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¹ Change of support effects in spatial variance-based sensitivity anal-

 $_2$ ysis¹

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Variance-based global sensitivity analysis (GSA) aims at study-Abstract 18 ing how uncertainty in the output of a model can be apportioned to different 19 sources of uncertainty in its inputs. GSA is an essential ingredient in model 20 building: it helps to identify model inputs that account for most of model 21 output variability. Yet this approach is not really appropriate for spatial 22 models, as it cannot describe how uncertainty interacts with another key 23 issue in spatial modeling: the issue of model upscaling and change of spa-24 tial support. In many environmental models, the end-user is interested in 25 the spatial average or sum of model output over a given spatial unit (e.g. 26 the average porosity of a geological block). Under a change of spatial sup-27 port, the relative contribution of uncertain model inputs to the variance of 28 aggregated model output may change. We propose in this paper a simple for-29 malism to discuss this question within GSA framework by defining *point* and 30 *block* sensitivity indices. We show that the relative contribution of an un-31 certain spatially distributed model input increases with its covariance range 32 and decreases with the size of the spatial unit considered for model output 33 aggregation. Results are briefly illustrated by a simple example. 34

Keywords Sensitivity analysis · Sobol' indices · Model upscaling · Change
 of support · Regularization theory · Spatial model

37 1 Introduction

Variance-based global sensitivity analysis (GSA) aims at studying how un-38 certainty in the output of a model can be apportioned to different sources of 39 uncertainty in its inputs. Here *model* denotes any computer code in which a 40 response variable is calculated as a deterministic function of input variables. 41 Born in the 1990ies (Sobol' 1993), GSA is now recognized as an essential in-42 gredient in model building (European Commission 2009; US Environmental 43 Protection Agency 2009) and is widely used in different fields (Cariboni et 44 al 2007; Tarantola et al 2002). It is based on the decomposition of model 45 output variance into conditional variances. So-called first-order sensitivity 46 indices measure the main effect contribution of each uncertain model input 47 to the model output variance. Based on these sensitivity indices, ranking of 48 model inputs helps 1) identifying inputs that account for most of model out-49 put variability and need to be better scrutinized with extra data-gathering 50 2) simplifying model by identifying model inputs that have little influence on 51 model output variance. 52

Although GSA was initially designed for models with scalar inputs and scalar output only, some work has been recently carried out on extending it to environmental models where both inputs and output are spatially distributed

over a 2D domain (Lilburne and Tarantola 2009, for a review). In these 56 works, spatial model inputs are usually maps derived from sampled field-57 data (e.g. digital elevation model, landuse map). They are uncertain due to 58 measurement errors, lack of knowledge or aleatory variability (Brown and 59 Heuvelink 2007; Refsgaard et al 2007), and are modeled as random fields. 60 Model output is also spatially distributed (e.g. a flood map, a pollution map). 61 Authors use geostatistical simulation to include spatially distributed model 62 inputs into GSA approach (Ruffo et al 2006; Saint-Geours et al 2010)63 and display efficient estimation procedures to compute sensitivity indices in 64 a spatial context, either with respect to the spatial average of model out-65 put (Lilburne and Tarantola 2009), or with respect to the values of model 66 output at each site of a study area (Heuvelink et al 2010; Marrel et al 2011; 67 Pettit and Wilson 2010). 68

Yet, to date none of these studies has reported on a key issue: the link between uncertainty propagation and model upscaling/downscaling. *Model upscaling* consists in the application of a spatial model, developed at a specific scale, to a larger scale. In many environmental models, physical quantities considered are additive (e.g. porosity, evapotranspiration), i.e. their large scale properties derive from small scale properties by simple averaging. In this case, model end-user is usually interested in the spatial linear average or sum

of spatial output over a given spatial unit (e.g. the average porosity of a block, 76 the total evapotranspiration over a plot of land) and model upscaling is thus 77 reduced to a *change of support* problem. Heuvelink (1998) pointed out that 78 under a change of spatial support of model output, the relative contribution 79 of uncertain model inputs to the variability of aggregated model output may 80 change. Exploring how sensitivity analysis results interact with change of 81 support issue is thus of great importance to check the robustness of model-82 based environmental impact assessment studies and give better confidence in 83 their results. It would allow the modeler to answer the following questions: 84 what are the most influential model inputs over a given spatial support? For 85 which support size does a spatially distributed model input contribute the 86 most to model output uncertainty? Does spatial structure of uncertainty of 87 a model input influence its contribution to model output variability? 88

⁸⁹ Change of support effect has been extensively discussed in geostatistics with ⁹⁰ the regularization theory (Journel and Huijbregts 1978, p.77). Hence, we try ⁹¹ in this paper to bring together regularization theory and variance-based GSA ⁹² frameworks. Our idea is to define *site sensitivity indices* and *block sensitivity* ⁹³ *indices*, in order to i) provide a simple formalism to extend variance-based ⁹⁴ GSA to spatial models, when the modeler's interest is in spatial average or ⁹⁵ sum of model output over a given spatial support (section 2); ii) discuss the ⁹⁶ influence of model upscaling on the relative contribution of uncertain model ⁹⁷ inputs to the variance of model output (section 3). We limit our study to ⁹⁸ point-based models, i.e. models where the computation of model output at ⁹⁹ some location uses the value of spatial inputs at that same location only ¹⁰⁰ (Heuvelink, Brus, and Reinds 2010). An example is used throughout the ¹⁰¹ paper to illustrate formal definitions and properties. We finally discuss the ¹⁰² limits of our approach and its links with related work in section 4.

¹⁰³ 2 Variance-based sensitivity indices for a spatial model

104 2.1 Description of spatial model \mathcal{M}

Let $\mathcal{D} \subset \mathbb{R}^2$ denote a 2D spatial domain, $\mathbf{x} \in \mathcal{D}$ a site, **h** the lag vector 105 between two sites \mathbf{x} and \mathbf{x}' , and $v \in \mathcal{D}$ some spatial support of area |v|. For 106 sake of clarity, we consider a spatial model $Y = \mathcal{M}(\mathbf{U}, Z)$ with n uncertain 107 scalar inputs U_1, \ldots, U_n that are grouped into a vector $\mathbf{U} \in \mathbb{R}^n$ of joint 108 pdf $p(\mathbf{U})$, and a single uncertain spatial input $\{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}$, that we will 109 often simply denote by $Z(\mathbf{x})$. $Z(\mathbf{x})$ is supposed to be a strictly stationary 110 random field (SRF) of mean μ with finite variance and covariogram $C(\cdot)$. Let 111 assume its covariance structure, characterized by range $a \in \mathbb{R}$ and nugget 112

effect $\eta \in [0; 1[$, is isotropic and of the form:

$$C(\mathbf{h}) = \begin{cases} C(0) & \text{if } \mathbf{h} = \mathbf{0} \\ \\ (1 - \eta) \cdot C(0) \cdot \rho_a \left(\|\mathbf{h}\| \right) & \text{if } \mathbf{h} \neq \mathbf{0} \end{cases}$$
(1)

with $\rho_a(\cdot)$ some valid correlogram (Cressie 1993, p.67). Model output is a 2D random field $\{Y(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}$, that we will simply denote by $Y(\mathbf{x})$. As discussed in the introduction, we limit our study to *point-based* models, hence we assume there exists a mapping $\psi : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ such that:

$$\forall \mathbf{x} \in \mathcal{D}, \quad Y(\mathbf{x}) = \psi \left[\mathbf{U}, Z(\mathbf{x}) \right]$$
(2)

We also assume that ψ is such that for any site $\mathbf{x} \in \mathcal{D}$, random variables $Y(\mathbf{x})$, 118 $\mathbb{E}[Y(\mathbf{x}) \mid Z(\mathbf{x})]$ and $\mathbb{E}[Y(\mathbf{x}) \mid \mathbf{U}]$ have finite expectation and finite variance. 119 Sensitivity analysis of model \mathcal{M} must be performed with respect to a scalar 120 quantity of interest derived from spatially distributed model output $Y(\mathbf{x})$. 121 Here we consider two different outputs of interest: the value $Y(\mathbf{x}^*)$ at some 122 specific site $\mathbf{x}^* \in \mathcal{D}$ and the aggregated value $Y_v = 1/|v| \int_v Y(\mathbf{x}) d\mathbf{x}$ over 123 support v. As model inputs U and $Z(\mathbf{x})$ are uncertain, $Y(\mathbf{x}^*)$ and Y_v are both 124 random variables: sensitivity analysis will discuss the relative contribution 125 of uncertain model inputs U and $Z(\mathbf{x})$ to their respective variances. 126

127 2.2 Site sensitivity indices and block sensitivity indices

Before defining sensitivity indices for spatial model \mathcal{M} , we very briefly review the mathematical basis of variance-based GSA. Consider a model $Y = f(X_1, \ldots, X_n)$ where X_i are independent random variables. First-order sensitivity index S_i of model input X_i is defined by:

$$S_{i} = \frac{\operatorname{Var}\left[E(Y|X_{i})\right]}{\operatorname{Var}\left(Y\right)} \tag{3}$$

 $S_i \in [0; 1]$ measures the main effect contribution of uncertain model input X_i 132 to the variance of model output Y. It is the expected part of output variance 133 Var(Y) that could be reduced if input X_i was perfectly known. Sensitivity 134 indices can be used to identify the model inputs that account for most of 135 model output variability (model inputs X_i with high first order indices S_i). 136 Sum of S_i is lower than 1: difference $1 - \sum_i S_i$ accounts for the contribution 137 of interactions between model inputs X_i to model output variance Var(Y). 138 If needed, Saltelli et al (2008) will provide more details on GSA theory and 139 on estimation of sensitivity indices. 140

To extend GSA to spatial model \mathcal{M} , we propose to use different types of sensitivity indices to describe the relative contribution of uncertain model inputs **U** and $Z(\mathbf{x})$ to the variability of model output: at site scale (i.e. with respect to output of interest $Y(\mathbf{x}^*)$) and at larger scale (i.e. with respect to output of interest Y_v). First-order sensitivity indices of model inputs with respect to $Y(\mathbf{x}^*)$ are called *site sensitivity indices*. Under stationary hypothesis on SRF $Z(\mathbf{x})$, they don't depend on site \mathbf{x}^* , thus will simply be denoted by $S_{\mathbf{U}}$ and S_Z :

$$S_{\mathbf{U}} = \frac{\operatorname{Var}\left[\mathbb{E}(Y(\mathbf{x}^*) \mid \mathbf{U})\right]}{\operatorname{Var}\left[Y(\mathbf{x}^*)\right]} \quad ; \quad S_Z = \frac{\operatorname{Var}\left[\mathbb{E}(Y(\mathbf{x}^*) \mid \{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\})\right]}{\operatorname{Var}\left[Y(\mathbf{x}^*)\right]} \quad (4)$$

First-order sensitivity indices of model inputs with respect to block average Y_v are called *block sensitivity indices* and are denoted by $S_{\mathbf{U}}(v)$ and $S_Z(v)$:

$$S_{\mathbf{U}}(v) = \frac{\operatorname{Var}\left[\mathbb{E}(Y_v \mid \mathbf{U})\right]}{\operatorname{Var}\left[Y_v\right]} \quad ; \quad S_Z(v) = \frac{\operatorname{Var}\left[\mathbb{E}(Y_v \mid \{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\})\right]}{\operatorname{Var}\left[Y_v\right]} \quad (5)$$

Ratio $S_Z(v)/S_{\mathbf{U}}(v)$ gives the relative contribution of uncertain model inputs $Z(\mathbf{x})$ and \mathbf{U} to the variability of the output of interest Y_v : when $S_Z(v)/S_{\mathbf{U}}(v) > 1$, variance of Y_v is mainly explained by uncertainty on 2D input field $Z(\mathbf{x})$; when $S_Z(v)/S_{\mathbf{U}}(v) < 1$, it's the uncertainty on non-spatial input \mathbf{U} that accounts for most of Var (Y_v) .

156 2.3 Illustrative example

The proposed formalism for spatial GSA is illustrated through the following example. A model $Y = \mathcal{M}(\mathbf{U}, Z)$ is used for economic assessment of flood risk. $Z(\mathbf{x})$ is the map of maximal water levels (m) reached during a flood event over a given area \mathcal{D} . It is assumed to be a Gaussian random field with mean $\mu = 50$ and exponential covariance $C(\mathbf{h})$ with C(0) = 100, range a = 5 and nugget $\eta = 0.1$. U is a set of three economic parameters U_1 , U_2 and U_3 , assumed to be independent random variables following Gaussian distributions $\mathcal{N}(1.5, 0.5)$, $\mathcal{N}(55, 5)$ and $\mathcal{N}(10, 10)$ respectively. Model output $Y(\mathbf{x})$ is the map of expected economic damages due to the flood over the area, which depend on U and $Z(\mathbf{x})$ through mapping ψ :

$$\forall \mathbf{x} \in \mathcal{D}, \quad Y(\mathbf{x}) = \psi \left[\mathbf{U}, Z(\mathbf{x}) \right] = U_1 \cdot Z(\mathbf{x}) - U_2 \cdot e^{-0.036 \cdot Z(\mathbf{x})} - U_3 \qquad (6)$$

Stakeholders are interested in two outputs: flood damage $Y(\mathbf{x}^*)$ on a specific 167 building $\mathbf{x}^* \in \mathcal{D}$, and total damage $|v| \cdot Y_v$ over a district v (here a disc of ra-168 dius r = 50). Here, analytical expression of model \mathcal{M} may be simple enough 169 to derive exact values of sensitivity indices, but it is usually not the case in 170 real applications. Thus we considered model \mathcal{M} as a *black box* and estimated 171 site sensitivity indices and block sensitivity indices with a sampling-based ap-172 proach (Lilburne and Tarantola 2009), using N = 4096 model runs (Table 1). 173 All calculations were carried out in R (R Development Core Team 2009). 174 It appears that at site scale, uncertainty on the map of water levels explains 175 most of the variance of $Y(\mathbf{x}^*)$: $S_Z = 0.89$. At a larger scale, uncertainty 176 on total flood damage $|v| \cdot Y_v$ is mainly due to the uncertainty on economic 177 parameters U_1 , U_2 and U_3 : $S_{\mathbf{U}}(v) = 0.86$. To improve accuracy of damage 178

estimation on a specific building, uncertainty should thus be first reduced on the map of water levels $Z(\mathbf{x})$; on the contrary, to improve accuracy of total damage estimation over a large district v, modeler should focus on reducing uncertainty on economic parameters U_1 , U_2 and U_3 .

¹⁸³ 3 Change of support effect on block sensitivity indices

We assess in this section how the ranking of uncertain model inputs based on their block sensitivity indices vary under a change of support v.

¹⁸⁶ 3.1 Relation between site sensitivity indices and block sensitivity indices

¹⁸⁷ Site sensitivity indices and block sensitivity indices are related. Let $\mathbb{E}_Z Y(\mathbf{x})$ ¹⁸⁸ denote the conditional expectation of $Y(\mathbf{x})$ knowing $Z(\mathbf{x})$, that is:

$$\forall \mathbf{x} \in \mathcal{D}, \quad \mathbb{E}_Z Y(\mathbf{x}) = \mathbb{E}\left[Y(\mathbf{x}) \mid Z(\mathbf{x})\right] \tag{7}$$

¹⁸⁹ $\mathbb{E}_Z Y(\mathbf{x})$ is the transform of input stationary random field $Z(\mathbf{x})$ through func-¹⁹⁰ tion $\bar{\psi}(z) = \int \psi(\mathbf{u}, z) p(\mathbf{u}) d\mathbf{u}$ [Eq. (2)]. Under our assumptions on ψ , $\mathbb{E}_Z Y(\mathbf{x})$ ¹⁹¹ is a SRF with finite variance. Let $C^*(\cdot)$ denote its covariogram, $\sigma^2 = C^*(0)$ ¹⁹² its variance and σ_v^2 its block variance over support v, that is, the variance ¹⁹³ of block average $1/|v| \int_v \mathbb{E}_Z Y(\mathbf{x}) d\mathbf{x}$. Block variance σ_v^2 is equal to the mean ¹⁹⁴ value of $C^*(\mathbf{h})$ when the two extremities of lag vector \mathbf{h} describe support v, which we denote by $\overline{C^*}(v, v)$ (Journel and Huijbregts 1978, p.78). Using these notations, it follows from Equations (4) and (5) that site sensitivity indices and block sensitivity indices are related by (see Appendix A for a proof):

$$\frac{S_Z(v)}{S_{\mathbf{U}}(v)} = \frac{S_Z}{S_{\mathbf{U}}} \cdot \frac{\sigma_v^2}{\sigma^2} = \frac{S_Z}{S_{\mathbf{U}}} \cdot \frac{\overline{C^*}(v,v)}{C^*(0)}$$
(8)

199 3.2 Change of support effect

Consider now that model \mathcal{M} was initially developed to study spatial average Y_v over support v, and that after model upscaling the modeler is interested in spatial average Y_V over support V such that $V \gg v$. We know from Krige's relation (Journel and Huijbregts 1978, p.67) that block variance σ_v^2 decreases with the size of support: $\sigma_V^2 \leq \sigma_v^2$. It follows from Equation (8) that:

$$\frac{S_Z(V)}{S_{\mathbf{U}}(V)} \le \frac{S_Z(v)}{S_{\mathbf{U}}(v)} \tag{9}$$

The relative contribution of input random field $Z(\mathbf{x})$ to the variability of aggregated model output - compared to the contribution of uncertain scalar input \mathbf{U} - is thus smaller on support V than on support v. Model upscaling results in a lower influence of uncertain spatial input $Z(\mathbf{x})$ on model output uncertainty. More specifically, let suppose that covariogram $C^*(\cdot)$ of $\mathbb{E}_Z Y(\mathbf{x})$ random field has finite range and that support v is large with respect to this range. To a first approximation, block variance σ_v^2 is of the form $\sigma_v^2 \simeq \sigma^2 A/|v|$ where A is the so-called *integral range* of $C^*(\cdot)$ defined by $A = 1/\sigma^2 \int C^*(\mathbf{h}) d\mathbf{h}$ (Chilès and Delfiner 1999, p.73). It follows from Equation (8) that:

$$\frac{S_Z(v)}{S_{\mathbf{U}}(v)} \simeq \frac{|v|_{\lim}}{|v|} \quad \text{with} \quad |v|_{\lim} = A \cdot \frac{S_Z}{S_{\mathbf{U}}} \tag{10}$$

Equation (10) shows that ratio $|v|_{\rm lim}/|v|$ drives the relative contribution of 215 model inputs $Z(\mathbf{x})$ and U to output variance $\operatorname{Var}(Y_v)$. The larger this ratio, 216 the larger the part of output variance $Var(Y_v)$ explained by the uncertainty 217 on input random field $Z(\mathbf{x})$. For a low ratio (i.e. when the area of support 218 v is large compared to critical size $|v|_{\text{lim}}$, variability of $Z(\mathbf{x})$ is mainly local, 219 and spatial correlation of $Z(\mathbf{x})$ over support v is weak. This local variabil-220 ity averages over support v when aggregated model output Y_v is computed: 221 hence the uncertainty on input 2D-field $Z(\mathbf{x})$ has a small influence on output 222 variance $\operatorname{Var}(Y_v)$. On the contrary, for a greater ratio (i.e. when the area of 223 support v is small compared to critical size $|v|_{\text{lim}}$, spatial correlation of $Z(\mathbf{x})$ 224 over v is strong. The averaging-out effect is weaker, hence the uncertainty 225 on model input $Z(\mathbf{x})$ has a larger influence on output variance $\operatorname{Var}(Y_v)$. 226

227 3.3 Influence of covariance range and nugget effect

Critical size $|v|_{\text{lim}} = A \cdot \frac{S_Z}{S_U}$ depends on the covariance structure $C^*(\cdot)$ of $\mathbb{E}_Z Y(\mathbf{x})$ random field, which is itself driven by covariogram $C(\cdot)$ of input SRF $Z(\mathbf{x})$. Let us assume now that $Z(\mathbf{x})$ is a Gaussian random field (GRF). As $\mathbb{E}_Z Y(\mathbf{x})$ is a transform of GRF $Z(\mathbf{x})$ through function $\bar{\psi}$ [Eq. (7)], it can be decomposed into an Hermitian expansion and its covariogram $C^*(\cdot)$ can be written as (Chilès and Delfiner 1999, p.396-399; see Appendix B for a proof):

$$C^*(\mathbf{h}) = \sum_{k=0}^{\infty} \lambda_k^2 \cdot [C(\mathbf{h})]^k$$
(11)

For most usual transition covariogram models (e.g. spherical, exponential, Gaussian models), covariance $C(\mathbf{h})$ is a monotically increasing function of range parameter a. In this case, it follows from Equation (11) that integral range $A = 1/\sigma^2 \int C^*(\mathbf{h}) d\mathbf{h}$ also grows with range a. An increase in range parameter a thus leads to a growth of critical size $|v|_{\text{lim}}$, and ratio of block sensitivity indices $S_Z(v)$ and $S_U(v)$ verifies [Eq. (10)]:

$$\frac{\partial}{\partial a} \left[\frac{S_Z(v)}{S_{\mathbf{U}}(v)} \right] \ge 0 \tag{12}$$

The relative contribution of uncertain model input $Z(\mathbf{x})$ to the variance of output of interest Y_v gets larger when covariance range of $Z(\mathbf{x})$ increases. Indeed, when range *a* increases, the averaging-out effect that occurs when ²⁴⁴ model output is aggregated over spatial support v gets weaker, thus the ²⁴⁵ influence of input random field $Z(\mathbf{x})$ on output variance $\operatorname{Var}(Y_v)$ grows.

The impact of nugget effect on block sensitivity indices can be interpreted the same way. Nugget parameter η controls the relative part of *pure noise* in input random field $Z(\mathbf{x})$ [Eq. (1)]. The lower η , the weaker the averaging-out effect will be when block average Y_v is computed over support v, hence the larger the part of output variance $Var(Y_v)$ that will be explained by $Z(\mathbf{x})$. Critical size $|v|_{\text{lim}}$ is thus a decreasing function of nugget parameter η , and ratio of block sensitivity indices $S_Z(v)$ and $S_U(v)$ verifies [Eq. (1), (8), (11)]:

$$\frac{\partial}{\partial \eta} \left[\frac{S_Z(v)}{S_{\mathbf{U}}(v)} \right] \le 0 \tag{13}$$

253 3.4 Illustrative example

To illustrate change of support effects on sensitivity analysis results, we performed spatial GSA on our numerical example in the following settings: varying disc-shaped support v of increasing size (Fig. 2); varying range from a = 1to a = 10 (Fig. 3); varying nugget parameter from $\eta = 0$ to $\eta = 0.9$ (Fig. 4). For each setting, we computed estimates of output variance $Var(Y_v)$, block sensitivity indices $S_{\mathbf{U}}(v)$, $S_Z(v)$ and ratio $S_Z(v)/S_{\mathbf{U}}(v)$ over N = 4096 model runs. The whole process was repeated 100 times and mean values with 95%

confidence interval are shown for each estimate. In accordance with Equa-261 tions (9), (12) and (13), it appears that block sensitivity index $S_Z(v)$ (i) 262 decreases when support v gets larger (Fig. 2b) (ii) increases with covariance 263 range a (Fig. 3b) (iii) decreases with nugget parameter η (Fig. 4b), while 264 sensitivity index $S_{\mathbf{U}}(v)$ has the opposite behaviour. Change of support effect 265 is clearly highlighted in Figure 2b: contribution of economic parameters U_1 , 266 U_2 and U_3 to the variability of total flood damage $|v| \cdot Y_v$ exceeds the contri-267 bution of water level map $Z(\mathbf{x})$ when the radius r of support v is greater than 268 $r_{\rm lim} \simeq 18$; for radius $r < r_{\rm lim}$, uncertainty on total flood damage over support 269 v is mainly due to the uncertainty on water levels $Z(\mathbf{x})$. Finally, Figure 2c 270 illustrates that ratio $S_Z(v)/S_U(v)$ is proportional to 1/|v| when support v is 271 large enough. Theoretical curve $S_Z(v)/S_U(v) = |v|_{\text{lim}}/|v|$ [Eq. 10] was fitted 272 (least squares - $R^2 = 0.99$) on data points (for $r \ge 20$ only), yielding an 273 estimate of critical size $|v|_{\text{lim}} \simeq 1068$. 274

275 4 Discussion

Our first goal was to provide a formalism to extend variance-based GSA approach to spatial models when the modeler is mainly interested in the linear average or the sum of model output $Y(\mathbf{x})$ over some spatial unit v. Our approach is strongly inspired from previous related works. Other authors had already computed site sensitivity indices (Marrel et al 2011; Pettit and
Wilson 2010) and block sensitivity indices (Lilburne and Tarantola 2009),
but without naming them nor exploring their analytical properties or their
relationship. Our paper is an attempt to do so. Equation (8) gives an exact
relation between site and block sensitivity indices: it may prove useful in the
case of a model with a simple enough analytical expression.

Our research also sought to account for change of support effects in the prop-286 agation of uncertainty through spatial models, within variance-based GSA 287 framework. We proved that the relative influence of spatially distributed 288 model input $Z(\mathbf{x})$ decreases under model upscaling: when support v is large 289 enough, the ratio of block sensitivity index of spatially distributed input with 290 block sensitivity index of scalar inputs is proportional to $|v|_{\rm lim}/|v|$. Critical 291 size $|v|_{\text{lim}}$ depends on the covariance structure of input SRF $Z(\mathbf{x})$: it usually 292 grows with an increase of range parameter a or a decrease of nugget parame-293 ter η . These findings are translation into GSA formalism of the averaging-out 294 effect clearly portrayed by Journel and Huijbregts (1978) in the regulariza-295 tion theory. Our contribution is to discuss this issue from the point of view 296 of GSA practitioners. Formalizing the effect of a change of support on sen-291 sitivity analysis results may well help modelers when they consider model 298 upscaling: it will orientate future data gathering by identifying model inputs 299

that will have major influence on model output variability over a new spatial support. It also promotes an increased awareness on the issue of choosing the appropriate accuracy of spatial model inputs for a given scale: when block sensitivity index of spatial input $Z(\mathbf{x})$ is small ($S_Z(v) < 0.1$), it may mean that it is over-accurate compared to the uncertainty of other model inputs, and that costs associated with field data gathering could have been avoided.

It should be noted that our approach is based on conditions that may not 306 be met in some pratical cases. First, we considered a simple model \mathcal{M} with 307 a single spatially distributed input $Z(\mathbf{x})$. In real applications, modelers of-308 ten have to deal with several spatial inputs $Z_1(\mathbf{x}), \ldots, Z_m(\mathbf{x})$, with different 309 covariance structures $C_i(\cdot)$, ranges a_i and nuggets η_i . In this case, it can be 310 shown that Equation (8) still holds separately for each spatial input $Z_i(\mathbf{x})$. 311 Yet no conclusion can be drawn a priori on how a change of support im-312 pacts the relative ranking of two spatial inputs $Z_i(\mathbf{x})$ and $Z_j(\mathbf{x})$: ratio of 313 their block sensitivity indices $S_{Zi}(v)/S_{Zj}(v)$ will depend on the ratio of block 314 variances $\sigma_{v,i}^2/\sigma_{v,j}^2$. Second, some environmental models are not point-based 315 and involve spatial interactions (e.g. erosion, groundwater flow models). In 316 this case, it still may be possible to build a point-based surrogate model as 317 a coarse approximation of the original model; if not, then change of support 318 properties discussed in section 3 may not hold. Third, we assumed input 319

random field $Z(\mathbf{x})$ to be stationary: if not, site sensitivity indices depend on site \mathbf{x}^* [Eq. (4)]. It is then possible to compute maps of these indices (Marrel et al 2011; Pettit and Wilson 2010) to discuss the spatial variability of model inputs sensitivities.

Finally, we focused on the case where the modeler's interest is in the spatial 324 linear average or the sum of model output $Y(\mathbf{x})$ over support v. As dis-325 cussed by Lilburne and Tarantola (2009), other outputs of interest may be 326 considered, such as maximum value of $Y(\mathbf{x})$ over v (e.g. maximal pollutant 327 concentration over a zone), some quantile of $Y(\mathbf{x})$ over v (Heuvelink et al 328 2010), the percentage of v where $Y(\mathbf{x})$ exceeds a certain threshold, etc. Up to 329 our knowledge, no investigation has been done on the properties of sensitivity 330 indices computed with respect to such outputs of interest. 331

332 5 Conclusion

This paper provides a formalism to apply variance-based global sensitivity analysis to spatial models when the modeler's interest is in the average or the sum of model output $Y(\mathbf{x})$ over a given spatial unit v. Site sensitivity indices and block sensitivity indices allow us to discuss how a change of support influence the relative contribution of uncertain model inputs to the variance of the output of interest. We give an analytical relationship between these

two types of sensitivity indices. Our results show that block sensitivity index 339 of input random field $Z(\mathbf{x})$ increases with ratio $|v|_{\text{lim}}/|v|$, where |v| is the area 340 of spatial support v and critical size $|v|_{\text{lim}}$ depends on the covariance structure 341 of $Z(\mathbf{x})$. Our formalization is made with a view towards promoting the use 342 of sensitivity analysis in model-based spatial decision support systems. Yet 343 further research is needed to explore the case of non point-based models and 344 extend our study to outputs of interest other than the average value of model 345 output over zone v. 346

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379

Appendix A: proof for relation between site sensitivity indices and
 block sensitivity indices

As mentioned in section 2, we assume that mapping ψ is such that for any site $\mathbf{x} \in \mathcal{D}$, random variables $Y(\mathbf{x})$, $\mathbb{E}[Y(\mathbf{x}) | Z(\mathbf{x})]$ and $\mathbb{E}[Y(\mathbf{x}) | \mathbf{U}]$ have finite expectation and finite variance. Ratio of block sensitivity indices writes [Eq. (5)]:

$$\frac{S_Z(v)}{S_{\mathbf{U}}(v)} = \frac{\operatorname{Var}\left(\mathbb{E}\left[Y_v \mid \{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}\right]\right)}{\operatorname{Var}\left(\mathbb{E}\left[Y_v \mid \mathbf{U}\right]\right)}$$
(14)

Conditional expectation of block average Y_v knowing $\{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}$ writes:

$$\mathbb{E}\left[Y_{v} \mid Z\right] = \mathbb{E}\left[1/|v| \int_{v} Y(\mathbf{x}) d\mathbf{x} \mid \{Z(\mathbf{x}') : \mathbf{x}' \in \mathcal{D}\}\right] \quad \text{(definition of } Y_{v}\text{)}$$
$$= 1/|v| \int_{v} \mathbb{E}\left[Y(\mathbf{x}) \mid \{Z(\mathbf{x}') : \mathbf{x}' \in \mathcal{D}\}\right] d\mathbf{x}$$
$$= 1/|v| \int_{v} \mathbb{E}\left[Y(\mathbf{x}) \mid Z(\mathbf{x})\right] d\mathbf{x} \quad \text{(for a point-based model)}$$
$$= 1/|v| \int_{v} \mathbb{E}_{Z} Y(\mathbf{x}) d\mathbf{x} \quad \text{(definition of } \mathbb{E}_{Z} Y(\mathbf{x})\text{)}$$

Thus we have $\operatorname{Var}\left(\mathbb{E}\left[Y_v \mid Z\right]\right) = \operatorname{Var}\left(1/|v| \int_v \mathbb{E}_Z Y(\mathbf{x}) d\mathbf{x}\right) = \sigma_v^2$ (definition of σ_v^2). Moreover, conditional expectation of block average Y_v knowing scalar input **U** writes:

$$\mathbb{E}\left[Y_v \mid \mathbf{U}\right] = \mathbb{E}\left[1/|v| \int_v Y(\mathbf{x}) \, d\mathbf{x} \mid \mathbf{U}\right] \quad \text{(definition of } Y_v\text{)}$$
$$= 1/|v| \int_v \mathbb{E}\left[Y(\mathbf{x}) \mid \mathbf{U}\right] \, d\mathbf{x}$$

⁴⁰⁵ $\mathbb{E}[Y(\mathbf{x}) | \mathbf{U}]$ does not depend on site \mathbf{x} under stationarity of SRF $Z(\mathbf{x})$, ⁴⁰⁶ thus we have in particular $\mathbb{E}[Y_v | \mathbf{U}] = \mathbb{E}[Y(\mathbf{x}^*) | \mathbf{U}]$, and $\operatorname{Var}(\mathbb{E}[Y_v | \mathbf{U}]) =$ ⁴⁰⁷ $\operatorname{Var}(\mathbb{E}[Y(\mathbf{x}^*) | \mathbf{U}])$. Combining these expressions with Equation (14) yields:

$$\frac{S_Z(v)}{S_{\mathbf{U}}(v)} = \frac{\sigma_v^2}{\operatorname{Var}(\mathbb{E}\left[Y(\mathbf{x}^*) \mid \mathbf{U}\right])}$$
(15)

⁴⁰⁸ Ratio of site sensitivity indices writes [Eq. (4)]:

$$\frac{S_Z}{S_{\mathbf{U}}} = \frac{\operatorname{Var}(\mathbb{E}\left[Y(\mathbf{x}^*) \mid \{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}\right])}{\operatorname{Var}(\mathbb{E}\left[Y(\mathbf{x}^*) \mid \mathbf{U}\right])}$$
(16)

We notice that for point-based models, $\operatorname{Var} [\mathbb{E}(Y(\mathbf{x}^*) | \{Z(\mathbf{x}) : \mathbf{x} \in \mathcal{D}\}] =$ $\operatorname{Var} [\mathbb{E}_Z Y(\mathbf{x}^*)] = \sigma^2$ (definition of $\mathbb{E}_Z Y(\mathbf{x})$ [Eq. (7)]). It finally follows from Equations (15) and (16) that:

$$\frac{S_Z(v)}{S_{\mathbf{U}}(v)} = \frac{S_Z}{S_{\mathbf{U}}} \cdot \frac{\sigma_v^2}{\sigma^2}$$

409 Appendix B: Hermitian expansion of random field $\mathbb{E}_Z Y(\mathbf{x})$

 $\mathbb{E}_Z Y(\mathbf{x})$ random field can be written [Eq. (2), (7)] as a transformation of $Z(\mathbf{x})$ Gaussian random field through function $\overline{\psi} : z \mapsto \int_{\mathbb{R}^n} \psi(\mathbf{u}, z) \cdot p(\mathbf{u}) d\mathbf{u}$:

$$\mathbb{E}_Z Y = \bar{\psi}\left(Z\right)$$

We previously assumed that for any site $\mathbf{x} \in \mathcal{D}$, $\mathbb{E}_Z Y(\mathbf{x})$ has finite expectation and finite variance. Under this condition, function $\bar{\psi}$ belongs to Hilbert space $L^2(\mathcal{G})$ of functions $f : \mathbb{R} \to \mathbb{R}$ which are square-integrable with respect to Gaussian density g(.). Hence $\bar{\psi}$ can be expanded on the sequence of Hermite polynomials $(\chi_k)_{k\in\mathbb{N}}$, which forms an orthonormal basis of $L^2(\mathcal{G})$ (Chilès and Delfiner 1999, p.399):

$$\bar{\psi} = \sum_{k=0}^{\infty} \alpha_k \cdot \chi_k$$
 with $\chi_k(z) = \frac{1}{\sqrt{k!}} \cdot \frac{1}{g(z)} \cdot \frac{\partial^k}{\partial z^k} g(z)$

where coefficients α_k are given by: $\alpha_k = \int_{\mathbb{R}} \chi_k(z) \overline{\psi}(z) g(z) dz$. It follows that $\mathbb{E}_Z Y(\mathbf{x})$ can be written as an infinite expansion of polynomials of $Z(\mathbf{x})$:

$$\forall \mathbf{x} \in \mathcal{D}, \quad \mathbb{E}_Z Y(\mathbf{x}) = \sum_{k=0}^{\infty} \alpha_k \cdot \chi_k \left[Z(\mathbf{x}) \right]$$

Its covariance then writes (Chilès and Delfiner 1999, p.396 Eq. (6.23) and p.399 Eq. (6.25)):

$$\operatorname{Cov}\left(\mathbb{E}_{Z}Y(\mathbf{x}), \mathbb{E}_{Z}Y(\mathbf{x}+\mathbf{h})\right) = \sum_{k=0}^{\infty} \alpha_{k}^{2} \cdot \left[\frac{C(\mathbf{h})}{C(0)}\right]^{k} = \sum_{k=0}^{\infty} \lambda_{k}^{2} \cdot \left[C(\mathbf{h})\right]^{k}$$

where $C(\mathbf{h})$ is the covariogram of GRF $Z(\mathbf{x})$ and $\lambda_k = \alpha_k \cdot C(0)^{-k/2}$.

411 Captions of tables

⁴¹² **Tab. 1** Sensitivity analysis results over N = 4096 model runs with respect ⁴¹³ to the outputs of interest $Y(\mathbf{x}^*)$ and $|v| \cdot Y_v$. Mean values with $\pm s.d.$ over ⁴¹⁴ 100 replicas.

TABLE 1

 $\overline{27}$

Output of interest	Mean	Variance	Type of indices	Sensitivity indices
$Y(\mathbf{x}^*)$	66.5 ± 4.2	1393 ± 188	Site S.I.	$S_{U} = 0.09 \pm 0.02$ $S_{Z} = 0.89 \pm 0.02$
$ v \cdot Y_v$	68.6 ± 0.4	145 ± 4	Block S.I.	$S_{\mathbf{U}}(v) = 0.86 \pm 0.01$ $S_{Z}(v) = 0.12 \pm 0.02$

416 Captions of figures

Fig. 1 Spatial model with uncertain inputs U and $Z(\mathbf{x})$ and spatial output $Y(\mathbf{x})$. The modeler is interested in the block average of $Y(\mathbf{x})$ over some spatial unit v

Fig. 2 GSA results depending on the size of disc-shaped support ν (with radius r and area $|\nu| = \pi r^2$), for a = 5, $\eta = 0.1$: (a) total variance of output of interest Y_v , (b) block sensitivity indices $S_{\mathbf{U}}(v)$ (solid line) and $S_Z(v)$ (dashed line), (c) ratio $S_Z(v)/S_{\mathbf{U}}(v)$ with fitted curve $S_Z(v)/S_{\mathbf{U}}(v) =$ $|v|_{\text{lim}}/|v|$ (dashed line). Error bars show 95 % confidence interval over 100 replicas

⁴²⁶ Fig. 3 GSA results depending on covariance range a, for $\eta = 0.1$ and a ⁴²⁷ disc-shaped support v of radius r = 50: (a) total variance of Y_v , (b) block ⁴²⁸ sensitivity indices $S_{\mathbf{U}}(v)$ (solid line) and $S_Z(v)$ (dashed line). Error bars ⁴²⁹ show 95 % confidence interval over 100 replicas

Fig. 4 GSA results depending on covariance nugget η , for a = 5 and a disc-shaped support v of radius r = 50: (a) total variance of Y_v , (b) block sensitivity indices $S_{\mathbf{U}}(v)$ (solid line) and $S_Z(v)$ (dashed line). Error bars show 95 % confidence interval over 100 replicas





436

FIGURE 2







439



