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# Feasible set estimation under functional uncertainty by Gaussian Process modelling

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## Abstract

In this paper we deal with the estimation of a feasible set defined by an inequality constraint on the output of a time-consuming black-box simulator. We focus on the setting where the black-box simulator takes as inputs both a set of scalar controlled variables and a functional uncontrolled variable. We then place ourselves in a probabilistic framework, modelling the functional uncontrolled variable by a random process. The inequality constraint is formulated as the expectation of the output of the simulator conditional on the values taken by the set of controlled variables. We propose an original method to solve the above feasibility problem with a reduced number of evaluations of the costly simulator. A Gaussian Process model of the simulator is learned in the joint space of controlled and uncontrolled input variables, on the basis of a set of simulations which is enriched through a sequential procedure. This procedure aims to reduce the estimation error of the feasible set by evaluating the simulator on new points chosen sequentially in the joint input space according to specific enrichment criteria. It involves as a preliminary step the reduction of the dimension of the uncontrolled input space. A variation of this strategy is also proposed, which increases adaptively the dimension of the reduced space, leading to an improvement in terms of number of calls to the simulator. The procedure we propose is compared with other sampling procedures and another modelling approach on analytical examples. Finally our methodology is implemented on an automotive industrial application. For this application, the feasible set to be recovered is the set of values of controlled variables of a gas after-treatment device leading to the respect of pollutant emission standards of a vehicle under driving profile uncertainties.

*Keywords:* feasible set estimation; Gaussian Process model; dimension reduction; functional uncertainty.

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## 1. Introduction

In recent years, engineers and scientists are increasingly relying on computer models as surrogates for physical experimentation generally too costly or impossible to execute ([1, 2]). In particular, practitioners using these numerical simulations are not only interested in the response of their model for a given set of inputs (forward problem) but also in recovering the set of input

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6 values leading to a prescribed value or range for the output of interest. The problem of estimating  
7 such a set is called hereafter feasible set estimation.

8 In our context, the numerical simulator, denoted  $f$ , takes two types of input variables: a set  
9 of controlled variables  $\mathbf{x} \in \mathbb{X}$ , and a set of uncontrolled variables  $\mathbf{v} \in \mathcal{V}$ . Without considering  
10 any assumptions on the set of uncontrolled variables  $\mathbf{v}$ , robust feasible set estimation consists in  
11 seeking the set of controlled variables  $\mathbf{x} \in \mathbb{X}$  such that  $\sup_{\mathbf{v} \in \mathcal{V}} f(\mathbf{x}, \mathbf{v})$  is smaller than a threshold  
12  $c$ . Then, the difficulty of solving this estimation problem strongly depends on the set  $\mathcal{V}$ .

13 In our setting, the simulator  $f$  takes as inputs a set of scalar controlled variables and a func-  
14 tional uncontrolled variable. Then we place ourselves in a probabilistic framework, modelling the  
15 functional uncontrolled variable by a random process  $\mathbf{V}$ . We are interested in the estimation of  
16 the feasible set defined as  $\Gamma^* := \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) = \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})] \leq c\}$ , with  $c \in \mathbb{R}$ . It is important to  
17 note here that our study is driven by an industrial application on automotive depollution. More  
18 precisely, we study an after-treatment device of diesel vehicles, depending on controlled variables,  
19 in an uncertain environment corresponding to the uncontrolled driving profile. Knowledge on the  
20 driving profile is provided through a finite set of realizations of moderate size (see Section 4.4 for  
21 more details). In order to fit this setting, we make the assumption that the process  $\mathbf{V}$  is only  
22 known through a finite set, denoted  $\Xi$ , of its realizations. Note that to estimate the expectation  
23  $\mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})]$  appearing in the definition of  $\Gamma^*$ , a brute force Monte Carlo is out of reach as each  
24 evaluation of the simulator is time consuming. Therefore we propose in the following a more  
25 elaborate sampling strategy.

26 Feasible set estimation has already been carried out in many applications, notably reliability  
27 engineering (see, e.g., [1], [2]), climatology (see, e.g., [3], [4]) and many other fields. In the literature,  
28 one way to solve the problem is to adopt a sequential sampling strategy based on a Gaussian Process  
29 (GP) model for  $g : \mathbf{x} \mapsto \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})]$ . The underlying idea is that Gaussian Process models, which  
30 capture prior knowledge about the regularity of the unknown function, make it possible to assess  
31 the estimation error of  $\Gamma^*$  given a set of evaluations of  $g$ . More specifically, for the estimation  
32 of a feasible set, these sequential strategies are closely related to the field of Bayesian global  
33 optimization (see, e.g., [5]). In the case of feasible set estimation, specific Stepwise Uncertainty  
34 Reduction (SUR) strategies were introduced in [6]. More recently, a parallel implementation of  
35 these strategies has been proposed in [2] and applied to the recovery of a feasible set. Briefly,  
36 the strategy SUR gives sequentially the next location in the controlled space where to run the  
37 simulator in order to minimize a function (called uncertainty function hereafter) measuring the  
38 estimation error of the feasible set.

39 In the field of robust optimization where uncertainty comes from a real-valued (or vector-valued)  
40 random input, various methods exist and aim at optimizing the expectation taken with respect  
41 to the probability distribution of the random input (see [7] or [8]). These methods are based on  
42 the modelling of  $f$  by a Gaussian Process built in the joint space of controlled and uncontrolled  
43 variables. Then a "projected" (integrated) Gaussian Process is defined by taking the expectation  
44 with respect to the probability distribution of the random input, leading to an approximation of the  
45 expected response  $g$ . Finally a sequential design of experiments (DoE) is proposed for optimizing  
46 the objective function  $g$ . In the same spirit, we propose an original method to solve a probabilistic  
47 feasible set estimation problem with the aim of reducing at most the number of evaluations of the  
48 simulator required. In this work  $f$  is approximated by a Gaussian Process model built on  $\mathbb{X} \times \mathbb{R}^m$ ,  
49 a finite-dimensional approximation of  $\mathbb{X} \times \mathcal{V}$ . The choice of the truncation argument  $m$  will be  
50 discussed further. For the iterative approximation of  $\Gamma^*$ , the sampling strategy in the joint space  
51 is based on two steps. Firstly a SUR approach is applied to the "projected" Gaussian Process  
52 to determine the next evaluation point  $\mathbf{x}_{n+1} \in \mathbb{X}$ . Secondly, in the uncontrolled space, the next  
53 realization  $v_{n+1}$  of the random process  $\mathbf{V}$  is chosen such that the standard error of the "projected"  
54 process evaluated at  $\mathbf{x}_{n+1}$  is minimized.

55 As already mentioned, our procedure relies on a preliminary step which aims, for a truncation

56 argument  $m$ , at estimating the  $m$ -truncated Karhunen-Loève (KL) decomposition of the random  
 57 process  $\mathbf{V}$  from the finite set  $\Xi$  of realizations of  $\mathbf{V}$ . Building the sampling strategy on a GP model  
 58 built on the finite-dimensional space  $\mathbb{X} \times \mathbb{R}^m$  certainly involves a loss of information. However,  
 59 we propose to mitigate this loss of information in the following manner: once the next point is  
 60 selected in  $\mathbb{X} \times \mathbb{R}^m$ , we evaluate the simulator on its closest neighbor in  $\mathbb{X} \times \Xi$ , where we recall  
 61 that  $\Xi$  is the available finite sample of realizations of  $\mathbf{V}$  (for more details, see the description of  
 62 **step 8** after the statement of Algorithm 1). By the way, we recover partial knowledge of the full  
 63 variability of the untruncated process  $\mathbf{V}$ , leading to a procedure which is robust with respect to  
 64 the truncation argument  $m$ . Also, we propose in Algorithm 2 a variation of our procedure, by  
 65 increasing adaptively the truncation argument  $m$  over the iterates.

66 Another procedure for solving the feasible set estimation problem described in this introduction  
 67 was proposed in [9]. The main difference with our work is that the sequential enrichment strategy  
 68 is defined on  $\mathbb{X}$ , the space of controlled variables and not on the joint space of controlled and  
 69 uncontrolled variables. Then, at each iteration, once the new point  $\mathbf{x}_{n+1}$  is selected, an accurate  
 70 approximation of  $\mathbb{E}_{\mathbf{V}}[f(\mathbf{x}_{n+1}, \mathbf{V})]$  is computed via quantization. The procedure we propose in the  
 71 present work outperforms the one in [9] by allowing to reduce even more the number of evaluations  
 72 of the costly simulator (see Figure 6 Section 4.2).

73 The article is structured as follows. In Section 2, we recall the problem formulation and we  
 74 extend the concept of Gaussian Process modelling to the case where one of the inputs is a random  
 75 process known only through a finite set of realizations. In Section 3, we introduce a new sequential  
 76 sampling strategy targeted for robust feasible set estimation to choose the next point in the joint  
 77 space:  $(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$  (Sections 3.1 and 3.2). In Section 3.3, together with numerical implementation  
 78 details, we summarize our strategy to tackle robust feasible set estimation in two algorithms: with  
 79 fixed KL parameter  $m$  (Algorithm 1) and its adaptive counterpart (Algorithm 2). The results of  
 80 these algorithms on two analytical test cases are presented in Section 4.1 to 4.3. In particular,  
 81 concerning the sampling enrichment in uncertain space, we compare our sampling strategy, based  
 82 on the standard deviation of the "projected" process evaluated at  $\mathbf{x}_{n+1}$ , with a uniform sampling  
 83 of  $v_{n+1}$  among the finite set of available realizations of the random process  $\mathbf{V}$ . We also compare  
 84 our procedure with the one introduced in [9] which combines the fitting of a Gaussian Process  
 85 model on the controlled space  $\mathbb{X}$  with a quantization estimation of the expectation of the output  
 86 conditional on the values taken by the controlled variables. In Section 4.4, our new procedure is  
 87 tested on the industrial application of a car pollution control system. Finally further discussion  
 88 on the modelling assumptions is postponed to Appendix A.

## 89 2. Problem formulation

90 We model the output of the industrial simulator by a function  $f : \mathbb{X} \times \mathcal{V} \rightarrow \mathbb{R}$  with  $\mathbb{X}$  a bounded  
 91 subset of  $\mathbb{R}^p$  being the controlled variable space and  $\mathcal{V}$  the functional space in which the random  
 92 process  $\mathbf{V}$ , modelling uncertainties, takes its values. We are interested in estimating the feasible  
 93 set

$$\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) \leq c\}, \quad (1)$$

94 where  $c \in \mathbb{R}$  is a threshold and  $g : \mathbb{X} \rightarrow \mathbb{R}$  such that  $g(\mathbf{x}) = \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})]$ . An additional constraint  
 95 is that the random process  $\mathbf{V}$  is known only through a finite set of realizations, denoted by  $\Xi$ . The  
 96 implication of this constraint will be specified in Section 3.3. The proposed sequential strategy to  
 97 estimate  $\Gamma^*$  involves three main ingredients introduced hereafter: dimension reduction to reduce  
 98 the random process  $\mathbf{V}$  to a  $m$ -dimensional random vector, Gaussian Process modelling in the joint  
 99 space  $\mathbb{X} \times \mathbb{R}^m$  and a wise selection of next point  $(\mathbf{x}_{n+1}, \mathbf{u}_{n+1}) \in \mathbb{X} \times \mathbb{R}^m$  at which to evaluate the  
 100 simulator. Although the Gaussian Process model is defined on the finite-dimensional truncated  
 101 space  $\mathbb{X} \times \mathbb{R}^m$ , robustness with respect to truncation level  $m$  is mitigated through the sequential  
 102 enrichment procedure of the design of experiments as for each selected point, the simulator is

103 evaluated at point  $(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$  where  $\mathbf{v}_{n+1}$  is the realization in  $\Xi$  corresponding to the truncated  
 104 vector  $\mathbf{u}_{n+1}$  in a sense to be precised in the following subsections.

105 *2.1. Random process finite dimensional representation*

Let  $(\Omega, \mathcal{F}, \mathbb{P})$  be a probability space. We assume that the random process  $\mathbf{V}$  belongs to  $\mathcal{H} = \mathbb{L}^2(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{V})$  with

$$\mathcal{V} = \left\{ \mathbf{v} : [0, T] \rightarrow \mathbb{R}, \|\mathbf{v}\| = (\langle v, v \rangle)^{1/2} = \left( \int_0^T \mathbf{v}(t)^2 dt \right)^{1/2} < +\infty \right\}.$$

106 We assume that  $\mathbf{V} \in \mathcal{H}$  has zero mean and continuous covariance function  $C(t, s)$ . Then

$$\forall t \in [0, T], \mathbf{V}(t) = \sum_{i=1}^{\infty} U_i \psi_i(t), \quad (2)$$

107 where  $\{\psi_i\}_{i=1}^{\infty}$  is an orthonormal basis of eigenfunctions of the integral operator corresponding to  
 108  $C$  such that:

$$\lambda_i \psi_i(t) = \int_0^T C(t, s) \psi_i(s) ds, \quad (3)$$

109 and with  $\{U_i\}_{i=1}^{\infty}$  denoting a set of uncorrelated random variables with zero mean and variance  $\lambda_i$ .  
 110 Decomposition (2) is known as the Karhunen-Loève (KL) expansion of  $\mathbf{V}$  ([10]). In the following  
 111 we denote the truncated version of  $\mathbf{V}$  as  $\mathbf{V}_m$ :

$$\forall t \in [0, T], \mathbf{V}_m(t) = \sum_{i=1}^m U_i \psi_i(t), \quad (4)$$

112 which represents, in the mean square error sense, the optimal  $m$ -term approximation of  $\mathbf{V}$  ([10]).  
 113 The value of the parameter  $m$  should be chosen such that the approximation is accurate enough.  
 114 Its influence in practice is discussed in Section 4.2.

115 *2.2. Gaussian Process modelling*

116 We assume that  $f(\mathbf{x}, \mathbf{v})$  is a realization of a Gaussian Process  $Z_{(\mathbf{x}, \mathbf{u})}$  defined on  $\mathbb{X} \times \mathbb{R}^m$ , where  
 117  $\mathbf{u} = (\langle \mathbf{v}, \psi_1 \rangle, \dots, \langle \mathbf{v}, \psi_m \rangle)^\top$ . Let  $m_Z$  be the mean function of  $Z_{(\mathbf{x}, \mathbf{u})}$  and  $k_Z$  its covariance  
 118 function,

$$\begin{aligned} \mathbb{E}[Z_{(\mathbf{x}, \mathbf{u})}] &= m_Z(\mathbf{x}, \mathbf{u}), \\ \text{Cov}(Z_{(\mathbf{x}, \mathbf{u})}, Z_{(\mathbf{x}', \mathbf{u}')}} &= k_Z((\mathbf{x}, \mathbf{u}); (\mathbf{x}', \mathbf{u}')). \end{aligned} \quad (5)$$

119 Let us denote  $Z^n$ , the GP  $Z$  conditioned on the set of  $n$  observations  $\mathbf{Z}_n =$   
 120  $\{f(\mathbf{x}_1, \mathbf{v}_1), \dots, f(\mathbf{x}_n, \mathbf{v}_n)\}$  of  $Z$  at  $(\mathcal{X}_n, \mathcal{U}_n) = \{(\mathbf{x}_1, \mathbf{u}_1), \dots, (\mathbf{x}_n, \mathbf{u}_n)\}$  where  $\mathbf{u}_i = (\langle \mathbf{v}_i, \psi_1 \rangle$   
 121  $, \dots, \langle \mathbf{v}_i, \psi_m \rangle)^\top$

$$Z_{(\mathbf{x}, \mathbf{u})}^n = [Z_{(\mathbf{x}, \mathbf{u})} | Z_{(\mathcal{X}_n, \mathcal{U}_n)} = \mathbf{Z}_n]. \quad (6)$$

The conditional mean and covariance are given by

$$\begin{aligned} \mathbb{E}[Z_{(\mathbf{x}, \mathbf{u})}^n] &= m_Z(\mathbf{x}, \mathbf{u}) + k_Z((\mathbf{x}, \mathbf{u}); (\mathcal{X}_n, \mathcal{U}_n)) \Sigma_{Z, n}^{-1} (\mathbf{Z} - m_Z(\mathcal{X}_n, \mathcal{U}_n)), \\ \text{Cov}(Z_{(\mathbf{x}, \mathbf{u})}^n, Z_{(\mathbf{x}', \mathbf{u}')}^n) &= k_Z((\mathbf{x}, \mathbf{u}); (\mathbf{x}', \mathbf{u}')) - k_Z((\mathbf{x}, \mathbf{u}); (\mathcal{X}_n, \mathcal{U}_n)) \Sigma_{Z, n}^{-1} k_Z((\mathcal{X}_n, \mathcal{U}_n); (\mathbf{x}', \mathbf{u}')). \end{aligned}$$

122 where  $\Sigma_{Z, n} = k_Z((\mathcal{X}_n, \mathcal{U}_n); (\mathcal{X}_n, \mathcal{U}_n))$ . The Gaussian Process  $Z_{(\mathbf{x}, \mathbf{u})}$  is defined on the finite-  
 123 dimensional truncated space  $\mathbb{X} \times \mathbb{R}^m$ . However, it is worth underlying that we recollect partial  
 124 knowledge of the full variability of the untruncated process  $\mathbf{V}$ , despite the truncation of the KL  
 125 expansion, by evaluating the simulator on design points in  $\mathbb{X} \times \Xi$ . A discussion about this model  
 126 is proposed in Appendix A.

127 *2.3. Integrated Gaussian Process*

128 Recall that  $\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) = \mathbb{E}[f(\mathbf{x}, \mathbf{V})] \leq c\}$ . Therefore, to model the function  $g$ , we  
 129 introduce the integrated process

$$Y_{\mathbf{x}}^n = \mathbb{E}_{\mathbf{U}}[Z_{(\mathbf{x}, \mathbf{U})}^n] = \int_{\mathbb{R}^m} Z_{(\mathbf{x}, \mathbf{u})}^n d\rho(\mathbf{u}), \quad (7)$$

130 where  $\rho$  is the probability distribution of  $\mathbf{U} = (U_1, \dots, U_m)^\top$  introduced in (4). The process  $Y_{\mathbf{x}}^n$  is  
 131 a Gaussian Process ([7]) fully characterized by its mean and covariance functions which are given  
 132 by

$$\mathbb{E}[Y_{\mathbf{x}}^n] = \int_{\mathbb{R}^m} m_Z(\mathbf{x}, \mathbf{u}) + k_Z((\mathbf{x}, \mathbf{u}); (\mathcal{X}_n, \mathcal{U}_n)) \Sigma_{Z,n}^{-1} (\mathbf{Z} - m_Z(\mathcal{X}_n, \mathcal{U}_n)) d\rho(\mathbf{u}), \quad (8)$$

133 and

$$\text{Cov}(Y_{\mathbf{x}}^n, Y_{\mathbf{x}'}^n) = \iint_{\mathbb{R}^m} k_Z((\mathbf{x}, \mathbf{u}); (\mathbf{x}', \mathbf{u}')) - k_Z((\mathbf{x}, \mathbf{u}); (\mathcal{X}_n, \mathcal{U}_n)) \Sigma_{Z,n}^{-1} k_Z((\mathcal{X}_n, \mathcal{U}_n); (\mathbf{x}', \mathbf{u}')) d\rho(\mathbf{u}) d\rho(\mathbf{u}'). \quad (9)$$

134 **3. Data driven infill strategy for robust feasible set estimation**

135 In this section we propose a two-step infill strategy in the joint space. The first step consists  
 136 in choosing a point in the controlled space while the second one aims at enriching the design with  
 137 a new point in the uncertain space.

138 *3.1. Minimization of the Vorob'ev deviation: choice of next  $\mathbf{x}$*

139 The objective of the first step is to wisely choose the points in the controlled space  $\mathbb{X}$  in order  
 140 to accurately estimate the set  $\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) = \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})] \leq c\}$ . For this purpose, we  
 141 consider the statistical model of the non-observable function  $g$  given by  $Y_{\mathbf{x}}^n$  introduced in Section  
 142 2.3. In the following, we assume that the Gaussian Process  $(Z_{(\mathbf{x}, \mathbf{u})})_{(\mathbf{x}, \mathbf{u}) \in \mathbb{X} \times \mathbb{R}^m}$  is separable with  
 143 continuous mean function  $m_Z$  and Matérn (5/2 or 3/2) covariance function  $k_Z$ . Then the feasible  
 144 set defined as  $\Gamma = \{\mathbf{x} \in \mathbb{X}, Y_{\mathbf{x}}^n \leq c\}$  is a random closed set (see, e.g., [11] p.4, 23).

From the assumption that  $g$  is a realization of  $Y_{\mathbf{x}}^n$ , the true unknown set  $\Gamma^*$  can be seen as a  
 realization of the random closed set  $\Gamma$ . The book of [11] gives many possible definitions for the  
 variance of a random closed set. In the present work we focus on the Vorob'ev deviation ([12, 13])  
 and we adapt the Stepwise Uncertainty Reduction (SUR) strategy introduced in [5] which aims  
 at decreasing an uncertainty function defined as the Vorob'ev deviation ([12, 13]) of the random  
 set. More precisely the uncertainty function at step  $n$  is defined as

$$\mathcal{H}_n^{\text{uncert}} = \mathbb{E}[\mu(\Gamma \Delta Q_{n, \alpha_n^*}) \mid Z_{(\mathcal{X}_n, \mathcal{U}_n)} = \mathbf{Z}_n],$$

where  $\mu$  is the Lebesgue measure on  $\mathbb{X}$ ,  $\Delta$  the symmetric difference operator between two sets, the  
 Vorob'ev quantiles are given by  $Q_{n, \alpha} = \{\mathbf{x} \in \mathbb{X}, \mathbb{P}(Y_{\mathbf{x}}^n \leq c) \geq \alpha\}$ , and the Vorob'ev expectation  
 $Q_{n, \alpha_n^*}$  can be determined by tuning  $\alpha$  to a level  $\alpha^*$  such that  $\mu(Q_{n, \alpha_n^*}) = \mathbb{E}[\mu(\Gamma) \mid Z_{(\mathcal{X}_n, \mathcal{U}_n)} = \mathbf{Z}_n]$ .  
 Let

$$\mathcal{H}_{n+1}^{\text{uncert}}(\mathbf{x}) = \mathbb{E}[\mu(\Gamma \Delta Q_{n+1, \alpha_{n+1}^*}) \mid Z_{(\mathcal{X}_n, \mathcal{U}_n)} = \mathbf{Z}_n, Y_{\mathbf{x}}^n].$$

145 The objective of the SUR strategy is thus to enrich the current design with a new point  $\mathbf{x}_{n+1}$   
 146 satisfying

$$\begin{aligned} \mathbf{x}_{n+1} &\in \operatorname{argmin}_{\mathbf{x} \in \mathbb{X}} \mathbb{E}_{n, \mathbf{x}}[\mathcal{H}_{n+1}^{\text{uncert}}(\mathbf{x})] \\ &:= \operatorname{argmin}_{\mathbf{x} \in \mathbb{X}} \mathcal{J}_n(\mathbf{x}), \end{aligned} \quad (10)$$

147 where  $\mathbb{E}_{n,\mathbf{x}}$  denotes the expectation with respect to  $Y_{\mathbf{x}}^n$ . For the computation of  $\mathcal{J}_n(\mathbf{x})$ , we use the  
 148 formula given in [14, Eq. (4.43) in Section 4.2] (see also [5, Section 3.1]).

149 The enrichment of the DoE consists in selecting a couple  $(\mathbf{x}_{n+1}, \mathbf{u}_{n+1})$  in the joint space  $\mathbb{X} \times \mathbb{R}^m$ .  
 150  $\mathbf{x}_{n+1}$  has just been defined by (10), it remains now to choose a new point  $u_{n+1}$  in the uncertain  
 151 space.

### 152 3.2. Minimization of the variance: choice of next $\mathbf{u}$

153 The process  $Y^n$  approximates the expectation  $\mathbb{E}_{\mathbf{V}}[f(\cdot, \mathbf{V})]$ . It can be seen as a projection of  
 154  $Z^n$  from the joint space onto the controlled space. We propose to sample the point  $\mathbf{u}_{n+1}$  in the  
 155 uncertain space in order to reduce at most the one-step-ahead variance at point  $\mathbf{x}_{n+1}$ ,  $\text{VAR}(Y_{\mathbf{x}_{n+1}}^{n+1})$ ,  
 156 whose expression is obtained from Eq. (9). More precisely,

$$\mathbf{u}_{n+1} = \operatorname{argmin}_{\tilde{\mathbf{u}} \in \mathbb{R}^m} \text{VAR}(Y_{\mathbf{x}_{n+1}}^{n+1}), \quad (11)$$

157 with

$$\begin{aligned} \text{VAR}(Y_{\mathbf{x}_{n+1}}^{n+1}) &= \vartheta(\tilde{\mathbf{u}}), \\ &= \iint_{\mathbb{R}^m} k_Z((\mathbf{x}_{n+1}, \mathbf{u}); (\mathbf{x}_{n+1}, \mathbf{u}')) d\rho(\mathbf{u}) d\rho(\mathbf{u}') \\ &\quad - \iint_{\mathbb{R}^m} k_Z((\mathbf{x}_{n+1}, \mathbf{u}); (\mathcal{X}_{n+1}, \mathcal{U}_{n+1})) \Sigma_{Z,n+1}^{-1} k_Z((\mathcal{X}_{n+1}, \mathcal{U}_{n+1}); (\mathbf{x}_{n+1}, \mathbf{u}')) d\rho(\mathbf{u}) d\rho(\mathbf{u}'), \end{aligned} \quad (12)$$

158 where  $\Sigma_{Z,n+1} = k_Z((\mathcal{X}_{n+1}, \mathcal{U}_{n+1}); (\mathcal{X}_{n+1}, \mathcal{U}_{n+1}))$  and  $(\mathcal{X}_{n+1}, \mathcal{U}_{n+1}) = (\mathcal{X}_n, \mathcal{U}_n) \cup \{(\mathbf{x}_{n+1}, \tilde{\mathbf{u}})\}$ .

### 159 3.3. Implementation

160 We present in this section two algorithms. Algorithm 1 is the global algorithm summarizing  
 161 the strategy we propose for robust feasible set estimation. The truncation argument is fixed once  
 162 for all in the algorithm. Algorithm 2 is a variation of Algorithm 1 with a data driven procedure  
 163 for increasing the truncation argument  $m$  over the iterations. This last algorithm allows to further  
 164 reduce the number of calls to the simulator.

165 The setting of our procedure is driven by our industrial application where the random process  
 166  $\mathbf{V}$  is known only through a finite set of realizations  $\Xi = \{\check{\mathbf{v}}_1, \dots, \check{\mathbf{v}}_N\}$ . In this framework, points  
 167 a) and b) below detail the computation of KL decomposition and the minimization of the one-  
 168 step-ahead variance.

169 a) *Computational method for functional PCA.* We consider the empirical version of  $C(s, t)$  defined

170 as  $C^N(s, t) = \frac{1}{N} \sum_{i=1}^N \check{\mathbf{v}}_i(s) \check{\mathbf{v}}_i(t)$ . The eigenvalue problem defined by Eq. (3) is then solved by

171 discretizing the trajectories  $\{\check{\mathbf{v}}_i\}_{i=1, \dots, N}$  on  $[0, T]$  and replacing  $C$  by  $C^N$ . Denoting by  $\hat{\psi}_i$ ,  $i =$   
 172  $1, \dots, m$ , the  $m$  first estimated eigenfunctions, we define

$$\mathcal{G}_m = \{\check{\mathbf{u}}_1, \dots, \check{\mathbf{u}}_m\} \quad (13)$$

173 where  $\check{\mathbf{u}}_i = (\langle \check{\mathbf{v}}_i, \hat{\psi}_1 \rangle, \dots, \langle \check{\mathbf{v}}_i, \hat{\psi}_m \rangle)^\top$ .

174 b) *Minimization of the one-step-ahead variance.* Since  $\mathbf{V}$  is known through a finite set  $\Xi$ , Eq. (11)  
 175 is solved on the finite set  $\mathcal{G}_m$ .

176 We now state the global algorithm we propose for robust feasible set estimation (Algorithm 1)  
 177 and its variation with a data driven increase of the truncation argument (Algorithm 2).  
 178

179 *3.3.1. A first algorithm for robust feasible set estimation*

180 In this section we provide a global algorithm for the implementation of our methodology. Then  
 181 we comment some of its steps.

---

**Algorithm 1** Robust feasible set estimation via joint space modelling

---

**Require:** The truncation argument  $m$ , the initial DoE of  $n_0$  points  $(\mathcal{X}_n, \mathcal{U}_n)$  in  $\mathbb{X} \times \mathcal{G}_m$ , and a maximal simulation budget

- 1: Set  $n = n_0$ .
  - 2: Calculate  $\mathbf{Z}$  the simulator responses at the design points  $(\mathcal{X}_n, \mathcal{U}_n)$
  - 3: **while**  $n \leq \text{budget}$  **do**
  - 4:   Fit the GP model  $Z^n$
  - 5:   Induce the integrated GP  $Y_{\mathbf{x}}^n$
  - 6:    $\mathbf{x}_{n+1} \leftarrow$  sampling criterion  $\mathcal{J}_n$
  - 7:    $\mathbf{u}_{n+1} \leftarrow \operatorname{argmin}_{\bar{\mathbf{u}} \in \mathcal{G}_m} \mathbb{V}\mathbb{A}\mathbb{R}(Y_{\mathbf{x}_{n+1}}^{n+1})$
  - 8:   Simulation at  $(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$ , where  $\mathbf{v}_{n+1} \in \Xi$  is the curve corresponding to  $\mathbf{u}_{n+1}$
  - 9:   Update DoE :  $(\mathcal{X}_{n+1}, \mathcal{U}_{n+1}) = (\mathcal{X}_n, \mathcal{U}_n) \cup \{(\mathbf{x}_{n+1}, \mathbf{u}_{n+1})\}$
  - 10:   Update  $\mathbf{Z} = \mathbf{Z} \cup \{f(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})\}$
  - 11:   Set  $n = n + 1$
  - 12: **end while**
  - 13: Fit the final GP model  $Z^n$
  - 14: Approximate  $\Gamma^*$  by the Vorob'ev expectation
- 

182 **step 1** Let  $\mathbb{U}$  be the smallest  $m$ -rectangle containing  $\mathcal{G}_m$ ,  $\mathbb{U} = \prod_{i=1}^m [\min(\langle \Xi, \hat{\psi}_i \rangle), \max(\langle \Xi, \hat{\psi}_i \rangle)]$ .  
 183 For the initial DoE, we first build a Random Latin Hypercube Design of  $n$  points  $(\mathcal{X}_n, \mathcal{U}_n)$  in the  
 184 joint space  $(\mathbb{X}, \mathbb{U})$ . Then the set of points  $\mathcal{U}_n$  is determined such that for  $i = 1, \dots, n$ ,  $\mathbf{u}_i \in \mathcal{G}_m$  is the  
 185 closest point from  $\bar{\mathbf{u}}_i \in \bar{\mathcal{U}}_n$  (with respect to the euclidean norm in  $\mathbb{R}^m$ ).

186 **step 4** The covariance kernel of the GP is chosen as a Matérn-5/2 covariance and we add a noise modelled  
 187 with a constant variance term. The homoscedastic modelling of the noise is discussed in Appendix A.  
 188 The mean function of the GP is modelled by a constant function. All types of parameters (mean,  
 189 correlation lengths, variance and noise) are estimated by maximum likelihood [15].

190 **step 5** In the framework where the uncertain vector  $\mathbf{U}$  is Gaussian as well as the covariance kernel, closed  
 191 form solutions of the integrals in (8) and (9) are given in [7]. In our framework, the integrals in (8)  
 192 and (9) are approximated by Monte Carlo.

193 **step 6**  $\mathbf{x}_{n+1}$  is obtained by solving (10) with a continuous global optimization algorithm: GENetic Opti-  
 194 mization Using Derivatives (GENOUD) [16].

195 **step 7** Once more the integrals in (12) are approximated by Monte Carlo. More details on the estimation  
 196 of (12) can be found in [7]. Here the minimization problem is solved by an exhaustive search on the  
 197 finite set  $\mathcal{G}_m$  defined in (13).

198 **step 8** The simulator is evaluated at point  $(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$  where  $\mathbf{v}_{n+1}$  is the curve of the initial set of curves  
 199  $\Xi$  corresponding to the truncated vector of coefficients  $\mathbf{u}_{n+1}$ . Note that evaluating the simulator at  
 200 a curve in the initial set of realizations whose coordinate in the uncertain space is  $\mathbf{u}_{n+1}$  and not a  
 201 projected curve on the basis composed with first eigenfunctions brings robustness with respect to  
 202 the truncation argument.

203 *3.3.2. A variant of the proposed algorithm with a varying size of the reduced uncertain space*

204 One limitation of our methodology is the prior choice of the truncation argument  $m$ . It can  
 205 be based on a sufficient level of explained variance. But, depending on the stochastic process  
 206 involved, this parameter can be high (up to 60 for the industrial application). Increasing  $m$

207 implies increasing the dimension of the GP space. A high number of design points is then needed  
 208 to produce an accurate response surface, which is very costly in simulation calls. To overcome  
 209 the simulation extra cost, another variant of our strategy is hereafter introduced. The approach  
 210 consists in augmenting the uncertain space sequentially when needed. More precisely, a first  
 211 Gaussian Process is defined in the  $p + m$  dimensional space, with  $m$  chosen small. Once the  
 212 enrichment strategy (given by Algorithm 1) no longer provides information - a rough or bias  
 213 approximation of the feasible set is achieved - the dimension of the uncertain space is increased  
 214 and the GP is updated in the  $p + m + 1$  dimensional space. It is important to underline that this  
 215 approach does not require additional calls to the numerical simulator. This alternative strategy is  
 216 summarized by Algorithm 2:

---

**Algorithm 2** Robust feasible set estimation via sequential joint space modelling

---

**Require:** The initial truncation argument  $m$  and the DoE of  $n$  points  $(\mathcal{X}_n, \mathcal{U}_n)$  in  $\mathbb{X} \times \mathcal{G}_m$

- 1: Set  $n = n_0$ .
  - 2: Calculate  $\mathbf{Z}$  the simulator responses at the design points  $(\mathcal{X}_n, \mathcal{U}_n)$
  - 3: **while**  $n \leq \text{budget}$  **do**
  - 4:    $m \leftarrow \text{Update.Dimension}()$
  - 5:   Fit the GP model  $Z^n$
  - 6:   Induce the integrated GP  $Y_{\mathbf{x}}^n$
  - 7:    $\mathbf{x}_{n+1} \leftarrow \text{sampling criterion } \mathcal{J}_n$
  - 8:    $\mathbf{u}_{n+1} \leftarrow \arg \min_{\mathbf{u} \in \mathcal{G}_m} \text{VAR}(Y_{\mathbf{x}_{n+1}}^{n+1})$
  - 9:   Simulator response at  $(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})$ , where  $\mathbf{v}_{n+1} \in \Xi$  is the curve corresponding to  $\mathbf{u}_{n+1}$
  - 10:   Update DoE :  $(\mathcal{X}_{n+1}, \mathcal{U}_{n+1}) = (\mathcal{X}_n, \mathcal{U}_n) \cup \{(\mathbf{x}_{n+1}, \mathbf{u}_{n+1})\}$
  - 11:   Update  $\mathbf{Z} = \mathbf{Z} \cup \{f(\mathbf{x}_{n+1}, \mathbf{v}_{n+1})\}$
  - 12:   Set  $n = n + 1$
  - 13: **end while**
  - 14: Fit the GP model  $Z^n$
  - 15: Approximate  $\Gamma^*$  by the Vorob'ev expectation
- 

217 In **step** 4 of Algorithm 2, the uncertain space dimension is updated based on a stagnation  
 218 criterion of the Vorob'ev Deviation. More precisely, the dimension is updated from  $m$  to  $m + 1$  if  
 219 the following stopping criterion is verified

$$\forall 0 \leq j < n_0^{\text{SUR}}, e_{n-j}^{\text{SUR}} \leq \epsilon^{\text{SUR}}, \quad (14)$$

220 where  $e_n^{\text{SUR}} = | \mathcal{H}_n^{\text{uncert}} - \mathcal{H}_{n-1}^{\text{uncert}} |$  is the absolute error between Vorob'ev deviations estimated  
 221 for two successive iterations. The condition in Eq. (14) tests if the variation of the Vorob'ev  
 222 deviation is smaller than a tolerance  $\epsilon^{\text{SUR}}$  on  $n_0^{\text{SUR}}$  consecutive steps, with  $n_0^{\text{SUR}}$  to be tuned by  
 223 the practitioner.

## 224 4. Numerical experiments

225 In the following, we first introduce in Section 4.1 two analytical examples on which we will  
 226 test our strategy. Then in Section 4.2 we present the results obtained by implementing Algorithm  
 227 1. In Section 4.3 we present the improvements we get by increasing adaptively the truncation  
 228 argument in the KL decomposition over iterations (Algorithm 2). Finally Section 4.4 is devoted  
 229 to the implementation of our strategy on an industrial application of automotive depollution.

230 *4.1. Two analytical examples - set-up*

231 To illustrate the behaviour of the proposed method, we consider two analytical examples. We  
 232 suppose that a sample  $\Xi$  of size  $N = 200$  realizations of the random process  $\mathbf{V}$  is available and  
 233 its probability distribution is unknown. To highlight the robustness of our method regarding the  
 234 random distribution of the uncertainties, we consider two types of random processes: max-stable  
 235 process and the well-known brownian motion. Regarding the max-stable process, we consider the  
 236 Schlather model with powered exponential correlation function, i.e.,  $\ell(h) = \exp\{-(h/\lambda)^\kappa\}$ , where  
 237  $\kappa = 1$  and  $\lambda = 10$ . This process is also known as the extremal Gaussian process [17]. The function  
 238 `rmaxstab` from the R-package `SpatialExtremes` is used to generate a sample of realizations. As  
 239 Algorithm 1 depends on the truncation argument  $m$ , different values are tested (see Table 1) to  
 240 better understand the effect of the uncertain space dimension.

	$m = 2$	$m = 4$	$m = 8$
$\mathbf{V}$ : brownian motion	90.1%	95.2%	97.6%
$\mathbf{V}$ : max-stable process	58.8%	63.3%	70%

Table 1: Variance explained by the truncated KL decomposition according to  $m$  for two different random processes.

241 For all analytical examples, we consider a Gaussian Process prior  $Z_{(\mathbf{x}, \mathbf{u})}$  with constant mean  
 242 and Matérn covariance kernel with  $\nu = 5/2$ . Random Latin Hypercube Designs (RLHD) are used  
 243 as initial DoEs in all the experiments. The number of points of the initial DoE is 20 for the first  
 244 analytical example and 30 for the second one. RLHD induce variability in the behaviour of the  
 245 algorithms. To account for this variability, the performance is averaged over 30 (respectively 10)  
 246 independent runs for brownian motion (respectively max-stable process).

**Analytical example 1.** We consider an additive function, sum of the two-dimensional Bo-  
 hachevsky function and a random term, defined as

$$f : (\mathbf{x}, \mathbf{V}) \mapsto (x_1^2 + 2x_2^2 - 0.3 \cos(3\pi x_1) - 0.4 \cos(4\pi x_2) + 0.7) + \int_0^T e^{\mathbf{V}_t} dt,$$

247 where  $\mathbf{x} \in \mathbb{X} = [-100, 100]^2$ . The objective is to approximate the set  $\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) =$   
 248  $\mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})] \leq 3500\}$  for the two different types of random processes (brownian motion and max-  
 249 stable process).

**Analytical example 2.** For the second example we define a function that is not separable  
 with respect to the controlled variables  $\mathbf{x}$  and the random process  $\mathbf{V}$ . The function involves the  
 maximum and the minimum of  $(V_t)_{t \geq 0}$ , so catching the whole variability of  $\mathbf{V}$  becomes important.  
 The function  $f$  is given by

$$f : (\mathbf{x}, \mathbf{V}) \mapsto \max_t \mathbf{V}_t |0.1 \cos(x_1 \max_t \mathbf{V}_t) \sin(x_2)(x_1 + x_2 \min_t \mathbf{V}_t)^2| \int_0^T (30 + \mathbf{V}_t)^{\frac{x_1 x_2}{20}} dt,$$

250 where the controlled variables lie in  $\mathbb{X} = [1.5, 5] \times [3.5, 5]$ . The objective is to approximate the set  
 251  $\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) = \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})] \leq c\}$ , when  $c = 1.2$  for the brownian motion and  $c = 0.9$  for  
 252 the max-stable process.

253 Note that for both examples the reference solution  $\Gamma^*$  is obtained from a  $30 \times 30$  grid experiment,  
 254 where at each grid point the expectation is empirically approximated using the whole sample  $\Xi$ . In  
 255 the following, we measure the performance of the different strategies with the ratio of the volume of  
 256 the symmetric difference between the reference set  $\Gamma^*$  and the estimated one  $Q_{n, \alpha^*}$  to the volume  
 257 of the reference set:  $\mu(\Gamma^* \Delta Q_{n, \alpha^*}) / \mu(\Gamma^*)$  to which we will refer as the quality-ratio.

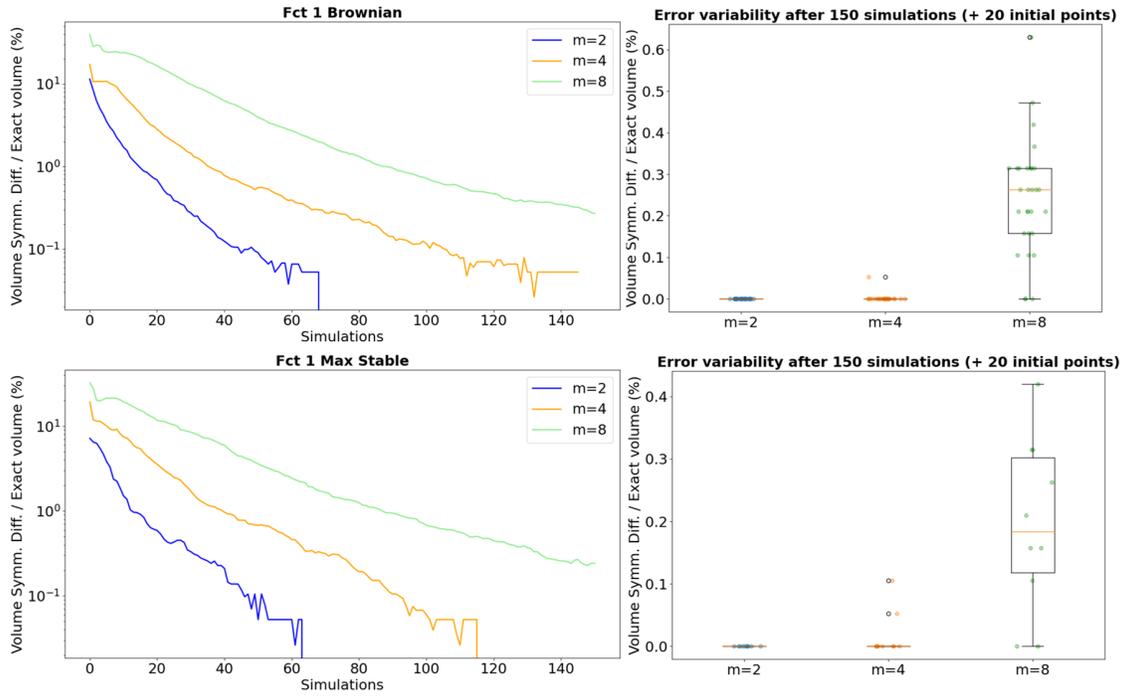


Figure 1: Analytical example 1 with brownian motion (top) and with max-stable process (bottom). Convergence of Algorithm 1 for  $m = \{2, 4, 8\}$ . Left: quality-ratio mean as function of the number of simulator calls in log scale. The mean is taken over the independent runs of initial RLHD. Right: quality-ratios associated with the random initial DoEs at the maximal simulation budget.

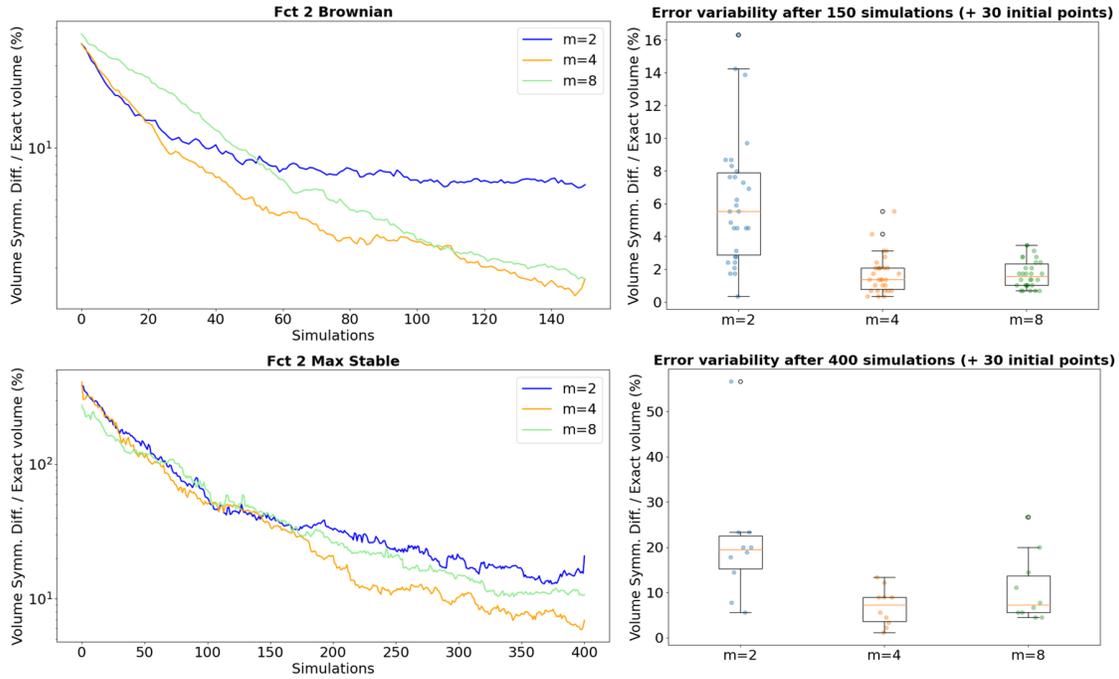


Figure 2: Analytical example 2 with brownian motion (top) and with max-stable process (bottom). Convergence of Algorithm 1 for  $m = \{2, 4, 8\}$ . Left: quality-ratio mean as function of the number of simulator calls in log scale. The mean is taken over the independent runs of initial RLHD. Right: quality-ratios associated with the random initial DoEs at the maximal simulation budget.

259 In Figures 1 and 2, we show the evolution of the averaged quality-ratio with respect to the  
 260 number of simulations involved in the Algorithm 1 on the two analytical examples with the two  
 261 types of functional uncertainties (brownian and max-stable processes). The average is taken over  
 262 the repeated runs of the complete approach corresponding to the 30 random initial designs (10 for  
 263 the max-table process), and for 3 values of the truncation argument  $m$ .

264 For the first analytical example, the smaller values of  $m$ , the faster is the convergence. This  
 265 observation can be explained by the fact that, in higher dimensional joined space (due to larger  
 266 values of  $m$ ), much more evaluation points are necessary to learn an accurate GP model (more  
 267 hyper-parameters to determine). It is worth noting that even for 90% (for brownian motion) or  
 268 58.8% (for max-stable process) of explained variance with  $m = 2$  the proposed algorithm provides  
 269 an efficient estimate of the true set  $\Gamma^*$ . Indeed, on stage 8 in Algorithm 1 the full curve  $\mathbf{v}_{n+1} \in \Xi$   
 270 associated to  $\mathbf{u}_{n+1}$  is recovered, such that the information lost after the dimension reduction is  
 271 reduced, thereby further robustifying the method.

272 Regarding the second analytical example, the output depends on local behaviours of the stochastic  
 273 process. The truncation argument  $m = 2$  is too small to catch these dependencies, the function  
 274 is sensitive to higher KL order. For the brownian motion, more than 95% of variance is explained  
 275 with  $m = 4$ . It seems sufficient to obtain an accurate approximation of  $\Gamma^*$ . The improvement  
 276 between  $m = 2$  and  $m = 4$  is noticeable. The improvement is not as important when the uncertain-  
 277 tainties are driven by a max-stable process since the percentage of explained variance increases  
 278 slowly. Better results should be observed with  $m = 8$ . It is not the case because a higher dimension  
 279 leads to difficulties in the estimation of the GP except by increasing consequently the number of  
 280 observation points. Figure A.14 in Appendix shows the evolution of the feasible domain estimation  
 281 with respect to the iterations of Algorithm 1 for the second analytic case and the brownian motion,  
 282 and for different truncation levels.

283 As shown in Figure 3, the higher the dimension of the GP space is, the longer the internal  
 284 computations last. Moreover, the computational time needed to provide the next evaluation point  
 285 increases with the number of simulator calls, and thus with the number of iterations, the cost of  
 286 kriging being directly linked to the learning sample size. For example in the case of  $m = 8$  (resp.  
 287  $m = 2$ ), iteration 80 requires 203 (resp. 126) seconds to provide the next evaluation point whereas  
 288 iteration 150 requires 275 (resp. 164) seconds.

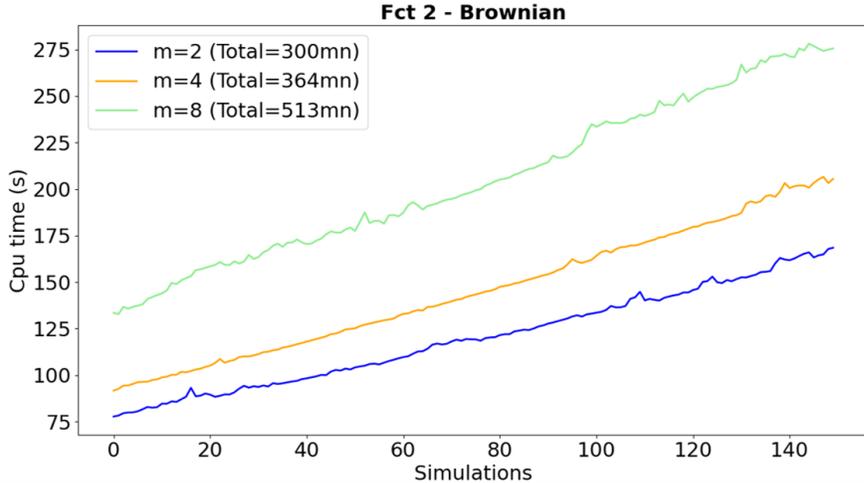


Figure 3: The computational time (sec.) needed to provide the next evaluation point as a function of iterations for the second analytic example with brownian motion. The values are averaged computational times for 5 runs of each strategy:  $m = 2, 4, 8$ .

289 To highlight the interest of the sampling criterion (11), we compared our approach to the  
 290 one where  $\mathbf{u}_{n+1}$  is chosen accordingly to a uniform distribution. The results obtained for both  
 291 analytical cases with the brownian motion are shown on Figure 4. We note that our criterion leads  
 292 to a faster decrease of the quality-ratio and to a much smaller error variability, in comparison to  
 293 a uniform sampling in the uncertain space. As shown in Figure 5, the points selected with the  
 294 criterion based on (11) seem to concentrate in interest areas, in comparison to the points selected  
 295 uniformly. Thus, the guided sampling in the uncertain space, that reduces the variance of the  
 296 expectation estimation, leads to a faster convergence towards the feasible domain.

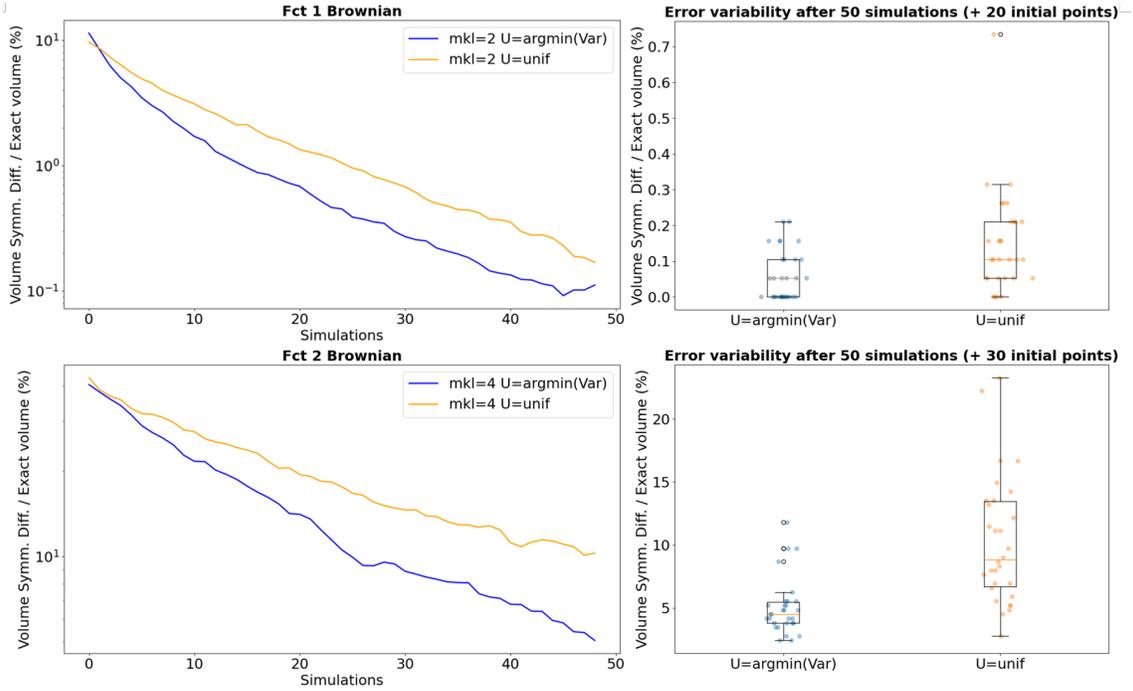


Figure 4: Analytical examples with the uncertainty modelled by a brownian motion. Decrease of the mean quality-ratio as function of the number of simulator calls (left) and boxplots for quality-ratios associated with the different random initial DoEs at the maximal simulation budget (right) for the first analytical case (top) and the second one (bottom), comparing criterion based on (11) with the uniform sampling in the uncertain space.

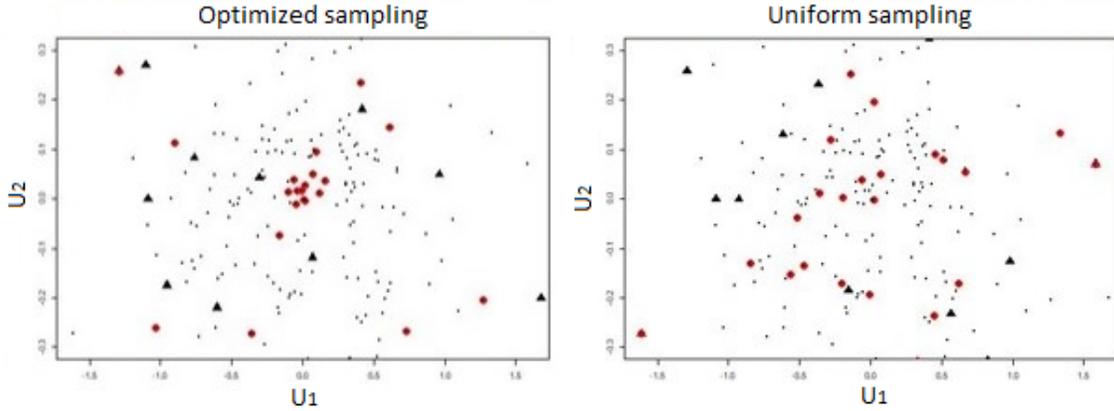


Figure 5: Analytical example 1 with the uncertainty modelled by a brownian motion. Black triangles correspond to the coefficients of the initial RLHD plotted in the uncertain truncated space ( $m = 2$ ). Red points are the added points based on our criterion (left) and uniformly sampled (right) up to 50 simulations.

297 Finally we compare our joint modelling based method with the approach introduced in [9] which  
 298 combines GP modelling in the controlled space with quantization to estimate the expectation in  
 299 the uncontrolled space. Even without taking into account the costs induced by the initial designs in  
 300 the controlled space (RLHD of size 9), the current approach based on joint GP modelling performs  
 301 better regardless of the truncation argument  $m$  (Figure 6). Adding the costs induced by the

302 quantization on the initial sample points would disadvantage even more the approach introduced  
 303 in [9] as the size of the quantizer is around 20 for each of the 9 points of the initial design, i.e. 180  
 304 simulator calls in average.

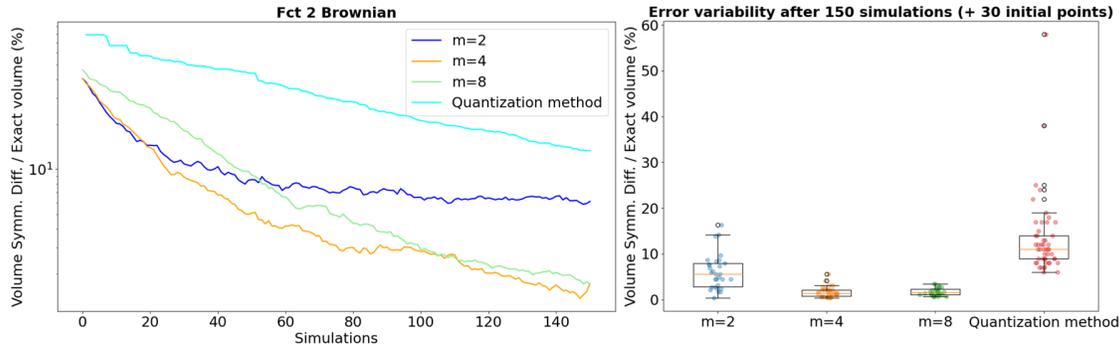


Figure 6: Comparison between the current approach based on joint GP modelling and the approach introduced in [9] combining GP modelling in the controlled space with quantization in the uncertain space. The costs induced by the initial designs (RLHD of size 9) are not compatibilized. The uncertainty is modelled by a brownian motion.

305 *4.3. Evaluation of the adaptive strategy of Algorithm 2*

306 We now evaluate the adaptive strategy presented in Algorithm 2. We focus on the second  
 307 analytical function of Section 4.1 which is the most complex one. A small initial value of  $m$  is  
 308 chosen,  $m = 2$ , and it is then increased when the variation of the Vorob'ev deviation remains  
 309 smaller than a given threshold  $\epsilon = 0.005$  during  $n_0 = 4$  consecutive iterations (see Eq. (14) in  
 310 Section 3.3). It allows to increase the dimension of the KL reduced space only when it is necessary  
 311 to obtain a better accuracy. As illustrated on Figure 7 it allows to save simulations and reduce  
 312 computational time. The accuracy reached with this strategy is similar to the one obtained with  
 313 the strategy with fixed  $m = 8$  but with a gain of  $\approx 12\%$  in terms of computational time (Figure  
 314 8). We notice that the first iterations are performed with  $m = 2$  and only the last iterations with  
 315  $m = 8$ .

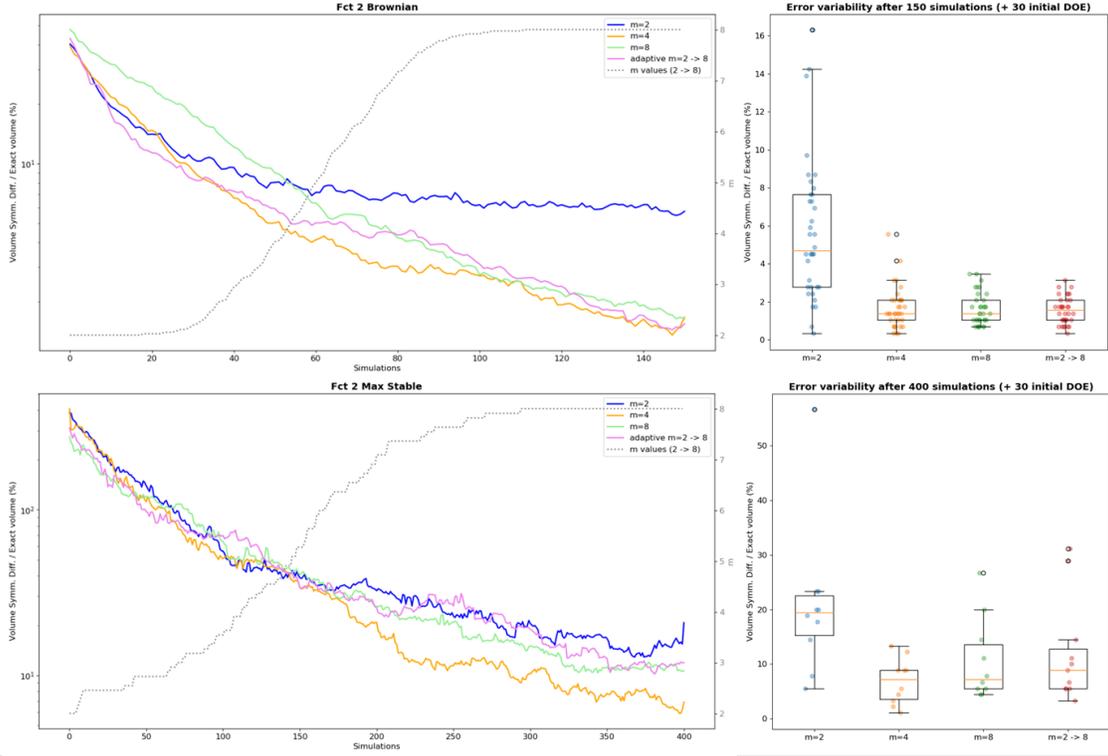


Figure 7: Analytical example 2 with brownian motion (top) and with max-stable process (bottom). Convergence of Algorithm 1 for  $m = \{2, 4, 8\}$  and for adaptive choice of  $m$  value (Algorithm 2). Left: mean quality-ratio as function of the number of simulator calls in log scale. The dashed grey curve is the mean of  $m$  values in the case of an adaptive choice of its value. The mean is taken over the independent runs of initial RLHD. Right: boxplots for the quality-ratios associated with the different random initial DoEs at the maximal simulation budget.

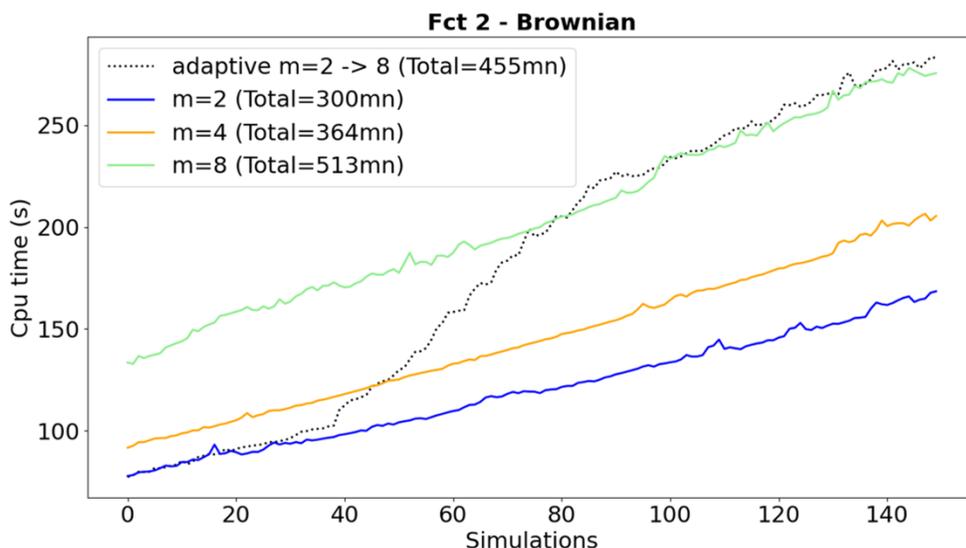


Figure 8: The computational time (sec.) needed to provide the next evaluation point as a function of iterations for the second analytic example with brownian motion. The values are averaged computational times for 5 runs of each strategy:  $m = 2, 4, 8$  and adaptive choice of  $m$  value.

316 *4.4. Application to a pollution control system SCR*

317 In this section we test the proposed method on an automotive test case from IFPEN. The  
 318 problem concerns an after-treatment device of diesel vehicles, called Selective Catalytic Reduction  
 319 (SCR). This latter consists of a basic process of chemical reduction of nitrogen oxides (NOx) to  
 320 diatomic nitrogen (N<sub>2</sub>) and water (H<sub>2</sub>O) by the reaction of NOx and ammonia NH<sub>3</sub>. The reaction  
 321 itself occurs in the SCR catalyst. Ammonia is provided by a liquid-reductant agent injected  
 322 upstream of the SCR catalyst. The amount of ammonia introduced into the reactor is a critical  
 323 quantity: overdosing causes undesirable ammonia slip (unreacted ammonia) downstream of the  
 324 catalyst, whereas under-dosing causes insufficient NOx reduction. In practice, ammonia slip is  
 325 restricted to a prescribed threshold. We use an emission-oriented simulator developed by IFPEN,  
 326 which models the vehicle, its engine and the exhaust after-treatment system. This latter takes  
 327 as input the vehicle driving cycle profile and provides the time-series of corresponding exhaust  
 328 emissions as output. A realistic SCR control law is used in this simulator (see [18] for more  
 329 details). In this study, the two controlled variables are parameters of the SCR control law and lie  
 330 in  $\mathbb{X} = [0, 0.6]^2$ . The random process describes the evolution of vehicle speed on  $I = [0, 5400s]$  and  
 331 is known through an available sample of 100 real driving cycles. A few samples are represented in  
 332 Figure 9.

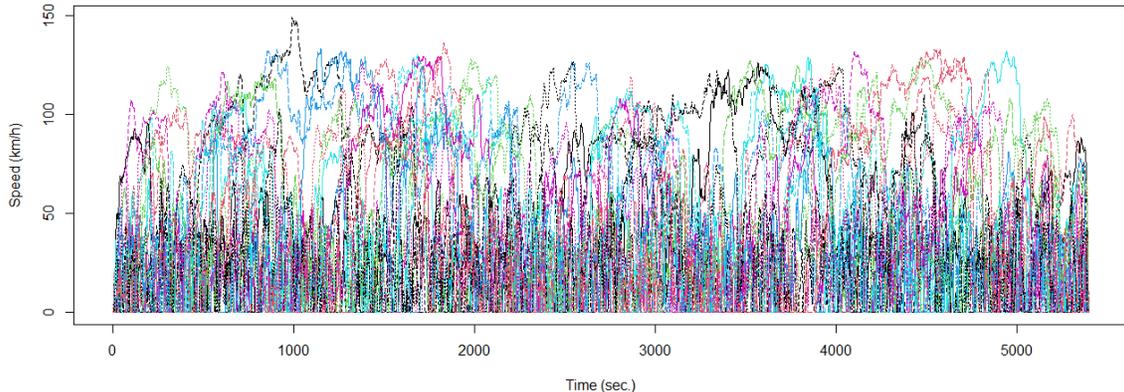


Figure 9: Seven real-driving cycles extracted from the available sample of size 100.

333 In short, the ammonia emissions peak during a driving cycle is modelled as a function

$$f : \begin{cases} \mathbb{X} \times \mathcal{V} & \rightarrow \mathbb{R} \\ (\mathbf{x}, \mathbf{V}) & \mapsto f(\mathbf{x}, \mathbf{V}) = \max_{t \in I} \text{NH}_3(t) \end{cases} \quad (15)$$

334 We are interested in recovering the set  $\Gamma^* = \{\mathbf{x} \in \mathbb{X}, g(\mathbf{x}) = \mathbb{E}_{\mathbf{V}}[f(\mathbf{x}, \mathbf{V})] \leq c\}$ , with  $c = 30\text{ppm}$ .  
 335 Conducting this study on a full grid would consist in covering the space  $[0, 0.6]^2$  with a fine mesh  
 336 and evaluating the code 100 times at each point. Knowing that each simulation takes about two  
 337 minutes, such study would require many hours of computational time, and thus using meta-models  
 338 allows to tackle this computational issue.

Truncation argument	$m = 15$	$m = 17$	$m = 19$	$m = 21$	$m = 23$	$m = 25$	$m = 64$
Explained variance	63.11%	66.64%	69.64%	72.45%	74.86%	76.87%	95.32%

Table 2: SCR pollution control system. The Variance explained by the KL decomposition according to  $m$  for the random cycle process  $\mathbf{V}$ .

339 In this industrial case, the explained variance grows very slowly as shown in the Table 2.  
 340 Therefore, to represent at best the driving cycle  $\mathbf{V}$  one should consider a high-dimensional threshold  
 341 ( $m = 64$ ). In order to avoid the curse of dimensionality involved by a high choice of  $m$ , we will  
 342 adopt the adaptive strategy introduced in section 3.3.2 and tested in subsection 4.3 on a toy  
 343 problem. More precisely, we start modeling the numerical simulator in a reduced space by taking  
 344  $m = 15$ . We increase the dimension of the uncertain space as soon as the condition in Eq. (14)  
 345 is satisfied. We set the condition parameters at  $\epsilon^{\text{SUR}} = 5 \times 10^{-3}$  and  $n_0^{\text{SUR}} = 4$ . We consider a  
 346 Gaussian Process prior  $Z_{(\mathbf{x}, \mathbf{u})}$ , with constant mean function and Matérn covariance kernel with  
 347  $\nu = 5/2$ . The initial DoE consists of a  $n = 60$  points LHS design optimized with respect to  
 348 the maximin criterion. The covariance kernel hyper-parameters are estimated by maximizing the  
 349 likelihood. Figure 10 shows the so-called excursion probability function defined by  $\mathbf{x} \mapsto \mathbb{P}(Y_{\mathbf{x}}^n \leq c)$ ,  
 350 with  $Y_{\mathbf{x}}^n$  the integrated Gaussian Process  $Y_{\mathbf{x}}$  conditionally to the  $n$  available observations. The  
 351 initial estimate of  $\Gamma^*$  is given by the green set with blue boundary. In the following and as for the  
 352 analytical examples, we proceed to add one point at each iteration of the SUR strategy.

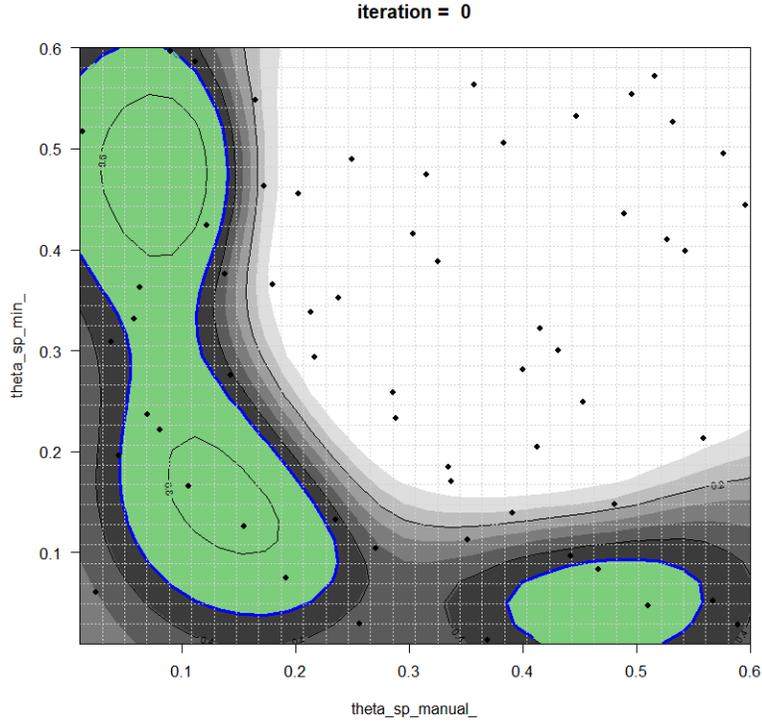


Figure 10: SCR pollution control system. The initial DoE (black triangles) and the initial estimate set (green). The contour plot in grey represents the excursion probability: darker corresponding to higher probability for the integrated process to be under the threshold.

353 Figure 11 shows the evolution of the Vorobev deviation and the dimension during the iterations.  
 354 Initially, we reduce the Vorobev deviation based on GP modeling in a 17-dimensional joint space.  
 355 At iteration 754, we increase the dimension  $m$  since we no longer improve the set estimation. This  
 356 step of increasing the dimension allows us to reduce bias and to bring more information from the  
 357 additional dimension. Fixing the maximal budget of iterations to 1000, we observe a stagnation of  
 358 the Vorobev deviation from dimension  $m = 24$ . The estimated set at different iterations is given  
 359 in Figure A.15 in Appendix. From Figure 12, we note that the SUR algorithm heavily visits the  
 360 boundary region of  $\Gamma^*$  and explore also other potentially interesting regions. Actually, after 1000  
 361 iterations the whole domain  $\mathbb{X}$  has an excursion probability close to either 0 or 1.

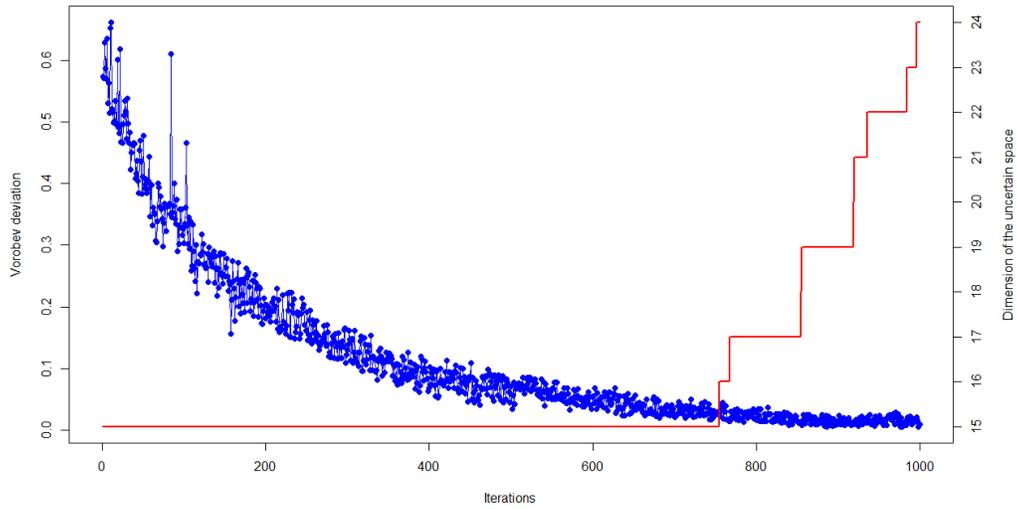


Figure 11: SCR pollution control system. The Vorob'ev deviation and the uncertain space dimension in function of the number of simulations.

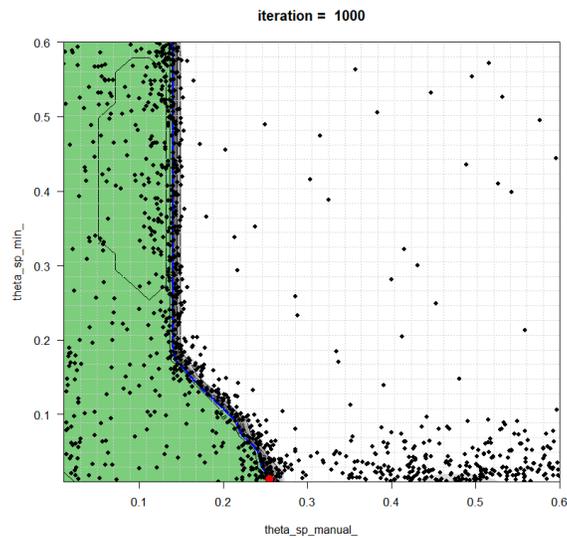


Figure 12: SCR pollution control system. The coverage probability function, the last proposed point by the algorithm (red point) and the estimate set (green set) after 1000 added points (black points). The contour plot in grey represents the excursion probability.

## 362 5. Conclusion

363 The aim of this paper is to propose a new feasible set estimation procedure for an automotive  
 364 control system in presence of functional uncontrolled variables modelled by a random process.  
 365 Our procedure outperforms the one recently introduced in [9], as it requires less evaluations of the  
 366 high-fidelity and expensive-to-evaluate model used to simulate the behaviour of the automotive  
 367 control system to achieve a similar accuracy.

368 Our procedure is based on a new enrichment strategy whose main ingredient is to fit a Gaussian  
369 Process model to the initial expensive-to-evaluate code in the joint input space of controlled and  
370 uncontrolled variables. In our framework, the uncontrolled variable is modelled by a random  
371 process  $\mathbf{V}$  to which a preliminary step of dimension reduction is applied. Moreover our knowledge  
372 of  $\mathbf{V}$  is limited to a finite set of realizations  $\Xi$ . Note that our approach guarantees robustness with  
373 respect to the order of reduction. Indeed, partial knowledge of the full variability of  $\mathbf{V}$  is recovered  
374 by evaluating the simulator on design points in  $\mathbb{X} \times \Xi$ . More precisely, at each step of the enrichment  
375 procedure, the simulator is evaluated in the point in  $\mathbb{X} \times \Xi$  whose projection corresponds to the  
376 point obtained by optimizing the criterion in the truncated joint input space. The enrichment  
377 procedure guides the sampling toward informative regions for the feasible set, allowing by the way  
378 an accurate estimation with less evaluations of the expensive-to-evaluate code. We also propose  
379 a variation of our strategy, in which the order of reduction of  $\mathbf{V}$  is increased adaptively. This  
380 approach consists in increasing the order of reduction sequentially, only when necessary, leading  
381 to even more computational savings.

382 Two bi-dimensional analytical examples are considered for which a reference solution can be  
383 computed. Then our procedure is validated by computing the quality-ratio defined as the ratio  
384 of the volume of the symmetric difference between the reference set and the estimated one to the  
385 volume of the true set. On these analytical examples, our procedure outperforms the one in [9] by  
386 achieving similar accuracy with much less evaluations of the expensive-to-evaluate code. Finally,  
387 we apply our procedure to an industrial problem related to the pollution control system of an  
388 automotive. A feasible set solution is found within a reasonable number of simulations.

389 The paper focuses on a formulation of the excursion set involving a unique constraint and where  
390 the uncertainty is summarized via its expectation. Nevertheless, as perspective, other reliability  
391 measures may also be of great interest. For example, one may be interested in ensuring a certain  
392 level of reliability with high probability or in considering multiple constraints, e.g., on the mean  
393 and the variance.

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#### 442 **Appendix A. Discussion on the GP model on the finite-dimensional truncated space**

We discuss here the assumption stated in Section 2.2 that  $f(\mathbf{x}, \mathbf{v})$  is a realization of a Gaussian Process  $Z_{(\mathbf{x}, \mathbf{u})}$  defined on the truncated space  $\mathbb{X} \times \mathbb{R}^m$ . Considering a  $m$ -truncation of the random process KL expansion, we reduce the hyperspace on which the GP is defined. Let us consider two truncation arguments  $m$  and  $L > m$ , with  $L$  large enough to ensure that the part of variance explained by the KL terms indexed by  $i > L$  is negligible. For a given realization  $\mathbf{v}$  of  $\mathbf{V}$ , let us introduce the notation  $(\mathbf{u}, \tilde{\mathbf{u}}) \in \mathbb{R}^m \times \mathbb{R}^{L-m}$  where  $\mathbf{u} = (\langle \mathbf{v}, \hat{\psi}_1 \rangle, \dots, \langle \mathbf{v}, \hat{\psi}_m \rangle)^\top$  and  $\tilde{\mathbf{u}} = (\langle \mathbf{v}, \hat{\psi}_{m+1} \rangle, \dots, \langle \mathbf{v}, \hat{\psi}_L \rangle)^\top$ . In that setting  $f(\mathbf{x}, \mathbf{V})$  can be expressed as

$$f(\mathbf{x}, \mathbf{V}) = f(\mathbf{x}, \hat{\mathbf{V}}_L) + \epsilon_T = f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{U}})\hat{\Phi}_L) + \epsilon_T$$

443 where  $\hat{\mathbf{V}}_L$  is the empirical version (estimated from  $C^N$ ) of the KL approximation of  $\mathbf{V}$  given by  
444 (4) (replacing  $m$  by  $L$ ),  $\hat{\Phi}_L = (\hat{\psi}_1, \dots, \hat{\psi}_L)^\top$  and  $\epsilon_T$  is the error associated to the KL truncation  
445 and empirical approximation, supposed small by construction.

Then, the best  $L^2$ -approximation of  $f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{U}})\hat{\Phi}_L)$  by a measurable function of  $\mathbf{U}$  only is the conditional expectation  $\mathbb{E}_{\tilde{\mathbf{U}}} [f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{U}})\hat{\Phi}_L) | \mathbf{U}]$ . We thus write:

$$f(\mathbf{x}, \mathbf{V}) = \mathbb{E}_{\tilde{\mathbf{U}}} [f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{U}})\hat{\Phi}_L) | \mathbf{U}] + \epsilon_P + \epsilon_T$$

with  $\epsilon_P$  the  $L^2$ -projection error. We can further approximate the conditional expectation by

$$f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{u}}(\mathbf{U}))\hat{\Phi}_L) + \epsilon_E$$

446 where  $\tilde{\mathbf{u}}(\mathbf{U})$  is one realization of  $\tilde{\mathbf{U}} | \mathbf{U}$  and  $\epsilon_E$  accounts for the expectation approximation. The  
447 latter approximation is motivated by the fact that, since  $\mathbf{V}$  is only known through a finite sample,  
448 we only have access to one  $\tilde{\mathbf{u}}(\mathbf{u})$  realization for each  $\mathbf{u}$  corresponding to  $\mathbf{v}$  in the initial finite set  
449  $\Xi$ . Thus we can write:

$$f(\mathbf{x}, \mathbf{V}) = f(\mathbf{x}, (\mathbf{U}, \tilde{\mathbf{u}}(\mathbf{U}))\hat{\Phi}_L) + \epsilon \tag{A.1}$$

with  $\epsilon = \epsilon_T + \epsilon_P + \epsilon_E$ . According to this last equation, the modelling assumption in Section 2.2 should include a noise term. However, the estimation of this heteroscedastic noise comes with an extra estimation cost and as it can be seen in Figure A.13, no significant model improvement is observed. Indeed in Figure A.13, for  $m = 2$ , we present the evolution of the symmetric difference for the noisy GP model  $Z_{(\mathbf{x}, \mathbf{u})}$  introduced from equation (A.1) when the noise  $\epsilon$  is Gaussian and heteroscedastic with a variance function of  $(\mathbf{x}, \mathbf{u})$ :

$$\tau^2(\mathbf{x}, \mathbf{u}) = \text{Var}_{\tilde{\mathbf{U}}} [f(\mathbf{x}, (\mathbf{u}, \tilde{\mathbf{U}}(\mathbf{u}))\hat{\Phi}_L) | \mathbf{U} = \mathbf{u}].$$

Moreover, supposing  $\mathbf{V}$  Gaussian or "nearly Gaussian", that is assuming that  $\tilde{\mathbf{U}}$  can be considered in first approximation as independent of  $\mathbf{U}$ , then  $\tau^2(\mathbf{x}, \mathbf{u})$  can be estimated by

$$\hat{\tau}^2(\mathbf{x}, \mathbf{u}) = \sum_{k=1}^l w_k [f(\mathbf{x}, \mathbf{V}_k^{\text{Quant}}) - \sum_{j=1}^l w_j f(\mathbf{x}, \mathbf{V}_j^{\text{Quant}})]^2$$

450 where  $l = 5$  and the  $\mathbf{V}_k^{Quant}$  are greedy functional quantizers and  $w_k$  associated weights (see [9]  
451 for more details). These quantizers are built from a set of  $N$  curves  $\{(\mathbf{u}, \tilde{\mathbf{u}}_k) \hat{\Phi}_L, k = 1, \dots, N\}$   
452 where  $\tilde{\mathbf{u}}_k$  are independent samples of  $\tilde{\mathbf{U}}$  which in practice are uniformly sampled in the finite set  
453  $\tilde{\mathcal{G}}_{m,L} = \{\tilde{\mathbf{u}}_1, \dots, \tilde{\mathbf{u}}_N\}$  where  $\tilde{\mathbf{u}}_i = (\langle \tilde{v}_i, \hat{\psi}_{m+1} \rangle, \dots, \langle \tilde{v}_i, \hat{\psi}_L \rangle)$ . Numerically we select 20  $(\mathbf{x}, \mathbf{u})$ -  
454 points from the initial DoE set of size  $n = 30$  and estimate the corresponding  $\hat{\tau}^2$ . To avoid further  
455 estimation of  $\tau^2$  at new locations (the remaining DoE points and during the infill strategy), we  
456 build a second GP model of  $\log(\hat{\tau}^2)$  based on the 20 initial estimations. Finally the noisy GP  
457 model  $Z$  is built using as noise variance  $\exp(\log(\hat{\tau}^2))$ . Overall we need additional  $l \times 20 = 100$   
458 costly evaluations of  $f$  to estimate the heteroscedastic noise.

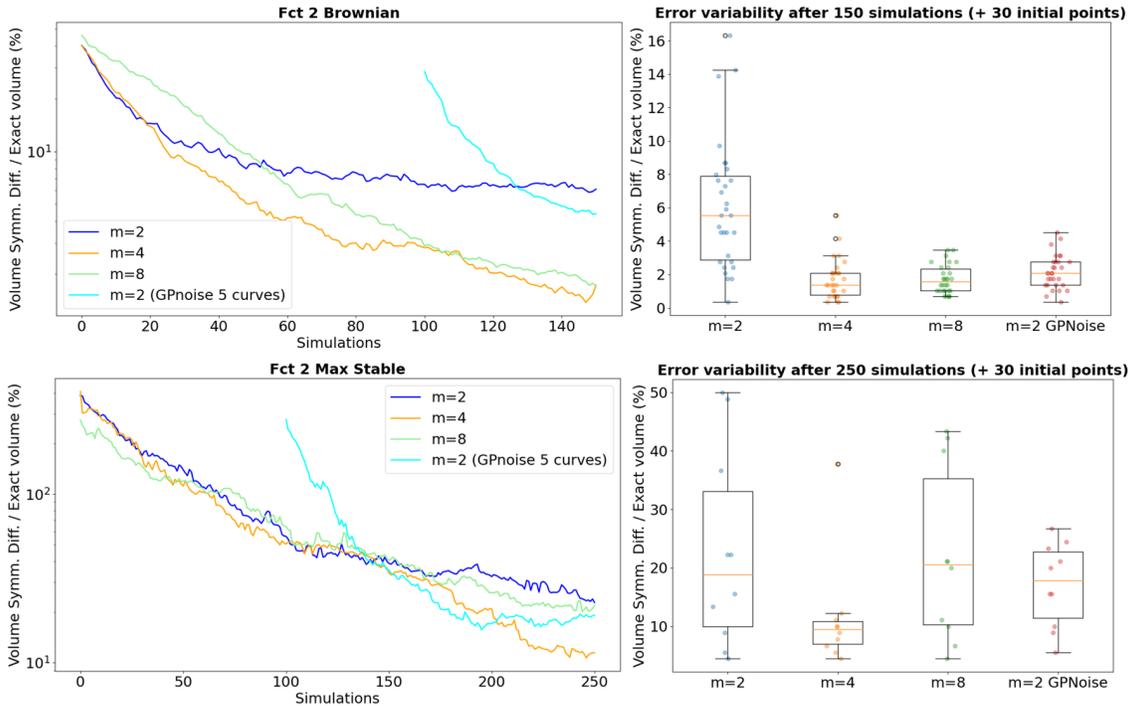


Figure A.13: Function 2 with brownian (top) and max-stable processes (bottom) with a comparison with the heteroscedastic GP model. Convergence of Algorithm 1 for  $m = \{2, 4, 8\}$ . Left: mean of the symmetric difference vs. number of simulator calls. The mean is taken over the independent runs of initial RLHD. The additional curve (cyan) corresponds to  $m = 2$  with the heteroscedastic model, it is translated to take into account the extra-cost of 100 simulations for the noise estimation. Right: symmetric differences associated with the random initial DoEs at the maximal simulation budget.

459 In Figure A.13 we notice that compared to the homoscedastic model with  $m = 2$ , the model  
460 with heteroscedastic noise achieves a faster symmetric difference volume reduction but the overcost,  
461 for the variance estimation, makes this approach interesting only for a large simulation budget:  
462 at least 130 simulations. For the brownian case, on function 2, the homoscedastic models with  
463 higher  $m$  still perform better for a budget up to 150 than the heteroscedastic one. A model with a  
464 small  $m$ , that is to say with a rough truncation error, involves a larger bias. Nevertheless, refining  
465 the heteroscedastic noise estimation should bring the method to a similar level but much further  
466 on the axis corresponding to the number of simulations. But on function 2 with a max-stable  
467 process, the heteroscedastic model slightly outperforms the homoscedastic models ( $m = 2, 4, 8$ )  
468 when approaching the 150 simulations (Figure A.13). We can understand this improvement by  
469 the fact that even with higher  $m$  a homoscedastic model does not make up for a wider truncation

470 error which is better approximated by a heteroscedastic model. Note that it is possible to relax  
 471 the "nearly Gaussian" hypothesis on  $\mathbf{V}$ . In that case the same kind of heteroscedastic variance  
 472 estimator could be used but would require an empirical estimation of the conditional distribution  
 473 of  $\tilde{\mathbf{U}}|\mathbf{U}$  which seems difficult in the context of our partial knowledge of  $\mathbf{V}$  imposing on us to work  
 474 on finite predefined sets  $\mathcal{G}$  and  $\tilde{\mathcal{G}}_{m,L}$ .

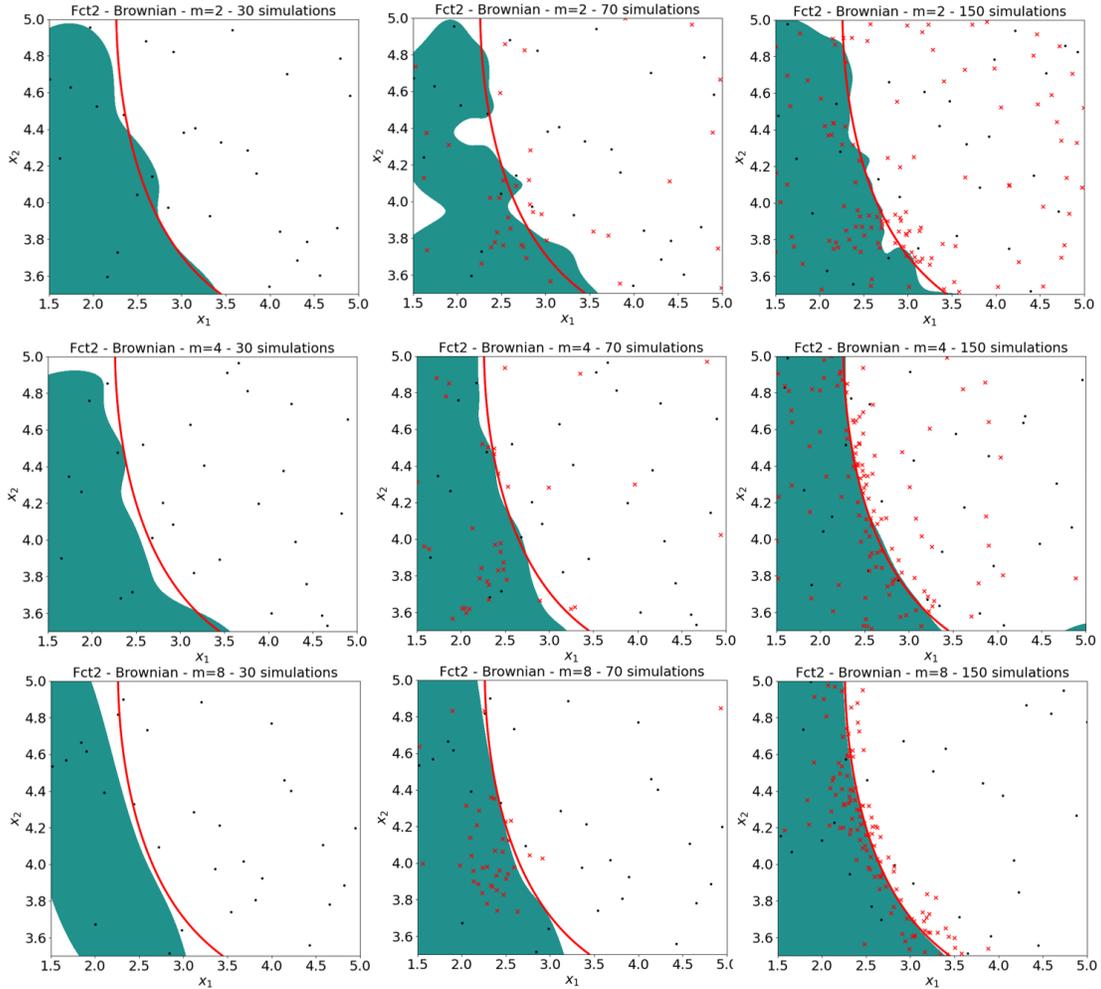


Figure A.14: Feasible domain estimation for analytical example 2 with brownian motion in green and its boundary in red for 3 different iterations (30, 70 and 150 from left to right) and for the 3 values of  $m = 2, 4$  and  $8$  (from top to bottom). The black dots are the  $\mathbf{x}$  coordinates of the points in the initial design of experiments, the red crosses are the additional points chosen by the algorithm.

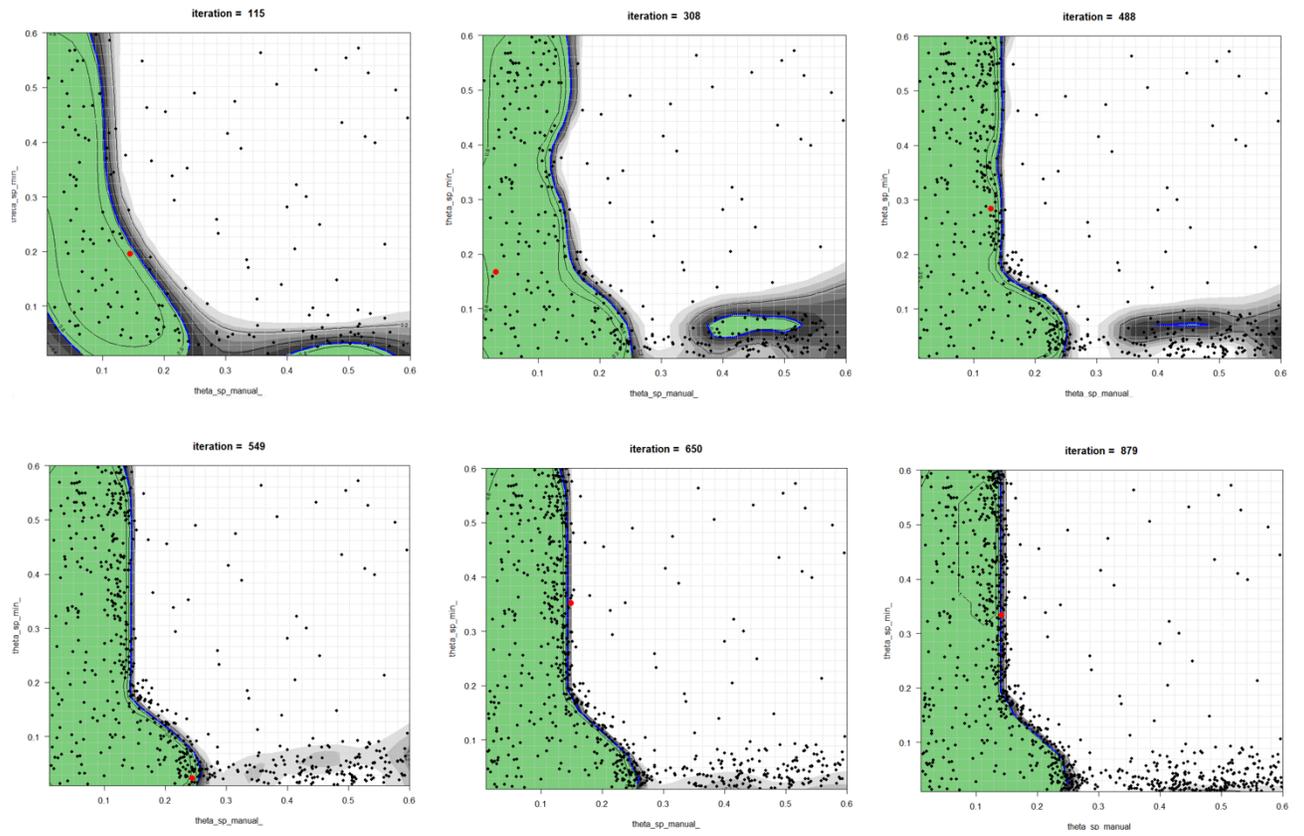


Figure A.15: SCR pollution control system. The estimated feasible domain at 6 different iterations.