (2015), which has the high fidelity function as

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

$$x \in \{0, 0.1, 0.2, \dots, 99.9, 100\}.$$
(13)

There alternative low-fidelity models were also proposed (Xu et al. 2015):

$$\tilde{g}_1(x) = \frac{\sin^6(0.09\pi x)}{2^{2((x-10)/80)^2}}, x \in \{0, 0.1, 0.2, \dots, 99.9, 100\}.$$
(14)

$$\tilde{g}_2(x) = \frac{\sin^6\left(0.09\pi(x-1.2)\right)}{2^{2((x-10)/80)^2}}, \ x \in \{0, 0.1, 0.2, \dots, 99.9, 100\}.$$
(15)

$$\tilde{g}_3(x) = \frac{\sin^6(0.09\pi(x-5))}{2^{2((x-10)/80)^2}}, x \in \{0, 0.1, 0.2, \dots, 99.9, 100\}.$$
(16)

Figures 4–6 compare the average performance in terms of achieved High Fidelity Value, resulting from 300 macro-replications, (OTVS uses one macro-replication since there is no random component in the algorithm iterates) with respect to the total budget used by the algorithms. MO^2TOS was implemented using a different number of groups (i.e., $k = \{2, 5, 10, 20\}$). In general, we observe that the proposed algorithm perform better than the original MO^2TOS , independently from the group size (that is a user-defined parameter) for low values of simulation budgets.

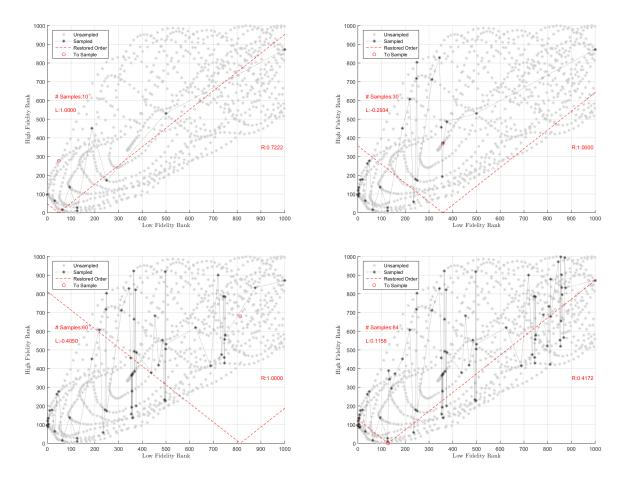


Figure 3: Example of OTVS iterates.

In particular, OTVS shows to be fast in identifying the promising area of solutions and then we observe that it requires more iterations to refine the solution and converge to the global optimum.

Nevertheless, OTVS advantage of not requiring the user to set any input parameter concerning the number of groups and the good performance reached by the algorithm compared to the original MO²TOS are very promising.

5 CONCLUSION

In this paper, building on the work on multi-fidelity optimization by Xu et al. (2014a), we inherit the Ordinal Transformation framework to construct an efficient algorithm that is able to look for the best solution only relying on low fidelity and high fidelity rank information.

In particular, we propose a V-shaped approach, which assigns a score to candidate solutions on the low-fidelity space, based on their "likelihood" to be rank-1 (i.e., best) solutions. Such a rank is constructed using the Kendall- τ distance concept inherited from ranking theory in machine learning algorithms for recommendation systems.

Thanks to this score, we are able to make a sampling decision which does not require to define groups of solutions in the low fidelity space as in the original algorithm proposed in Xu et al. (2014a). Numerical results show that the proposed approach has outperformed the original algorithm for low values of the budget and is consistently competitive as the budget increases.

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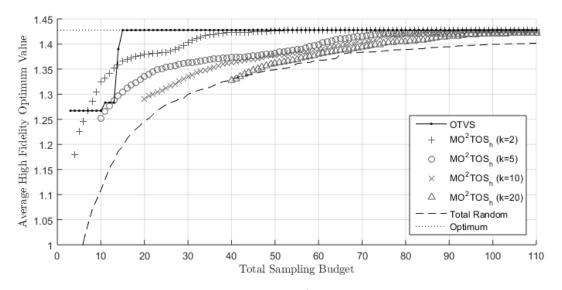


Figure 4: Compare OTVS and MO²TOS with different k on \tilde{g}_1 .

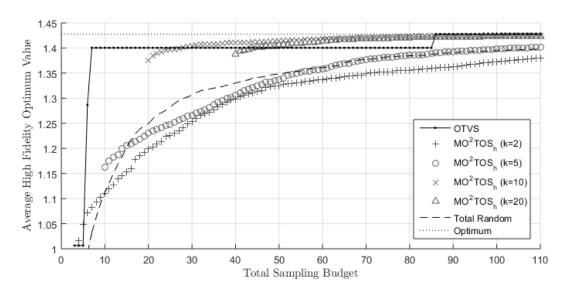


Figure 5: Compare OTVS and MO²TOS with different k on \tilde{g}_2 .

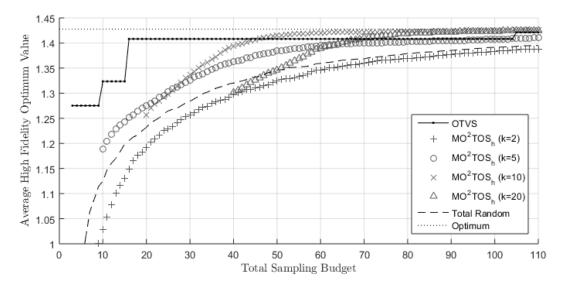


Figure 6: Compare OTVS and MO²TOS with different k on \tilde{g}_3 .

Future works will provide a rigorous foundation for the OTVS algorithm in term of convergent rate, and extend it to continuous optimization problems. In that case, consider that low-fidelity model cannot be run for all candidate solutions, we need to rethink and improve the framework of MO^2TOS .

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