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Support indices: Measuring the effect of input variables over their support

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Abstract

Two new sensitivity indices are presented which give an original solution to the known question in sensitivity analysis of how to determine regions within in the input space for which the model variation is high. The indices, as functions over the input domain, give insight into the local influence of input variables over the whole domain when the other variables lie in the global domain. They can serve as an informative extension to a standard analysis and in addition are especially helpful in the specification of the input domain, a critical, but often vaguely handled issue in sensitivity analysis. In the usual framework of independent continuous input variables, we present theoretical results that show an asymptotic connection between the presented indices and Sobol indices, valid for general probability distribution functions. Finally, we show how the indices can be successfully applied in an analytical as well as a real example.

Keywords: sensitivity analysis, support analysis, Sobol indices, DGSM

Global sensitivity analysis is an essential tool in many of the steps in the analysis of computer experiments, like screening, investigation, model building, or optimization [1]. Variance-based indices have become the method of choice among practitioners, as they offer a clear interpretable quantification of the

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5 influence of variables on the output variance. Different types of variance-based indices have been proposed in the literature. The single influence of a variable is e.g. measured by the first-order Sobol index [2]. The total sensitivity index [3] quantifies the joint influence of a variable and all its interactions and thus can be used to detect unessential variables. A screening of interactions can be
 10 obtained by the total interaction index ([4], [5]), which captures the total impact of the second-order interaction of a pair of variables.

An alternative concept to global sensitivity are derivate-based global indices (DGSM) [6]. The indices use the integrated square derivative of the model output over the domain of the inputs as indicator of the influence and, like total
 15 sensitivity indices, can be used to detect unessential variables.

For the estimation of both, variance-based indices and DGSM, input variables are usually treated as random variables following a distribution defined by the user. The minimum and maximum value of the support of this distribution is usually specified from the region of interest of the parameter in question.
 20 They are often chosen vaguely, but can have an important impact.

As an example, let us consider the Ishigami function by [7],

$$f(x_1, x_2, x_3) = \sin(x_1) + 7 \sin^2(x_2) + 0.1x_3^4 \sin(x_1).$$

This function is often chosen in sensitivity analysis due to its strong non-linearities and interactions. The usual setting is to assume that X_1, X_2, X_3 are independent random variables, drawn uniformly on $[-\pi, \pi]$, and to investigate
 25 the Sobol indices of $f(X_1, X_2, X_3)$. A direct computation (see e.g. [1]) shows that the unscaled total sensitivity indices of the Ishigami function are equal to $D_1^T = 7.72$, $D_2^T = 6.13$, and $D_3^T = 3.37$. Now, if we reduce the support of the distribution of X_3 by 10 percent, $X_3^* \sim U[-\pi + \frac{\pi}{10}, \pi - \frac{\pi}{10}]$, we get $D_1^{T*} = 4.05$, $D_2^{T*} = 6.13$, and $D_3^{T*} = 1.45$. The first and the last variable have rapidly lost
 30 influence in comparison to the second one, the ranking of variables has changed. This can be explained by the interaction between X_1 and X_3 , which is much stronger at the borders than in the rest of the function. The index of X_2 stays unchanged as it does not interact with X_3 . The change in the output when

changing X_2 stays the same.

35 As very cheap-to-evaluate metamodels are often used in practice, it is possible to compute more than the common one or two simple numbers, the Sobol and the total sensitivity index, for each input variable. We present a method that extends those two scalar indices to functions of sensitivities as an extension to the traditional sensitivity analysis. They explore the local influence behavior
40 over the support of the input variables and thus show the impact of the choice of the input distribution.

In their book on sensitivity analysis, Saltelli et al. [1] name as one goal of sensitivity analysis “to determine the optimal regions within the space of the factors for which the model variation is maximum”. The presented method
45 performs this task by returning the local influences over the whole domain. It is related to the idea of *local sensitivities* as mentioned e.g. in [8, Section 2.5.1.]. There, local sensitivities are defined as partial derivatives at fixed baseline points. Our method shares with them that partial derivatives are used to obtain local influences. The main difference is that in local sensitivity analysis,
50 the influence of a variables is studied in a local space of the other inputs whereas our method studies the local influence of a variable in a global space of the other variables. The local influences are studied over the whole input space, so no space is ignored. Welch et al. [9] suggest to plot curves of the *main effects*, i.e. the expectation of the model conditional on each input, in a framework
55 with a Gaussian process metamodel. They argue that these plots give a visual indication of the effects and provide insight into their relative magnitude. Our idea shares these aims, but gives two different local sensitivities corresponding to first-order Sobol indices and total indices, which has to our knowledge not been done before.

60 With our method, effects of the choice of the input distribution can be visible. In addition, it gives further insight into the function by presenting a *function of sensitivities* as extension to Sobol and total sensitivity indices. It can also be a helpful tool in sequential optimization, where the input behavior of certain optimal regions is of interest, which might differ extensively from the

65 global behavior. After an overview on global sensitivity measures in Section 1,
we define the support index functions and show that they are connected to
classical indices when the variable in question is restricted to an interval whose
size goes to zero (Section 2). In Section 3, we present further connections to
classical indices, obtained by integration over the functions. To illustrate the
70 method, it is applied to the Ishigami function and a real life application in sheet
metal forming in Section 4. We conclude with Section 5.

1. Overview of global sensitivity measures

We consider a black-box function $Y = f(X)$ of independent random variables
 $X = (X_1, \dots, X_d)$ with distribution $\mu = \mu_1 \otimes \dots \otimes \mu_d$. The function f is defined
75 on $\Delta \subseteq \mathbb{R}^d \rightarrow \mathbb{R}$ such that $f(X) \in L^2(\mu)$.

1.1. Variance-based sensitivity measures

The FANOVA decomposition [10, 2] gives a decomposition of the function
 f into additive terms which are centered and orthogonal:

$$f(\mathbf{X}) = f_0 + \sum_{i=1}^d f_i(X_i) + \sum_{1 \leq i < j \leq d} f_{i,j}(X_i, X_j) + \dots + f_{1,\dots,d}(X_1, \dots, X_d) \quad (1)$$

The terms represent first-order effects ($f_i(X_i)$), second-order interactions
80 ($f_{i,j}(X_i, X_j)$), and all higher combinations of input variables. From the orthog-
onality in Eq. (1), the variance of the f can be decomposed accordingly,

$$\text{var}(f(\mathbf{X})) = \sum_{I \subseteq \{1, \dots, d\}} \text{var}(f_I(\mathbf{X}_I)), \quad (2)$$

where the overall variance is denoted by $D = \text{var}(f(\mathbf{X}))$, and the variance
terms by $D_I = \text{var}(f_I(\mathbf{X}_I))$. These terms quantify the influence of the set of
variables X_I on the output variance. The Sobol sensitivity indices S_I are defined
85 as the following ratios, ensuring the indices to fall in $[0, 1]$,

$$S_I = \frac{D_I}{D}. \quad (3)$$

In a sensitivity analysis procedure, the first-order Sobol indices $S_i, i = 1, \dots, d$ are usually estimated to quantify the single influences of the input variables. In addition, often the total sensitivity indices S_i^T are estimated, which give the influence of each variable including all interactions and thus are suitable
90 for variable screening,

$$D_i^T = \sum_{J \supseteq \{i\}} D_J, \quad S_i^T = \frac{D_i^T}{D} \quad (4)$$

1.2. Derivative-based measures

A further sensitivity measure, the *derivate-based global sensitivity measures (DGSM)*, was introduced by [6]. Here, the notion of sensitivity is based on the derivative of the function, rather than on the output variance. It thus
95 summarizes the local variation instead of the global one. The DGSM are defined by

$$\nu_i = \int \left(\frac{\partial f(\mathbf{X})}{\partial X_i} \right)^2 d\mu(\mathbf{X}). \quad (5)$$

It can be connected to total sensitivity indices through

$$D_i^T \leq C(\mu_i)\nu_i, \quad (6)$$

provided that μ belongs to a class of distributions that satisfy a Poincaré inequality,

$$\int g(\mathbf{X})^2 d\mu(\mathbf{X}) \leq C(\mu) \int \|\nabla g(\mathbf{X})\|^2 d\mu(\mathbf{X}),$$

for all functions g in $L^2(\mu)$ such that $\int g(\mathbf{X}) d\mu(\mathbf{X}) = 0$, and $\|\nabla g\| \in L^2(\mu)$, where ∇g denotes the gradient of g . See [11] or [12] for a comprehensive summary. Equation (6) implies that the DGSM can be used as upper boundaries
100 for the total sensitivity indices. It can thus serve as a cheaper method for the screening of noninfluential input variables, especially when the computer experiment additionally provides partial derivatives.

2. Support index functions

We now develop new sensitivity measures to quantify the changing effect of
105 the input variables over their support. In addition to the previous notation, we

assume that $\Delta = [0, 1]^d$, f of class C^1 , and that X_1, \dots, X_d have continuous density functions with support $[0, 1]$. Remark that since f is of class C^1 on the compact set $[0, 1]^d$, f and all its first-order derivatives are bounded, ensuring
 110 that $f(\mathbf{X})$ and $\frac{\partial f}{\partial \mathbf{x}_\bullet}(\mathbf{X})$ are in L^2 .

The support index functions are then defined as follows.

Definition 1. *Support index functions*

The first-order support index $D_i(t)$ of an input variable X_i at a point t , $t \in [0, 1]$, is defined as the square of the expected value of the first derivative of f ,

$$D_i(t) = \left(E \left(\frac{\partial f}{\partial \mathbf{x}_i}(t, \mathbf{X}_{-i}) \right) \right)^2.$$

115 The total support index $D_i^T(t)$ of an input variable X_i at a point t , $t \in [0, 1]$, is defined as the expected value of the squared derivative of f ,

$$D_i^T(t) = E \left(\left(\frac{\partial f}{\partial \mathbf{x}_i}(t, \mathbf{X}_{-i}) \right)^2 \right).$$

The support variance $D^{X_i}(t)$ corresponding to a support index of an input variable X_i at a point t , $t \in [0, 1]$, is defined as the overall variance for $X_i = t$,

$$D^{X_i}(t) = \text{var}(f(t, \mathbf{X}_{-i})).$$

Thus, the local influence is measured through the partial derivative of X_i
 120 at each point t , summarized over the global variable space by the expectation. The role of the square will be clearer later through the connection to first-order and total indices in Proposition 1.

The functions can be evaluated and plotted for a sufficiently large number of discrete points $t = 0, \dots, 1$ over the support. If the gradient of f is known the
 125 functions can be calculated directly. If not, the gradient can be approximated by finite differences. For instance the *first-order support index* of X_i at point t using Monte Carlo samples of \mathbf{X}_{-i} , $\mathbf{x}_{-i}^{(1)}, \dots, \mathbf{x}_{-i}^{(n)}$, and a small value of δ^* can be estimated by

$$\widehat{D}_i(t) = \left(\frac{1}{n} \sum_{k=1}^n \frac{f(t + \delta^*, \mathbf{x}_{-i}^{(k)}) - f(t - \delta^*, \mathbf{x}_{-i}^{(k)})}{2\delta^*} \right)^2.$$

An interpretation of the support functions can be obtained, when we look
 130 at the first-order and total influence of the specific point in the support of the
 variable. Indeed, the functions are connected to the classical index estimation
 when we restrict X_i to vary only over a small interval around t and let the size
 of the interval go to zero.

135 **Proposition 1.** *Let X_1, \dots, X_d be independent random variables with con-
 tinuous density functions with support $[0, 1]$. Let f be a function defined on
 $\Delta = [0, 1]^d$ compact and assume that f is of class C^2 , ensuring that $f(\mathbf{X})$,
 $\frac{\partial f}{\partial \mathbf{x}_\bullet}(\mathbf{X})$, $\frac{\partial^2 f}{\partial \mathbf{x}_\bullet \partial \mathbf{x}_\bullet}(\mathbf{X})$ are in L^2 . Now let one of the random variables, say X_i ,
 be restricted to $X_i^h \sim X_i | X_i \in [t - h/2, t + h/2]$ for $t \in]0, 1[$ and $h > 0$. Then we
 140 have that*

$$\frac{\text{var}(X_i^h - t)}{h^2} \xrightarrow{h \rightarrow 0} \frac{1}{12},$$

and for the limits of the overall variance, the Sobol index of X_i^h , denoted by
 $D_{X_i^h}$, and the total sensitivity index of X_i^h , denoted by $D_{X_i^h}^T$, it holds that

1. $\text{var}(f(X_i^h, \mathbf{X}_{-i})) \xrightarrow{h \rightarrow 0} \text{var}(f(t, \mathbf{X}_{-i})) = D^{X_i}(t)$,
2. $D_{X_i^h} = \text{var}(E[f(X_i^h, \mathbf{X}_{-i}) | X_i^h]) / h^2 \xrightarrow{h \rightarrow 0} \frac{1}{12} \left(E \left(\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) \right) \right)^2 = D_i(t) / 12$,
3. $D_{X_i^h}^T = E(\text{var}[f(X_i^h, \mathbf{X}_{-i}) | \mathbf{X}_{-i}]) / h^2 \xrightarrow{h \rightarrow 0} \frac{1}{12} E \left(\left(\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) \right)^2 \right) = D_i^T(t) / 12$.

Remark. *The factor $\frac{1}{12}$ is common to all probability density functions.*

Proof. Let us first show that

$$\frac{\text{var}(X_i^h - t)}{h^2} \xrightarrow{h \rightarrow 0} \frac{1}{12}.$$

Let g be the density function of $X_i - t$, $g(x) = f_{X_i}(x + t)$. By assumption,
 145 g is continuous in 0, $g(0) > 0$. Consider the density of the truncated variable
 $X_i^h - t$, $g_h(x) = \frac{g(x)}{\int_{-\frac{h}{2}}^{\frac{h}{2}} g(t) dt} 1_{[-\frac{h}{2}, \frac{h}{2}]}(x)$.

Let $\ell_h = \inf_{x \in [-\frac{h}{2}, \frac{h}{2}]} g(x)$ and $u_h = \sup_{x \in [-\frac{h}{2}, \frac{h}{2}]} g(x)$. With continuity of f in 0, we have $u_h \xrightarrow{h \rightarrow 0} g(0)$ and $\ell_h \xrightarrow{h \rightarrow 0} g(0)$. By standard integral computations we get

$$h\ell_h \leq \int_{-\frac{h}{2}}^{\frac{h}{2}} g(x) dx \leq hu_h \quad \text{and} \quad \frac{h^3}{12}\ell_h \leq \int_{-\frac{h}{2}}^{\frac{h}{2}} g(x)x^2 dx \leq \frac{h^3}{12}u_h$$

so that for $E((X_i^h - t)^2) = \frac{\int_{-\frac{h}{2}}^{\frac{h}{2}} g(x)x^2 dx}{\int_{-\frac{h}{2}}^{\frac{h}{2}} g(x) dx}$ it holds that

$$\frac{\ell_h}{u_h} \frac{h^3/12}{h} \leq E((X_i^h - t)^2) \leq \frac{u_h}{\ell_h} \frac{h^3/12}{h}.$$

By dividing by h^2 this leads to

$$\frac{E((X_i^h - t)^2)}{h^2} \xrightarrow{h \rightarrow 0} \frac{1}{12}.$$

It remains to show that $\frac{E(X_i^h - t)}{h} \xrightarrow{h \rightarrow 0} 0$. As

$$\int_{-\frac{h}{2}}^{\frac{h}{2}} g(x)x dx = \int_0^{\frac{h}{2}} (g(x) - g(-x))x dx$$

it holds that

$$\begin{aligned} |E(X_i^h - t)| &\leq \frac{1}{\ell_h h} \int_0^{\frac{h}{2}} |g(x) - g(-x)|x dx \leq \frac{1}{\ell_h h} \int_0^{\frac{h}{2}} (u_h - \ell_h)x dx \\ &= \frac{u_h - \ell_h}{\ell_h h} \int_0^{\frac{h}{2}} x dx = \frac{u_h - \ell_h}{\ell_h h} \frac{h^2}{8}. \end{aligned}$$

Thus

$$\frac{|E(X_i^h - t)|}{h} \leq \frac{u_h - \ell_h}{8\ell_h} \xrightarrow{h \rightarrow 0} 0.$$

In the following, denote $B_i = \frac{X_i^h - t}{h}$. Remark that B_i is bounded by $|B_i| \leq \frac{1}{2}$ and that $\text{var}(B_i) \xrightarrow{h \rightarrow 0} \frac{1}{12}$.

Proof of 1. Write the mean value theorem between a real number $x_i \in [t - h/2, t + h/2] \subseteq [0, 1]$ and t

$$f(\mathbf{x}) = f(x_i, \mathbf{x}_{-i}) = f(t, \mathbf{x}_{-i}) + (x_i - t) \frac{\partial f}{\partial x_i}(c, \mathbf{x}_{-i})$$

for a c between x_i and t , thus $c \in [t - h/2, t + h/2]$. Replacing by random variables, we get

$$f(X_i^h, \mathbf{X}_{-i}) = f(t, \mathbf{X}_{-i}) + (X_i^h - t) \frac{\partial f}{\partial x_i}(C, \mathbf{X}_{-i}),$$

160 where C is a random variable such that $C \in [t - h/2, t + h/2]$. Denoting $Q = B_i \frac{\partial f}{\partial x_i}(C, \mathbf{X}_{-i})$, we then have

$$f(X_i^h, \mathbf{X}_{-i}) = f(t, \mathbf{X}_{-i}) + hQ.$$

Now remark that Q is bounded since both B_i and $\frac{\partial f}{\partial x_i}$ are bounded (by continuity of $\frac{\partial f}{\partial x_i}$ on the compact set $[0, 1]^d$). This implies that $\mathbb{E}(f(X_i^h, \mathbf{X}_{-i})) \xrightarrow{h \rightarrow 0} \mathbb{E}(f(t, \mathbf{X}_{-i}))$ by Lebesgue theorem as well as $\mathbb{E}(f(X_i^h, \mathbf{X}_{-i})^2) \xrightarrow{h \rightarrow 0} \mathbb{E}(f(t, \mathbf{X}_{-i})^2)$.

165 The result follows.

Proof of 2. The proof is similar to the one of 1. Write the Taylor-Lagrange expansion of f between a real number $x_i \in [t - h/2, t + h/2] \subseteq [0, 1]$ and t

$$f(\mathbf{x}) = f(x_i, \mathbf{x}_{-i}) = f(t, \mathbf{x}_{-i}) + (x_i - t) \frac{\partial f}{\partial x_i}(t, \mathbf{x}_{-i}) + \frac{1}{2}(x_i - t)^2 \frac{\partial^2 f}{\partial x_i^2}(c, \mathbf{x}_{-i})$$

for a c between x_i and t , thus $c \in [t - h/2, t + h/2]$. Replacing by random variables, we have

$$f(X_i^h, \mathbf{X}_{-i}) = f(t, \mathbf{X}_{-i}) + hB_i \frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) + h^2 \tilde{R},$$

with $\tilde{R} = \frac{1}{2} B_i^2 \frac{\partial^2 f}{\partial x_i^2}(C, \mathbf{X}_{-i})$, where C is a random variable, $C \in [t - h/2, t + h/2]$. Then, using the independence between X_i^h and \mathbf{X}_{-i} , we have

$$\mathbb{E}[f(X_i^h, \mathbf{X}_{-i}) | X_i^h] = \beta_0 + h\beta_1 B_i + h^2 R,$$

with $\beta_0 = \mathbb{E}(f(t, \mathbf{X}_{-i}))$, $\beta_1 = \mathbb{E}\left(\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i})\right)$, and $R = \mathbb{E}[\tilde{R} | X_i^h]$. Finally

$$\text{var}(\mathbb{E}[f(X_i^h, \mathbf{X}_{-i}) | X_i^h]) = h^2 \beta_1^2 \text{var}(B_i) + 2h^3 \beta_1 \text{Cov}(B_i, R) + h^4 \text{var}(R).$$

Now remark that \tilde{R} is a bounded random variable by continuity of $\frac{\partial^2 f}{\partial x_i^2}$ on the compact set $[0, 1]^d$, and thus R is bounded as well. This implies that $\text{var}(R) = O(1)$ and $\text{Cov}(B_i, R) = O(1)$, and the result follows.

Proof of 3. With the same notations as in the proof of 2., we have

$$\mathbb{E}[f(X_i^h, \mathbf{X}_{-i}) | \mathbf{X}_{-i}] = f(t, \mathbf{X}_{-i}) + h\mathbb{E}(B_i) \frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) + h^2 \mathbb{E}[\tilde{R} | \mathbf{X}_{-i}]$$

and thus

$$f(X_i^h, \mathbf{X}_{-i}) - \mathbb{E}[f(X_i^h, \mathbf{X}_{-i}) | \mathbf{X}_{-i}] = h(B_i - \mathbb{E}(B_i)) \frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) + h^2 S,$$

with $S = \tilde{R} - \mathbb{E}[\tilde{R} | \mathbf{X}_{-i}]$. Since S is centered, we have by independence of B_i and $\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i})$

$$\begin{aligned} & \mathbb{E} \left((f(X_i^h, \mathbf{X}_{-i}) - \mathbb{E}[f(X_i^h, \mathbf{X}_{-i}) | \mathbf{X}_{-i}])^2 \right) = \\ & \beta_2 \text{var}(B_i) h^2 + 2h^3 \text{Cov} \left((B_i - \mathbb{E}(B_i)) \frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}), S \right) + h^4 \text{var}(S), \end{aligned}$$

180 with $\beta_2 = \mathbb{E} \left(\left(\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i}) \right)^2 \right)$. The result follows in the same way as in the proof of 2. by using that $\frac{\partial f}{\partial x_i}(t, \mathbf{X}_{-i})$ and S are bounded random variables. \square

3. Further connections to existing indices

Taking the expected value over the support index functions reveals interesting connections to other indices, which give a little more insight into the
185 interpretation of the functions.

For the total support index, we immediately get that the equality to the DGSM index. On the other hand, the expected value over the first-order support index function can be connected to variance-based indices when we replace f as underlying function by the partial derivative of f with respect to x_i . Then the
190 expected value can be obtained as first-order index plus its global mean.

Proposition 2. 1. For the total support index $D_i^T(t)$ and the DGSM ν_i (see Eq. (5)) of a variable X_i , we have

$$\mathbb{E}[D_i^T(X_i)] = \nu_i.$$

2. Denote by $\left(\frac{\partial f}{\partial x_i}\right)_0$ the global mean of the derivative function $\frac{\partial f}{\partial x_i}(\cdot)$ and by $D_i\left(\frac{\partial f}{\partial x_i}(\mathbf{X})\right)$ its first-order Sobol index of variable X_i , then we obtain

$$\mathbb{E}[D_i(X_i)] = D_i\left(\frac{\partial f}{\partial x_i}(\mathbf{X})\right) + \left(\left(\frac{\partial f}{\partial x_i}\right)_0\right)^2.$$

Proof. The first part is obtained directly by writing

$$\mathbb{E} [D_i^T(X_i)] = \mathbb{E} \left[\mathbb{E} \left[\left(\frac{\partial f}{\partial \mathbf{x}_i}(X_i, \mathbf{X}_{-i}) \right)^2 \middle| X_i \right] \right] = \nu_i.$$

For the second point, compute the first-order Sobol index of $\frac{\partial f}{\partial x_i}(\cdot)$ corresponding to the input variable X_i by using the pick-freeze formula [2] with \mathbf{Z}_{-i} an independent copy of \mathbf{X}_i ,

$$D_i \left(\frac{\partial f}{\partial x_i}(\mathbf{X}) \right) = \mathbb{E} \left[\frac{\partial f}{\partial x_i}(X_i, \mathbf{X}_{-i}) \frac{\partial f}{\partial x_i}(X_i, \mathbf{Z}_{-i}) \right] - \left(\left(\frac{\partial f}{\partial x_i} \right)_0 \right)^2.$$

As both factors in the expectation are independent conditionally on X_i , we can write

$$\begin{aligned} D_i \left(\frac{\partial f}{\partial x_i}(\mathbf{X}) \right) &= \mathbb{E} \left[\mathbb{E} \left(\frac{\partial f}{\partial x_i}(X_i, \mathbf{X}_{-i}) \frac{\partial f}{\partial x_i}(X_i, \mathbf{Z}_{-i}) \middle| X_i \right) \right] - \left(\left(\frac{\partial f}{\partial x_i} \right)_0 \right)^2 \\ &= \mathbb{E} \left[\left(\mathbb{E} \left[\frac{\partial f}{\partial x_i}(X_i, \mathbf{X}_{-i}) \middle| X_i \right] \right) \left(\mathbb{E} \left[\frac{\partial f}{\partial x_i}(X_i, \mathbf{Z}_{-i}) \middle| X_i \right] \right) \right] - \left(\left(\frac{\partial f}{\partial x_i} \right)_0 \right)^2, \end{aligned}$$

and due to the same distribution of \mathbf{X}_{-i} and \mathbf{Z}_{-i} , we obtain

$$D_i \left(\frac{\partial f}{\partial x_i}(\mathbf{X}) \right) = \mathbb{E} \left[\left(\mathbb{E} \left[\frac{\partial f}{\partial x_i}(X_i, \mathbf{X}_{-i}) \middle| X_i \right] \right)^2 \right] - \left(\left(\frac{\partial f}{\partial x_i} \right)_0 \right)^2.$$

□

195 From 1., it follows that the expected value of the total support index serves as an upper bound for the total sensitivity index,

$$C(\mu_i) \mathbb{E} [D_i^T(X_i)] \geq D_i^T,$$

with $C(\mu_i)$ the Poincaré constant of μ_i as before.

4. Example and application

200 We first continue the example from the introduction and show how the new indices capture the changing impact of the variables over the support. Then we give a complete sensitivity analysis of a real-life application in the field of sheet metal forming.

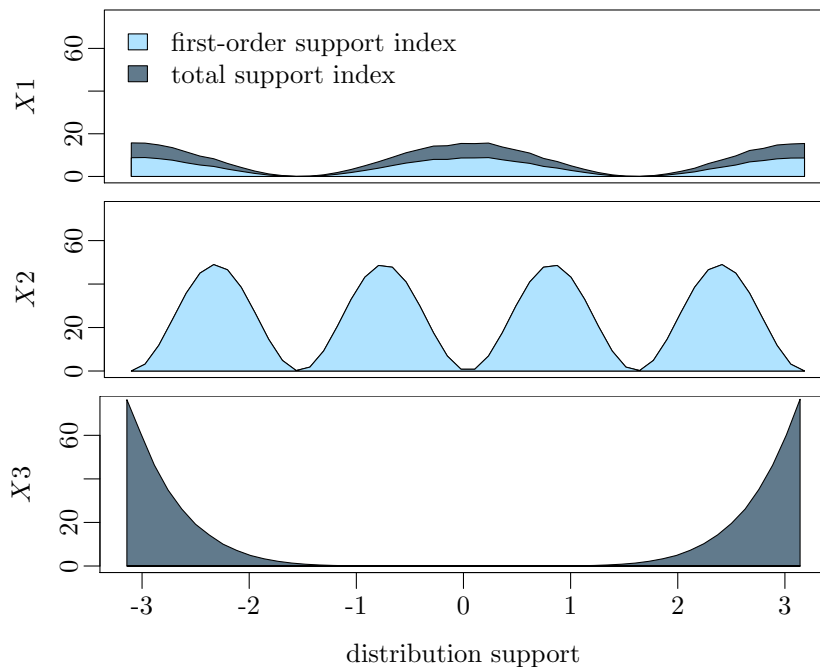


Figure 1: Support analysis of the Ishigami function.

4.1. A numerical example

Applying the described support analysis to the Ishigami function, $f(x_1, x_2, x_3) =$
 205 $\sin(x_1) + 7 \sin^2(x_2) + 0.1x_3^4 \sin(x_1)$, reveals the effect observed in the introduc-
 tion. For the estimation, the estimators based on finite differences, $\widehat{D}_i(t)$ and
 $\widehat{D}_i^T(t)$, were computed at 40 regularly spread points in $]-\pi, \pi[$ for Monte Carlo
 samples of size $n = 5000$. Notice that for this simple function, the support in-
 210 dexes could have been computed analytically. The results are shown in Figure 1.
 The influence of the input variable X_3 is increasing strongly at the borders,
 which explains the observed strong change in the total effect, when the support
 size is changed. Beside this the sinusoidal behavior of X_1 and X_2 can be ob-
 served as well as the facts already known from the standard analysis that X_1
 and X_3 interact and that the main influence of X_2 is the strongest.

215 *4.2. Application to sheet metal forming*

The industrial process of deep drawing is a fundamental procedure for forming sheet metal into desired shapes. It is for example extensively applied in the automotive industry in the production of car bodies. In the deep drawing process, a flat sheet metal is pressed with a punch into a die while so-called blankholders keep the metal fixed at the metal borders. The application aims at analyzing the influence of several input parameters on the thickness reduction of the formed part. A high thickness reduction at a region of the sheet metal means a strong local thinning, which can lead to structural deformations or actual tearing. Is it thus of interest to know, which parameters influence the thinning and in which way as well as modeling and optimization.

Eight input variables are varied in this study, listed in Table 1 together with ranges assumed by the practitioners. The variables flow stress, initial sheet thickness, hardening exponent and sheet layout concern the material, blankholder force and friction can be varied during the process. In practice, friction can be changed during the process by adding or removing lubricant with high pressure air and oil removing agents. To roughly integrate this change of friction over the process time, friction is modeled as three independent variables corresponding to three stages of the process time over which friction is kept constant. The output value is the maximal thickness reduction, that is the thickness reduction of the point of the formed part with the strongest thinning. It is given as the ratio between thickness reduction and initial thickness which leads to a scalar value between 0 and 1.

As the duration of the simulation lies between two and six hours per run, it is out of the scope of a direct analysis. A common approach to reduce the number of evaluations is to replace the original exact model by a fast-to-evaluate metamodel, which is fitted on a comparatively small amount of evaluations (see e.g. [13]). For the design of these evaluations, space-filling designs like Latin hypercube design [14] are well suited. In this application, a Latin hypercube design with 50 runs is applied. The input variables are scaled to lie between 0 and 1. While this does not affect the sensitivity analysis, it simplifies computations

	input variable	feasible region
X_1	flow stress	100-200 MPa
X_2	initial sheet thickness	0.5-1.7 mm
X_3	blankholder force	50-200 kN
X_4	friction; 1 st third of process time	0-0.14
X_5	friction: 2 nd third of process time	0-0.14
X_6	friction: 3 rd third of process time	0-0.14
X_7	hardening exponent	0.1-0.3
X_8	sheet layout	100-150%

Table 1: Input variables of the thickness reduction application.

and is necessary for the comparisons in the support analysis. On the results, a Gaussian process metamodel with a standard product kernel, a single constant trend, and Matérn 5/2 covariance functions is fitted (see e.g. [15] or [16]). The accuracy of the metamodel is validated by leave-one-out cross-validation. The root mean square deviation of the cross-validated predictions from the exact values lies at 0.11, which, considering the range of the thickness reduction [0.2, 0.9], we regard as sufficient.

Using the obtained Gaussian process metamodel, the standard single indices, first-order Sobol and total sensitivity indices, are estimated by applying independent uniform distributions to the input variables. For the computation and visualization the R package `sensitivity` [17] is used. The results are shown in Figure 2. According to this, variable X_8 , the sheet layout, has the strongest influence followed by the two last parts of the friction X_5 and X_6 . The total sensitivity indices show strong interactions for those variables.

As we are working with the very fast-to-evaluate Gaussian process metamodel, we can explore this main effect analysis further by looking at the support indices of the three most influential variables X_5 , X_6 and X_8 . This analysis shows us the local influence of the variables over the domain and can in particular check if the chosen input ranges influence the results critically. Support

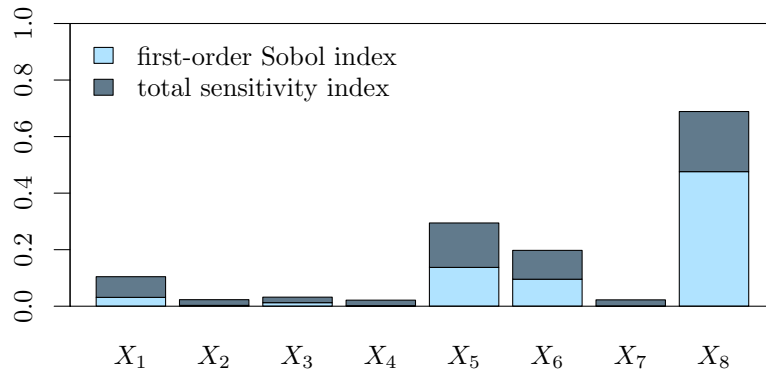


Figure 2: Thickness reduction application, first-order Sobol and total sensitivity indices.

265 indices are estimated at 50 equally distributed points over the scaled domain
 $[0, 1]$ via finite differences with a Monte Carlo sample of size 2 000 for each point.
 The resulting support functions are drawn in Figure 3. The plots show that the
 chosen ranges indeed seem appropriate, as the output variation is not strong
 at the borders of the input supports. The wavy shape of the support index
 270 function of variable X_8 reveals strong nonlinearities in the relation between this
 variable and the thickness reduction. For instance, the local influence of X_8 —
 when X_5, X_6 lie in $[0, 1]$ — is strong around 0.2 and 0.8, but vanishes around
 0.4, 0.6, and 0.9. The two friction parameters X_5 and X_6 show rather similar
 support functions, underlining that both describe the same type of parameter.
 275 The interactions seem to be rather equally spread over the support.

5. Conclusion and perspectives

Two new sensitivity indices, the first-order support index and the total sup-
 port index, have been presented that extend the Sobol index and the total
 sensitivity index, respectively. They give an original and global solution to

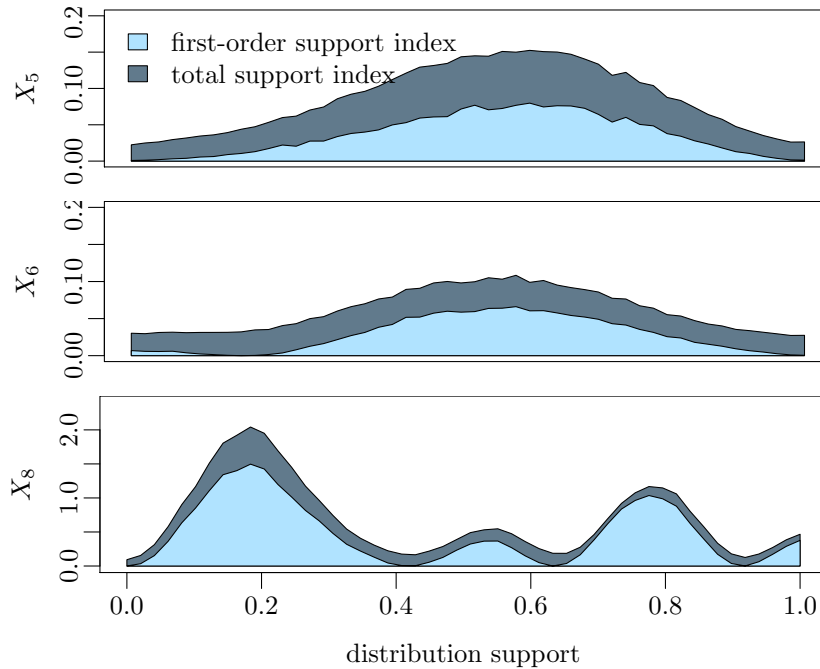


Figure 3: Support analysis of the sheet metal application.

280 one of the challenges of sensitivity analysis named in [1]: to determine regions within in input space for which the model variation is maximum. By returning a function of sensitivities over the input space, the indices give insight into the first-order and the total local behavior of input variables.

285 On the theoretical level, we showed that the two support index functions are asymptotically connected to their corresponding scalar indices when the support approaches zero. Furthermore, we showed that the expected value over the support of the functions is linked to derivative-based indices and variance-based indices, respectively. The results are general as they only require independence and work for every probability density functions of the input variables.

290 The functions give insight into the local influence of variables and thus can be used as an extension to a sensitivity analysis via standard scalar indices. They can be especially helpful in the specification of the input distribution, a possibly highly influential, but often vaguely determined point in sensitivity

analysis. They can further be useful in optimization to explore potential regions
295 in the input domain.

We have noticed two limitations of support indices, which correspond to those observed for the Sobol indices and derivative-based Sobol measures. First, the estimation of the indices is expensive and thus can only be used with rather cheap-to-evaluate models like metamodels. Second, as the support indices represent functions of partial derivatives, strongly varying models will lead to higher
300 support indices than smooth ones, an effect which is not reflected in the scalar indices which just summarize the output variance. This is due to the focus on local sensitivities and only important in the case of strongly varying models, in which careful interpretation is necessary. Finally, the definition is restricted to
305 independent input variables. An interesting perspective would be to extend the approach to the case of dependent inputs.

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