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Maximizing Regional Sensitivity Analysis indices to find sensitive model behaviors

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Abstract

We address the question of sensitivity analysis for model outputs of any dimension using Regional Sensitivity Analysis (RSA). Classical RSA computes sensitivity indices related to the impact of model inputs variations on the occurrence of a target region of the model output space. In this work, we put this perspective one step further by proposing to find, for a given model input, the region whose occurrence is best explained by the variations of this input. When it exists, this region can be seen as a model behavior whose occurrence is particularly sensitive to the variations of the model input under study. We name this method mRSA (for maximized RSA).

mRSA is formalized as an optimization problem using region-based sensitivity indices. Two formulations are studied, one theoretically and one numerically using a dedicated algorithm. Using a 2D test model and an environmental model producing time series, we show that mRSA, as a new model exploration tool, can provide interpretable insights on the sensitivity of model outputs of various dimensions.

Keywords: Multivariate sensitivity analysis, Cluster analysis, Factor mapping setting, Sobol' indices

1. Introduction

The analysis of models with multidimensional outputs (temporal, spatial, heterogeneous) is one of the current challenges of sensitivity analysis [1, 2].

The most natural way to handle such outputs is to apply classical sensitivity analysis on each of their components in order to generate multidimensional sensitivity indices (e.g. spatial maps or temporal evolution of sensitivity indices, as in [3, 4]). This approach however produces only local information while many other characterizations of the outputs distributions can be of interest in case of multi-dimensional outputs, for instance the influence of model inputs on the change in shape of model outputs. Two main approaches tackle multidimensional outputs in a non purely local way. The first one aims at computing a set

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33 of indices associated to coordinates along a basis of functions on which the model outputs
34 are projected ([5, 6, 7]). Its flexibility and interpretability are limited by the choice of the
35 basis. The second approach summarizes the impact of the model inputs on the variability
36 of all the model outputs using a single index [8, 9, 10, 11]. It provides useful aggregated
37 indices but does not allow a fine understanding of model outputs sensitivity.

38 Spear and Hornberger introduced in [12] the concept of model behavior in sensitivity
39 analysis through the Regional Sensitivity Analysis (RSA) approach.

40 The principle is to start from the definition of a target region of the output space (de-
41 noted as "behavioral") and to analyze the impact of the variations of model inputs on its
42 occurrence. Using model behaviors expressed as regions of the output space appears to be an
43 efficient method to get interpretable characterizations of model properties [13]. It has also
44 the property to scale to any dimension of the output space. Among the last developments
45 on RSA, two are of particular interest in the present study: i) the application of RSA in the
46 context of reliability engineering to characterize parameter sensitivity in relation to a critical
47 domain of the output space (e.g. the failure domain of a system) using sensitivity measures
48 compatible with rare events and taking into account interactions (Target SA, [14, 15]), ii) its
49 application in combination with a clustering procedure in order to characterize parameter
50 sensitivity with respect to the dominant model behaviors detected in the model output space
51 (Distance-Based Generalized SA [16], Cluster-based GSA, [13]).

52 These approaches rely on an a priori characterization of the behaviors (regions of the
53 output space) to be analyzed. Behaviors are identified either by experts or by automatic
54 clustering of the simulations. Pannier and Graf [17] for instance introduced sectional sen-
55 sitivity analysis to study the functional interrelations between model inputs and outputs
56 based on a priori defined subdivisions of the model inputs and outputs spaces. In this work,
57 we propose a new perspective on the link between behaviors and sensitivity analysis based
58 on an extension of the recent developments on RSA. Instead of trying to a priori charac-
59 terize target regions of the output space, we propose to use an optimization procedure in
60 order to reveal the region of the output space whose occurrence is best explained by the
61 variations of this input. We name this approach mRSA (for maximized Regional Sensitivity
62 Analysis). The formalization of mRSA in terms of principles and numerical algorithm is
63 presented in Section 2. The results of the method application are presented in Section 3 on
64 two examples: a model with 2D outputs and an environmental model producing time series.
65 Software availability is described in Section 5.

66 2. mRSA methods and algorithm

67 2.1. Notation

68 We consider a model whose inputs are noted X_i , for $i = 1, \dots, n$. We assume that $X =$
69 (X_1, \dots, X_n) is a set of independent random variables. We suppose that they follow an
70 uniform distribution in $[0, 1]$. The model output is noted $Y = f(X_1, \dots, X_n)$ and is typically
71 a multivariate output in \mathbb{R}^d . Model behaviors in the context of RSA are defined as regions
72 of the model output space $Im(f) = \{f(X), X \in [0, 1]^n\}$.

73 *2.2. Principle*

74 The objective of this work is to find, for a given input X_i , the region C^* of the output
75 space whose occurrence is most influenced by the variations of X_i . Note that it is equivalent
76 to look for the partition $(C^*, \overline{C^*})$ (where $\overline{C^*}$ is the complement of C^*) such that the transition
77 of model outputs from C^* to $\overline{C^*}$ (or equivalently from $\overline{C^*}$ to C^*) is best explained by the
78 variations of X_i .

79 We formalize this question as an optimization problem using the region-based sensitivity
80 indices proposed in [13]. These indices are based on membership functions characterizing
81 the level of membership of any element of the output space to a given region C of the
82 output space. They are defined by applying the variance-based Sobol' indices [18, 19] to
83 the membership functions and quantify the impact of a given input factor on the occurrence
84 of C . In the context of this article, we consider first order indices and binary membership
85 functions that are written using indicator functions (i.e. the function returning 1 if the
86 element of the output space is in the considered region, 0 otherwise). For an input X_i , the
87 region-based index under study, noted S_i^C and associated to a region C , is then defined as:

$$S_i^C = \frac{\mathbb{V}[\mathbb{E}[\mathbb{1}_C(Y)|X_i]]}{\mathbb{V}[\mathbb{1}_C(Y)]} \quad (1)$$

88 where \mathbb{V} is the variance, \mathbb{E} the expectation, and $\mathbb{1}_C(\cdot)$ the indicator function of set C .

89 In this case, the mRSA approach aims at finding for each input X_i a partition $(C_i^*, \overline{C_i^*})$ so
90 that C_i^* (or equivalently $\overline{C_i^*}$) maximizes S_i^C . Note that this maximization does not necessarily
91 gives $S_i^{C_i^*} > 0.5$, in other words, X_i is not necessarily the most influential input to explain
92 the occurrence of the optimal region C_i^* .

93 *2.3. First Formulation: unconstrained mRSA*

A natural way of formalizing the sensitivity indices maximization problem is to consider
the following unconstrained formulation (P1):

$$(P1) : \max_{C \subset \text{Im}(f)} S_i^C$$

94
95 The maximum value that can take S_i^C is 1. While this maximum might not often occur
96 for real world problems, studying conditions such that solutions of (P1) reach this maximum
97 gives insights on the mRSA approach. This study is presented in section 2.3.1. We then
98 show in Section 2.3.2 some limitations in (P1) that will lead to another formulation (P2) on
99 which the rest of the article focuses.

100 *2.3.1. Characterization of partitions such that $S_i^{C^*} = 1$*

We note as E_i^* the set of optimal solutions of (P1):

$$E_i^* = \{C \subset \text{Im}(f) \mid S_i^C = 1\}$$

We introduce a multi-valued function φ_i defined on $\text{Im}(f)$ by:

$$\varphi_i(y) = \{x_i \in [0, 1] \mid \exists x_{-i} \in [0, 1]^{n-1} \text{ such that } y = f(x_i, x_{-i})\}$$

101 The set $\varphi_i(y)$ contains all values x_i that can lead to y and contains at least one value (as
 102 $y \in \text{Im}(f)$). But $\varphi_i(y)$ can also contain several values or even an infinity depending on the
 103 model properties.

104 Let us now give a characterization of the set E_i^* of optimal solutions (see Proof in
 105 Appendix A).

106 **Proposition 1.** $(C \in E_i^*) \Leftrightarrow$ There exists a function F defined on $[0, 1]$ and valued in $\{0, 1\}$
 107 such that:

$$108 \quad \left\{ \begin{array}{l} C = \{y \in \text{Im}(f) \mid \forall z \in \varphi_i(y), F(z) = 1\} \\ C \neq \emptyset \text{ and } C \neq \text{Im}(f) \end{array} \right.$$

110 Proposition 1 states that an optimal partition of $\text{Im}(f)$ verifying $S_i^{C^*} = 1$ is associated
 111 to a partition (defined by function F) of the domain of X_i . Note that on the other hand, a
 112 partition F of the domain of X_i does not necessarily defines a partition of $\text{Im}(f)$.

113 *Remark 1* (Example with $E_i^* = \emptyset$). Let us consider a purely insensitive input factor X_i , a
 114 function F valued in $\{0, 1\}$ and the set $C = \{y \mid \forall z \in \varphi_i(y), F(z) = 1\}$. As $\forall (x_i, x'_i, x_{-i})$,
 115 $f(x_i, x_{-i}) = f(x'_i, x_{-i})$, we deduce that for any $y \in \text{Im}(f)$, $\varphi_i(y)$ is equal to $[0, 1]$. F is
 116 therefore necessarily constant and equal to one. But this implies that $C = \text{Im}(f)$, which is
 117 excluded in Proposition 1. Proposition 1 thus shows that there exists no set C^* verifying
 118 $S_i^{C^*} = 1$ in this case. Actually, in this example, for every $C \subset \text{Im}(f)$, we have $S_i^C = 0$.

119 *Remark 2* (Example with an infinite sets of optimal solutions). Let us now consider a model
 120 verifying that each point y of the output space can be uniquely reached from a single
 121 possible value x_i . In this case, $\varphi_i(\cdot)$ is a single valued function. Then let us consider any
 122 non-degenerated partition of $[0, 1]$. Any such partition defines a non-degenerated partition
 123 of $\text{Im}(f)$ by applying model f . The resulting partition is characterized by the fact that every
 124 output point reached using a same value x_i is in the same set of the partition. Following
 125 Proposition 1, any such partition is optimal. In this case, as there is an infinite number of
 126 non-degenerated partitions of $[0, 1]$, there is also an infinite set of solutions in E_i^* .

127 *Remark 3* (Example with $S_i = 0$ and $S_i^{C^*} = 1$). Let us consider the model $Y = \text{Sign}(X_1) \cdot$
 128 $|X_2|$, with X_1 and X_2 following uniform distributions on $[-1, 1]$ with a focus on X_2 . The
 129 first order Sobol' index of X_2 , noted S_2 , is equal to zero. We now apply Proposition 1: as for
 130 any $y \in [-1, 1]$, $\varphi_2(y) = \{-y, y\}$, all not-degenerated partitions of the output space $[-1, 1]$
 131 gathering y and $-y$ in the same set of the partition are optimal. Among others, the set
 132 $C^* = \{y \in [-1, 1] \mid |y| < \alpha, \text{ with } \alpha \in]0, 1[\}$ defines a partition $(C^*, \overline{C^*})$ verifying $S_2^{C^*} = 1$.
 133 X_2 has therefore the effect of leading the output from the center of the domain toward its
 134 boundaries (or equivalently from the boundaries to the center). This example shows the
 135 potential of mRSA in revealing the strong influence of a model input on the occurrence of
 136 specific patterns of model outputs ($S_i^{C^*} = 1$) while the standard application of sensitivity
 137 analysis methods may have led to consider it as non-important ($S_i = 0$).

138 2.3.2. Limits of the unconstrained formulation

139 Let us consider the function $f(x_1, x_2) = \frac{1}{x_1 + \lfloor 2 \cdot x_2^{-0.5} \rfloor}$ where $\lfloor x \rfloor$ is the integer part
 140 of x , and let us study $Y = f(X_1, X_2)$, with X_1 and X_2 following independent uniform
 141 distributions on $[0, 1]$. We consider problem (P1) on this model and input X_1 . A sample of
 model responses is presented in Figure 1.

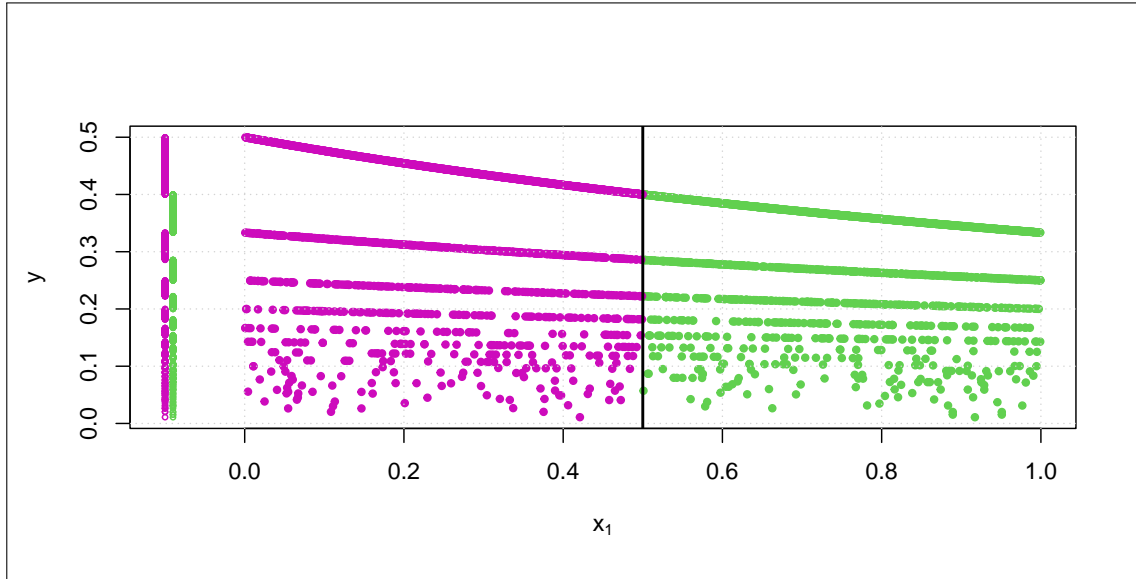


Figure 1: An optimal solution of problem (P1) on model $f(X_1, X_2) = \frac{1}{X_1 + \lfloor 2 \cdot X_2^{-0.5} \rfloor}$. Samples of Y as a function of X_1 are represented. A particular partition of the output space is showed vertically on the left, defined from a partitioning of the x_1 domain above (green values) and below 0.5 (pink values). The partition is optimal from Proposition 1, but difficult to interpret as it is made of an infinite set of sub-intervals when y tends towards zero.

142 This model has several interesting properties for a mRSA exploration with the uncon-
 143 strained formulation (P1):
 144

- 145 • First, neither X_1 nor X_2 is purely insensitive. Indeed, we find numerically that their
 146 first Sobol' indices are respectively about $S_1 = 0.086$ and $S_2 = 0.886$.
- 147 • This model has, for X_1 , the property mentioned in *Remark 2*: any point of the output
 148 space $Im(f) = [0, \frac{1}{2}]$ is reached from a single possible value x_1 . Thus the multi-valued
 149 function $\varphi_1(\cdot)$ produces in this case only single values and can be noted as a function
 150 $f_1^{-1}(\cdot)$. Let us consider the partitioning (C, \overline{C}) of $[0, \frac{1}{2}]$ defined by:

$$C = \{y \in Im(f) \mid F(f_1^{-1}(y)) = 1\} \text{ with } F(x_1) = \begin{cases} 0 & \text{if } x_1 > 0.5 \\ 1 & \text{if } x_1 \leq 0.5 \end{cases}$$

151 This partition is plotted vertically on Figure 1. Following Proposition 1, we have
 152 $S_1^C = 1$, which means that X_1 perfectly explains the transition of the model output
 153 between sets C and \overline{C} .

154 Nevertheless, this solution lacks interpretability, in particular because it is made of an infinite
 155 set of connected components when y tends towards 0 (see Figure 1). Moreover, when y
 156 tends toward 0, there is a full mixing of sets C and \overline{C} in the sense that $\forall \epsilon > 0$, we can
 157 find $0 < y_1 < y_2 < y_3 < \epsilon$ such that $y_1 \in C, y_2 \in \overline{C}, y_3 \in C$. The region whose occurrence
 158 is best explained by the variation of X_1 is thus difficult to characterize in this case. This
 159 example shows that additional constraints must be added to the formulation of Problem
 160 (P1) in order to increase the interpretability of the solutions, in particular regarding the risk
 161 of near-overlapping between C and \overline{C} .

162 2.4. Improved Formulation: constrained mRSA

To overcome the limitations described in the previous section, we now add constraints to
 Problem (P1) by searching only solutions belonging to a set denoted as \mathcal{I} (Problem (P2)):

$$(P2) : \max_{C \subset \text{Im}(f), C \in \mathcal{I}} S_i^C$$

163 This set \mathcal{I} is introduced to increase the chances that a solution is interpretable by an
 164 expert of the model. There is no general definition of this interpretability, but we propose
 165 a trick to improve the method in this direction. We first suppose that a set of K_Y non-
 166 overlapping clusters (C_1, \dots, C_{K_Y}) covering $\text{Im}(f)$ has been defined. We denote as *elementary*
 167 *clusters* these K_Y clusters. A *meta-cluster* is defined as a union of elementary clusters. \mathcal{I}
 168 is then defined as the set of all possible meta-clusters. This choice: i) allows to avoid the
 169 mixing effect illustrated in the 1D example presented in the previous section by choosing
 170 an appropriate value for K_Y , ii) adds an indirect constraint on the number of connected
 171 components of the solution (depending on the number of elementary clusters), iii) adds the
 172 possibility to define elementary clusters either from expert knowledge or using an automatic
 173 algorithm. For these reasons, we found that Problem (P2) is more relevant in practice
 174 than Problem (P1). However, Problem (P2) must be solved numerically using a dedicated
 175 algorithm, since the cost of testing all possible meta-clusters ($2^{K_Y-1} - 1$) is prohibitive.

177 2.5. Algorithm for the constrained formulation (P2)

179 2.5.1. Required simulated data

180 The numerical resolution of Problem (P2) requires a simulation sample noted (\mathbf{X}, \mathbf{Y}) ,
 181 where \mathbf{X} is a matrix of parameters values, and \mathbf{Y} the matrix of multivariate simulated values
 182 obtained by applying the model under study on \mathbf{X} . For the sake of simplicity, we suppose
 183 here that \mathbf{X} is made of N i.i.d parameters values, but note that the algorithm presented in
 184 Section 2.5.3 can also be applied on not i.i.d samples with the only consequence that this
 185 can lead to sub-optimal results.

186 *2.5.2. Aggregation of elementary clusters (C_1, \dots, C_{K_Y})*

187 We designed a hierarchical clustering procedure using an aggregating property in order
188 to merge iteratively elementary clusters (C_1, \dots, C_{K_Y}).

189 Let us introduce a partition of $[0, 1]$ into n_X bins (B_1, \dots, B_{n_X}), typically with $B_j =]\frac{j-1}{n_X}, \frac{j}{n_X}]$,
190 for $j = 1, \dots, n_X$. For a subset C of the simulated output values and a bin B_j , let us define
191 h_j^C such that:

$$h_j^C = \text{Card}\{y \in C \mid \exists x_i \in B_j \text{ such that } y = f(x_i, x_{-i})\}$$

192 The vector $h^C = (h_1^C, \dots, h_{n_X}^C)$ is an approximate representation of the distribution $\mathcal{L}(X_i \mid Y \in$
193 $C)$ and is a (non normalized) histogram associated to cluster C . Let us note \tilde{S}_i^C the estimate
194 of S_i^C obtained by using histogram h^C (its expression can be found in Appendix B).
195

196 **Proposition 2.** *Let us consider two elementary clusters C and C' with histograms h and*
197 *h' satisfying $h' = \theta h$, with $\theta > 0$. Let us denote $(C^*, \overline{C^*})$ the partition of the output space*
198 *maximizing \tilde{S}_i^C over the set \mathcal{I} . Then clusters C and C' belong both to C^* or to $\overline{C^*}$.*

199 Proposition 2 (see Proof in Appendix C) states that elementary clusters having propor-
200 tional histograms cannot be in different sets of the optimal partition $(C^*, \overline{C^*})$ for criterion
201 \tilde{S}_i^C . It therefore suggests that meta-clusters should be defined by aggregating elementary
202 clusters whose histograms are the closest to be proportional. We proposed to do that by us-
203 ing a clustering method based on the histogram correlation distance $d(h, h') = 1 - \text{Cor}(h, h')$.
204 This procedure will be used in Algorithm mRSA presented in the coming section. Note that
205 while the estimator \tilde{S}_i^C was useful to establish Proposition 2, it is however not as pre-
206 cise as classical Sobol' indices estimators. It is therefore not used in practice to make any
207 computation.

208 *2.5.3. Algorithm mRSA*

209 Algorithm mRSA is based on: i) the restriction of the search space to meta-clusters
210 defined from (C_1, \dots, C_{K_Y}) to handle the constraint $C \in \mathcal{I}$, ii) the use of the aggregation
211 method described in the previous section.

212 The first step of Algorithm mRSA consists in clustering the simulated values using an
213 automatic or user-defined clustering procedure ClustFun^Y to get K_Y elementary clusters.
214 Then a clustering of these K_Y elementary clusters into K_H meta-clusters is done using
215 the method noted ClustFun^H . ClustFun^H is a classical hierarchical clustering method
216 using the aggregation procedure described in the previous section. As the last step of
217 the algorithm, an exhaustive search for the best partition over all the $(2^{K_H-1} - 1)$ possible
218 merging of the K_H meta-clusters is performed by estimating $S_i^{P_k}$ for each candidate partition
219 $(P_k, \overline{P_k})$. This algorithm has the following parameters: the index i of the input under study,
220 the pre-clustering method ClustFun^Y , the number K_Y of clusters for the pre-clustering step,
221 the number n_X of bins for the histograms computations, the number of meta-clusters K_H
222 and a size parameter γ which is introduced to exclude meta-clusters having too few elements.

	Input data: (\mathbf{X}, \mathbf{Y})
Algorithm mRSA	Parameters: $(i, ClustFun^Y, K_Y, n_X, K_H, \gamma)$
	Output : $(P_{k^*}, \overline{P_{k^*}}), \widehat{S}_i^{P_{k^*}}$

Apply $ClustFun^Y$ on \mathbf{Y} to get K_Y elementary clusters (C_1, \dots, C_{K_Y})
Compute all histograms $(h^{C_k})_{k=1..K_Y}$ for input X_i discretized with n_X bins
Apply $ClustFun^H$ on $(h^{C_1}, \dots, h^{C_{K_Y}})$ to get K_H meta-clusters $(\widehat{C}_1, \dots, \widehat{C}_{K_H})$
for all 2-partitions $(P_k, \overline{P_k})$ of $(\widehat{C}_1, \dots, \widehat{C}_{K_H})$ **do**
 Compute an estimate $\widehat{S}_i^{P_k}$ of $S_i^{P_k}$ from (\mathbf{X}, \mathbf{Y})
 Compute $\gamma_k = \frac{1}{N} \min (Card(P_k), Card(\overline{P_k}))$, where N =number of rows in \mathbf{X}
end for
 $k^* = \arg \max_{k, \gamma_k \geq \gamma} \widehat{S}_i^{P_k}$

223 *2.5.4. Parameter tuning guidelines*

224 We propose in Table 1 guidelines to set the parameters of Algorithm mRSA based on
225 parameters definitions and numerical experiments.

226 The sample size N (number of rows in \mathbf{X} and \mathbf{Y}) has to be i) large enough for precise
227 estimation of first order indices using (\mathbf{X}, \mathbf{Y}) , but also ii) large enough for a good covering
228 of the output space in order to obtain partitions as close as possible to an optimal solution.
229 There is no general rule for this tuning. For the two case studies, samples of size 4000 and
230 5000 were enough to reveal interpretable partitions of the output space associated with high
231 first order sensitivity indices.

232
233 Parameter K_H which drives the exhaustive search should be set to the highest value
234 allowed by the computational budget (typically lower than 20). Parameter γ was typically
235 set to 0.1 (10% of the number of simulated points). Parameter n_X should be set in order
236 to avoid histograms with too few values per bin, which was satisfied with n_X around 10-
237 20 in our tests. It also turned out to be quite insensitive in the numerical experiments we
238 carried out. On the other hand, the pre-clustering is a critical step. As explained previously,
239 the elementary clusters can be defined by the user to constrain the shape of the solution
240 according to a prior knowledge. An automatic clustering can also be used, such as the
241 hierarchical clustering using euclidean distances used in the numerical examples presented
242 in Section 3. Note that depending on the output space and user knowledge, other procedures
243 may lead to better results. The number of elementary clusters K_Y for this pre-clustering step
244 was found very sensitive in the numerical experiments (see Section 3). Its optimal setting
245 appeared to be a trade-off between the interpretability of the partition (better for low K_Y)
246 and the sensitivity score of the partition (better for large K_Y). A value of $K_Y = 500$ was
247 found to be satisfactory for the different case studies.

Name	Function	Guideline	Value	
			models \mathcal{M}_{2D} (§ 3.1, 3.2)	model CANTIS (§ 3.3)
N	initial sample size	large enough for Sobol' indices estimation and for good covering of output space	4000	5000
K_Y	number of elementary clusters	trade-off between interpretability (small K_Y) and optimality (large K_Y); $K_Y \leq N$	2000, 500, 30	500
$ClustFun^Y$	method for pre-clustering the output space	to be adapted to the output space/ user expertise	HCA^{euc}	HCA^{euc}
K_H	number of meta-clusters	maximum value allowed by computing time budget	12	12
n_X	number of histogram bins	10-20	18	18
γ	relative minimum size of meta-clusters	user requirement	0.1	0.1

Table 1: Guidelines for setting the parameters of the mRSA algorithm and values used for the different tests. HCA^{euc} is a classical hierarchical clustering algorithm used with an euclidean distance.

248 3. Numerical applications

249 3.1. Noise-free 2D test model

250 3.1.1. Model definition and properties

251 We first consider the following test model $(Y_1, Y_2) = \mathcal{M}_{2D}(X_1, X_2, X_3)$, where:

$$\begin{aligned}
 Y_1 &= c_1 + 0.25 \cdot \sqrt{X_3} \cdot \cos(2\pi X_2) \\
 Y_2 &= c_2 + 0.25 \cdot \sqrt{X_3} \cdot \sin(2\pi X_2)
 \end{aligned}
 \quad \text{with } (c_1, c_2) = \begin{cases} (0.5, 0.316), & \text{if } X_1 < 0.33 \\ (0.25, 0.75), & \text{if } 0.33 \leq X_1 < 0.66 \\ (0.75, 0.75), & \text{if } X_1 \geq 0.66 \end{cases}$$

252 Model \mathcal{M}_{2D} is studied for X_1, X_2, X_3 following independent uniform distributions on $[0, 1]$.

253 Basically, the model draws a point in the plane at a distance from a reference point related

254 to the value of X_3 and with an angle to the horizontal line related to the value of X_2 . The
 255 coordinates of the three possible reference points are defined from the value of X_1 . The set
 256 of possible positions for (Y_1, Y_2) is the union of three disks $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$ centered on the reference
 257 points (see Figure 2). We choose the coordinates of the reference points so that any point
 258 of the output space is obtained from exactly one set of values of the parameters.

259 By applying Proposition 1, we know what the solutions to Problem (P1) are for model
 260 \mathcal{M}_{2D} :

- 261 • X_1 : $\varphi_1(y)$ is one of the three intervals $I_1 = [0, \frac{1}{3}[$, $I_2 = [\frac{1}{3}, \frac{2}{3}[$, $I_3 = [\frac{2}{3}, 1]$, each associated
 262 to one of the three disks $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$. There are therefore three non-degenerated solutions
 263 of (P1) for model \mathcal{M}_{2D} : $(\mathcal{C}_1, \overline{\mathcal{C}_1}), (\mathcal{C}_2, \overline{\mathcal{C}_2}), (\mathcal{C}_3, \overline{\mathcal{C}_3})$.
- 264 • X_2, X_3 : for each of these inputs and for each $y \in Im(\mathcal{M}_{2D})$, $\varphi_i(y)$ has a single value.
 265 Thus, from Remark 2 following Proposition 1, any non-degenerated partition of the X_2
 266 (resp. X_3) domain defines an optimal partition of the output space. For both X_2 and
 267 X_3 , the optimal solution is made of a sub-partition replicated on all disks $\mathcal{C}_1, \mathcal{C}_2, \mathcal{C}_3$.
 268 For X_2 , optimal partitions have an angular pattern (i.e. all outputs y having the same
 269 angle to the closest center are in the same set of the partition) resulting in partitions
 270 made of angular sectors. For X_3 , optimal partitions have a radial pattern (i.e. all y at
 271 the same distance from the closest center are in the same set of the partition) resulting
 272 in partitions made of rings.

273 3.1.2. Results

274 We applied Algorithm mRSA to the model \mathcal{M}_{2D} for problem (P2). A set of 2000 elemen-
 275 tary clusters is used to define the set \mathcal{I} . Elementary clusters are obtained using a hierarchical
 276 clustering algorithm with an euclidean distance on \mathbb{R}^2 . The values of the parameters used for
 277 the application of Algorithm mRSA are given in Table 1. The sensitivity indices are com-
 278 puted using the estimation method based on ranks [20] implemented in sobolrank function
 279 of the R package sensitivity [21], applied on a Monte Carlo sample of size $N = 4000$.

280 The results are displayed as a 35×35 image with the following convention: red pixels
 281 contain only points belonging to C^* , blue pixels contain only points belonging to $\overline{C^*}$, yellow
 282 pixels include points from C^* and $\overline{C^*}$. This display allows to quickly assess regions where
 283 many points of the two clusters are close together (which leads to poor interpretability).

284 The results are presented in Figure 2. As we can see, the optimized values of \widehat{S}^{C^*} are
 285 equal to one for each input, showing that the algorithm is able to find optimal solutions
 286 for $i = 1, 2, 3$. The partitions found are consistent with the set of optimal solutions of
 287 (P1), meaning that in this simple example and with the quite large number of elementary
 288 clusters used, (P1) and (P2) are equivalent, and the solutions obtained are interpretable.
 289 This example shows the ability to find optimal numerical solutions in a favorable case.

290 3.2. 2D test model with noise

291 3.2.1. Model definition and properties

292 In order to test the algorithm properties in a more complicated case, we add a noise in
 293 the formulation of model \mathcal{M}_{2D} to define a new model $(Y_1^{(r)}, Y_2^{(r)}) = \mathcal{M}_{2D}^{(r)}(X_1, X_2, X_3, X_4)$.

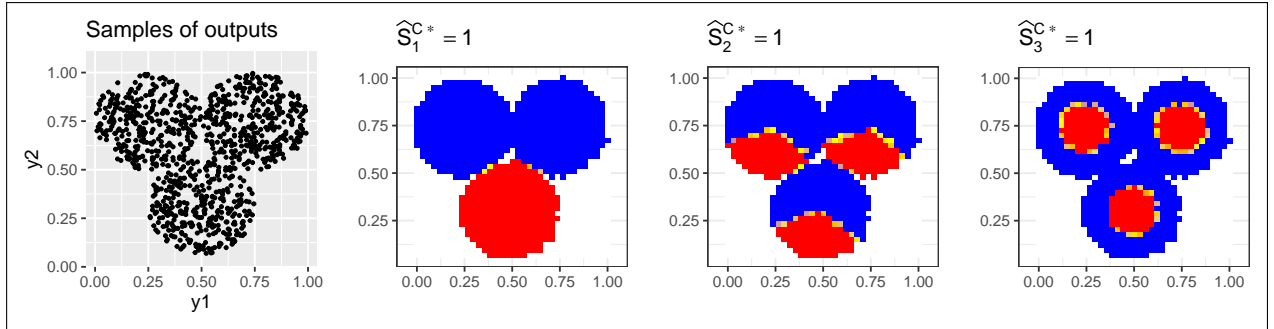


Figure 2: Results of the mRSA algorithm on model \mathcal{M}_{2D} (model with 2D outputs without noise). Left: sample of model outputs, Right: optimized partitions found for each model input (red: pixels belonging to C^* , blue: pixels belonging to $\overline{C^*}$, yellow: pixels including points from C^* and points from $\overline{C^*}$). For each X_i , the values of $\widehat{S}_i^{C^*}$ are equal to 1.

294 The idea is to have a fourth parameter X_4 (following a uniform distribution in $[0, 1]$) that
 295 adds a small displacement to the output of \mathcal{M}_{2D} .

296 In order to avoid ending up with a stochastic model (which would raise additional issues
 297 for the definition and estimation of the Sobol' indices [22], outside the scope of the present
 298 study), the perturbation is defined in a deterministic way by taking the row of index $\lfloor 100 \cdot X_4 \rfloor$
 299 of a pre-defined matrix Υ . Matrix Υ is of size $(100, 2)$ and made of small 2D displacements
 300 sampled from random distributions. $(Y_1^{(r)}, Y_2^{(r)}) = \mathcal{M}_{2D}^{(r)}(X_1, X_2, X_3, X_4)$ is therefore defined
 301 as:

$$\begin{aligned} Y_1^{(r)} &= Y_1 + \Upsilon_{\lfloor 100 \cdot X_4 \rfloor, 1} \\ Y_2^{(r)} &= Y_2 + \Upsilon_{\lfloor 100 \cdot X_4 \rfloor, 2} \end{aligned}$$

302 Due to the perturbations, Problem (P1) no longer has simple solutions when consid-
 303 ering model $\mathcal{M}_{2D}^{(r)}$. Indeed, for many points y of the output space, $\varphi_i(y)$ is multi-valued:
 304 there are many different settings leading to a same value y (actually all (x_1, x_2, x_3) such as
 305 $\mathcal{M}_{2D}(x_1, x_2, x_3) = y - \Upsilon_{i, \cdot}$, where $\Upsilon_{i, \cdot}$ is one row of Matrix Υ). We therefore do not know a
 306 priori the solutions of (P1) or (P2) in this case. Nevertheless, as the amplitude of the noise
 307 decreases, we expect to retrieve the solutions found for the model \mathcal{M}_{2D} .

308 3.2.2. Results

309 We applied Algorithm mRSA on problem (P2) for model $\mathcal{M}_{2D}^{(r)}$ for $K_Y = \{2000, 500, 30\}$
 310 elementary clusters in the pre-clustering phase of the algorithm. The results are presented
 311 in Figure 3 for all the inputs (including the one driving the perturbations).

312 As expected, the partitions found are related to the ones obtained with model \mathcal{M}_{2D} ,
 313 but are blurred. We can also notice that the level of noise depends on the setting of the
 314 parameter K_Y : there is more noise for high values of K_Y , which makes the interpretation of
 315 the results more difficult. On the other hand, lowering K_Y too much leads to more clearly
 316 defined partitions but at the expense of their optimality. For example, when looking at the

317 sensitivity scores \widehat{S}_2^{C*} as a function of K_Y , we have $\widehat{S}_3^{C*}(2000) = 0.435$, $\widehat{S}_3^{C*}(500) = 0.315$,
 318 and $\widehat{S}_3^{C*}(30) = 0.234$. As mentioned in the guidelines given in Table 1, there is a compromise
 319 to be found in the value of K_Y to obtain results that are both precise and interpretable. In
 320 this example, $K_Y = 500$ seems to be a relevant choice.

321 Another notable result is that the patterns found are not the same depending on the value
 322 of K_Y . However, we can note that they all correspond to an optimal solution of the previous
 323 problem. For example there are different angular patterns for the solutions found for X_2 .
 324 Lastly, it is interesting to look at the patterns and associated sensitivity scores obtained for
 325 the perturbation parameter X_4 . As expected, the scores are low and the patterns made of
 326 a lot of connected components even for $K_Y = 500$. The algorithm therefore does not create
 327 a falsely interpretable structure associated with this perturbation parameter.

328 3.3. Environmental model simulating temporal outputs

329 3.3.1. Model and input distributions

330 We applied the mRSA algorithm on the environmental model CANTIS [23], which sim-
 331 ulates the decomposition of organic biomass in crop residues over time based on a set of
 332 differential equations. We use the same model setting as in [13]. The model setting consists
 333 in ten uncertain model inputs and the analysis of one time-varying output: the zymogenous
 334 microbial biomass, here-after referred to as ZYB . The reader is invited to refer to [13] for
 335 more details. The sensitivity indices are computed using the estimation method based on
 336 ranks [20] implemented in sobolrank function of the R package sensitivity [21], applied on
 337 a Monte Carlo sample of size $N = 5000$ producing 5000 output curves of ZYB . The other
 338 parameters values used to apply Algorithm mRSA are given in Table 1.

339 3.3.2. Results

340 We present in Table 2 the sensitivity indices \widehat{S}_i^{C*} obtained when applying the Algorithm
 341 mRSA on each input of the CANTIS model in the considered uncertainty setting. Only X_8
 342 and X_9 exhibits large values that deserve further analysis. For these two inputs, we plotted
 343 in Figure 4 the optimal clusters found.

344 For input X_8 , we obtained $\widehat{S}_8^{C*} = 0.851$. Looking at Figure 4, we can see that the
 345 two clusters identified differ the most at the beginning of the simulation time period. The
 346 two clusters then overlap rapidly. The application of the method indicates that X_8 drives
 347 the occurrence of biomass dynamics that start by increasing (or equivalently that start by
 348 decreasing).

349 For input X_9 , a very high score ($\widehat{S}_9^{C*} = 0.874$) was also obtained. For this input, when
 350 examining Figure 4, it appears that what best distinguishes the two clusters is the level
 351 of ZYB values over the entire simulated time period, and particularly the final values. We
 352 conclude that X_9 drives the occurrence of dynamics with the highest (or the lowest) biomass
 353 levels all along the considered time scale and particularly for the final value.

354 4. Conclusion

355 In this work, a new sensitivity analysis approach extending Regional Sensitivity Analysis
 356 and named mRSA was introduced with the aim of automatically identifying the model

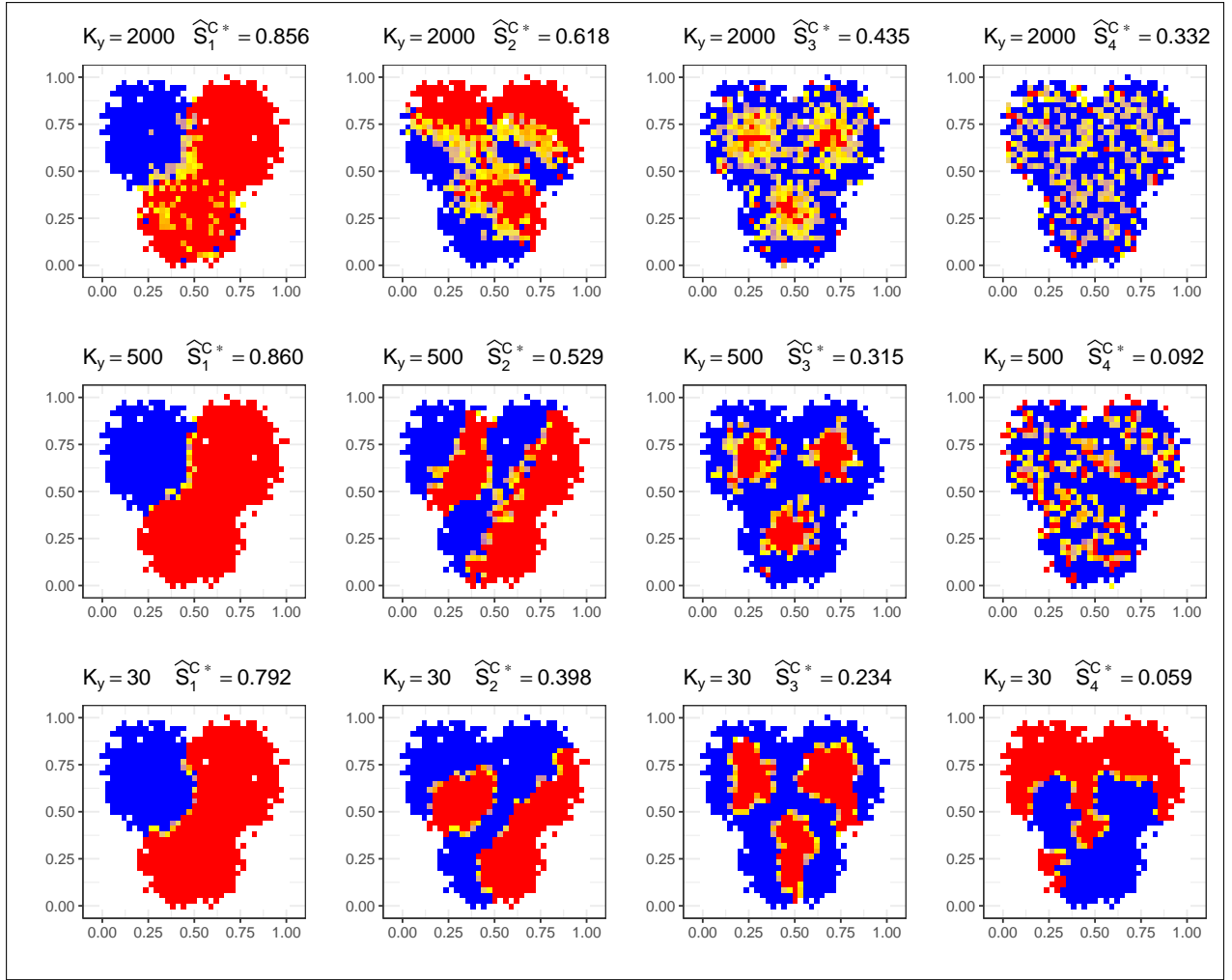


Figure 3: Results of the mRSA algorithm on the 2D model with noise $\mathcal{M}_{2D}^{(r)}$ with $K_Y = \{2000, 500, 30\}$ for the four model inputs. Red: pixels belonging to C^* , blue: pixels belonging to $\overline{C^*}$, yellow: pixels including points from C^* and points from $\overline{C^*}$.

357 behaviors best explained by the variations of the different model inputs. A first formalization
 358 of mRSA as an unconstrained maximization problem using a sensitivity based criterion was
 359 theoretically studied. An improved formulation (constrained mRSA), more interesting in
 360 practice, was introduced and solved numerically with a dedicated algorithm. The application
 361 of this algorithm on an environmental model producing biomass dynamics showed the ability
 362 of mRSA to reveal, both in a quantitative and graphical way, some impact of the model
 363 inputs variations that would not have been easy to detect without strong prior knowledge.
 364 This approach opens new perspectives, particularly for the study of complex models with
 365 multivariate outputs.

366 In this study, only first order indices were considered in the optimization procedure.

X_i	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
\widehat{S}_i^{C*}	0.069	0.066	0.083	0.069	0.078	0.059	0.069	0.851	0.874	0.062

Table 2: Optimized region-based sensitivity indices obtained for each input X_i for the environmental model CANTIS.

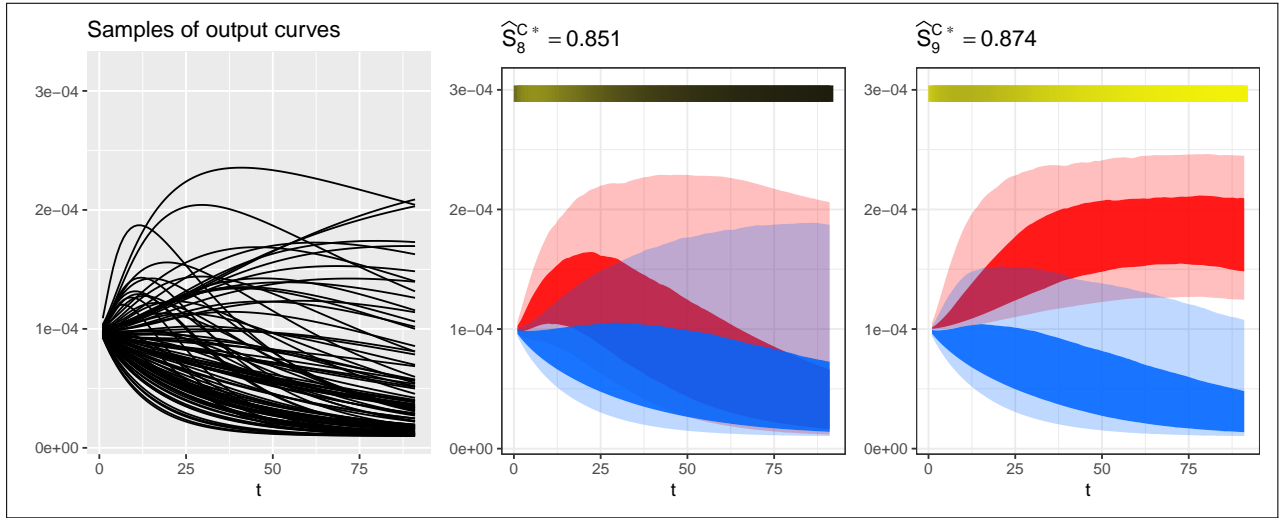


Figure 4: Clustering obtained with Algorithm mRSA on the CANTIS model. Left: samples of output curves. Right: results of the mRSA application for input X_8 and X_9 . Sensitivity scores and optimal partitions are represented. The optimal partitions are plotted using quantiles (0.05,0.25,0.75,0.95) as a function of time. The horizontal colorbar indicates the significance of the difference between the two partitions at a given time: yellow (resp. black) corresponds to a high (resp. low) difference as given by Kolmogorov–Smirnov statistic.

367 Other indices could have been considered, such as indices of groups of parameters, or indices
368 quantifying some interaction effects of interest. Looking for partitions optimizing such in-
369 dices would enlarge the possible model properties explored. The question of having efficient
370 algorithm to find solutions in such cases is however challenging and is a direction for future
371 work.

372

373 5. Software availability

374 R codes for applying Algorithm mRSA on the toy model and on the CANTIS model
375 are available from a Gitlab repository located at https://forgemia.inra.fr/sebastien.roux/mrsa_paper/.
376

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426 **Appendix A: Proof of Proposition 1**

427 We first recall the Sobol' Hoeffding decomposition over $[0, 1]^n$, which states that any
 428 function g square-integrable over $[0, 1]^n$ can be uniquely decomposed in the following form:

$$g(X) = g_0 + \sum_{i_1=1}^n g_{i_1}(X_{i_1}) + \sum_{i_2>i_1} g_{i_1 i_2}(X_{i_1}, X_{i_2}) + \dots + g_{i_1 \dots i_n}(X_{i_1}, \dots, X_{i_n})$$

429 where

$$\begin{aligned} \mathbb{E}[g_{i_1 \dots i_s}(X_{i_1}, \dots, X_{i_s})] &= 0, \forall \{i_1 \dots i_s\} \subseteq \{1, 2, \dots, n\} \\ \mathbb{E}[g_{i_1 \dots i_s}(X_{i_1}, \dots, X_{i_s}) g_{j_1 \dots j_t}(X_{j_1}, \dots, X_{j_t})] &= 0, \forall \{i_1, \dots, i_s\} \neq \{j_1, \dots, j_t\} \end{aligned}$$

430 We also recall that $S_i = 1$ (where S_i is the first Sobol' index associated to X_i) implies that
 431 for all multi-index $j \neq \{i\}$, the total Sobol' index $S_j^T = 0$, which implies that all terms in
 432 decomposition except g_i have null variances. Therefore, $S_i = 1$ implies that:

$$g(X) = g_0 + g_i(X_i) \tag{2}$$

Necessary Condition We suppose $C \in E_i^*$ (thus $C \neq \emptyset$ and $C \neq \text{Im}(f)$). As $S_i^C = 1$, when
 applying Equation (2) to $\mathbb{1}_C(\cdot)$, we find that there exists a function $F_i(\cdot)$ valued in $\{0, 1\}$,
 such that $\forall (X_1, \dots, X_n)$ in their variation domain:

$$\mathbb{1}_C(f(X_1, \dots, X_n)) = F_i(X_i)$$

433 If $y \in C$ (resp. \overline{C}), any (x_i, x_{-i}) such that $y = f(x_i, x_{-i})$ verifies $F_i(x_i) = 1$ (resp. 0).
 434 Therefore $y \in C$ (resp. \overline{C}) implies that $\forall z \in \varphi_i(y), F_i(z) = 1$ (resp. 0). Therefore F_i
 435 satisfies the conditions of Proposition 1.

Sufficient Condition We suppose the existence of a set C satisfying the right hand side of
 Proposition 1 and calculate S_i^C . There exists a function F such that $\forall (X_1, \dots, X_n)$ in their
 variation domain:

$$\mathbb{1}_C(f(X_1, \dots, X_n)) = F(X_i)$$

This implies that:

$$\mathbb{V}[\mathbb{E}[\mathbb{1}_C(f(X_1, \dots, X_n)) | X_i]] = \mathbb{V}[F]$$

436 Moreover, as $C \neq \emptyset$ and $C \neq \text{Im}(f)$, we have $\mathbb{V}[\mathbb{1}_C(f(X_1, \dots, X_n))] = \mathbb{V}[F] \neq 0$. Therefore
 437 $S_i^C = 1$.

438 **Appendix B: Expression of \widetilde{S}_i^C , an approximation of S_i^C using h^C**

Equation (1) can be written as:

$$S_i^C = \frac{1}{\mathbb{V}[\mathbb{1}_C(Y)]} \mathbb{E}_{X_i} [\mathbb{E}[\mathbb{1}_C(Y) | X_i] - \mathbb{E}[\mathbb{E}[\mathbb{1}_C(Y) | X_i]]]^2$$

439 We note that, with the discretization of X_i into n_X bins:

$$\begin{aligned} \mathbb{E}[\mathbb{E}[\mathbb{1}_C(Y)|X_i]] &= \frac{1}{n_X} \sum_{j=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j] \\ \mathbb{V}[\mathbb{1}_C(Y)] &= \mathbb{E}[(\mathbb{E}[\mathbb{1}_C(Y)|X_i] - \mathbb{E}[\mathbb{E}[\mathbb{1}_C(Y)|X_i]])^2] \\ &= \frac{1}{n_X} \sum_{j=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j] - \left(\frac{1}{n_X} \sum_{j=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j]\right)^2 \end{aligned}$$

440 S_i^C can be rewritten with the discretization of X_i into n_X bins by:

$$S_i^C = \frac{\frac{1}{n_X} \sum_{j=1}^{n_X} \left(\mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j] - \frac{1}{n_X} \sum_{l=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_l] \right)^2}{\frac{1}{n_X} \sum_{j=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j] \cdot \left(1 - \frac{1}{n_X} \sum_{j=1}^{n_X} \mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j]\right)}$$

Moreover, using the simulation sample of size N , we have the approximation:

$$\mathbb{E}[\mathbb{1}_C(Y)|X_i \in B_j] \approx \frac{n_X \cdot h_j^C}{N}$$

441 Using this approximation, we deduce that the following expression noted \tilde{S}_i^C is an ap-
442 proximation of S_i^C :

$$\tilde{S}_i^C = \frac{n_X}{\sum_{j=1}^{n_X} h_j^C \cdot (N - \sum_{j=1}^{n_X} h_j^C)} \sum_{j=1}^{n_X} \left(h_j^C - \frac{1}{n_X} \sum_{l=1}^{n_X} h_l^C \right)^2 = \frac{\|h^C - H^C\|^2}{H^C \cdot (N - n_X H^C)}$$

443 where $H^C = \frac{1}{n_X} \sum_{j=1}^{n_X} h_j^C$.

444 Appendix C: Proof of Proposition 2

445 Let us consider a cluster C_0 (having histogram h^0 with mean H_0) that we either merge
446 with a cluster C (having histogram h and histogram mean H) to form cluster $C_1 = C_0 \cup C$,
447 or with two clusters C and C' having respective histograms h and $h' = \theta h$ to form cluster
448 $C_2 = C_0 \cup C \cup C'$. The region-based sensitivity criteria based on histograms for these three
449 sets are $\tilde{S}_i^{C_0}$, $\tilde{S}_i^{C_1}$ and $\tilde{S}_i^{C_2}$.

450 We suppose that $\tilde{S}_i^{C_0} \leq \tilde{S}_i^{C_1}$, i.e. that merging C_0 and C , forming partition $(C_1, \overline{C_1})$
451 leads to a better partition than $(C_0, \overline{C_0})$. The principle of the proof is to show that there
452 is an improvement in merging C' with C_1 , i.e. that $\tilde{S}_i^{C_1} < \tilde{S}_i^{C_2}$. Hence we will conclude

453 that, supposing now that two elementary clusters have proportional histograms, then they
 454 are necessarily of the same side of the optimal partition.

455 We denote: $N_0 = \frac{N}{n_X}$, and $u = h^0 - H_0, v = h - H$.

456 From $C_0 \cup C \cup C' \subsetneq \text{Im}(f)$ we deduce $\sum_j (h_j^0 + (1 + \theta)h_j) < N$ and $H_0 + (1 + \theta)H < N_0$.

457 Then, with these notations, we express the sensitivity criteria based on histograms:

$$\begin{aligned} n_X \tilde{S}_i^{C_0} &= \frac{1}{H_0(N_0 - H_0)} \|u\|^2 \\ n_X \tilde{S}_i^{C_1} &= \frac{1}{(H_0 + H)(N_0 - (H_0 + H))} \|u + v\|^2 \\ n_X \tilde{S}_i^{C_2} &= \frac{1}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + (1 + \theta)H))} \|u + (1 + \theta)v\|^2 \end{aligned}$$

458 From $\tilde{S}_i^{C_0} \leq \tilde{S}_i^{C_1}$ we deduce:

$$\|u + v\|^2 \geq \frac{(H_0 + H)(N_0 - (H_0 + H))}{H_0(N_0 - H_0)} \|u\|^2 \quad (3)$$

459 As $H_0 + (1 + \theta)H < N_0$, we consider $\frac{\tilde{S}_i^{C_2}}{\tilde{S}_i^{C_1}}$:

$$\begin{aligned} \frac{\tilde{S}_i^{C_2}}{\tilde{S}_i^{C_1}} &= \frac{\|u + (1 + \theta)v\|^2}{\|u + v\|^2} \frac{(H_0 + H)(N_0 - (H_0 + H))}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + (1 + \theta)H))} \\ &= \frac{\|u + v\|^2 + (\theta^2 + 2\theta)\|v\|^2 + 2\theta u \cdot v}{\|u + v\|^2} \frac{(H_0 + H)(N_0 - (H_0 + H))}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + (1 + \theta)H))} \end{aligned}$$

460 From $(\theta^2 + 2\theta)\|v\|^2 + 2\theta u \cdot v = \theta(\|u + v\|^2 - \|u\|^2 + (1 + \theta)\|v\|^2)$ and Equation (3) we deduce:

$$\begin{aligned} (\theta^2 + 2\theta)\|v\|^2 + 2\theta u \cdot v &\geq \theta \left(1 - \frac{H_0(N_0 - H_0)}{(H_0 + H)(N_0 - (H_0 + H))}\right) \|u + v\|^2 \\ \|u + v\|^2 + (\theta^2 + 2\theta)\|v\|^2 + 2\theta u \cdot v &\geq \left(1 + \theta - \frac{\theta H_0(N_0 - H_0)}{(H_0 + H)(N_0 - (H_0 + H))}\right) \|u + v\|^2 \end{aligned}$$

461 Hence:

$$\begin{aligned} \frac{\tilde{S}_i^{C_2}}{\tilde{S}_i^{C_1}} &\geq \frac{(1 + \theta)(H_0 + H)(N_0 - (H_0 + H)) - \theta H_0(N_0 - H_0)}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + (1 + \theta)H))} \\ \frac{\tilde{S}_i^{C_2}}{\tilde{S}_i^{C_1}} &\geq \frac{(H_0 + (1 + \theta)H)(N_0 - (H_0 + H)) - \theta H_0 H}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + H)) - \theta H(H_0 + (1 + \theta)H)} \\ \frac{\tilde{S}_i^{C_2}}{\tilde{S}_i^{C_1}} &\geq 1 + \frac{\theta(1 + \theta)H^2}{(H_0 + (1 + \theta)H)(N_0 - (H_0 + (1 + \theta)H))} > 1 \end{aligned}$$

462 so $\tilde{S}_i^{C_1} < \tilde{S}_i^{C_2}$.