2022 European Control Conference (ECC)
July 12-15, 2022. London, United Kingdom

Cost-aware Adaptive Sampling for Global Metamodeling Using Voronoi Tessellation

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Abstract— **Metamodeling has become a common approach to replace costly and time-consuming physical experiments or computer experiments (e.g., numerical simulation, training of AI models) by an easy-to-evaluate metamodel, which is trained on samples of the experiment. Since the choice of sample points significantly impacts model accuracy, these are in many cases determined using adaptive sampling methods. In addition, the cost of conducting an experiment often depends decisively on the choice of its parameters. However, only few strategies for selecting the sample points have been proposed, that take into account parameter-dependent costs. In this work, we introduce a novel Voronoi-based cost-aware adaptive sampling algorithm for global metamodeling that is independent of the choice of sampling strategy and metamodel. The method is evaluated on a variety of randomly generated black-box and cost functions, where it has shown to vastly outperform existing sampling strategies.**

I. Introduction

In many engineering applications, physical experiments (e.g., crash test [1], wind tunnel [2]), or computer experiments experiments (e.g., numerical simulations [3], training of AI models [4]) need to be carried out to gain insight into the process, understand the effects of the parameters in the design space on the system output, or to identify optimal parameters. These experiments are often expensive or time-consuming, making it impossible to evaluate a large number of parameter combinations in design space [5]. Global metamodeling tries to reduce the experimental costs by replacing the experiment with an easy-to-evaluate metamodel, that approximates the behavior of the original experiment based on a limited number of samples [6], [7].

However, the accuracy of the model depends decisively on the choice of points in the design space [8], [9]. Design of Experiments (DoE) generate points in the design space in such a way that the effects of parameter changes on the quantity to be modeled are reflected as precisely as possible [10].

One-shot approaches like fractional designs, latin hypercubes, and orthogonal arrays [7], [11], [12] try to achieve this by evenly covering the design space [11]. The advantage of these methods is their simplicity. Since, however, only information known before the first experiment can be considered for the choice of sample points [12], too many or too few samples might be taken [13], and it is not clear what needs to be done if the desired model accuracy after sampling is not sufficient [10].

*This work is supported by the German Federal Ministry of Education and Research (BMBF) within the ROBDEKON project and has been researched at the Karlsruhe Institut of Technology (KIT). westermann@kit.edu, lucas.alber@student.kit.edu.

In many cases, one-shot approaches are used to create a few points (initial design) as a basis for more sophisticated adaptive design approaches [10], [11], [14], which determine one or more new points per iteration based on the already existing samples. Thus, they also allow for a termination criterion (e.g., reaching a desired estimated model accuracy) and hence, a variable number of samples adapted to the specific setting.

All adaptive sampling methods (also called sequential designs [11] or active learning [12]) need to perform a trade-off between exploration and exploitation [7], [13], where exploitation increases the local model accuracy and exploration ensures that no relevant regions of the design space are omitted. Numerous distance-, variance-, gradient-, and cross-validation-based adaptive exploration and exploitation strategies have been researched [6].

Some of these methods construct Voronoi cells based on the existing samples and leverage the properties of Voronoi diagrams to select the next sample point. For instance, the vertices of the Voronoi cells are used to discretize a continuous objective function and thus serve as candidates for the next sample point [15]. In the CV-Voronoi approach [13], leave-one-out cross-validation is applied to existing samples where the sample furthest from the model is used for choosing the next sample. A Voronoi tessellation is constructed on all existing samples and the next sample is sequentially chosen as the furthest vertex of the associated Voronoi cell. The LOLA-Voronoi algorithm [11] estimates the local nonlinearity of the unknown function at each sample point. Just like in the CV-Voronoi method, the next sample point is then chosen to be the furthest vertex of the Voronoi cell corresponding to the largest estimated nonlinearity. The advantage of this method is its independence from the applied metamodel. In general, the performance of the respective algorithm depends on the characteristics of the black-box function [6]. However, it has been shown that CV-Voronoi outperforms LOLA-Voronoi for various black-box functions [13].

In many applications, sampling costs depend on the specific parameter combinations. Accordingly, in addition to the trade-off between exploration and exploitation, cost-aware adaptive sampling algorithms must trade off between two further competing goals: maximizing information about the black-box function and minimizing sampling costs.

For example, in the ROBDEKON project [16], expensive and time-consuming sampling of contaminated sites with subsequent laboratory evaluation have to be carried out in order to reconstruct the pollutant distribution in the soil. To ensure that the pollutants can be removed precisely, an accu-

rate metamodel is required. In addition, sample locations that are difficult to access (e.g., buildings, vegetation, slopes) are costly and time consuming to sample and should therefore be avoided.

For computer experiments, the simulation time and the energy demand represent costs that depend on the parameters of the experiment (e.g., varying regularization, learning rates, number of iterations or layer sizes in neural networks [4], [17]).

To the best of our knowledge, there is only one cost-aware sampling method for global metamodeling and few in the context of global optimization. Crombeq et al. consider the parameter-dependent cost of choosing the next sample point by dividing various variance- and distance-based criteria by the cost function [2]. Here, the cost function can be interpreted as the parameter-dependent scaling of the criterion. The same approach is also used in the context of Bayes Opimization (BO). There, the acquisition function Expected Improvement (EI) is divided by the cost function to obtain the Expected Improvement per unit (EIpu). For their method Cost Apportioned BO (CArBO), Lee et al. extend EIpu by cost-cooling, which decreases the influence of the cost function with the number of samples [4]. By dividing by the cost function, cost often has too great of an impact on the choice of the next sample point [2] and the criterion becomes numerically unstable for costs close to zero due to the inversion of the cost function.

All adaptive sampling methods are started with an initial design [7]. However, with conventional space-filling methods, some of the initial points may fall into expensive regions of the design space. To prevent this, Lee et al. propose a space-filling cost-effective initial design [4]. For this, the design space is discretized, the cost function is evaluated at all discrete points, and the results are stored in a data set. In each iteration of the algorithm, the most expensive point and the point closest to the existing sample points are then alternately removed from the data set until only one point remains. This is then used as the next sample point. The procedure is repeated while the accumulated sampling cost is below a given budget. In the first iteration the cheapest of the discrete points is used as next sample point, since there is no existing sample points yet.

This paper proposes a Voronoi-based cost-aware adaptive adaptive sampling algorithm for global metamodeling of expensive-to-evaluate black-box functions with parameter-dependent cost functions. The algorithm is independent of the applied metamodel or cell selection criterion and can thus be used for both generation of a cost-aware initial design using a space-filling criterion and cost-aware adaptive sampling using an exploitation-based criterion. Unlike the literature methods, the algorithm can handle any positive valued cost function including zero. We show that our method yields higher model accuracy for a given budget than the cost-effective initial design of CArBO and the adaptive design CV-Voronoi.

The paper is structured as follows: Sec. II provides a formal description of the considered problem. The general procedure of global metamodeling is presented in Sec. III. Sec. IV introduces our novel cost-aware adaptive sampling algorithm. Finally, we present our evaluation in Sec. V and conclusions in Sec. VI.

II. Problem Formulation

An (unknown) expensive-to-evaluate black-box function $f : \mathbb{R}^n \to \mathbb{R}$ is to be approximated by a metamodel $\hat{f}$ within the bounded set $\mathcal{X} \subset \mathbb{R}^n$ based on evaluations (samples) $y_l \in \mathbb{R}$ of f at points $\underline{x}_l \in \mathcal{X}$ for $1 \leq l \leq m$, where m is the number of existing samples, n is the number of design parameters, and $\mathcal{X}$ is the design space. The samples

$$y_l = f(\underline{x}_l) \tag{1}$$

are given by the value of the true function $f(\underline{x})$ at points $\underline{x}_l$. Furthermore, the sampling costs depend on the location $\underline{x}$ in the design space $\mathcal{X}$ and are given by the positive valued cost function $c_l : \mathbb{R}^n \to \mathbb{R}_0^+$. For a series of m sequential samples, the accumulated cost

$$c_{\text{cum}} = \sum_{l=1}^{m} c_l(\underline{x}_l) \tag{2}$$

can be calculated as the sum of costs per iteration.

The goal is to sequentially determine the sample points $\underline{x}_l$ such that, for a given budget c_{max}, the global error between the metamodel $\hat{f}$ and the black-box function f becomes minimal w.r.t. a given metric. Accordingly, the budget represents the upper bound for the accumulated costs $c_{\text{cum}} \leq c_{\text{max}}$.

III. Adaptive Sampling for Global Metamodeling

Adaptive sampling methods determine the next sample point based on the existing samples or metamodel. Since initially no information about the black-box function is available, a space-filling initial design $\mathcal{D}_0$ is created to evenly cover the design space $\mathcal{X}$. Then, until a termination criterion (e.g., maximum number of iterations, estimated model accuracy, available budget) is met, the following steps are repeated:

- the metamodel $\hat{f}$ is updated with the current data set $\mathcal{D}$
- the next sample point $\underline{x}_{m+1}$ is determined based on some criterion
- the black-box function f is evaluated at $\underline{x}_{m+1}$
- the new data $(\underline{x}_{m+1}, y_{m+1})$ is added to the data set $\mathcal{D}$.

An illustration of the described procedure is shown in Fig. 1.

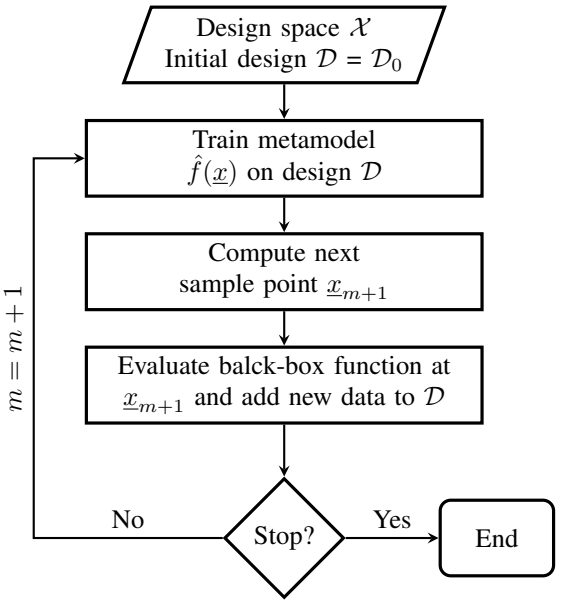


Fig. 1: General procedure for metamodeling using adaptive sampling, starting with a space-filling initial design.

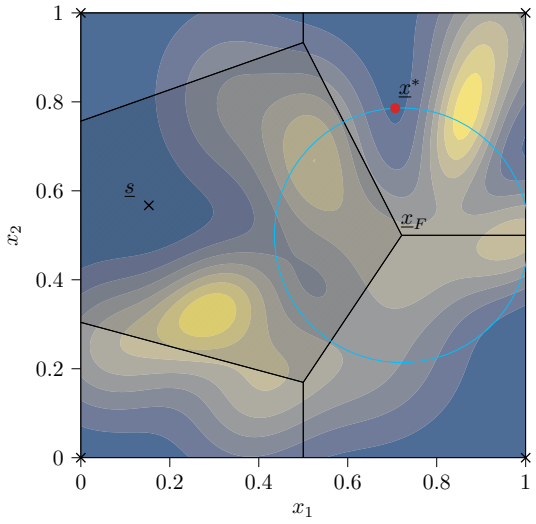


Fig. 2: Voronoi cells (black lines) and optimization region (blue circle) on top of the contour plot of the cost function. The shaded cell was selected by the cell selection criterion K_i. $\underline{s}$, $\underline{x}_F$ and $\underline{x}^*$ indicate the according sample point, furthest vertex and next sample point.

IV. Cost-aware Voronoi Sampling (CAV)

CAV is an adaptive sampling algorithm as illustrated in Fig. 1. It is warm-started with a non-empty initial data set $\mathcal{D}_0 = \{(\underline{x}_l, y_l)\}_{l=1}^{m_0}$, where m_0 is the number of initial samples. Accordingly, the cumulative costs $c_{\text{cum}} = c_0$ are initialized with the initial costs $c_0 = \sum_{l=1}^{m_0} c_l(\underline{x}_l)$ of the samples in $\mathcal{D}_0$. In each iteration i, a Voronoi tessellation (bounded on the design space $\mathcal{X}$) is constructed on the current data set $\mathcal{D}_i = \{(\underline{x}_l, y_l)\}_{l=1}^{m}$ containing the m existing samples. The Voronoi tessellation can either be computed exactly or, especially for higher dimensional design spaces, be approximated using a Monte Carlo approach [12]. This results in $\underline{v}_i$ and $\boldsymbol{F}_i$ containing volumes and furthest corners of each Voronoi cell j in iteration i. Note that the number of existing samples $m = m_0 + i$ equals the number of initial samples m_0 plus the iteration i. Using a cell selection criterion

$$K_i : \{1, \dots, m\} \to \mathbb{R} \tag{3}$$

a real value is assigned to each cell j based on the existing samples, Voronoi diagram, or metamodel. The cell

$$j^* = \arg\max_j \; K_i(j) \tag{4}$$

that has been assigned the highest value is then selected.

Conventional Voronoi-based adaptive sampling methods (e.g., CV-, LOLA-Voronoi) use the vertex $\underline{x}_{\text{F}} = \boldsymbol{F}[j^*]$ of the selected cell farthest from the associated sample point $\underline{s}$ as the next sample point. CAV, on the other hand, uses $\underline{x}_{\text{F}}$ as the starting point for a local optimization

$$\begin{aligned} &\underset{\underline{x} \in \mathcal{X}}{\text{minimize}} \; c(\underline{x}) \\ &\text{subject to } ||\underline{x} - \underline{x}_{\text{F}}|| < a \cdot ||\underline{s} - \underline{x}_{\text{F}}|| \end{aligned} \tag{5}$$

of the cost function within a hyper-ball around $\underline{x}_{\text{F}}$, whose radius can be set with a. The optimization result $\underline{x}^*$ is then used as the next sample point $\underline{x}_{m+1}$. As the number of samples increases, the expected distance between sample points decreases, so the optimization region also becomes smaller. Consequently, the influence of the cost function on the choice of the next sample point decreases with the distance between the samples and thus, on average, with the number of samples. This behavior is similar to the concept of cost-cooling, which is used for example in CArBO [4]. We found $a = 0.5$ to produce good results on 150 randomly generated black-box and cost function pairs and therefore suggest to use this value for application of the algorithm. Refer to Alg. 1 for the pseudocode of the described algorithm.

Algorithm 1 Cost-aware Voronoi Sampling (CAV)

Input: budget c_{max}, design space $\mathcal{X}$, initial cost function c_0, initial data set $\mathcal{D}_0 = \{(\underline{x}_l, y_l)\}_{l=1}^{m0}$
set $c_{\text{cum}} = \sum_{l=1}^{m_0} c_0(\underline{x}_l)$, $i = 0$, $m = m_0$
while $c_{\text{cum}} \leq c_{\text{max}}$ **do**
  $\underline{v}_i$, $\boldsymbol{F}_i \leftarrow$ Voronoi($\mathcal{D}_i$), $\underline{v}_i$: volumes, $\boldsymbol{F}_i$: furthest vertices
  select cell j^* according to (4) using criterion K_i
  compute next sample point $\underline{x}_{m+1}$ according to (5)
  $y_{m+1} \leftarrow f(\underline{x}_{m+1})$
  $\mathcal{D}_{i+1} \leftarrow \mathcal{D}_i \cup (\underline{x}_{m+1}, y_{m+1})$, $c_{\text{cum}} \leftarrow c_{\text{cum}} + c_i(\underline{x}_{m+1})$
  update metamodel and costfunction
  $i \leftarrow i + 1$, $m \leftarrow m + 1$
end while
Return: $\mathcal{D}_i$

Note that the proposed algorithm is independent of the metamodel, as long as the criterion K_i is model independent. The criterion K_i alone defines the dependencies on the metamodel or the type of metamodel. Moreover, the algorithm does not impose any condition on the cost function, except that it must not take negative values ($c_i : \mathbb{R}^n \to \mathbb{R}_0^+$). This applies to both given cost functions and cost models that are – in case of unknown cost functions – iteratively learned during the sampling procedure.

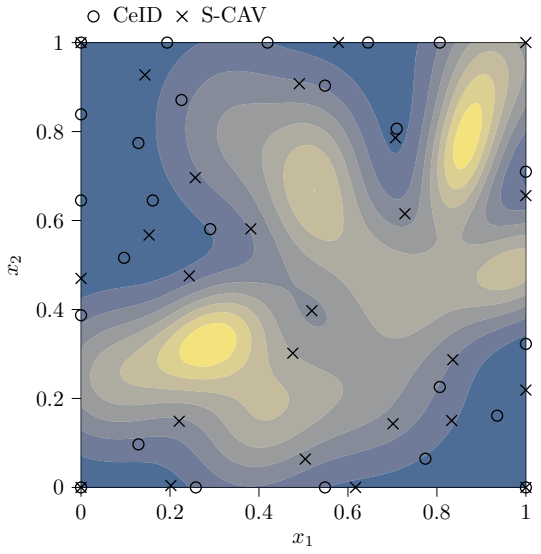


Fig. 3: First 25 samples generated by the cost-aware initial designs S-CAV (crosses) and CeID (circles) on top of the contour plot of the cost function.

A. Space-filling Cost-aware Voronoi (S-CAV)

S-CAV is a special variant of CAV that is suitable for creating space-filling initial designs. It obtains the space-filling properties by using the hypervolume of the cell as the cell selection criterion

$$K_i(j) = \underline{v}[j] \ . \tag{6}$$

This reduces the size of the largest Voronoi cell in each iteration i, resulting in evenly distributed sample points in the design space. At the same time, parameter-dependent costs are taken into account by the local optimization in (5). The algorithm can be initialized with any non-empty set of sample points located in the design space. If a single initial sample point is used, we recommend to use the minimum of the initial cost function c_0.

B. Cross-validation Cost-aware Voronoi (CV-CAV)

CV-CAV is a variant of CAV, in which the cross-validation error of CV-Voronoi is used as cell selection criterion

$$K_i(j) = \left| \hat{f}_{-j}(\underline{s}_j) - \hat{f}(\underline{s}_j) \right| \ , \tag{7}$$

where $\underline{s}_j$ is the sample point associated with the jth cell, $\hat{f}$ is the metamodel trained on the current data set $\mathcal{D}_i$, and $\hat{f}_{-j}$ is the metamodel trained on the current data set leaving out the sample of the jth Voronoi cell $\mathcal{D}_i \setminus \underline{s}_j$.

V. Evaluation

In the following section, the variants S-CAV and CV-CAV of our proposed algorithm CAV are evaluated. First, the experimental setup is described in Sec. V-A. Then, S-CAV is compared against the cost-effective initial design of CArBO [4], which we will refer to as CeID, and latin hypercube design (LHD) in Sec. V-B. The comparison of the cost-aware adaptive designs is presented in Sec. V-C.

A. Experimental Setup

To evaluate the algorithms, they were applied to $N^{\text{runs}} = 100$ randomly generated black-box and cost function pairs f_q, c_q, $q \in \{1, \dots, N^{\text{runs}}\}$ on the design space $\mathcal{X} = [0, 1] \times [0, 1]$. The cost functions were assumed to be known and were static, thus invariant w.r.t. the iteration of the algorithms. Each of the black-box functions was modeled as sum of five Gaussian distributions. The covariance matrices of the individual Gaussian distributions were generated by rotating a diagonal matrix with random entries between $[0.005, 0.05]$ by a random angle using a rotation matrix. This resulted in smooth distributions that could already be well approximated with 100 samples. The cost functions were generated in the same way as sum of 30 Gaussian distributions. However, the entries of the diagonal matrices were chosen between $[0.001, 0.02]$ and an offset between $(0, 1]$ was added to account for constant costs. These more complex cost functions should make it difficult for algorithms to take them into account when choosing sample points.

Two measures were used to evaluate the algorithms.

1) Normalized Root-mean-square Error (NRMSE): Model accuracy was determined using the NRMSE

$$\text{NRMSE} = \frac{\sqrt{\frac{1}{N^{\text{eval}}} \sum_{k=1}^{N^{\text{eval}}} \left(\hat{f}(\underline{x}_k) - f(\underline{x}_k) \right)^2}}{y_{\max} - y_{\min}} \ , \tag{8}$$
$$\text{where } y_{\max} = \max_k \ f(\underline{x}_k) \ ,$$
$$\text{and } y_{\min} = \min_k \ f(\underline{x}_k)$$

between the black-box function and the metamodel on a 100×100 regular grid ($N^{\text{eval}} = 10^4$) and was evaluated over the number of samples and the normalized budget. The normalized budget provides insight into the metamodel accuracy that can be achieved for a given budget $c_{\max}$. For each cost function c_q the budget

$$c_{\max,q} = M \cdot \mathrm{E}\{c_q(\underline{x})\} \tag{9}$$

was defined as a fixed number of samples M (here $M = 100$) times the expected cost, given the cost function c_q on the design space. Hence, M random samples could be taken in average. The normalized cost was computed by dividing the budgets $c_{\max,q}$ corresponding to the individual cost functions c_q by the maximal budget $\max_q \ c_{\max,q}$.

2) Normalized Cost per Sample (NCPS): For a cost function c and a sample point $\underline{x}$, the cost $c(\underline{x})$ is obtained. $c(\underline{x})$ is normalized by dividing it by the expected cost, which corresponds to the mean value of the cost function c on the design space. NCPS of 1.0 thus corresponds to the expected normalized cost of a random sample point. Normalization allows NCPS to be compared across multiple cost functions.

As metamodel a Gaussian Process [18] with a squared exponential kernel was used. In addition, we assumed the black-box functions to be deterministic.

Note that in Fig. 4 and Fig. 5 $\overline{\text{NRMSE}}$ and $\overline{\text{NCPS}}$ denote the mean values of NRMSE and NCPS over the N^{runs} runs.

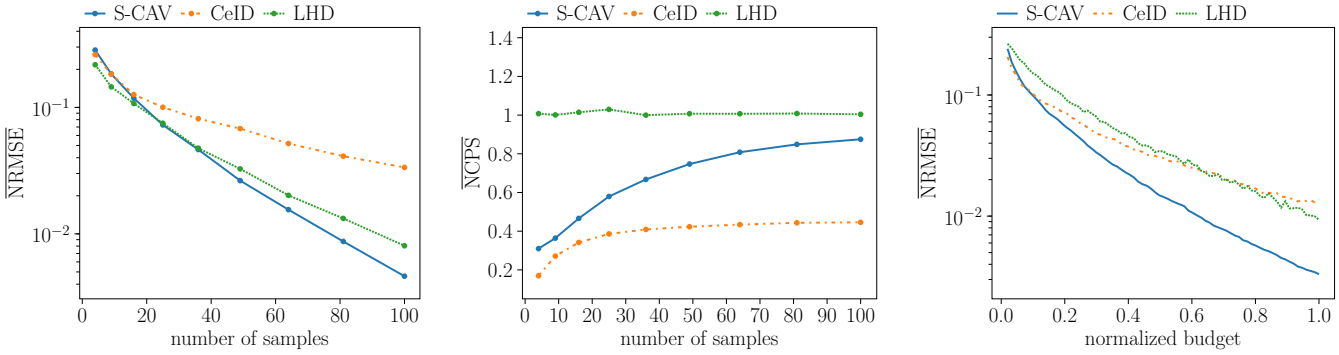


Fig. 4: Mean NRMSE and mean NCPS of the initial designs S-CAV, CeID and LHD over the number of samples and budget based on 100 randomly generated pairs of cost and black-box functions (see V-A).

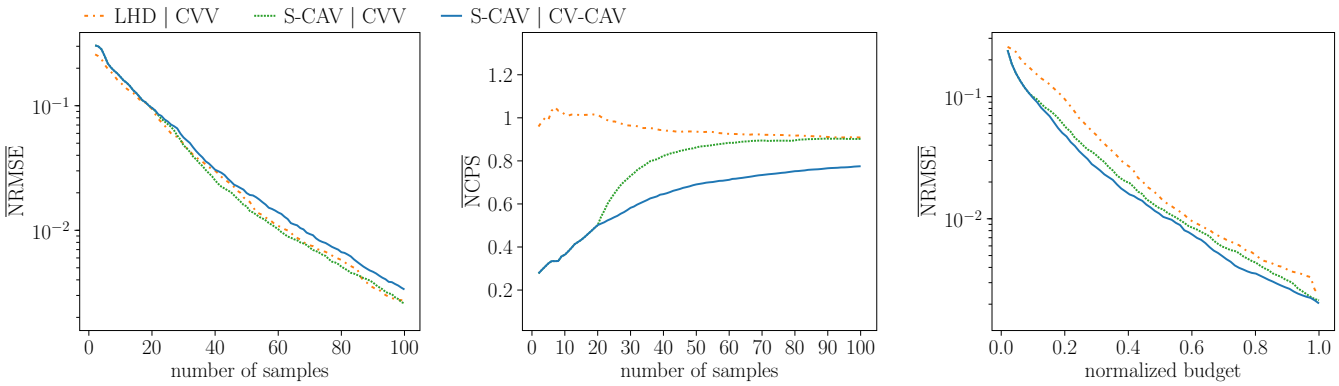


Fig. 5: Mean NRMSE and mean NCPS of LHD | CVV, S-CAV | CVV, and S-CAV | CV-CAV using an initial design size of 20 samples over the number of samples and budget based on 100 randomly generated pairs of cost and black-box functions (see V-A).

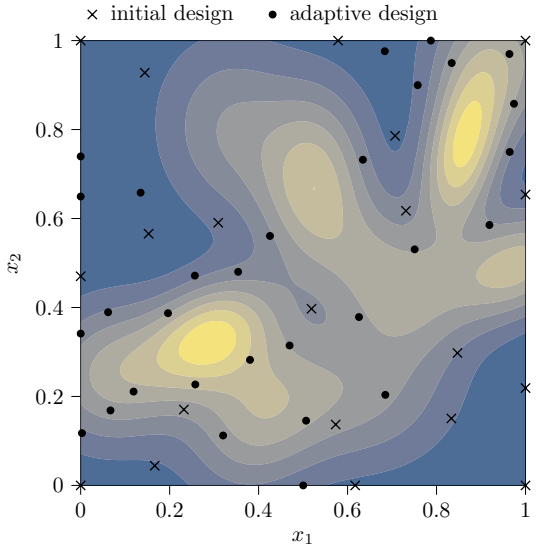
B. Cost-aware Initial Designs

In this section, the performance of S-CAV is compared against CeID and LHD. Fig. 4a shows that S-CAV and CeID start with comparable NRMSE up to about 16 samples, and LHD is slightly below that. With increasing number of samples, S-CAV achieves the best model accuracy, followed by LHD. CeID performs significantly worse than S-CAV and LHD. In Fig. 4b NCPS takes values close to 1.0 on average for LHD, since the samples are evenly distributed without cost considerations. NCPS of CeID remains strictly below the other methods and also below 0.5. This is because CeID strongly prefers low-cost regions (see Fig. 3). The resulting uneven distribution of sample points is also the reason for its large NRMSE compared to the other approaches in Fig. 4a. S-CAV starts with low NCPS that increase with the number of samples but remain below those of LHD. This is because the radius of the optimization region to account for the cost (and thus the impact of the cost function on the choice of the next sample point) depends on the spacing of the sample points, which decreases with the number of samples. Due to the low NCPS, CeID can generate more samples than S-CAV and LHD with the same budget (compare Fig. 4c). The uneven distribution of sample points of CeID results in the NRMSE being below that of LHD only for small budgets and above it for large budgets. S-CAV distinctly achieves the smallest NRMSE.

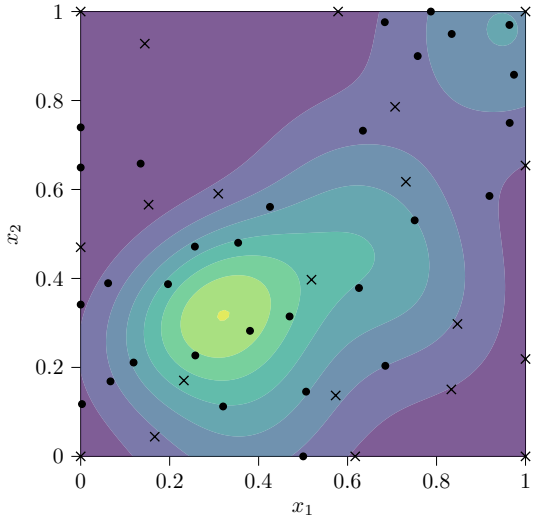
C. Cost-aware Adaptive Designs

To compare the adaptive sampling methods, we introduce the notation A | B, where A denotes the applied initial design and B denotes the adaptive design used. Each initial design included 20 samples. A Gaussian process with a squared exponential kernel was used as metamodel to compute the cross-validation error for CV Voronoi.

In Fig. 5, it can be seen that S-CAV | CV-CAV has much lower NCPS (see Fig. 5b) than the comparison methods with only slightly larger NRMSE (see Fig. 5a). The change from a cost-aware initial design to an adaptive design without cost consideration results in a rapid increase in NCPS for S-CAV | CVV. The NCPS of CV-CAV are much lower than the NCPS of the comparison methods despite the optimization region getting smaller with the number of samples. Analogous to the NCPS, the effect of S-CAV | CV-CAV can also be seen in Fig. 5c. For small budgets, the cost-aware algorithms achieve a significantly lower NRMSE. Only for larger budgets, when CV-CAV also samples more expensive points, the NRMSE converge. S-CAV | CV-CAV provides the best model accuracy for a given budget, followed by S-CAV | CVV and LHD | CVV. Fig. 6 shows the initial and adaptive samples of S-CAV | CV-CAV for one pair of cost function (see Fig. 6a) and black-box function (see Fig. 6b).



(a) Sample points of S-CAV | CV-CAV on the cost function



(b) Sample points of S-CAV | CV-CAV on the black-box function

Fig. 6: Initial design of 20 samples (crosses) and adaptive design of 30 samples (dots) of S-CAV | CV-CAV depicted on contour plots of a sample pair of cost and black-box functions.

VI. Conclusion

This paper introduces CAV, a cost-aware adaptive sampling algorithm for expensive-to-evaluate black-box functions. Based on a Voronoi tessellation of the existing sample points, a cell of interest is selected using a cell selection criterion. The vertex farthest from the associated sample point is then used as the starting point for a local optimization of the cost function. Since the radius of the optimization region depends on the distance between the sample point and the most distant vertex, it decreases with increasing number of samples. This also reduces the influence of the cost function on the choice of the sample point (cost-cooling). The space-filling variant S-CAV and the adaptive variant CV-CAV of CAV were compared against the cost-effective initial design of CArBO and CV-Voronoi. It has been shown that for a given budget, the proposed algorithms result in a smaller approximation error of the black-box function. S-CAV even achieves a lower approximation error based on the number of samples than the comparison methods. In future work, CAV will be used for global optimization and learned cost functions. In addition, the extension of the algorithm to discrete and categorical inputs is planned.

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