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Surrogate-Assisted Bounding-Box Approach Applied to Constrained Multi-Objective Optimisation Under Uncertainty

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Abstract

This paper is devoted to tackling constrained multi-objective optimisation under uncertainty problems. A Surrogate-Assisted Bounding-Box approach (SABBa) is formulated here to deal with approximated robustness and reliability measures, which can be adaptively refined.

A Bounding-Box is defined as a multi-dimensional product of intervals, centred on the estimated objectives and constraints, that contains the true underlying values. The accuracy of these estimations can be tuned throughout the optimisation so as to reach high levels only on promising designs, which allows quick convergence toward the optimal area. In SABBa, this approach is supplemented with a Surrogate-Assisting (SA) strategy, which permits to further reduce the overall computational cost. The adaptive refinement within the Bounding-Box approach is guided by the computation of the Pareto Optimal Probability (POP) of each box.

We first assess the proposed method on several analytical uncertainty-based optimisation test-cases with respect to an *a priori* metamodel approach in terms of a probabilistic modified Hausdorff distance to the true Pareto optimal set. The method is then applied to three engineering applications: the design of two-bar truss in structural mechanics, the shape optimisation of an Organic Rankine Cycle turbine blade and the design of a thermal protection system for atmospheric reentry.

Keywords:

Multi-objective optimisation, Uncertainty-based optimisation, Error bounding boxes, Imprecise Pareto front, Surrogate-Assisting strategy

1. Introduction

1 Optimisation under uncertainty is of particular interest for companies nowadays, since
2 robustness, reliability and cost optimality are critical factors for assessing the quality of a
3 product and the efficiency of a company. In this context, two main areas are of primary
4 interest: Robust Optimisation (RO) and Reliability-Based Design Optimisation (RBDO).
5 Although there exist several interpretations for these concepts, very often in an optimization
6 problem under uncertainty, statistics-based metrics appear in the objective function in the
7

8 case of robustness, whereas they appear in the constraint for reliability. One of the central
9 issues in conducting such analysis is the computational cost of attaining a prescribed level of
10 accuracy for these statistics. Most of the time, these optimisations are performed **in coupling**
11 **with numerical simulations, where run times can reach magnitudes of weeks or months. This**
12 **is notably the case in the context of Direct Numerical Simulation (DNS) or Large Eddy**
13 **Simulation (LES), as depicted in [1] despite running on a 4 gigaflops supercomputer. Such a**
14 **computational burden prohibits the use of** direct simulation-based methods such as nested
15 Monte Carlo Simulations (MCS).

16 RBDO formulations usually feature a failure probability or Reliability Index (RI) within
17 the optimisation constraint. The later is classically used in the First-Order Reliability
18 Method (FORM), and the Performance Measure Approach (PMA) [2, 3]. Recently, history-
19 based failure probability estimation have been proposed using quasi-optimal Importance
20 Sampling (IS) distributions [4, 5]. Some approaches rely on local approximations of the fail-
21 ure probability and its gradient to perform line search optimisation [6, 7]. More generally,
22 the idea of using a surrogate model to tackle the computational cost limitation has been
23 extensively exploited with Neural Networks [8], Polynomial Chaos Expansion (PCE) [9, 10]
24 and PCE-Kriging metamodels [11]. Kriging-based techniques have notably been compared
25 with FORM in [12] and allow for a natural computation of the RI in [13]. Recently, adaptive
26 kriging approaches are among the most successful techniques. The Stepwise Uncertainty Re-
27 duction (SUR) strategy [14] and Efficient Global Reliability Analysis (EGRA) [15, 16] allow
28 for very parsimonious reliability estimations. Support Vector Regression (SVR) models can
29 also be employed similarly, as proposed in [17] with parameterised Matern smoothness.

30 As for Robust Optimisation, several methods have been proposed, with and without
31 surrogate models. Examples of the latter for mean performance optimisation make use of
32 the Simultaneous Perturbation Stochastic Approximation (SPSA) [18, 19] with Stochastic
33 Subset Optimisation (SSO) and Importance Sampling (IS) respectively. As shown in [20],
34 surrogate models like PCE [9], and mostly kriging [21, 22, 23, 24] provide very efficient
35 techniques for solving uncertainty-based optimisation. The properties of kriging models,
36 also called Gaussian Processes (GP), are exploited in [25] to analytically perform mean
37 performance optimisation and in [26] by taking heterogeneous noises into account. They
38 are also used in the context of Taguchi optimisation through the construction of a dual
39 metamodel in [27] and of a gradient-enhanced kriging for Taylor-based measure estimations
40 in [28]. Finally, in [29] conditional simulations are exploited in the context of multi-objective
41 optimisation to sample possible Pareto optima.

42 In the vast majority of the above methods, statistics computations are prone to some
43 error, either coming from the numerical interpolation (*e.g.* Monte Carlo) scheme or the sur-
44 rogate model approximation. Both these sources are studied and estimated in [30], and the
45 surrogate-based estimation error is analytically tracked in [25] in the context of mean statis-
46 tical measures and GP models with Gaussian kernels. In this work, we propose estimating
47 these computation errors with a simple interval assumption and incorporating them into
48 the optimisation strategy. This choice is motivated by the fact that most of the time, only
49 bounds are available to quantify the error of an uncertainty propagation process [31, 32].

50 To this extent, the Bounding-Box approach [33, 34, 35] gives an efficient framework for per-
 51 forming multi-objective optimisation on cost functions affected with interval uncertainty. A
 52 histogram-based approach has even been proposed in [36] to extend Bounding-Boxes to non-
 53 parametric distribution shapes. An adaptive strategy has been proposed in [37] to tackle
 54 refinable interval uncertainty in the objective functions with tunable accuracy. Parsimony
 55 is notably obtained thanks to a Surrogate-Assisting strategy, and the overall strategy is
 56 referred to as the Surrogate-Assisted Bounding-Box approach (SABBa) framework.

57 The main contribution of the present paper is twofold. It first proposes suitable surrogate-
 58 based error estimations of the statistical measures to be used in SABBa for Robust Opti-
 59 misation. It also extends SABBa to constrained problems with interval uncertainty on the
 60 constraint functions, allowing to solve both robust and reliability-based optimisation prob-
 61 lems in a common framework.

62 We depict a general measure-based optimisation under uncertainty problem in Section 2,
 63 with some classical robustness and reliability measures. Then, we introduce the Bounding-
 64 Boxes and Pareto Optimal Probability (POP) in Section 3. We notably extend the existing
 65 concepts from [33, 34, 35, 37] to constrained optimisation problems. The global algorithm
 66 is depicted in Section 4 alongside computational insights for measure estimation. Three
 67 variants of SABBa are quantitatively compared in Section 5 on analytical test-case and
 68 the most efficient approach is applied on two engineering applications in Section 6. Some
 69 conclusions and perspectives are drawn in Section 7.

70 2. Problem formulation

71 The objective of this section is to formulate a general expression for an Optimisation
 72 under Uncertainty problem including both Robust and Reliability-Based Optimisation (RO
 73 and RBDO).

74 Without loss of generality, a deterministic constrained multi-objective optimisation prob-
 75 lem can be described as the following minimisation problem:

$$\begin{aligned}
 & \text{minimise: } && \mathbf{f}(\mathbf{x}), \\
 & \text{satisfying: } && \mathbf{g}(\mathbf{x}) \leq \mathbf{0}, \\
 & \text{by changing: } && \mathbf{x} \in \mathcal{X},
 \end{aligned} \tag{1}$$

76 where the m_1 objective functions are collected in a vector $\mathbf{f} \in \mathbb{R}^{m_1}$, the m_2 constraint
 77 functions in $\mathbf{g} \in \mathbb{R}^{m_2}$ and $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^n$ are the n design variables. Note that $\mathbf{g}(\mathbf{x}) \leq \mathbf{0}$
 78 stands for $\forall i, g_i(\mathbf{x}) \leq 0$.

79 The computation of \mathbf{f} and \mathbf{g} can also depend on a multitude of uncontrollable parameters
 80 (*e.g.* environmental, material, geometrical, ...), here denoted by $\boldsymbol{\xi} \in \Xi$. The most straight-
 81 forward setting to deal with these uncertain parameters is to consider them aleatoric. In
 82 this context, $\boldsymbol{\xi}$, $\mathbf{f}(\mathbf{x}, \boldsymbol{\xi})$ and $\mathbf{g}(\mathbf{x}, \boldsymbol{\xi})$ are random variables and Equation (1) is not suitable
 83 anymore to represent the problem.

84 Here, we tackle optimisation under uncertainty problems in a measure-based setting,
 85 where specific statistics of the random outputs $\mathbf{f}(\mathbf{x}, \boldsymbol{\xi})$ and $\mathbf{g}(\mathbf{x}, \boldsymbol{\xi})$ are optimised. We denote

86 these new objectives and constraints as robustness and reliability measures, written $\boldsymbol{\rho}_f$ and
 87 $\boldsymbol{\rho}_g$ respectively. An uncertainty-based optimisation problem can then be formulated as
 88 follows:

$$\begin{aligned} & \text{minimise: } \boldsymbol{\rho}_f(\mathbf{x}), \\ & \text{satisfying: } \boldsymbol{\rho}_g(\mathbf{x}) \leq \mathbf{0}, \\ & \text{by changing: } \mathbf{x} \in \mathcal{X}, \end{aligned}$$

89 with $\boldsymbol{\rho}_f \in \mathbb{R}^{m_1}$ and $\boldsymbol{\rho}_g \in \mathbb{R}^{m_2}$.

Remark. For conciseness, \mathbf{f} and \mathbf{g} are gathered in a vector $\mathbf{q} \in \mathbb{R}^{m_1+m_2}$. Namely,

$$\forall (\mathbf{x}, \boldsymbol{\xi}) \in \mathcal{X} \times \Xi, \mathbf{q}(\mathbf{x}, \boldsymbol{\xi}) = \begin{pmatrix} \mathbf{f}(\mathbf{x}, \boldsymbol{\xi}) \\ \mathbf{g}(\mathbf{x}, \boldsymbol{\xi}) \end{pmatrix}. \quad (2)$$

Similarly, $\boldsymbol{\rho}_f$ and $\boldsymbol{\rho}_g$ are gathered in a single vector $\boldsymbol{\rho} \in \mathbb{R}^{m_1+m_2}$,

$$\forall \mathbf{x} \in \mathcal{X}, \boldsymbol{\rho}(\mathbf{x}) = \begin{pmatrix} \boldsymbol{\rho}_f(\mathbf{x}) \\ \boldsymbol{\rho}_g(\mathbf{x}) \end{pmatrix}. \quad (3)$$

90 Many formulations are possible for $\boldsymbol{\rho}$. The following are tackled in this paper:

$$\begin{aligned} \text{Expectation: } & \boldsymbol{\rho}(\mathbf{x}) = \mathbb{E}_{\boldsymbol{\xi}}[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})], \\ \text{Variance: } & \boldsymbol{\rho}(\mathbf{x}) = \mathbb{V}_{\boldsymbol{\xi}}[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})], \\ \text{Worst case: } & \boldsymbol{\rho}(\mathbf{x}) = \max_{\boldsymbol{\xi}}[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})], \\ \text{Quantile: } & \boldsymbol{\rho}(\mathbf{x}) = \mathbf{q}_{\boldsymbol{\xi}}^p[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})], \quad p \in [0, 1]. \end{aligned}$$

91 Note that any other measure could also be treated similarly in the following as we choose
 92 to approximate statistical measures through Monte Carlo Simulations (MCS) on surrogate
 93 models. We consider the unitary evaluation of \mathbf{q} to be expensive, thus a compromise must be
 94 chosen between the accuracy and the computational cost associated with the evaluation of
 95 $\boldsymbol{\rho}$. This compromise is guided here by the number of evaluations of \mathbf{q} , which are the training
 96 data permitting to construct the surrogate model for MCS numerical integration.

97 The uncertainty-based optimisation problem hence reduces to a constrained multi-objective
 98 optimisation problem with tunable accuracy computations for all objectives and constraints.
 99 The concept of tunable accuracy in the unconstrained case has been introduced in [37] for
 100 multi-objective optimisation problems (≤ 3 objectives). Next section illustrates the concept
 101 of Bounding-Boxes and their applicability to constrained problems.

102 3. Bounding-Boxes

103 In this section, we first recall the definition of Bounding-Boxes. Their extension to
 104 constrained optimisation problems is then illustrated in Section 3.1.2. Finally, the concept
 105 of Pareto Optimal Probability is presented in Section 3.2 alongside computational insights.

106 *3.1. Bounding-Box definition*

107 A m -dimensional box is defined as follows, with $\mathbf{a} \in \mathbb{R}^m$ the center and $\mathbf{r} \in \mathbb{R}_+^m$ the
 108 positive half-width vector:

$$\mathcal{B}(\mathbf{a}, \mathbf{r}) = \{\mathbf{b} \in \mathbb{R}^m \mid \mathbf{b} \in [\mathbf{a} - \mathbf{r}, \mathbf{a} + \mathbf{r}]\} \in \wp(\mathbb{R}^m),$$

109 where $\wp(\mathbb{R}^m)$ is the power set of \mathbb{R}^m .

110 The Bounding-Box approach consists in approximating an unknown value, here statistical
 111 measures $\boldsymbol{\rho}$, by a conservative box containing the true values. More precisely, an approxi-
 112 mation $\tilde{\boldsymbol{\rho}}$ of the unknown value $\boldsymbol{\rho}$ is considered and the exact approximation error $\boldsymbol{\varepsilon} = \boldsymbol{\rho} - \tilde{\boldsymbol{\rho}}$
 113 is conservatively approximated by $\bar{\boldsymbol{\varepsilon}} \geq |\boldsymbol{\varepsilon}|$. Hence it comes that $\boldsymbol{\rho} \in \mathcal{B}(\tilde{\boldsymbol{\rho}}, \bar{\boldsymbol{\varepsilon}})$ (see Fig. 1).

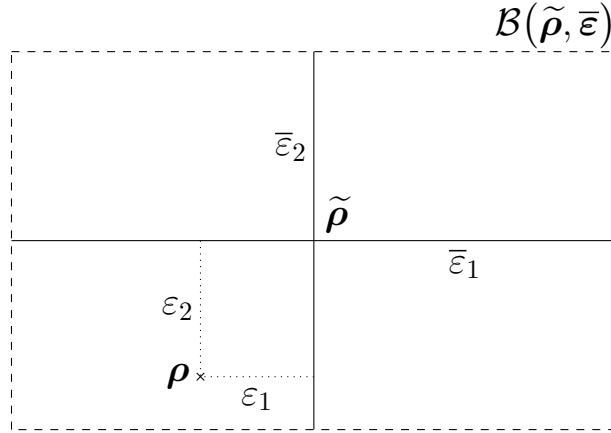


Figure 1: Bounding-Box approximation

114 *3.1.1. Boxed Pareto Dominance*

115 To perform multi-objective optimisation, the Pareto dominance rules are usually ex-
 116 ploited to assess dominance (\succ), strict dominance ($\succ\!\succ$) or indifference (\sim) between designs.
 117 In the Bounding-Box context, for comparing two boxes $(\mathcal{B}(\mathbf{a}, \mathbf{r}), \mathcal{B}(\mathbf{b}, \mathbf{r}')) \in \wp(\mathbb{R}^m)^2$, the
 118 *Boxed Pareto dominance* in the multi-minimisation case is defined as follows:

- $\mathcal{B}(\mathbf{a}, \mathbf{r})$ dominates $\mathcal{B}(\mathbf{b}, \mathbf{r}')$ in the *Boxed Pareto dominance* sense:

$$\mathcal{B}(\mathbf{a}, \mathbf{r}) \underset{\mathcal{B}}{\succ} \mathcal{B}(\mathbf{b}, \mathbf{r}') \iff \forall j \in \llbracket 1, m \rrbracket, a_j + r_j \leq b_j - r'_j \quad \text{and} \\ \exists j \in \llbracket 1, m \rrbracket, a_j + r_j < b_j - r'_j;$$

- $\mathcal{B}(\mathbf{a}, \mathbf{r})$ strictly dominates $\mathcal{B}(\mathbf{b}, \mathbf{r}')$ in the *Boxed Pareto dominance* sense:

$$\mathcal{B}(\mathbf{a}, \mathbf{r}) \underset{\mathcal{B}}{\succ\!\succ} \mathcal{B}(\mathbf{b}, \mathbf{r}') \iff \forall j \in \llbracket 1, m \rrbracket, a_j + r_j < b_j - r'_j;$$

- $\mathcal{B}(\mathbf{a}, \mathbf{r})$ and $\mathcal{B}(\mathbf{b}, \mathbf{r}')$ are indifferent in the *Boxed Pareto dominance* sense:

$$\mathcal{B}(\mathbf{a}, \mathbf{r}) \underset{\mathcal{B}}{\sim} \mathcal{B}(\mathbf{b}, \mathbf{r}') \iff \mathcal{B}(\mathbf{a}, \mathbf{r}) \not\underset{\mathcal{B}}{\succ} \mathcal{B}(\mathbf{b}, \mathbf{r}') \quad \text{and} \quad \mathcal{B}(\mathbf{b}, \mathbf{r}') \not\underset{\mathcal{B}}{\succ} \mathcal{B}(\mathbf{a}, \mathbf{r}).$$

119 Intuitively, $\mathcal{B}(\mathbf{a}, \mathbf{r})$ dominates $\mathcal{B}(\mathbf{b}, \mathbf{r}')$ if the worst outcome of $\mathcal{B}(\mathbf{a}, \mathbf{r})$ dominates in the
 120 classical sense the best outcome of $\mathcal{B}(\mathbf{b}, \mathbf{r}')$. An example is given hereafter in Fig. 2(a). In
 121 the case of bi-minimisation, $\mathcal{B}_1 \succcurlyeq_{\mathcal{B}} \mathcal{B}_6$, and the other boxes are indifferent with each other.
 122 Hence, among these six boxes, only \mathcal{B}_6 is dominated.

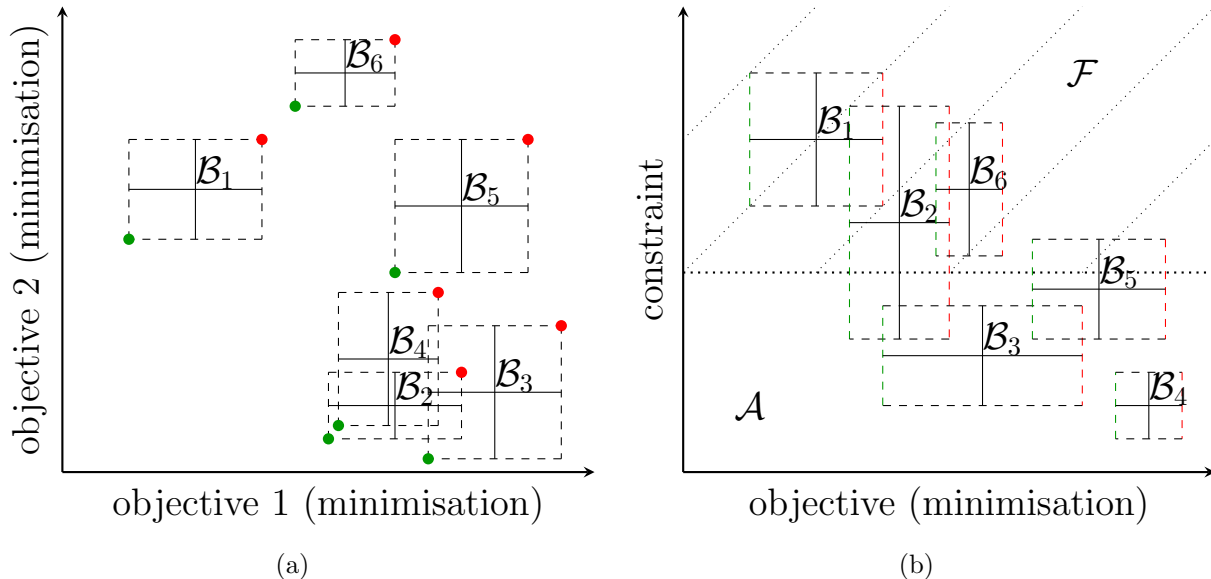


Figure 2: (a) *Boxed Pareto Dominance*, (b) *Constrained Boxed Pareto Dominance*. Comparison of six boxes, best and worst outcomes in green and red, respectively.

123 3.1.2. Constrained Boxed Pareto dominance

124 The *Boxed Pareto dominance* allows comparing boxes in a multi-objective optimisation
 125 context. For dealing with robust objectives as well as reliability-based constraints, the Pareto
 126 dominance should take into account constraint violation. To this extent, a *Constrained*
 127 *Pareto dominance* \succ_c is proposed, where again \succ refers to the classical Pareto dominance.

128 In the multi-objective constrained problem, let us denote by \mathbf{a}_f the objective values and
 129 \mathbf{a}_g the constraint values of design \mathbf{a} . Without loss of generality, these m_2 constraints can be
 130 considered of the form:

$$a_g \leq 0.$$

131 The admissible and failure sets are then defined as follows:

$$\mathcal{A} = \{\mathbf{a} \in \mathbb{R}^m \mid a_g \leq 0\},$$

$$\mathcal{F} = \{\mathbf{a} \in \mathbb{R}^m \mid a_g \not\leq 0\}.$$

132 Contrarily to the classical Pareto dominance, the *Constrained Pareto dominance* com-
 133 pares boxes from the coupled objective/constraint spaces. We propose to use the following

134 dominance rule in a classical constrained environment:

$$\begin{aligned}
\mathbf{a} \succ_c \mathbf{b} &\iff \mathbf{a} \in \mathcal{A} \text{ and } \mathbf{a}_f \succ \mathbf{b}_f \text{ or } \mathbf{b} \in \mathcal{F} \\
\mathbf{a} \succ_c \mathbf{b} &\iff \mathbf{a} \in \mathcal{A} \text{ and } \mathbf{a}_f \succ \mathbf{b}_f \text{ or } \mathbf{b} \in \mathcal{F} \\
\mathbf{a} \sim_c \mathbf{b} &\iff \mathbf{a} \not\succeq_c \mathbf{b} \text{ and } \mathbf{b} \not\succeq_c \mathbf{a}.
\end{aligned}$$

135 Note that in this case, $\mathcal{A} = \mathcal{F}^c$, where the superscript \cdot^c stands for complement. This relation
136 would not hold in the context of boxed objectives and constraints, as shown in the following.

137 When comparing boxes of \mathbb{R}^m , the admissible \mathcal{A}_B and failure \mathcal{F}_B sets contain the boxes
138 that lie entirely in \mathcal{A} and \mathcal{F} respectively:

$$\begin{aligned}
\mathcal{A}_B &= \{ \mathcal{B} \in \wp(\mathbb{R}^m) \mid \forall \mathbf{a} \in \mathcal{B}, \mathbf{a} \in \mathcal{A} \} \\
\mathcal{F}_B &= \{ \mathcal{B} \in \wp(\mathbb{R}^m) \mid \forall \mathbf{a} \in \mathcal{B}, \mathbf{a} \in \mathcal{F} \}
\end{aligned}$$

139 Hence, in the general case, $\mathcal{A}_B \neq \mathcal{F}_B^c$. A more computationally friendly formulation is
140 the following, using again the best and worst outcomes:

$$\begin{aligned}
\mathcal{A}_B &= \{ \mathcal{B}(\mathbf{a}, \mathbf{r}) \in \wp(\mathbb{R}^m) \mid \mathbf{a} + \mathbf{r} \in \mathcal{A} \}, \\
\mathcal{F}_B &= \{ \mathcal{B}(\mathbf{a}, \mathbf{r}) \in \wp(\mathbb{R}^m) \mid \mathbf{a} - \mathbf{r} \in \mathcal{F} \}.
\end{aligned}$$

141 The *Boxed Constrained Pareto dominance* is then defined as follows:

$$\begin{aligned}
\mathcal{B}(\mathbf{a}, \mathbf{r}) \succ_c \mathcal{B}(\mathbf{b}, \mathbf{r}') &\iff \mathcal{B}(\mathbf{a}_f, \mathbf{r}_f) \succ_B \mathcal{B}(\mathbf{b}_f, \mathbf{r}'_f) \text{ and } \mathcal{B}(\mathbf{a}, \mathbf{r}) \in \mathcal{A}_B \text{ or} \\
&\quad \mathcal{B}(\mathbf{b}, \mathbf{r}') \in \mathcal{F}_B, \\
\mathcal{B}(\mathbf{a}, \mathbf{r}) \succ_c \mathcal{B}(\mathbf{b}, \mathbf{r}') &\iff \mathcal{B}(\mathbf{a}_f, \mathbf{r}_f) \succ_B \mathcal{B}(\mathbf{b}_f, \mathbf{r}'_f) \text{ and } \mathcal{B}(\mathbf{a}, \mathbf{r}) \in \mathcal{A}_B \text{ or} \\
&\quad \mathcal{B}(\mathbf{b}, \mathbf{r}') \in \mathcal{F}_B, \\
\mathcal{B}(\mathbf{a}, \mathbf{r}) \sim_c \mathcal{B}(\mathbf{b}, \mathbf{r}') &\iff \mathcal{B}(\mathbf{a}, \mathbf{r}) \not\succeq_c \mathcal{B}(\mathbf{b}, \mathbf{r}') \text{ and } \mathcal{B}(\mathbf{b}, \mathbf{r}') \not\succeq_c \mathcal{B}(\mathbf{a}, \mathbf{r}).
\end{aligned}$$

142 With this Pareto dominance rule, two boxes in \mathcal{F}_B will mutually dominate each other. Such
143 a behaviour is desired to make sure that any box of the boxed failure set is completely
144 dominated, regardless of the performance of the other boxes. This will be exploited in the
145 next section, where the Pareto Optimal Probability of each box is computed.

146 In the general case, for a box to be dominated, the non-constrained *Boxed Pareto Dom-*
147 *inance* must be fulfilled in the objective dimensions and the dominant box must lie entirely
148 in the admissible set. An example is given in Fig. 2(b) with a constrained mono-objective
149 minimisation. Here, $\{\mathcal{B}_1, \mathcal{B}_6\} \subset \mathcal{F}_B$, $\{\mathcal{B}_3, \mathcal{B}_4\} \subset \mathcal{A}_B$ and $\{\mathcal{B}_2, \mathcal{B}_5\} \subset \mathcal{F}_B^c \cap \mathcal{A}_B^c$. In terms of
150 dominance, \mathcal{B}_1 and \mathcal{B}_6 are dominated by all other boxes for being entirely in the failure set.
151 \mathcal{B}_4 is also dominated by \mathcal{B}_3 , which is entirely in the admissible set.

152 3.2. Pareto Optimal Probability

153 In the above, dominance rules allow to discriminate dominated boxes from non-dominated
154 ones among a finite set of boxes. This rule is exploited in [35, 37] to refine only non-dominated

155 boxes. To discriminate in a more rigorous way between non-dominated boxes, we propose to
 156 compute for each Bounding-Box its probability of being non-dominated. Such a computation
 157 is based on the assumption that the true robustness and reliability measures $\boldsymbol{\rho}$ in Figure 1 can
 158 be modelled with an aleatory variable following a uniform distribution within the Bounding
 159 Box $\mathcal{B}(\tilde{\boldsymbol{\rho}}^l, \bar{\boldsymbol{\epsilon}}^l)$. The problem relapses to computing the Pareto Optimal Probability of aleatory
 160 variables with known uniform distributions.

161 With \mathcal{B}_{all} a given set of boxes $\{\mathcal{B}_i\}_i$, the exact POP computation follows the formula
 162 below:

$$POP_{true}(\mathcal{B}_i) = \mathbb{P}_{\{\mathbf{Z}_k\}_k} \left[\bigcap_{\substack{\mathcal{B}_j \in \mathcal{B}_{all} \\ j \neq i}} \mathbf{Z}_j \not\prec_c \mathbf{Z}_i \right], \quad (4)$$

163 where for all k , $\mathbf{Z}_k \sim \mathcal{U}(\mathcal{B}_k)$. As assumed earlier, the realisations \mathbf{Z}_k are drawn uniformly
 164 within the set \mathcal{B}_k .

165 Note however that this POP computation yields a combinatorial complexity that pro-
 166 foundly limits its calculation in closed form and would require Monte-Carlo approximation.
 167 Moreover, clustered boxes tend to dominate each other and result in low POP values, even
 168 when they are close to the Pareto front, which can be counter-intuitive. For this reason, we
 169 propose two approximations of the POP, that will be quantitatively compared.

170 Ref. [33] proposes the use of a box probabilistic ranking as the fitness function for ESPEA
 171 (Estimated Strength Pareto Evolutionary Algorithm). The score of a given box is computed
 172 by averaging the one-to-one domination probability with respect to all other boxes. Since
 173 we compute each probability between only two boxes, the computational burden is very low.
 174 However, clustered boxes still yield unintuitive scores.

175 In this work, we propose a new metric denoted as POP_{min} . It is defined as follows, with
 176 \mathcal{B}_{nd} the set of non-dominated designs (using the *Constrained Boxed Pareto dominance*):

$$POP_{min}(\mathcal{B}_i) = \min_{\substack{\mathcal{B}_j \in \mathcal{B}_{nd} \\ j \neq i}} \left(\mathbb{P}_{\mathbf{Z}_j, \mathbf{Z}_i} [\mathbf{Z}_j \not\prec_c \mathbf{Z}_i] \right). \quad (5)$$

177 This metric yields a good relative ranking between boxes and is efficiently computable.
 178 It also shows a more intuitive behaviour when dealing with clustered boxes. POP_{min} and
 179 POP_{true} metrics are quantitatively compared in Table 1 on the two small examples depicted
 180 in Figure 2, and show very similar scoring.

181 Thus, for its simplicity, interpretability and very low computational burden, POP_{min} will
 182 be used in the following.

183 4. SABBa framework

184 The objective of SABBa is to lower the computational cost of estimating the Pareto
 185 front by adaptively refining the approximations $\tilde{\boldsymbol{\rho}}$ only at the most promising designs. The
 186 unconstrained version of this framework is developed in [37] and relies on the coupling
 187 between the Bounding-Box approach and a Surrogate-Assisting (SA) model built directly
 188 on the objective values. SABBa can be coupled to generic optimisation algorithm and any

	Figure 2(a) example		Figure 2(b) example	
	POP_{true}	POP_{min}	POP_{true}	POP_{min}
\mathcal{B}_1	1.0	1.0	0.0	0.0
\mathcal{B}_2	0.902	0.912	0.254	0.254
\mathcal{B}_3	0.39	0.419	0.724	0.746
\mathcal{B}_4	0.621	0.622	0.0	0.0
\mathcal{B}_5	0.017	0.07	0.022	0.031
\mathcal{B}_6	0.0	0.0	0.0	0.0

Table 1: POPs comparison on both examples from Figure 2

189 surrogate model can be employed for the SA strategy. This feature allows the approach to
 190 be readily applicable and to benefit from new optimisation or metamodeling techniques.

191 In this paper, we make use of the NOMAD [38] optimisation technique for its reliable
 192 management of multiple objectives and constraints within a derivative-free framework (ver-
 193 sion 3.6.2). All surrogate models are Gaussian Processes, constructed using the python
 194 Gaussian Process package GPy [39] (version 1.8.5).

195 In the following, we provide the global algorithm and necessary numerical ingredients for
 196 the implementation of SABBa. Specifically, Section 4.1 presents the structure and algorithm
 197 of the framework in details, Section 4.2 deals with the computation and refinement of the
 198 Bounding-Boxes and Section 4.3 proposes a quality indicator for quantitative comparison on
 199 analytical test-cases.

200 4.1. Algorithm

201 The framework follows the structure depicted in Figure 3. The optimiser manages the
 202 design space exploration with the aim of covering the whole Pareto front.

203 We illustrate now the typical sequence of operations within an iteration of the algorithm.
 204 Let us assume to have already computed measures $\tilde{\rho}$ at a set \mathcal{X}_c of design so far in the
 205 optimisation process. The current SA model ρ_{SA} is constructed on these $\tilde{\rho}$ estimations. At
 206 each optimisation iteration, and for each new design \mathbf{x} :

- 207 • If the chosen SA model yields accurate prediction, *i.e.* $\bar{\epsilon}_{SA}(\mathbf{x}) \leq \mathbf{s}_1$, the SA-based
 208 measures estimations $\rho_{SA}(\mathbf{x})$ are returned to the optimiser. Gaussian process-based
 209 computations of ρ_{SA} and $\bar{\epsilon}_{SA}$ are proposed in Section 4.2.2.
- 210 • Else, measures must be estimated. Design \mathbf{x} is thus added to the set \mathcal{X}_c . Outputs
 211 $\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})$ are computed for some values of $\boldsymbol{\xi}$ in order to build the surrogate model $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$
 212 on which the robustness and reliability measures $\tilde{\rho}(\mathbf{x})$ can be estimated for free. The
 213 associated accuracy mainly depends on the number of $\boldsymbol{\xi}$ training samples. The Gaus-
 214 sian Process surrogate models also permits to compute an approximation $\bar{\epsilon}(\mathbf{x})$ of the
 215 estimation error. Accuracy can then be improved by increasing the size of the training
 216 data $\{\boldsymbol{\xi}_i, \mathbf{q}(\mathbf{x}, \boldsymbol{\xi}_i)\}$ on which the surrogate $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$ is built.

217 In the case of a set of designs \mathcal{X}_{new} estimated simultaneously, gathered, such as for
 218 the initial Design of Experiments (DoE) or for a generation in evolutionary algorithms, we
 219 propose to guide the refinements with the Pareto Optimal Probability (POP) of the estimated
 220 boxes, in decreasing order. Intuition behind the choice of decreasing order is that the most
 221 promising boxes, once highly refined, might dominate most of the remaining boxes, thus
 222 rendering their refinement unnecessary. This refinement is performed until each box of \mathcal{X}_{new}
 223 is either dominated, or has reached an estimated error $\bar{\epsilon}$ below a user-defined threshold s_2 .
 224 POP computation is presented in section 3.2.

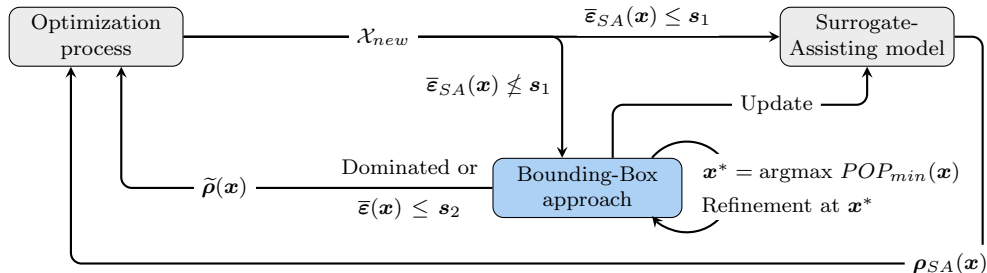


Figure 3: Structure of the SABBa framework

225 The strategy presented above and pictured in Figure 3 is made explicit in Algorithm 1.
 226 The tunable parameters are listed below and the Bounding-Box computational details are
 227 given in the following section.

Algorithm 1 Algorithm overview

```
1: Loop over values of  $\mathbf{s}_1$  and  $\mathbf{s}_2$ 
2: Initialise  $\mathcal{X}_c$  empty
3: while Optimisation running do
4:   Read new designs  $\mathcal{X}_{new}$ 
5:   for each  $\mathbf{x} \in \mathcal{X}_{new}$  do
6:     if  $\bar{\epsilon}_{SA}(\mathbf{x}) \leq \mathbf{s}_1$  then
7:       Return  $\boldsymbol{\rho}_{SA}(\mathbf{x})$  to the optimiser
8:     else
9:       Add  $\mathbf{x}$  in  $\mathcal{X}_c$ 
10:      Compute a first approximation  $\tilde{\boldsymbol{\rho}}(\mathbf{x})$  of  $\boldsymbol{\rho}(\mathbf{x})$ 
11:    end if
12:  end for
13:  while  $\mathcal{X}_r = \{\mathbf{x} \in \mathcal{X}_{\tilde{\boldsymbol{\rho}_B}} \cap \mathcal{X}_c \mid \bar{\epsilon}(\mathbf{x}) > \mathbf{s}_2\}$  is non-empty do
14:    Find  $\mathbf{x}^* = \underset{\mathbf{x} \in \mathcal{X}_r}{\operatorname{argmax}} POP_{min}(\mathbf{x})$ 
15:    Compute  $\mathbf{q}(\mathbf{x}^*, \boldsymbol{\xi})$  at some  $\boldsymbol{\xi}$ 
16:    Update surrogate  $\hat{\mathbf{q}}(\mathbf{x}^*, \cdot)$ 
17:    Compute new estimates  $\tilde{\boldsymbol{\rho}}(\mathbf{x}^*)$  and  $\bar{\epsilon}(\mathbf{x}^*)$ 
18:  end while
19:  Update  $\boldsymbol{\rho}_{SA}$  and  $\bar{\epsilon}_{SA}$  with the new  $\tilde{\boldsymbol{\rho}}$  and  $\bar{\epsilon}$  values
20:  Return  $\tilde{\boldsymbol{\rho}}(\mathbf{x})$  for  $\mathbf{x} \in \mathcal{X}_{new}$  to the optimiser
21: end while
```

228 $\mathcal{X}_{\tilde{\boldsymbol{\rho}_B}}$ contains all designs which associated boxes are non-dominated and \mathcal{X}_c refers to the
229 designs which measures have not been returned by the SA model. Hence, the boxes in \mathcal{X}_r
230 are all estimated without the SA model and both non-dominated and not refined up to \mathbf{s}_2 .

231 *Remark.* We consider to loop over finer and finer values of \mathbf{s}_1 and \mathbf{s}_2 . This allows more
232 accurate intermediate results and slightly cheaper overall convergence. Practically, vectors
233 of thresholds can be specified by the user.

234

235 The algorithm relies on a quite small set of parameters, namely:

- 236 • The predefined sequence of pair of thresholds $(\mathbf{s}_1, \mathbf{s}_2)$;
- 237 • The number of function evaluations N_{first} for the first approximations $\tilde{\boldsymbol{\rho}}$ and N_{new} the
238 number of additional evaluations for refinement;
- 239 • The number of designs N at each optimisation iteration and N_{init} at the first iteration.
240 The optimiser may impose these parameters.

241 4.2. Bounding-Boxes computation and refinement

242 To compute the boxes, robustness and reliability measures must be estimated, and the
243 associated error must be quantified. In particular, we focus in this paper on the following

244 measures: Expectation, variance, minimum, maximum and quantile. The values returned to
 245 the optimiser are denoted by $\hat{\boldsymbol{\rho}}(\mathbf{x})$ and $\hat{\boldsymbol{\varepsilon}}(\mathbf{x})$. As shown in Fig. 3 and Alg. 1, they can be
 246 computed from the $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$ surrogate with numerical integration or read from the SA model.
 247 These two computations are presented in details in the following sections.

248 Note that we make use of Gaussian Processes as surrogate models, giving both a predictive
 249 value and an associated predictive variance. Box widths are then computed based on this
 250 variance, relaxing the conservative assumption to a $\pm 3\sigma$ paradigm. Practically, with $\boldsymbol{\sigma}^2(\mathbf{z})$
 251 the predictive variance of a GP surrogate model, an error can be computed as:

$$\bar{\boldsymbol{\varepsilon}}(\mathbf{z}) = 3\boldsymbol{\sigma}(\mathbf{z}).$$

252 Although this does not imply $\bar{\boldsymbol{\varepsilon}}(\mathbf{z}) \geq |\boldsymbol{\varepsilon}(\mathbf{z})|$, with $\boldsymbol{\varepsilon}$ the true error of the surrogate, the
 253 probability of dissatisfying the conservative assumption is very low.

254 Other surrogate modelling techniques could be employed, as long as a specific strategy
 255 is given for computing $\bar{\boldsymbol{\varepsilon}}$.

256 4.2.1. Computed boxes

257 For each design \mathbf{x} where the SA model is not exploited, the boxes must be directly
 258 computed from samples of \mathbf{q} in the uncertain space. This step requires: (i) constructing
 259 a surrogate model $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$ of the quantities of interest, (ii) estimating the statistical mea-
 260 sures $\tilde{\boldsymbol{\rho}}(\mathbf{x})$ and associated error $\bar{\boldsymbol{\varepsilon}}(\mathbf{x})$ and (iii) refining these estimations until the prescribed
 261 accuracy is reached.

262 *Surrogate model.* Here, the underlying functions $\mathbf{q}(\mathbf{x}, \cdot)$ are approximated by GP models.
 263 Two approaches are considered:

- 264 • *Separated Spaces:* At a given \mathbf{x} , a GP is constructed only in Ξ on a set of samples
 265 $\{\mathbf{q}(\mathbf{x}, \boldsymbol{\xi}_i)\}_i$. This GP directly corresponds to $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$. In this setting, a set of N_{first}
 266 evaluations must be computed for getting the first approximation $\tilde{\boldsymbol{\rho}}$ at line 10 of Alg.
 267 1.
- 268 • *Coupled Space:* Here, a GP is built in $\mathcal{X} \times \Xi$ using all previous samples $\{\mathbf{q}(\mathbf{x}_i, \boldsymbol{\xi}_i)\}_i$.
 269 From this approximation $\hat{\mathbf{q}}$ of \mathbf{q} , the cut $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$ can be returned for measure estimation.
 270 Except at the very first loop, N_{first} can thus be set to 0.

271 Note that while the Separated Spaces (SS) approach builds a GP in a space of lower
 272 dimension ($Card(\Xi)$) than the Coupled Space (CS) approach ($Card(\mathcal{X} \times \Xi)$), thus easing
 273 the surrogate modelling task, it does not use surrounding samples in the design space and
 274 restarts from scratch at each new design point \mathbf{x} . These strategies will be compared on
 275 analytical test-cases in Section 5.

276 *Measure and error estimation.* Both SS and CS approaches allow having a predictive model
 277 $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$, that will be written $\hat{\mathbf{q}}_{\mathbf{x}}$, and the associated predictive variance $\boldsymbol{\sigma}_{\mathbf{q}}(\mathbf{x}, \cdot)$. The $\pm 3\sigma$
 278 paradigm provides the box widths, denoted as $\bar{\boldsymbol{\varepsilon}}_{\mathbf{q}_{\mathbf{x}}} = 3\boldsymbol{\sigma}_{\mathbf{q}}(\mathbf{x}, \cdot)$. For each output measure,
 279 indexed by k , the classical empirical estimators are exploited on the surrogate model $\hat{\mathbf{q}}_{\mathbf{x}}$ for

280 the computation of $\tilde{\rho}_k(\mathbf{x})$, such as the sample mean $\frac{1}{N} \sum_i \hat{\mathbf{q}}_x(\boldsymbol{\xi}_i)$ with *i.i.d.* samples $\boldsymbol{\xi}_i$. The
 281 associated errors $\bar{\varepsilon}_k(\mathbf{x})$ are then estimated using Eq. (6):

$$\bar{\varepsilon}_k(\mathbf{x}) = \begin{cases} \mathbb{E}_{\boldsymbol{\xi}} [\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})] & \text{for expectation} \\ \mathbb{E}_{\boldsymbol{\xi}} [(\bar{\varepsilon}_{\mu}(\mathbf{x}) + \bar{\varepsilon}_{q_x}(\boldsymbol{\xi}))^2 + 2|\hat{\mathbf{q}}_x(\boldsymbol{\xi}) - \tilde{\boldsymbol{\mu}}(\mathbf{x})|(\bar{\varepsilon}_{\mu}(\mathbf{x}) + \bar{\varepsilon}_{q_x}(\boldsymbol{\xi}))] & \text{for variance} \\ \max(|\tilde{\mathbf{m}}(\mathbf{x}) - \min_{\boldsymbol{\xi}}[\hat{\mathbf{q}}_x^-(\boldsymbol{\xi})]|, |\tilde{\mathbf{m}}(\mathbf{x}) - \min_{\boldsymbol{\xi}}[\hat{\mathbf{q}}_x^+(\boldsymbol{\xi})]|) & \text{for minimum} \\ \max(|\tilde{\mathbf{M}}(\mathbf{x}) - \max_{\boldsymbol{\xi}}[\hat{\mathbf{q}}_x^-(\boldsymbol{\xi})]|, |\tilde{\mathbf{M}}(\mathbf{x}) - \max_{\boldsymbol{\xi}}[\hat{\mathbf{q}}_x^+(\boldsymbol{\xi})]|) & \text{for maximum} \\ \max(|\tilde{\mathbf{q}}^p(\mathbf{x}) - \mathbf{q}_{\boldsymbol{\xi}}^p[\hat{\mathbf{q}}_x^-(\boldsymbol{\xi})]|, |\tilde{\mathbf{q}}^p(\mathbf{x}) - \mathbf{q}_{\boldsymbol{\xi}}^p[\hat{\mathbf{q}}_x^+(\boldsymbol{\xi})]|) & \text{for quantile} \end{cases} \quad (6)$$

282 where $\hat{\mathbf{q}}_x^+(\boldsymbol{\xi}) = \hat{\mathbf{q}}_x(\boldsymbol{\xi}) + \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})$ and $\hat{\mathbf{q}}_x^-(\boldsymbol{\xi}) = \hat{\mathbf{q}}_x(\boldsymbol{\xi}) - \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})$. In practice, the quantiles and
 283 expected values above are approximated by means of Monte Carlo Sampling (MCS) on surro-
 284 gate model at very low cost. A formal justification of these box sizes is given in Appendix B.

285

286 *Refinement.* We also provide guidance for refining the surrogate model $\hat{\mathbf{q}}_x(\boldsymbol{\xi})$ that permits
 287 low-cost MCS. While one could rely on a space-filling paradigm, we choose here to use
 288 GP-based refinement criteria. In practice, the proposed criterion should explore areas of
 289 high probability featuring significant uncertainty. In addition, this criterion should prioritise
 290 refinement of the least well-estimated measures. To this extent, we propose partial criteria
 291 associated with each statistical measure that shall then be combined within a weighted sum
 292 to obtain the global criterion. These partial criteria are given hereafter:

$$c_k(\boldsymbol{\xi}) = \begin{cases} \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})\phi(\boldsymbol{\xi}) & \text{for expectation} \\ \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})\phi(\boldsymbol{\xi}) & \text{for variance} \\ \left[\frac{\tilde{\mathbf{m}} - \hat{\mathbf{q}}_x^-(\boldsymbol{\xi})}{2\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})} \right]_+ & \text{for minimum} \\ \left[\frac{\hat{\mathbf{q}}_x^+(\boldsymbol{\xi}) - \tilde{\mathbf{M}}}{2\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})} \right]_+ & \text{for maximum} \\ \left[\frac{\tilde{\mathbf{q}}^p - \hat{\mathbf{q}}_x^-(\boldsymbol{\xi})}{2\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})} \right]_+ \left[\frac{\hat{\mathbf{q}}_x^+(\boldsymbol{\xi}) - \tilde{\mathbf{q}}^p}{2\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})} \right]_+ \phi(\boldsymbol{\xi}) & \text{for quantile} \end{cases} \quad (7)$$

293 with the same definition of $\hat{\mathbf{q}}_x^+(\boldsymbol{\xi})$ and $\hat{\mathbf{q}}_x^-(\boldsymbol{\xi})$ as before and where $[\cdot]_+ = \max(0, \cdot)$. To
 294 promote areas of high probability, we choose here to multiply the criteria for the mean,
 295 variance and quantile measures by the input Probability Density Function (PDF) $\phi(\boldsymbol{\xi})$ in
 296 order to put more weight on the most likely area. Justifications for these formulas are
 297 provided in Appendix C.

298 These partial criteria are then combined into the final refinement criterion through the
 299 following weighted sum:

$$c(\boldsymbol{\xi}) = \sum_{k=1}^m w_k \bar{c}_k(\boldsymbol{\xi}) \quad (8)$$

300 with $\bar{c}_k(\boldsymbol{\xi})$ the normalised partial criteria, m the number of measures and w_k the weights.
 301 The normalised partial criteria are computed as follows:

$$\bar{c}_k(\boldsymbol{\xi}) = \frac{c_k(\boldsymbol{\xi}) - \min_{\boldsymbol{\xi}}[c_k(\boldsymbol{\xi})]}{\max_{\boldsymbol{\xi}}[c_k(\boldsymbol{\xi})] - \min_{\boldsymbol{\xi}}[c_k(\boldsymbol{\xi})]} \in [0, 1].$$

302 Finally, we propose here to compute the weights as the ratio between the conservative
 303 error $\bar{\epsilon}_k$ and the target accuracy. In this manner, any partial criterion associated with high
 304 error compared to the target accuracy will heavily influence the final criterion. Practically,
 305 to emphasise this behaviour, the dependence to the conservative error is chosen quadratic:

$$w_k = \left(\frac{\bar{\epsilon}_k}{s_{2k}} \right)^2.$$

306 Note that in the case of multi-point refinement, we conduct a greedy sequential approach
 307 by assuming that previous refinements are performed, fixing the predictive values of the GP
 308 surrogate model and recomputing the predictive variance to obtain the updated refinement
 309 criterion. We can then perform Black-box evaluations in parallel on these points. This
 310 approach is usually called the Kriging Believer strategy and allows performing multi-point
 311 refinement efficiently without the need of any clustering or local penalisation heuristics.
 312 However, this strategy makes a lot of assumptions and is often sub-optimal when performing
 313 many refinements in parallel.

314 4.2.2. SA-based boxes

315 When the SA model error is low enough, below \mathbf{s}_1 in all output dimension, the predictive
 316 value $\boldsymbol{\rho}_{SA}(\mathbf{x})$ is directly returned to the optimiser. As stated previously, we propose here to
 317 use Gaussian Processes as SA model, which gives access to the predictive variance in order
 318 to compute box widths.

319 The SA model is built on the previously computed boxes to return an approximation
 320 $\boldsymbol{\rho}_{SA}$ of $\boldsymbol{\rho}$ in \mathcal{X} . In practice, the available data for constructing this model are boxes of
 321 various sizes. These boxes can be considered as noisy evaluations of $\boldsymbol{\rho}$ at different \mathbf{x} , with
 322 heterogeneous noises. Using again the $\pm 3\sigma$ paradigm, these noises can be translated into
 323 heterogeneous variances $\sigma_i^2 = \left(\frac{\bar{\epsilon}^l(\mathbf{x}_i)}{3} \right)^2$. This allows to make use of heteroscedastic Gaus-
 324 sian Processes, which naturally take into account heterogeneous noise variances, under a
 325 gaussianity assumption. The measure estimations $\boldsymbol{\rho}_{SA}$ and associated error $\bar{\epsilon}_{SA}$ at a new
 326 design \mathbf{x} are computed as follows:

$$\begin{aligned} \boldsymbol{\rho}_{SA}(\mathbf{x}) &= \mathbf{k}_*^T (K + \Delta)^{-1} \tilde{\boldsymbol{\rho}} \\ \bar{\epsilon}_{SA}(\mathbf{x}) &= 3\sigma_{SA}(\mathbf{x}) = 3(k_{**} - \mathbf{k}_*^T (K + \Delta)^{-1} \mathbf{k}_*). \end{aligned} \quad (9)$$

327 The matrix $K = K(\{\mathbf{x}_i\}_i, \{\mathbf{x}_i\}_i)$ represents the autocovariance matrix between training
 328 points, $k_{**} = k(\mathbf{x}, \mathbf{x})$ at the new design and $\mathbf{k}_* = \mathbf{k}(\mathbf{x}, \{\mathbf{x}_i\}_i)$ the covariance vector between
 329 \mathbf{x} and training points. The diagonal matrix $\Delta = \text{diag}(\{\sigma_i^2\}_i)$ represents the heterogeneous
 330 gaussian noises presented previously. More details on GP surrogate models can be found in
 331 [40].

332 *4.3. Quality indicator*

333 Assessing and comparing the performance of several methods requires the computation
 334 of a quantitative quality indicator. To this extent, the Hausdorff distance d_H is a classical
 335 choice for computing the closeness of the found optimal set to the true one.

336 However, in practice, the modified Hausdorff distance d'_H proposed in [41] captures the
 337 similarities more efficiently by replacing a maximum with an expectation.

338 In the Bounding-Box context, there is no Pareto Optimal set but rather a set of non-
 339 dominated designs, each of them having a Pareto Optimal Probability. The approximated
 340 Pareto front $\tilde{\mathcal{P}}$ and Pareto optima $\mathcal{X}_{\tilde{\mathcal{P}}}$ are hence aleatory. We propose to compute the
 341 expected value of the modified Hausdorff distance with respect to realisations of $\tilde{\mathcal{X}}_{\mathcal{P}}$.

342 The deterministic modified Hausdorff distance d'_H writes follows:

$$\begin{aligned} d'_H(\mathcal{A}, \mathcal{B}) &= \max(d'_1(\mathcal{A}, \mathcal{B}), d'_1(\mathcal{B}, \mathcal{A})), \\ d'_1 &= \frac{1}{N} \sum_{a \in \mathcal{A}} d_2(a, \mathcal{B}), \\ d_2(a, \mathcal{B}) &= \min_{b \in \mathcal{B}} [\|a - b\|_2]. \end{aligned}$$

343 Under the box independence and uniformity assumptions, as in Section 3.2 we have $\forall \mathbf{x}$,

$$\boldsymbol{\rho}(\mathbf{x}) \sim \mathcal{U}\left(\mathcal{B}(\hat{\boldsymbol{\rho}}(\mathbf{x}), \hat{\boldsymbol{\varepsilon}}(\mathbf{x}))\right),$$

344 where $\hat{\boldsymbol{\rho}}(\mathbf{x})$ and $\hat{\boldsymbol{\varepsilon}}(\mathbf{x})$ are the values returned to the optimiser, either from the BB approach
 345 or the SA strategy. The proposed expected modified Hausdorff distance reads:

$$Q_{\mathcal{B}} = \mathbb{E}_{\tilde{\mathcal{X}}_{\mathcal{P}}} [d'_H(\mathcal{X}_{\mathcal{P}}, \tilde{\mathcal{X}}_{\mathcal{P}})]. \quad (10)$$

346 where a realisation of $\tilde{\mathcal{X}}_{\mathcal{P}}$ corresponds to a realisation of $\boldsymbol{\rho}(\mathbf{x})$ for all \mathbf{x} and the computation
 347 of the classical Pareto optima.

348 Intuitively, $Q_{\mathcal{B}}$ can be seen as an averaged distance between the real Pareto-optimal area
 349 and the preimage of a Pareto front realization. In a normalized input space such as the
 350 $[0, 1]^2$ square, a value of $Q_{\mathcal{B}} = 1$ corresponds to a terrible score, with approximated and real
 351 Pareto optima on opposite sides of the input space. On the contrary, a score of $Q_{\mathcal{B}} = 10^{-2}$
 352 reveals an excellent agreement between the approximated and the real optimal area.

353 *4.4. Summary of SABBa variants*

354 Based on the SABBa algorithm (Alg. 1), we explore potential variants according to some
 355 choices. First, as denoted at the beginning of Section 4.2.1, boxes centers and widths can
 356 either be computed using a *Coupled Space* (CS) surrogate model, or *Separated Spaces* (SS)
 357 surrogate models. Secondly, the user can use (or not) the Surrogate-Assisting (SA) strategy.
 358 These algorithmic variants are made explicit in Algorithm 2, where the use of the SA strategy
 359 is toggled at line 6, and the SS or CS variants are selected lines 16 to 19.

360

Algorithm 2 SABBa variants

```
1: Loop over values of  $\mathbf{s}_1$  and  $\mathbf{s}_2$ 
2: Initialise  $\mathcal{X}_c$  empty
3: while Optimisation running do
4:   Read new designs  $\mathcal{X}_{new}$ 
5:   for each  $\mathbf{x} \in \mathcal{X}_{new}$  do
6:     if using SA and  $\bar{\epsilon}_{SA}(\mathbf{x}) \leq \mathbf{s}_1$  then
7:       Return  $\boldsymbol{\rho}_{SA}(\mathbf{x})$  to the optimiser
8:     else
9:       Add  $\mathbf{x}$  in  $\mathcal{X}_c$ 
10:      Compute a first approximation  $\tilde{\boldsymbol{\rho}}(\mathbf{x})$  of  $\boldsymbol{\rho}(\mathbf{x})$ 
11:    end if
12:  end for
13:  while  $\mathcal{X}_r = \{\mathbf{x} \in \mathcal{X}_{\tilde{\mathcal{P}}_B} \cap \mathcal{X}_c \mid \bar{\epsilon}(\mathbf{x}) > \mathbf{s}_2\}$  is non-empty do
14:    Find  $\mathbf{x}^* = \underset{\mathbf{x} \in \mathcal{X}_r}{\operatorname{argmax}} POP_{min}(\mathbf{x})$ 
15:    Compute  $\mathbf{q}(\mathbf{x}^*, \boldsymbol{\xi})$  at some  $\boldsymbol{\xi}$ 
16:    if using SS surrogate model then
17:      Update  $\hat{\mathbf{q}}(\mathbf{x}^*, \cdot)$  in  $\Xi$ 
18:    else if using CS surrogate model then
19:      Update  $\hat{\mathbf{q}}(\cdot, \cdot)$  in  $\mathcal{X} \times \Xi$ 
20:    end if
21:    Compute new estimates  $\tilde{\boldsymbol{\rho}}(\mathbf{x}^*)$  and  $\bar{\epsilon}(\mathbf{x}^*)$ 
22:  end while
23:  Update  $\boldsymbol{\rho}_{SA}$  and  $\bar{\epsilon}_{SA}$  with the new  $\tilde{\boldsymbol{\rho}}$  and  $\bar{\epsilon}$  values
24:  Return  $\tilde{\boldsymbol{\rho}}(\mathbf{x})$  for  $\mathbf{x} \in \mathcal{X}_{new}$  to the optimiser
25: end while
```

361 These combinations lead to four main variants, denoted SA-CS, SA-SS, CS and SS, where
362 the two latest do not use the SA strategy. Note that the SS variant is the only one that does
363 not build any surrogate in the design space, making it very computationally expensive. For
364 this reason, it will not be further studied in the following of this paper. Parallels can be made
365 between these strategies and formulations 3 and 4 from [24]. Among the three remaining
366 variants, one can expect SA-CS to give better results than SA-SS and CS, taking advantage
367 of both the low-dimensional Surrogate-Assisting model and the coupled space correlation to
368 speed up box refinement.

369 In the following, we compare the performance of the proposed variants to an A Priori
370 MetaModel (APMM) strategy. A surrogate model $\hat{\mathbf{q}}(\mathbf{x}, \boldsymbol{\xi})$ is constructed in the coupled space
371 based on a given Design of Experiments (DoE). The robustness and reliability measures at
372 different locations \mathbf{x} are then numerically approximated using this surrogate throughout
373 the optimisation process. The overall computational cost of this strategy is thus entirely
374 dependent on the initial DoE.

375 In the next section, the variants described above are applied to analytical test-cases to

376 assess their performance. The quality of the optimisation outputs is quantified using the
 377 quantitative indicator presented above.

378 5. Analytical comparisons

379 We apply here SABBa to two analytical test-cases. The first one is low-dimensional
 380 and deals with a Taguchi multi-objective robustness formulation (mean optimisation and
 381 variance minimisation). The second test-case features a higher number of dimensions and
 382 consists in a mean optimisation under quantile constraint.

383 Ten runs are performed for each strategy to capture both the mean convergence curve and
 384 the associated variability, represented as a translucent band around the mean. For plotting
 385 purposes, the log distance is assumed to show a Gaussian distribution over the repeated runs,
 386 implying a log-normal distribution over the actual distance. Note that a high variability of
 387 the convergence curves reveals a lack of reliability of the associated approaches.

388 5.1. Test-case 1: Unconstrained Taguchi optimisation

389 This problem is a bi-objective robust optimisation proposed in [35]. There are two design
 390 variables \mathbf{x} and one uncertain parameter ξ , and the problem reads:

$$\begin{aligned}
 &\text{minimise: } \boldsymbol{\rho}_f(\mathbf{x}) = \begin{pmatrix} \mu(\mathbf{x}) \\ \sigma^2(\mathbf{x}) \end{pmatrix} \\
 &\quad \text{where: } \mu(\mathbf{x}) = \mathbb{E}_\xi[q(\mathbf{x}, \xi)] \\
 &\quad \quad \sigma^2(\mathbf{x}) = \mathbb{V}_\xi[q(\mathbf{x}, \xi)] \\
 &\quad \text{with: } q(\mathbf{x}, \xi) = \xi - x_1\xi^5 + \cos(2\pi x_2\xi) + 5 \\
 &\quad \quad \xi \sim \mathcal{U}([0, 1]) \\
 &\text{by changing: } (x_1, x_2) \in [1, 2]^2 \tag{11}
 \end{aligned}$$

391 The Pareto front associated with this problem is discontinuous, and the optimal set in
 392 the design space is the union of a segment and a point (see Fig. 4).

393 For this first test-case, we consider two different surrogate-modelling capabilities. The
 394 aim is to illustrate SABBa performance both when the surrogate is able to represent the
 395 underlying functions accurately and when it shows poor efficiency. This highly impacts
 396 the quality of the APMM $\hat{\mathbf{q}}$, the Surrogate-Assisting model $\boldsymbol{\rho}_{SA}(\mathbf{x})$ and the separated or
 397 Coupled-Space models $\hat{\mathbf{q}}(\mathbf{x}, \cdot)$.

398 5.1.1. With high-quality surrogate model

399 The unconstrained Taguchi optimisation problem is first solved using high-quality meta-
 400 modelling approaches. Practically, we build a heterogeneous GP surrogate model with an
 401 anisotropic RBF kernel (also called squared-exponential, exponential quadratic or Gaussian),

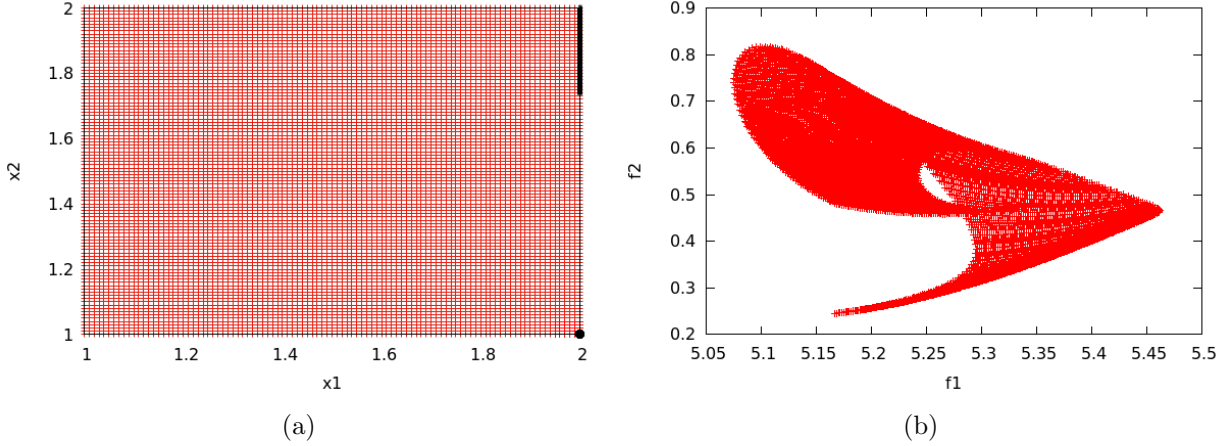


Figure 4: Test-case 1: a) Discretisation of the design space in red and Pareto optimal sets in black. b) Image of the discretised points in the objective (μ, σ^2) space.

402 and Automatic Relevance Determination (ARD):

$$k(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left(-\frac{r_l^2}{2}\right)$$

$$\text{with } r_l = \sqrt{\sum_{i=1}^m \left(\frac{x_i - x'_i}{l_i}\right)^2}$$

403 We recall that the kernel function gives the covariance matrix in Equation (9).

404 This model requires $m + 1$ hyperparameters $\{\sigma^2, l_1, \dots, l_m\}$ to be optimised but captures
 405 the characteristic lengthscale associated with each input dimension.

406 Note that here, the thresholds \mathbf{s}_1 and \mathbf{s}_2 are sequentially refined five times. To alleviate
 407 the tuning of these thresholds, SABBA can deal with normalised thresholds $\bar{\mathbf{s}}_1$ and $\bar{\mathbf{s}}_2$. At
 408 each iteration, the range h_i covered in the i^{th} -dimension is updated, namely,

$$\forall i, h_i = \max_{\mathbf{x}}[\rho_i(\mathbf{x})] - \min_{\mathbf{x}}[\rho_i(\mathbf{x})],$$

409 and the thresholds $\bar{\mathbf{s}}_1$ and $\bar{\mathbf{s}}_2$ are given in percentage of \mathbf{h} . Here, $\bar{\mathbf{s}}_1$ and $\bar{\mathbf{s}}_2$ are both
 410 sequentially taken as 50%, 40%, 30%, 20%, 10% and 5% in all dimensions. The chosen
 411 parameters of SABBA are as follows: $N_{init} = 10$, $N = 1$ (sequential optimiser), $N_{first} = 5$
 412 and $N_{new} = 1$ (sequential refinement).

413 Figure 5 pictures the convergence curves of the APMM strategy and the three studied
 414 SABBA variants (SA-CS, SA-SS and CS). The mean curves are mostly comparable, with a
 415 slight advantage for SA-CS. However, the associated variability is much smaller when using
 416 any SABBA variant with respect to the APMM strategy. The indicator is assumed to follow
 417 a normal distribution in log scale, hence to be log-normal. The high variance associated to
 418 the APMM strategy coupled with the heavy tail of the log-normal distribution makes the
 419 approach very unreliable. We picture this risk in Figure 6, where the worst result out of ten

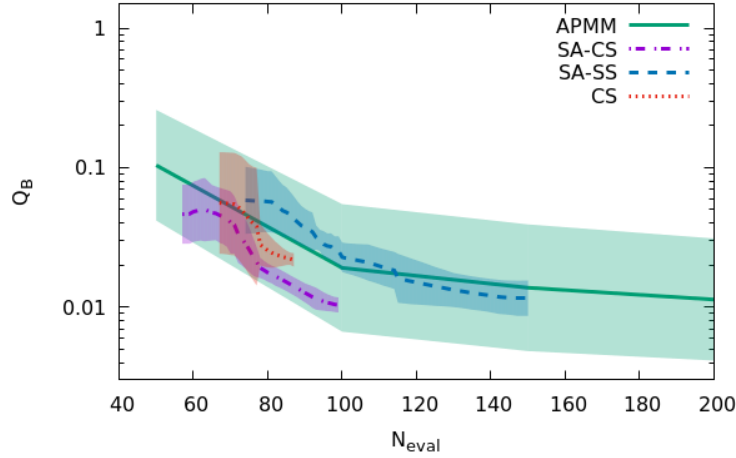


Figure 5: Test-case 1-a: Cost comparison between APMM and three SABBA variants.

420 repeated runs of SA-CS and the APMM strategy are plotted. These outputs correspond to
 421 $N_{eval} \approx 100$.

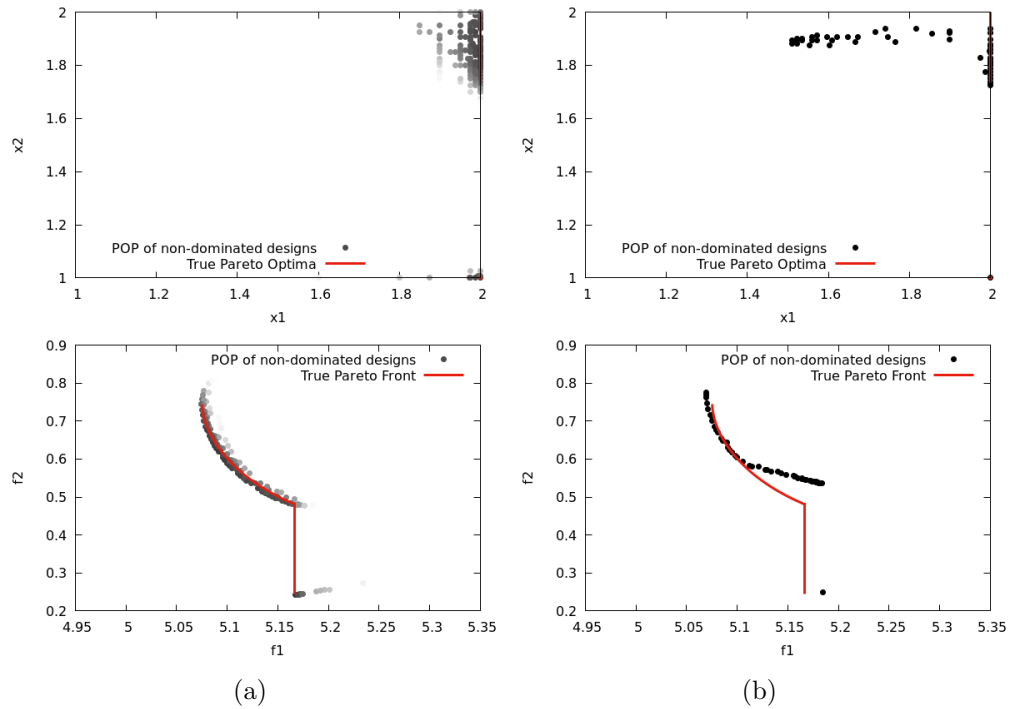


Figure 6: Worst optimisation results: (a) SABBA SA-CS, 93 evaluations , $Q_B = 1.29 \times 10^{-2}$. (b) APMM, 100 evaluations , $Q_B = 1.91 \times 10^{-1}$.

422 In these figures, optimal designs returned by SABBA are plotted in greyscale. This refers
 423 to the Pareto Optimal Probability (POP) of each design, ranging continuously from 0 (white)

424 to 1 (black).

425 In line with Figure 5, Figure 6 reveals that the APMM strategy may return very inaccurate
 426 results when the DoE that was used for constructing the coupled-space model is not well
 427 sampled in the optimal area. On the contrary, the adaptive surrogate model construction
 428 permits SABBa to return very stable results.

429 *5.1.2. With a low-quality surrogate model*

430 In the following, the same optimisation problem is solved using a low-quality surrogate
 431 model in both SABBa and the APMM strategy. Contrarily to the previous formulation, we
 432 build an isotropic GP surrogate model with only one lengthscale, that has to account for all
 433 dimensions. Practically,

$$k(\mathbf{x}, \mathbf{x}') = \sigma^2 \exp\left(-\frac{r_l^2}{2}\right)$$

$$\text{with } r_l = \frac{1}{l} \sqrt{\sum_{i=1}^m (x_i - x'_i)^2}$$

434 Only two hyperparameters $\{\sigma^2, l\}$ must be optimised. However, this model will notably
 435 fail when the characteristic lengths of the function in the different dimensions are very
 436 disparate. This test-case aims at simulating problems where the coupled space behaviour
 437 is hard to model. This would naturally arise when the number of dimensions is significant.
 438 Hence, one can expect the SA strategy to yield a significant cost improvement through
 439 low-dimensional measures surrogate modelling.

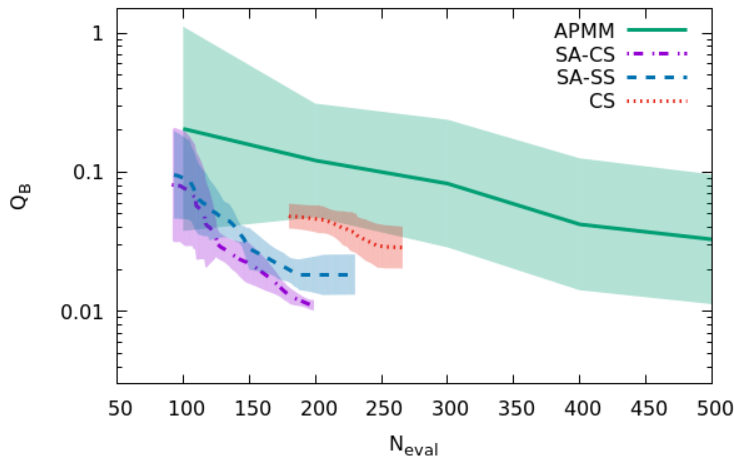


Figure 7: Test-case 1-b: Cost comparison between APMM and three SABBa variants.

440 Such improvement is indeed revealed in Figure 7. The use of the SA strategy has two
 441 consequences: (i) non-Surrogate-Assisted approaches (APMM and SABBa CS) show poor
 442 performance compared to the other strategies and (ii) the gap between SA-CS and SA-SS is

443 much narrower. Indeed, here, they both rely for the most part on the low-dimensional SA
 444 model.

445 As previously, the worst optimisation outputs are plotted for SABBa SA-CS and the
 446 APMM approach. In Figure 8, SABBa shows again much higher consistency and accuracy
 447 compared to APMM.

448 The use of coupled space surrogate models and Surrogate-Assisting strategy have shown
 449 to bring a significant cost reduction for the SABBa SA-CS framework. It performs better in
 450 average than the APMM strategy and shows far greater consistency and robustness.

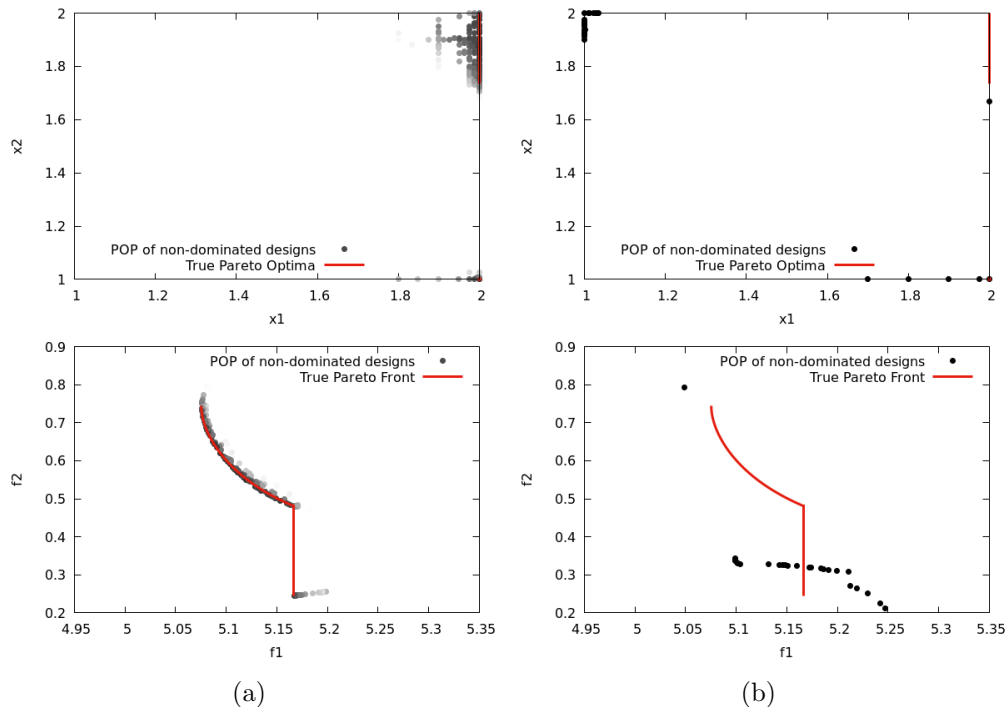


Figure 8: Worst optimisation results: (a) SABBa SA-CS, 196 evaluations , $Q_B = 1.23 \times 10^{-2}$. (b) APMM, 200 evaluations , $Q_B = 7.94 \times 10^{-1}$.

451 *5.2. Test-case 2: Quantile-constrained mean performance optimisation*

452 We propose this second test-case to assess the performance of SABBa in a higher dimen-
 453 sional case and in the presence of a reliability-based constraint (derived from the Six-Hump
 454 Camel function). The objective is a robustness measure derived from a simplified Rosen-
 455 brock function. We consider here four design variables and three uncertain parameters. The

456 problem is stated as follows:

$$\begin{aligned}
& \text{minimise: } \boldsymbol{\rho}_f(\mathbf{x}) = \mu(\mathbf{x}) \\
& \text{satisfying: } \boldsymbol{\rho}_g(\mathbf{x}) = \mathbf{q}^{95\%}(\mathbf{x}) \leq 1 \\
& \text{where: } \mu(\mathbf{x}) = \mathbb{E}_{\boldsymbol{\xi}}[q_1(\mathbf{x}, \boldsymbol{\xi})] \\
& \quad \mathbf{q}^{95\%}(\mathbf{x}) = \mathbf{q}_{\boldsymbol{\xi}}^{95\%}[q_2(\mathbf{x}, \boldsymbol{\xi})] \\
& \text{with: } q_1(\mathbf{x}, \boldsymbol{\xi}) = \sum_{i=1}^3 \left[(1 - x_i) + 3 \left(1 + \frac{\arctan(5(\xi_i - 0.5))}{2} \right) (x_{i+1} - x_i^2)^2 \right] \\
& \quad q_2(\mathbf{x}, \boldsymbol{\xi}) = \left(4 - 2.1x_1^2 + \frac{x_1^4}{3} \right) x_1^2 + x_1x_2 + (-4 + 4x_2^2)x_2^2 \\
& \quad \quad + \frac{\cos(2\pi\xi_1) - \sin(\frac{\pi}{2}\xi_1) - \xi_1 - (\cos(2\pi \cdot 0.05) - \sin(\frac{\pi}{2} \cdot 0.05) - 0.05)}{5} \\
& \quad \boldsymbol{\xi} \sim \mathcal{U}([0, 1]^3) \\
& \text{by changing: } \mathbf{x} \in [-0.2, 1.2]^4 \tag{12}
\end{aligned}$$

457 One can note that the robustness measure reduces to the classical formulation of the 4D
458 Rosenbrock function and the reliability measures to the Six-Hump Camel function. Analytically,
459 it holds that:

$$\begin{aligned}
\mu(\mathbf{x}) &= \sum_{i=1}^3 \left[(1 - x_i) + 3(x_{i+1} - x_i^2)^2 \right], \\
\mathbf{q}^{95\%}(\mathbf{x}) &= \left(4 - 2.1x_1^2 + \frac{x_1^4}{3} \right) x_1^2 + x_1x_2 + (-4 + 4x_2^2)x_2^2. \tag{13}
\end{aligned}$$

460 The optimum of this deterministic problem is found at $\mathbf{x}_* \approx (0.7033, 0.7035, 0.6212, 0.3859)$
461 with $\mathbf{q}^{95\%}(\mathbf{x}_*) = 1$ and $\mu(\mathbf{x}_*) \approx 0.4981$.

462 For this test case, both $\bar{\mathbf{s}}_1$ and $\bar{\mathbf{s}}_2$ are sequentially taken as 50%, 40%, 30%, 20%, 10%,
463 5%, 3%, 2%, 1% and 0.5%. As for the other parameters, $N_{init} = 10$, $N = 1$ (sequential
464 optimiser), $N_{first} = 5$ and $N_{new} = 1$ (sequential refinement).

465 Figure 9 shows a slight mean improvement when using SA-CS compared to the APMM
466 strategy. The variability of the output is also halved with all SABBa variants, which is
467 critical for real-world applications. Note that the plateau that is reached by the SA-CS
468 curve is actually a plotting artefact. All runs have different final number of evaluations,
469 and we considered the indicator $Q_{\mathcal{B}}$ constant when the optimum is reached. Therefore, the
470 average of these curves tends to flatten at the end.

471 Again, we plot the worst optimisation outputs in Figures 10. They are depicted in parallel
472 coordinates plots, with a POP_{\min} greyscale. Each efficient individual is represented by a grey
473 curve and the true optimum is in red. This comparison reveals again the high unreliability
474 of the APMM strategy with respect to the SABBa framework.

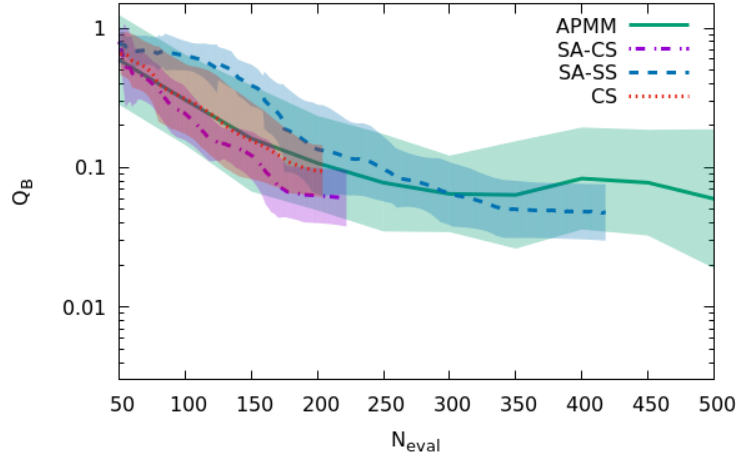


Figure 9: Test-case 2: Cost comparison between APMM and three SABBa variants.

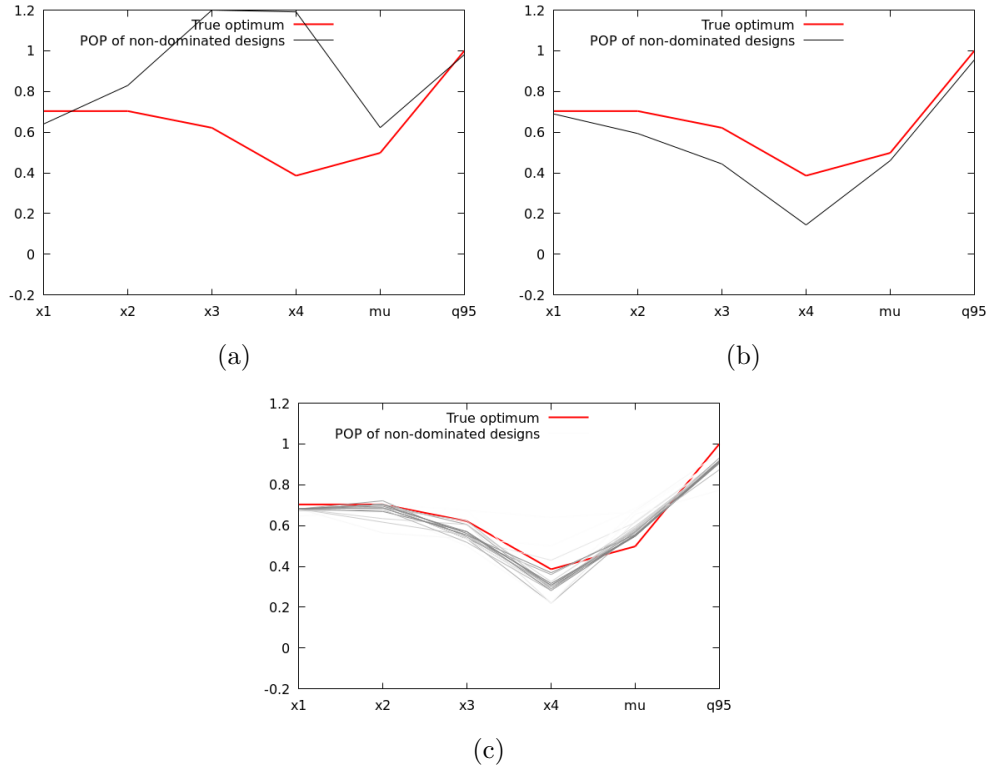


Figure 10: Worst optimisation results: (a) APMM, 150 evaluations, $Q_B = 1.0 \times 10^0$. (b) SABBa SA-CS, 161 evaluations, $Q_B = 1.12 \times 10^{-1}$. (c) APMM, 200 evaluations, $Q_B = 3.24 \times 10^{-1}$.

475 6. Physical applications

476 Three real-world test cases are tackled hereafter. The first one, Section 6.1, is the classi-
 477 cal two-bar truss structural test case, in which the external force and the Young modulus are

478 considered uncertain. This application features four design parameters and two uncertain
 479 variables. Then, shape optimization of an Organic Ranking Cycle (ORC) turbine is per-
 480 formed in Section 6.2, with nine design parameters and three uncertain parameters. Finally,
 481 the design of a Thermal Protection System (TPS) is optimized in Section 6.3, where the
 482 design space is of dimension two and the uncertain space of dimension twelve.

483 6.1. Two-bar truss

484 The two-bar truss optimization problem is notably illustrated in Refs. [42] and [20]. The
 485 uncertainty-based optimization problem is formulated as follows (with a schematic represen-
 486 tation in Figure 11(a)):

$$\begin{aligned}
 &\text{minimise: } \boldsymbol{\rho}_f(\mathbf{x}) = V(\mathbf{x}) \\
 &\text{satisfying: } \boldsymbol{\rho}_g(\mathbf{x}) = \begin{pmatrix} c_1(\mathbf{x}) \\ c_2(\mathbf{x}) \end{pmatrix} \leq \begin{pmatrix} s_{\max} \\ 0 \end{pmatrix} \\
 &\text{where: } c_1(\mathbf{x}) = q^{0.999}[s(\mathbf{x}, \boldsymbol{\xi})] \\
 &\quad c_2(\mathbf{x}) = q^{0.999}[s(\mathbf{x}, \boldsymbol{\xi}) - s_{crit}(\mathbf{x}, \boldsymbol{\xi})] \\
 &\text{with: } \boldsymbol{\xi} \sim \mathcal{N}\left(\begin{pmatrix} 150000 \\ 210000 \end{pmatrix}, \begin{pmatrix} 30000^2 & 0 \\ 0 & 21000^2 \end{pmatrix}\right) \\
 &\text{by changing: } \mathbf{x} \in [20, 80] \times [800, 1200] \times [700, 800] \times [2, 3] \tag{14}
 \end{aligned}$$

487 In the above, the design variables are: (x_1) the diameter of the cross section d , (x_2) the
 488 bar length L , (x_3) the structure half-width B and (x_4) the thickness of the cross section T .
 489 The uncertain parameters refer to (ξ_1) the external force F and (ξ_2) the elastic modulus E .
 490 The objective is to minimize the total volume $V(\mathbf{x}) = 2\pi x_1 x_2 x_4 \times 10^{-6}$ while verifying that
 491 the probability of $s(\mathbf{x}, \boldsymbol{\xi}) = \frac{x_2 \xi_1}{2\pi x_1 x_4 \sqrt{x_2^2 - x_3^2}}$ exceeding $s_{\max} = 400 \text{ N.mm}^{-2}$ and $s_{crit}(\mathbf{x}, \boldsymbol{\xi}) =$
 492 $\frac{\pi^2 \xi_2 (x_1^2 + x_4^2)}{8x_2^2}$ are both below 0.001.

493 The problem is represented in Fig. 11(b), where the objective value ($V(\mathbf{x})$, to be min-
 494 imised) is plotted in the constraints space with a colour scale. The abscissa and ordinate
 495 directions refer to the constraints $c_1(\mathbf{x})$ and $c_2(\mathbf{x})$; the associated thresholds are drawn with
 496 red lines. The admissible set is in the lower left quadrangle ($c_1 < 400 \text{ N.mm}^{-2}$ and $c_2 < 0$
 497 N.mm^{-2}) and one may note that the objective is nearly constant on the limit $c_1 = 400$
 498 N.mm^{-2} , with optimum value at $(c_1, c_2) = (400, 0)$.

499 This optimisation has been solved with the SA-CS variant. Thresholds \mathbf{s}_1 and \mathbf{s}_2 are
 500 sequentially reduced up to 0.1% of the total ranges, with four steps 3%, 1%, 0.3% and 0.1%.

501 Results are depicted in Figure 12 with parallel coordinates plots. The four thresholds
 502 are sequentially reached with a total number of **42**, **44**, **46** and **52** function evaluations, and
 503 an optimal objective value of roughly 0.698 is found. Uniform approximation errors from
 504 SABBa are represented as vertical intervals for each design with non-zero POP. Note that

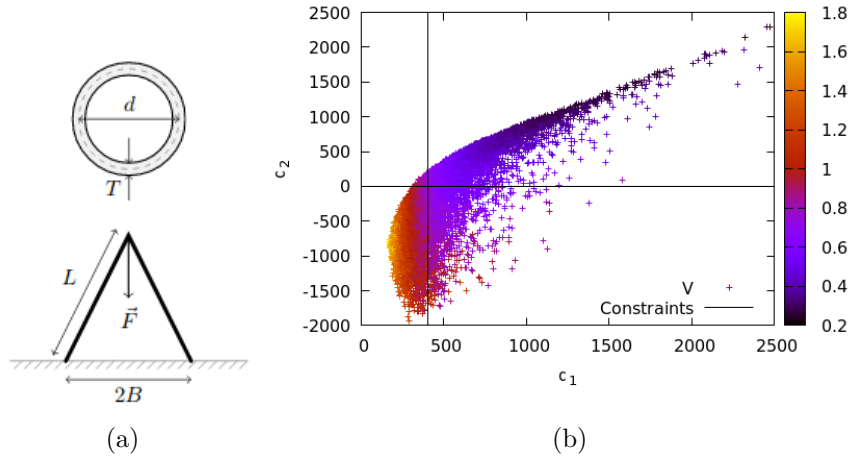


Figure 11: (a) Schematic representation of the two bars, with bar section above (from [42]). (b) Representation in the objective/constraints space, constraints in abscissa and ordinate, objective in color.

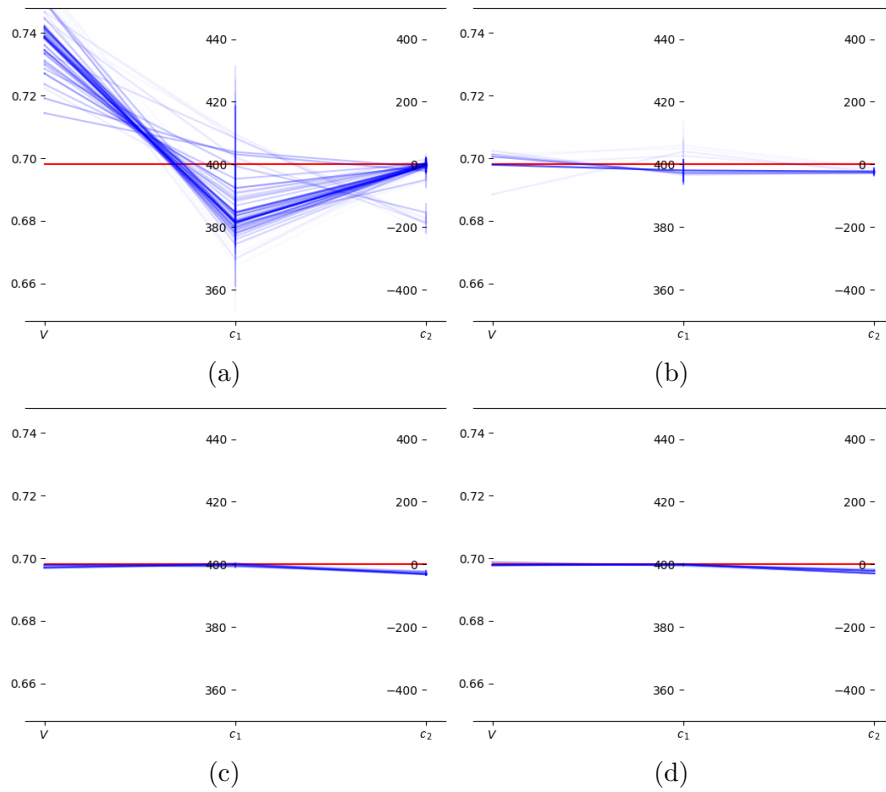


Figure 12: Objective and constraints values with (a) 42, (b) 44, (c) 46 and (d) 52 evaluations. Transparency driven by POP value and optimal value in red.

505 the second constraint c_2 is slightly off its optimal value 0 because the objective value V is
 506 nearly constant w.r.t. c_2 , as can be observed in Figure 11(b).

507 On this analytical engineering test-case, SABBa reveals very parsimonious. Uncertainty-
 508 based optimisation with 95% quantiles has been solved with only 40 to 50 evaluations.

509 6.2. ORC turbine shape optimisation

510 This test case aims to show the potential of SABBa in solving a problem formulation that
 511 includes the concepts of robustness and reliability. In particular, we focus on multi-objective
 512 shape optimization to reduce the mean and variance of a given quantity of interest with a
 513 statistical constraint.

514 Here, we consider the design of a 2D Organic Rankine Cycles (ORCs) turbine, which
 515 is a very relevant problem to exploit renewable energy sources. The studied blade profile
 516 is the Biere, which results in a convergent-divergent cascade passage to accelerate the fluid
 517 up to supersonic speed. Across the cascade, the fluid is expanded from superheated condi-
 518 tions. However, shocks appear past stator vanes, as depicted in Figure 13, and may induce
 519 significant losses in the turbine efficiency. The robust design of the trailing edge is thus
 520 critical. SABBa is here exploited for optimising the turbine blade profile under uncertain
 521 inlet and outlet conditions. To estimate the aerodynamic performances of the turbine, the
 522 2D Non-Ideal Compressible-Fluid Dynamics solver included in the SU2 suite is used [43]. In
 523 particular, for computational reasons, the in-house reduced model built in Ref. [43] is used
 524 here, allowing for a quick evaluation. Furthermore, an approximate Pareto front which is
 525 already known for the tackled OUU problem, is used to assess the performances of SABBa.

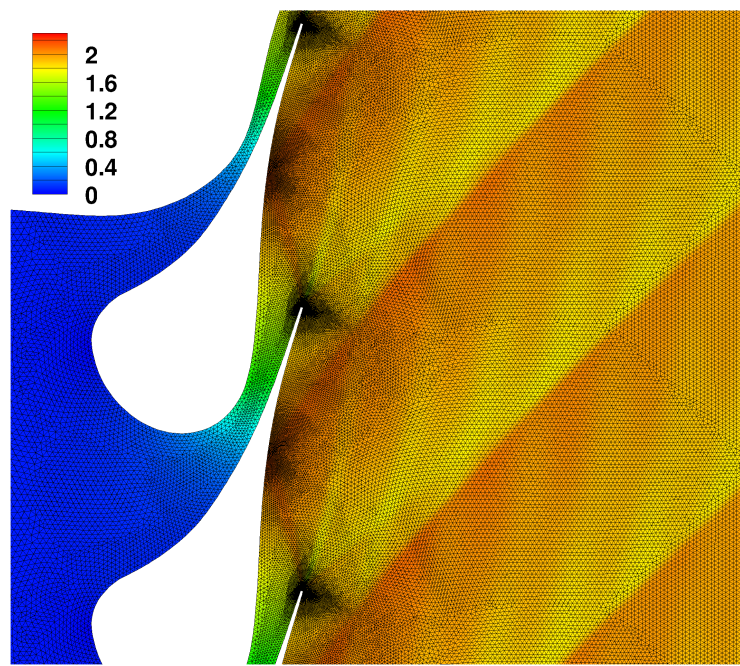


Figure 13: Mach contours at nominal conditions for the baseline profile and computational grid of 36k cells.

526 A spline-based geometry parameterisation is proposed. A B-spline curve of degree 3 is
 527 defined over a total number of 30 Control Points (CP) from which a subset of nine constitute

528 the design vector \mathbf{x} , denoted in red in Figure 14. These CPs are allowed to move in the
 529 direction normal to the baseline geometry.

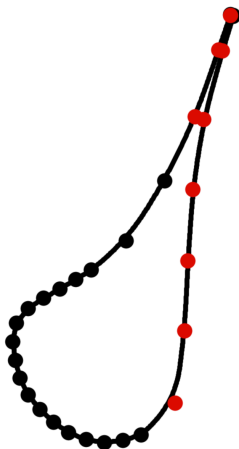


Figure 14: B-splines parameterisation. Fixed CP in black, moving CP in red.

530 The objective function ΔP is defined as the standard deviation of the azimuthal distri-
 531 bution of static pressure downstream of the blade. A low standard deviation should induce
 532 lower shocks in the outlet flow. A constraint is also imposed on the mass-flow rate per unit
 533 span \dot{m} , to remain close from the nominal value.

The tackled OUU problem reads then as follows:

$$\begin{aligned}
 &\text{minimise: } \boldsymbol{\rho}_f(\mathbf{x}) = \begin{pmatrix} \mu_1(\mathbf{x}) \\ \sigma^2(\mathbf{x}) \end{pmatrix} \\
 &\text{satisfying: } \boldsymbol{\rho}_g(\mathbf{x}) = \mu_2(\mathbf{x}) \in [0.98\dot{m}_0, 1.02\dot{m}_0] \\
 &\text{where: } \mu_1(\mathbf{x}) = \mathbb{E}_{\boldsymbol{\xi}}[\Delta P(\mathbf{x}, \boldsymbol{\xi})] \\
 &\quad \sigma^2(\mathbf{x}) = \mathbb{V}_{\boldsymbol{\xi}}[\Delta P(\mathbf{x}, \boldsymbol{\xi})] \\
 &\quad \mu_2(\mathbf{x}) = \mathbb{E}_{\boldsymbol{\xi}}[\dot{m}(\mathbf{x}, \boldsymbol{\xi})] \\
 &\quad \dot{m}_0 = 344.843 \\
 &\text{with: } \boldsymbol{\xi} \sim \mathcal{U}(\Xi) \\
 &\text{by changing: } \mathbf{x} \in \mathcal{X} \tag{15}
 \end{aligned}$$

534 where $\Xi = [7.95, 8.05] \times [541.15, 549.15] \times [1, 2]$. Note that the uncertain parameters corre-
 535 spond to the inlet and outlet conditions: $\boldsymbol{\xi} = [P_{in}^t, T_{in}^t, P_{out}^s]$. Overall, the problem features
 536 nine design parameters and three uncertainties.

537 SABBa is ran with parameters $N_{init} = 5$, $N_{new} = 1$ (sequential optimizer), $N_{first} = 4$ and
 538 $N_{ref} = 1$ (sequential refinement). The normalised thresholds \bar{s}_1 and \bar{s}_2 are both sequentially
 539 taken as 10%, 5%, 2% and 1% in all dimensions. The Pareto fronts associated with each of
 540 these thresholds are depicted hereafter in Figure 15. All boxes with non-zero POP are drawn
 541 with a transparency corresponding to the POP value. One can qualitatively see that these

542 promising boxes get closer and closer to the known Pareto front, depicted in red. SABBa
 543 SA-CS is able to get a very good approximation of the robust front at the cost of only **600**
 544 function evaluations, although missing the very left part of the front. This test case clearly
 545 illustrates the good performances of SABBa within a formulation combining robustness and
 546 reliability metrics.

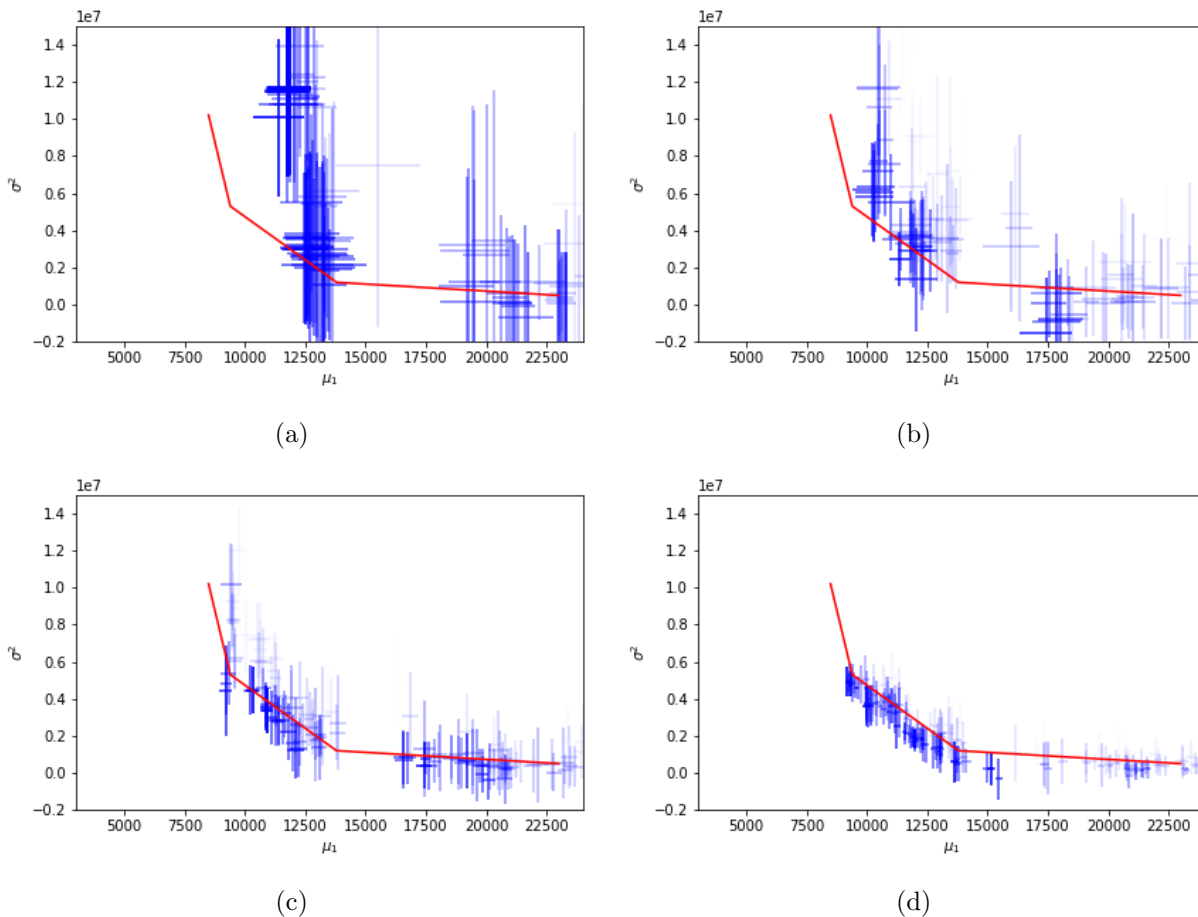


Figure 15: Outputs of the SABBa framework with (a) **156**, (b) **241**, (b) **418**, (b) **598** function evaluations. Transparency of the boxes driven by POP value and known front in red.

547 6.3. Design of a Thermal Protection System

548 The SABBa framework is then applied to the design of a thermal protection system for a
 549 re-entry vehicle. This test-case deals with 12 dimensions and aims at minimising the mean
 550 mass density under worst-case temperature constraint.

551 We study the re-entry of Stardust, that was the first mission using a low-density carbon-
 552 phenolic ablator in 2006. Stardust was the fastest man-made object re-entering the earth
 553 atmosphere, at a velocity of 12.7 km/s . A generic heat-shield for atmospheric reentry is
 554 depicted in Figure 16.

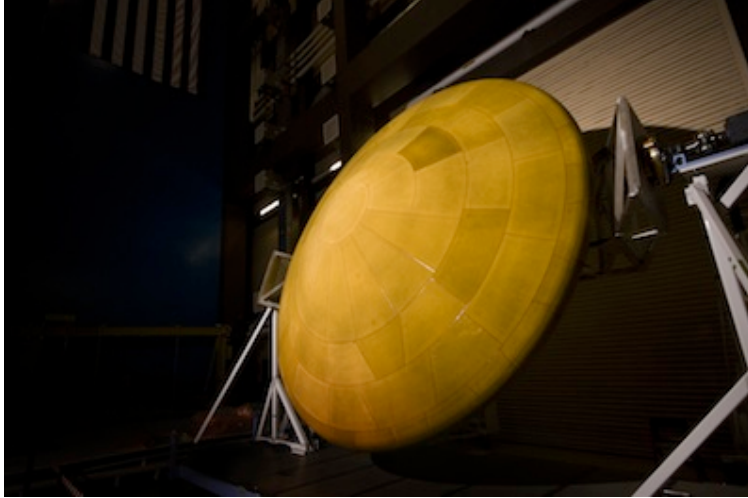


Figure 16: Thermal Protection System (TPS) of the Mars Science Laboratory (MSL) for atmospheric reentry.

555 Surface total pressure and heat flux were computed from hypersonic computational fluid
 556 dynamics (CFD) simulations. In accordance with the state-of-the-art design approach, we
 557 assume that the problem is locally mono-dimensional. The analysis is performed using
 558 the properties of the Theoretical Ablative Composite for Open Testing (TACOT). Nominal
 559 TACOT properties are available in the open literature. Volume-wise, TACOT is made of
 560 10% of carbon fibers, 10% of phenolic resin, and is 80% porous. The thickness of the ablative
 561 material is two inches and adiabatic conditions are used at the bondline.

562 The physical model used here is a generic heat and mass transfer model for porous media
 563 that is presented in [44]. The model is implemented in the Porous material Analysis Toolbox
 564 (PATO), distributed Open Source. First-order implicit finite-volume schemes in time and
 565 space were used for the simulations. The mono-dimensional problem was meshed with 300
 566 finite-volume cells with a logarithmic refinement of parameter 0.2 towards the surface. In
 567 this study, we used an equilibrium chemistry model. We study the material response at
 568 the stagnation point, which reaches the highest temperature during the reentry. Figure 17
 569 illustrates the typical evolution of the temperature inside the material (dashed lines) and at
 570 the heated surface (plain red line).

571 Formally, the optimisation problems reads as follows:

$$\begin{aligned}
 &\text{minimise: } \boldsymbol{\rho}_f(\boldsymbol{x}) = \mu(\boldsymbol{x}) \\
 &\text{satisfying: } \boldsymbol{\rho}_g(\boldsymbol{x}) = M(\boldsymbol{x}) \leq 473.15 \\
 &\quad \text{where: } \mu(\boldsymbol{x}) = \mathbb{E}_{\boldsymbol{\xi}}[\sigma(\boldsymbol{x}, \boldsymbol{\xi})] \\
 &\quad \quad \quad M(\boldsymbol{x}) = \max_{\boldsymbol{\xi}}[T_b(\boldsymbol{x}, \boldsymbol{\xi})] \\
 &\quad \text{with: } \boldsymbol{\xi} \sim \mathcal{U}(\Xi) \\
 &\text{by changing: } \boldsymbol{x} \in [0.01, 0.1] \times [3.5, 7]
 \end{aligned} \tag{16}$$

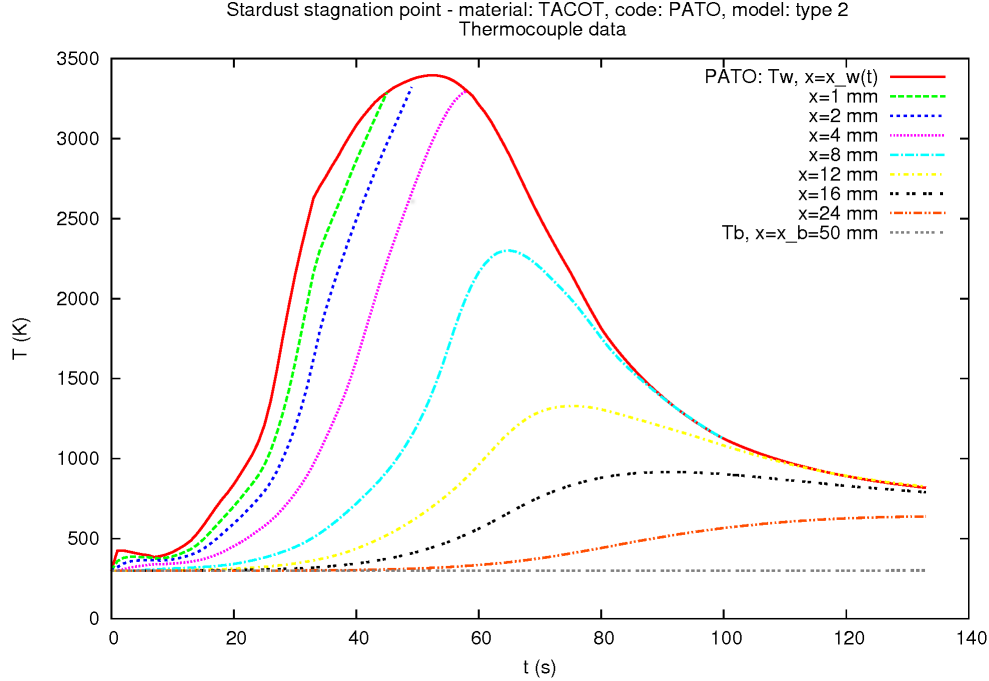


Figure 17: Surface and in-depth temperatures obtained with nominal parameters.

572 with x_1 the resin volume fraction (originally 10%) and x_2 the overall width of the system
 573 (originally 7.21 cm). We observe in Figure 17 that with initial parameters, the bottom
 574 temperature stays merely constant during the whole reentry. Hence, the search space is
 575 centred on lower x_1 and x_2 values, which tends to increase the bottom temperature.

576 In this test-case, Ξ is of dimension 12 and all uncertainties are assumed uniform. The
 577 choice of the uncertain parameters relies on a sensitivity analysis performed on this test-case
 578 in a previous paper [45]. Here, retained uncertain parameters are: 1) Density and volume
 579 fraction of the fibrous preform ($\pm 5\%$ uncertainty each); 2) Density and volume fraction of
 580 the phenolic resin ($\pm 5\%$ uncertainty each); 3) Thermal properties of the charred material:
 581 heat capacity, conductivity and emissivity ($\pm 5\%$ uncertainty each); 4) Oxygen fraction
 582 in the pyrolysis gases ($\pm 10\%$ uncertainty); 5) Pyrolysis reaction activation energy ($\pm 10\%$
 583 uncertainty); 6) Overall width of the system (± 0.1 cm uncertainty). Both design parameters
 584 are also affected by an uncertainty (± 0.005 for x_1 and ± 0.1 for x_2).

585 Each function evaluation requires the 1D simulation of heat transfer and shield ablation.
 586 This takes approximately 10 minutes to compute on a 2.90 GHz processor. An acceptable
 587 global cost should remain within a day, or equivalently below 100 to 150 evaluations.

588 SABBA is ran with parameters $N_{init} = 5$, $N_{new} = 1$ (sequential optimizer), $N_{first} = 4$ and
 589 $N_{ref} = 1$ (sequential refinement). As for the normalised thresholds \bar{s}_1 and \bar{s}_2 , they are both
 590 sequentially taken as 50%, 40%, 30%, 20%, 10%, 5%, 3%, 2% and 1% in all dimensions.

591 Three optima are found using SABBA with coupled-space surrogate model (SA-CS) for a

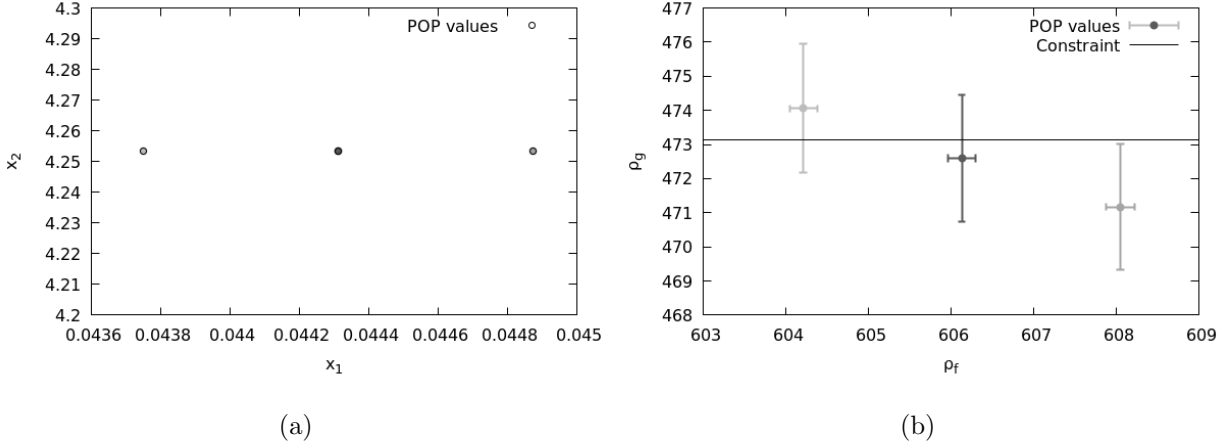


Figure 18: Outputs of the SABBa framework in (a) the input space, (b) the objective/constraint space.

592 computational cost of only **40** function evaluations. These Pareto optimal designs are plotted
 593 in Figure 18. The design $\mathbf{x}^* \approx (4.43 \times 10^{-2}, 4.25)$ has the highest Pareto Optimal Probability
 594 (POP), of approximately 65%. It corresponds to the middle box in Fig. 18(b), where ρ_f
 595 must be minimised and the admissible set is below the constraint threshold $\rho_g = 473.15$ K.

596 In Figure 19, we have reported the performance of all the designs evaluated during the
 597 optimisation. They are plotted in blue when dominated, red when entirely in the failure
 598 zone and green when non-dominated.

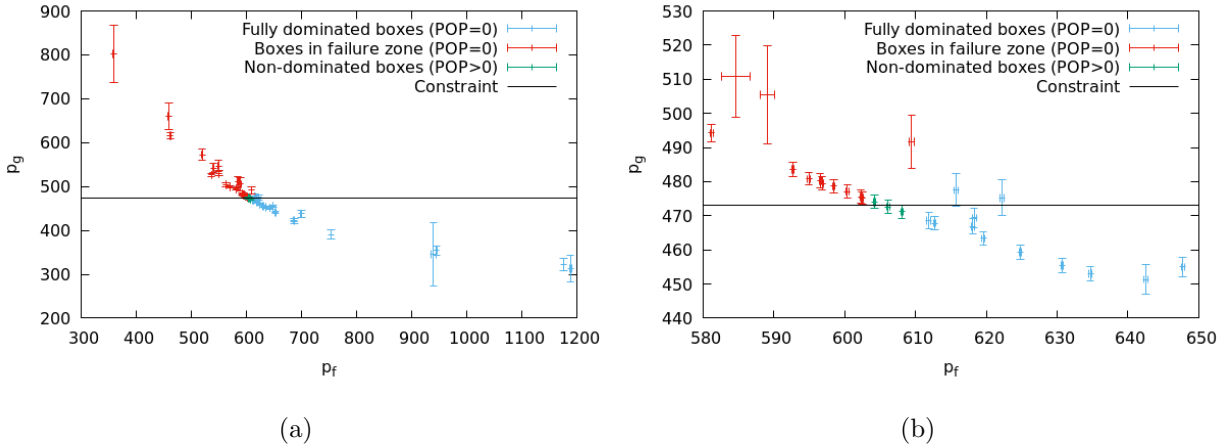


Figure 19: All constructed boxes, depicted in blue when dominated, in red when entirely in failure zone and in green when non-dominated. (a) Full view, (b) zoomed-in view.

599 Among the three optimal designs depicted in Figure 18, only the right one lies entirely
 600 in the admissible set, and thus belongs to \mathcal{A}_B . Contrarily to the two other optimal designs,
 601 it can dominate other boxes. In Figure 19, it can be observed that this design dominates all
 602 the blue boxes, that are not entirely in the failure zone but are strictly worse in the objective
 603 dimension. Contrarily, the red boxes belong to \mathcal{F}_B and lie entirely in the failure zone. Hence,

604 they are all considered dominated. This behaviour explains why only three designs are kept,
 605 as shown in Figure 18. It can be observed in Figure 19 that the Bounding-Box approach
 606 permits to exploit the tunable accuracy since extreme boxes (on the very left or very right)
 607 are estimated with very wide uncertainty.

608 Figure 20 provides a visualisation of the final SA model. In particular, we plot the SA
 609 mean surface density $\rho_{SA_f}(\mathbf{x})$, wherever the constraint $\rho_{SA_g}(\mathbf{x}) \leq 473.15$ k is satisfied. One
 610 can see that (i) the optima plotted in Figure 18 are coherent with this SA model, and (ii) the
 611 objective value $\rho_{SA_f}(\mathbf{x})$ seems merely constant on the constraint limit. The final accuracy
 612 is imposed at 1%, which may not be enough to discriminate designs on the constraint limit.
 613 The above found $\mathbf{x}^* \approx (4.43 \times 10^{-2}, 4.25)$ is returned by SABBa but the whole frontier from
 614 $(0.01, 5.1)$ to $(0.07, 4)$ is of high interest.

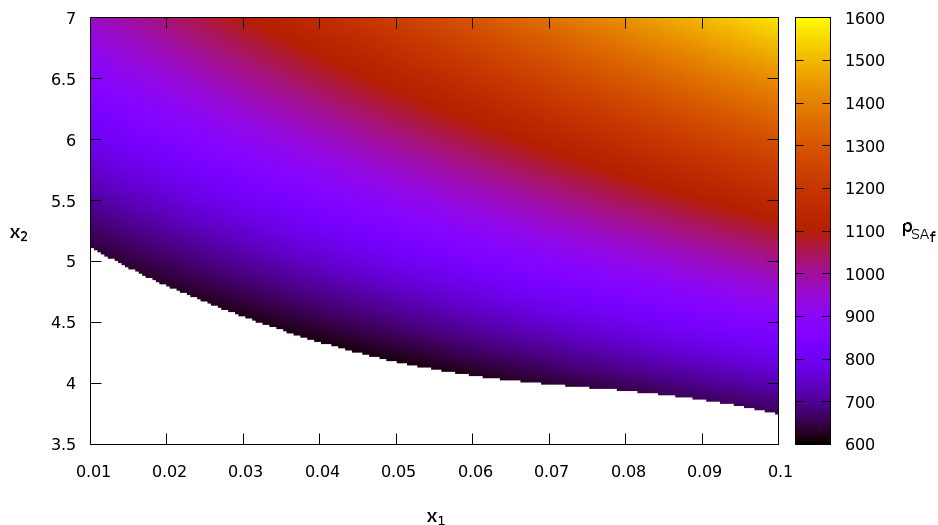


Figure 20: Final SA model, representing $\rho_{SA_f}(\mathbf{x})$ where the constraint $\rho_{SA_g}(\mathbf{x}) \leq 473.15$ K is satisfied.

615 7. Conclusions

616 In this work, we present an efficient framework, SABBa, for constrained optimisation
 617 under uncertainty problems. It handles most classical robustness and reliability measures,
 618 such as the Taguchi (mean and variance) robust optimisation or the quantile constrained
 619 optimisation problems. The parsimony of SABBa relies on several features presented in this
 620 paper. The Bounding-Box measure approximation is used to compare designs in a tunable
 621 accuracy context. It permits to compute the Pareto Optimal Probability (POP) associated
 622 to each design to perform a rigorous ranking among them. Gaussian Process (GP) surrogate
 623 models are exploited both for measure estimation and Surrogate-Assisting strategy, and
 624 allows to tract the estimation variability throughout the framework.

625 We have assessed the performance of the framework against a more classical A Priori
 626 MetaModel (APMM) strategy on several analytical test cases. To this extent, we have for-
 627 mulated a specific indicator based on a modified Hausdorff distance. Overall, SABBa shows
 628 both a faster convergence rate and a dramatic increase in the robustness of the optimisation
 629 process.

630 The proposed method has then been employed on three engineering test-cases to demon-
 631 strate its applicability for solving real-world uncertainty-based optimization problems with
 632 different reliability and robustness metrics. It has been successfully applied to a low-quantile
 633 reliability-based structural optimisation with six dimensions in the coupled space. The ac-
 634 curacy is very satisfactory, with an associated computational cost of 40 to 50 evaluations.
 635 It has also been employed for obtaining a bi-objective Pareto front approximation with the
 636 aim of minimising shocks past ORC turbine blades, that may induce significant losses. This
 637 constrained bi-objective Pareto front approximation only required around 600 function eval-
 638 uations. Finally, a 12-dimensional Thermal Protection System (TPS) design with worst-case
 639 constraints has been performed, with a high impact of the tunable accuracy setting, at the
 640 cost of only 40 evaluations.

641 This approach remains very general and broadly applicable to any optimisation process
 642 with statistics-based objectives and constraints. It shows very good parsimony, which is of
 643 primary importance for real world applications, where black-box evaluations can take several
 644 days to run. Most importantly, the optimiser is not imposed by the approach, allowing for an
 645 easy coupling with any existing method, given that it is able to deal with noised estimations
 646 of the cost functions.

647 Several steps in this work remain improvable. We used local refinement criteria, which
 648 are cheaper but less efficient than integral criteria. The use of GP surrogate models also
 649 limits the number of manageable input dimensions. Surrogate modelling on over few dozens
 650 of dimensions would require specific techniques such as feature selection or kernel adaptation.
 651 Likewise, in order to efficiently deal with very low probability constraints (*e.g.* 1×10^{-7}), one
 652 should couple SABBa to a dedicated tool for low quantile computation. Finally, the proposed
 653 method could benefit from multi-output GP models for taking advantage of dependencies
 654 between quantities of interest or statistical measures.

655 On-going work aims at proposing non-uniform error estimations so as to more closely
 656 represent the measure uncertainties.

657 Appendix A. POP computational details

658 The set of boxes $\mathcal{B} = \{\mathcal{B}_i\}_i$ is given, with $\mathcal{B}_i = \mathcal{B}(\mathbf{a}_i, \mathbf{r}_i)$. Every $\mathbf{Z}_i \sim \mathcal{U}(\mathcal{B}_i)$ is of
 659 dimension $m = m_1 + m_2$ where m_1 is the number of objectives and m_2 the number of con-
 660 straints. We write \mathbf{Z}_{i_f} the objectives values and \mathbf{Z}_{i_g} the constraints values. The probability
 661 in Equation (5) is computed as follows, using the independence assumptions between boxes

662 and between dimensions:

$$\begin{aligned}
\mathbb{P}_{\mathbf{Z}_j, \mathbf{Z}_i} [\mathbf{Z}_j \not\prec_c \mathbf{Z}_i] &= 1 - \mathbb{P}_{\mathbf{Z}_j, \mathbf{Z}_i} [\mathbf{Z}_j \succ_c \mathbf{Z}_i] \\
&= 1 - \left(\mathbb{P}_{\mathbf{Z}_{i_g}} [\mathbf{Z}_{i_g} \not\leq \mathbf{0}] \right. \\
&\quad \left. + \mathbb{P}_{\mathbf{Z}_{i_g}} [\mathbf{Z}_{i_g} \leq \mathbf{0}] \mathbb{P}_{\mathbf{Z}_{j_g}} [\mathbf{Z}_{j_g} \leq \mathbf{0}] \mathbb{P}_{\mathbf{Z}_{j_f}, \mathbf{Z}_{i_f}} [\mathbf{Z}_{j_f} \succ \mathbf{Z}_{i_f}] \right) \\
&= \mathbb{P}_{\mathbf{Z}_{i_g}} [\mathbf{Z}_{i_g} \leq \mathbf{0}] \left(1 - \mathbb{P}_{\mathbf{Z}_{j_g}} [\mathbf{Z}_{j_g} \leq \mathbf{0}] \mathbb{P}_{\mathbf{Z}_{j_f}, \mathbf{Z}_{i_f}} [\mathbf{Z}_{j_f} \succ \mathbf{Z}_{i_f}] \right)
\end{aligned} \tag{A.1}$$

663 where

$$\mathbb{P}_{\mathbf{Z}_{i_g}} [\mathbf{Z}_{i_g} \leq \mathbf{0}] = \prod_{k=m_1+1}^m \max \left(0, \min \left(1, \frac{-\mathcal{B}_{i_k}^-}{2r_{i_k}} \right) \right) = \prod_{k=m_1+1}^m \left[\frac{-\mathcal{B}_{i_k}^-}{2r_{i_k}} \right]_0^1,$$

664 and $[\cdot]_0^1$ means that values are taken between 0 and 1. The lower bound of the box is
665 written as $\mathcal{B}_i^- = \mathbf{a}_i - \mathbf{r}_i$. The second probability involved in the last line of Equation (A.1)
666 is computed as follows:

$$\begin{aligned}
\mathbb{P}_{\mathbf{Z}_{j_f}, \mathbf{Z}_{i_f}} [\mathbf{Z}_{j_f} \succ \mathbf{Z}_{i_f}] &= \prod_{k=1}^{m_1} \mathbb{P}_{Z_{j_k}, Z_{i_k}} [Z_{j_k} \leq Z_{i_k}] \\
&= \prod_{k=1}^{m_1} \left(\left[\frac{L_{1_k}}{2r_{j_k}} \right]_0^1 + \left[\frac{L_{2_k}}{2r_{j_k}} \right]_0^1 \left(\frac{1}{2} \left[\frac{L_{2_k}}{2r_{j_k}} \right]_0^1 + \left[\frac{L_{3_k}}{2r_{j_k}} \right]_0^1 \right) \right),
\end{aligned}$$

667 where

$$\begin{aligned}
L_{1_k} &= \mathcal{B}_{i_k}^- - \mathcal{B}_{j_k}^-, \\
L_{2_k} &= \min(\mathcal{B}_{i_k}^+, \mathcal{B}_{j_k}^+) - \max(\mathcal{B}_{i_k}^-, \mathcal{B}_{j_k}^-), \\
L_{3_k} &= \mathcal{B}_{i_k}^+ - \mathcal{B}_{j_k}^+.
\end{aligned}$$

668 In the above, $\mathcal{B}_i^+ = \mathbf{a}_i + \mathbf{r}_i$ is the upper bound of the box.

669 In each dimension, L_{1_k} can be interpreted as the portion of \mathcal{B}_j dominating \mathcal{B}_i , L_{3_k} the
670 portion of \mathcal{B}_i dominated by \mathcal{B}_j and L_{2_k} the overlapping area. We depict these lengths in Fig.
671 A.21. Note that these values can be negative and that the computation is not symmetric
672 between \mathcal{B}_j and \mathcal{B}_i .

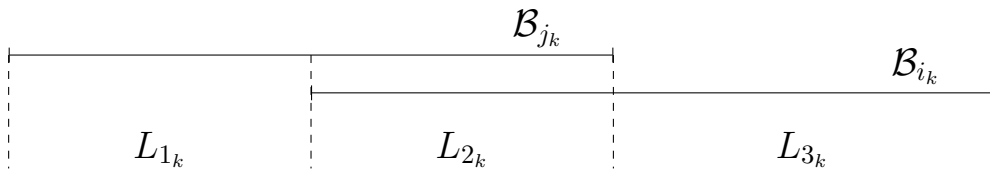


Figure A.21: Computational details

673 **Appendix B. Justification for box sizes**

674 Some developments are given here to explain the choice of the conservative error in
675 Equation (6) associated with measure approximations.

676 Note that in the following, empirical estimators are considered well converged, so that all
677 impreciseness comes from the surrogate model \widehat{q}_x of $q(\mathbf{x}, \cdot)$. For example, $\widetilde{\mu}(\mathbf{x})$ is considered
678 equal to $\mathbb{E}_\xi[\widehat{q}_x(\boldsymbol{\xi})]$ in the following formula although only the empirical value is used.

679 The expectation approximation conservative error $\bar{\varepsilon}_\mu$ is quite straightforward:

$$\begin{aligned} |\varepsilon_\mu(\mathbf{x})| &= |\boldsymbol{\mu}(\mathbf{x}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x})| = |\mathbb{E}_\xi[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})] - \mathbb{E}_\xi[\widehat{\mathbf{q}}_x(\boldsymbol{\xi})]| \\ &= |\mathbb{E}_\xi[\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) + \varepsilon_{q_x}(\boldsymbol{\xi})] - \mathbb{E}_\xi[\widehat{\mathbf{q}}_x(\boldsymbol{\xi})]| \\ &= |\mathbb{E}_\xi[\varepsilon_{q_x}(\boldsymbol{\xi})]| \\ &\leq \mathbb{E}_\xi[\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})] \\ &= \bar{\varepsilon}_\mu(\mathbf{x}) \end{aligned}$$

680 with $\boldsymbol{\mu}(\mathbf{x})$ the true statistical moment on \mathbf{q} at a given \mathbf{x} and $\widetilde{\boldsymbol{\mu}}(\mathbf{x})$ the approximated one,
681 computed on the surrogate model \widehat{q}_x . The true error ε_{q_x} is defined from $\mathbf{q}(\mathbf{x}, \boldsymbol{\xi}) = \widehat{\mathbf{q}}_x(\boldsymbol{\xi}) +$
682 $\varepsilon_{q_x}(\boldsymbol{\xi})$ and is conservatively approximated by $\bar{\varepsilon}_{q_x}(\boldsymbol{\xi}) \geq |\varepsilon_{q_x}(\boldsymbol{\xi})|$.

683 The same can be conducted for the variance measure, with a bit more risks of overesti-
684 mation:

$$\begin{aligned} |\varepsilon_{\sigma^2}(\mathbf{x})| &= |\boldsymbol{\sigma}^2(\mathbf{x}) - \widetilde{\boldsymbol{\sigma}}^2(\mathbf{x})| = |\mathbb{E}_\xi[(\mathbf{q}(\mathbf{x}, \boldsymbol{\xi}) - \boldsymbol{\mu}(\mathbf{x}))^2] - \mathbb{E}_\xi[(\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x}))^2]| \\ &= |\mathbb{E}_\xi[(\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x}) + \varepsilon_{q_x}(\boldsymbol{\xi}) - \varepsilon_\mu(\mathbf{x}))^2] - \mathbb{E}_\xi[(\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x}))^2]| \\ &= |\mathbb{E}_\xi[(\varepsilon_{q_x}(\boldsymbol{\xi}) - \varepsilon_\mu(\mathbf{x}))^2 + 2(\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x}))(\varepsilon_{q_x}(\boldsymbol{\xi}) - \varepsilon_\mu(\mathbf{x}))]| \\ &\leq \mathbb{E}_\xi[(\bar{\varepsilon}_{q_x}(\boldsymbol{\xi}) + \bar{\varepsilon}_\mu(\mathbf{x}))^2 + 2|\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \widetilde{\boldsymbol{\mu}}(\mathbf{x})|(\bar{\varepsilon}_{q_x}(\boldsymbol{\xi}) + \bar{\varepsilon}_\mu(\mathbf{x}))] \\ &= \bar{\varepsilon}_{\sigma^2}(\mathbf{x}) \end{aligned}$$

685 The conservative error associated with the expectation approximation could also be ex-
686 plained based on the monotonicity of the expectation operator. We write $f \geq g \iff$
687 $\forall \mathbf{x}, f(\mathbf{x}) \geq g(\mathbf{x})$. By definition $\mathbf{q}(\mathbf{x}, \cdot) \in [\widehat{\mathbf{q}}_x - \bar{\varepsilon}_{q_x}, \widehat{\mathbf{q}}_x + \bar{\varepsilon}_{q_x}]$. The monotonicity of the
688 expectation operator then gives $\mathbb{E}_\xi[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})] \in [\mathbb{E}_\xi[\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) - \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})], \mathbb{E}_\xi[\widehat{\mathbf{q}}_x(\boldsymbol{\xi}) + \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})]]$, or
689 equivalently $\boldsymbol{\mu}(\mathbf{x}) \in [\widetilde{\boldsymbol{\mu}}(\mathbf{x}) - \mathbb{E}_\xi[\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})], \widetilde{\boldsymbol{\mu}}(\mathbf{x}) + \mathbb{E}_\xi[\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})]]$, thus giving the conservative
690 error found in the above $\bar{\varepsilon}_\mu(\mathbf{x}) = \mathbb{E}_\xi[\bar{\varepsilon}_{q_x}(\boldsymbol{\xi})]$.

691 By defining $\widehat{q}_x^+(\boldsymbol{\xi}) = \widehat{q}_x(\boldsymbol{\xi}) + \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})$ and $\widehat{q}_x^-(\boldsymbol{\xi}) = \widehat{q}_x(\boldsymbol{\xi}) - \bar{\varepsilon}_{q_x}(\boldsymbol{\xi})$, the monotonicity of
692 the minimum, maximum and quantile operators can also be exploited to obtain conservative
693 error approximations. For the case of the minimum operator, with $\widetilde{\mathbf{m}} = \min_{\boldsymbol{\xi}}[\widehat{\mathbf{q}}_x(\boldsymbol{\xi})]$,

$$\begin{aligned} \mathbf{m}(\mathbf{x}) &= \min_{\boldsymbol{\xi}}[\mathbf{q}(\mathbf{x}, \boldsymbol{\xi})] \in [\min_{\boldsymbol{\xi}}[\widehat{\mathbf{q}}_x^-(\boldsymbol{\xi})], \min_{\boldsymbol{\xi}}[\widehat{\mathbf{q}}_x^+(\boldsymbol{\xi})]] \\ &= [\widetilde{\mathbf{m}}(\mathbf{x}) - |\widetilde{\mathbf{m}}(\mathbf{x}) - \min_{\boldsymbol{\xi}}[\widehat{\mathbf{q}}_x^-(\boldsymbol{\xi})]|, \widetilde{\mathbf{m}}(\mathbf{x}) + |\widetilde{\mathbf{m}}(\mathbf{x}) - \min_{\boldsymbol{\xi}}[\widehat{\mathbf{q}}_x^+(\boldsymbol{\xi})]|] \\ &\in [\widetilde{\mathbf{m}}(\mathbf{x}) - \bar{\varepsilon}_{\min}(\mathbf{x}), \widetilde{\mathbf{m}}(\mathbf{x}) + \bar{\varepsilon}_{\min}(\mathbf{x})] \end{aligned}$$

694 where $\bar{\epsilon}_{\min}(\mathbf{x}) = \max(|\widetilde{\mathbf{m}}(\mathbf{x}) - \min_{\xi}[\widehat{\mathbf{q}}_x^-(\xi)|, |\widetilde{\mathbf{m}}(\mathbf{x}) - \min_{\xi}[\widehat{\mathbf{q}}_x^+(\xi)|]$.

695 The same idea can be followed for the maximum and quantile approximations, resulting
696 in the following errors:

$$\begin{aligned}\bar{\epsilon}_{\max}(\mathbf{x}) &= \max(|\widetilde{\mathbf{M}}(\mathbf{x}) - \max_{\xi}[\widehat{\mathbf{q}}_x^-(\xi)|, |\widetilde{\mathbf{M}}(\mathbf{x}) - \max_{\xi}[\widehat{\mathbf{q}}_x^+(\xi)|]) \\ \bar{\epsilon}_{q^p}(\mathbf{x}) &= \max(|\widetilde{\mathbf{q}}^p(\mathbf{x}) - q_{\xi}^p[\widehat{\mathbf{q}}_x^-(\xi)|, |\widetilde{\mathbf{q}}^p(\mathbf{x}) - q_{\xi}^p[\widehat{\mathbf{q}}_x^+(\xi)|])\end{aligned}$$

697 Appendix C. Justification for refinement criteria

698 The chosen partial criteria for GP model refinement given in Equation (7) are also ex-
699 plained in the following.

700 Both the expectation and variance are global measures over the whole domain. For this
701 reason, it has been chosen to iteratively add a point at the maximum predictive conservative
702 error, to converge the model on the entire space. This strategy is usually called Maximum
703 Mean Square Predictive Error or MMSPE. Note that the partial criteria are multiplied by
704 the input pdf to weight the predictive error according to the probability of occurrence. Thus,
705 the final partial criteria are:

$$\begin{aligned}\mathbf{c}_{\mu}(\xi) &= \bar{\epsilon}_{q_x}(\xi)\phi(\xi) \\ \mathbf{c}_{\sigma^2}(\xi) &= \bar{\epsilon}_{q_x}(\xi)\phi(\xi)\end{aligned}$$

706 with ϕ the Probability Density Function (PDF) of the uncertain variables.

707 The minimum (resp maximum) measure partial criteria is simply the probability of ex-
708 ceeding the current minimal (resp. maximal) value $\widetilde{\mathbf{m}}$ (resp. $\widetilde{\mathbf{M}}$). This is performed with
709 an assumption of uniform distribution with the conservative error box. Hence, the criteria
710 can be written as such:

$$\begin{aligned}\mathbf{c}_{\min}(\xi) &= \left[\frac{\widetilde{\mathbf{m}} - \widehat{\mathbf{q}}_x^-(\xi)}{2\bar{\epsilon}_{q_x}(\xi)} \right]_+ \\ \mathbf{c}_{\max}(\xi) &= \left[\frac{\widehat{\mathbf{q}}_x^+(\xi) - \widetilde{\mathbf{M}}}{2\bar{\epsilon}_{q_x}(\xi)} \right]_+\end{aligned}$$

711 where $\widehat{\mathbf{q}}_x^+(\xi) = \widehat{\mathbf{q}}_x(\xi) + \bar{\epsilon}_{q_x}(\xi)$ and $\widehat{\mathbf{q}}_x^-(\xi) = \widehat{\mathbf{q}}_x(\xi) - \bar{\epsilon}_{q_x}(\xi)$ and with $[\cdot]_+ = \max(0, \cdot)$
712 referring to the value if positive, 0 either.

713 Finally, for the case of the quantile measure, it has been chosen to compute the product
714 of the aforementioned probability of exceeding the quantile value, multiplied by the input
715 density:

$$\mathbf{c}_{q^p}(\xi) = \left[\frac{\widetilde{\mathbf{q}}^p - \widehat{\mathbf{q}}_x^-(\xi)}{2\bar{\epsilon}_{q_x}(\xi)} \right]_+ \left[\frac{\widehat{\mathbf{q}}_x^+(\xi) - \widetilde{\mathbf{q}}^p}{2\bar{\epsilon}_{q_x}(\xi)} \right]_+ \phi(\xi)$$

716 This product is maximised on the hyperplane $\widehat{\mathbf{q}}_x = q^p$. Multiplying the criteria by $\phi(\xi)$
717 puts more weight according to the probability of occurrence. The spread may not be optimal,

718 but the optimisation of the criteria being performed on a fixed sampling, the tightening of
719 the conservative error is very likely to decrease the value of the criterion in the surrounding
720 area because samples are very unlikely to be localised exactly on the isoline of the function.

721 We can note that the chosen criteria are far from being optimal. However, these choices
722 give a fast determination of the refinement point, and the number of samples is usually low
723 enough so that the choice of the training point is not of significant importance compared to
724 the quality of the metamodeling strategy.

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