Estimating Sensitivity Indices from Computer Simulator Output

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Abstract

An overview is given of statistical methodology for estimating sensitivity indices, including moment-based, quadrature-based, and process-based estimators of global sensitivity indices. The paper, together with the on-line Supplementary material, derives the specific formulae needed for the computation of process-based Bayesian and empirical Bayesian global sensitivity indices for a broad class of regression plus stationary Gaussian process models using the Gaussian, Bohman, or cubic correlation functions. It is shown how to restrict the parameter space for the compactly supported Bohman and cubic correlation functions so that (at least) a given proportion of the training data correlation entries are zero. This feature is important in the situation where the set of training data is large. Formulae are given in a form suitable for computation, and the estimation methods are illustrated and compared via examples.

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1 Introduction

A *computer experiment* uses a computer simulator based on a mathematical model of a physical process as an experimental tool to determine "responses" or "outputs" at a set of user-specified input sites. These input sites constitute the design for the computer experiment. Sophisticated computer codes may take hours or even days to produce an output and, therefore, a flexible and rapidly-computable predictor, sometimes called a "code emulator", is often fitted to the inputs/outputs of the design, which are then called *training data*. An emulator allows the detailed, albeit approximate, exploration of the output over the entire experimental region. In preliminary stages of study using the simulator, emulators also allow the researcher to assess the sensitivity of the output to individual inputs or groups of inputs, i.e., to conduct a "sensitivity analysis".

The purpose of this paper is to give an overview of moment-based, quadrature-based, and process-based methods for assessing sensitivity which have appeared in disjoint form in the literature and to compare these via examples. The paper derives the specific formulae required to compute Bayesian and empirical (plug-in) Bayesian estimates of sensitivity indices for a broad class of regression plus stationary Gaussian process models.

Sensitivity indices, most especially total sensitivity indices, are one tool for "screening", that is for detecting influential inputs that have major impacts on an input-output system (see Hyejung Moon and Dean (2011) and also Linkletter, Bingham, Hengartner, Higdon, and Ye (2006) for contrasting approaches).

To introduce notation, assume that the computer simulator has d continuous input variables denoted by the vector $\boldsymbol{x} = (x_1, \ldots, x_d)$ and that the output of the simulator is denoted by $y(\boldsymbol{x}) = y(x_1, \ldots, x_d)$, which can be determined for $\boldsymbol{x}$ in the hyper-rectangle $\mathcal{X} = \prod_{j=1}^{d}[l_j, u_j]$. The *local change* in $y(\cdot)$ at $\boldsymbol{x}^0 = (x_1^0, \ldots, x_d^0)$ as the j^{th} input varies by a small amount parallel to the x_j axis can be determined from the partial derivatives of $y(\cdot)$ with respect to

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x_j, i.e., from knowledge of

$$\left.\frac{\partial y(\boldsymbol{x})}{\partial x_j}\right|_{\boldsymbol{x}^0} . \tag{1.1}$$

In contrast, *global sensitivity indices* measure the change in $y(\cdot)$ as one (or more) inputs vary over their entire range, when the remaining inputs are fixed. Global sensitivity indices can suggest when there are interactions among sets of inputs (see Section 2).

For estimating local sensitivity indices (1.1), Morris (1991) proposed a *one-at-time sampling design*. Assuming that the input space has been scaled to $[0,1]^d$, this method constructs a design on the grid $\{0, 1/(p-1), \ldots, 1\}^d$ of $[0,1]^d$ for a given positive integer p. For input $j \in \{1, \ldots d\}$ and $\Delta = q/(p-1)$ for some positive integer $q < p$, Morris's method selects as a design a random sample of n inputs $\boldsymbol{x} \in \{0, 1/(p-1), \ldots, 1\}^d$ for which both terms in the numerator of

$$d_j(\boldsymbol{x}) \equiv \frac{y(x_1, \ldots, x_{j-1}, x_j + \Delta, x_{j+1}, \ldots, x_d) - y(\boldsymbol{x})}{\Delta} \tag{1.2}$$

are defined. Using $2dn$ function evaluations, the design produces n independent $d_j(\cdot)$ estimates for each $j \in \{1, \ldots, d\}$; the estimates for different j are dependent. If the resulting set $\{d_j(\boldsymbol{x})\}_{\boldsymbol{x}}$ values has a *large* sample variance, this suggests that the influence of x_j on the output is highly dependent on the $\boldsymbol{x}$ at which $d_j(\boldsymbol{x})$ is evaluated; thus $y(\boldsymbol{x})$ is likely to be nonlinear in x_j or involve interactions of x_j with other inputs. If the sample mean and sample variance of the $\{d_j(\boldsymbol{x})\}_{\boldsymbol{x}}$ values are both *small*, this suggests that x_j has negligible influence on $y(\cdot)$. If the sample mean of the $\{d_j(\boldsymbol{x})\}_{\boldsymbol{x}}$ values is roughly a *non-zero constant* and the sample variance is *small*, this suggests that x_j has an additive linear influence on $y(\cdot)$.

This paper now focuses on global sensitivity indices (defined in Section 2), and compares a number of methods that have been used to estimate these. Section 3 reviews moment-based methods which use specific designs. A quadrature-based method of estimation that is not tied to a specific experimental design is described in Section 4. Section 5 presents Bayesian methods of estimating global sensitivity indices for a class of regression plus stationary Gaussian process models. Together with the on-line Supplementary Material, Section 5 derives specific formulae for these indices using Gaussian, Bohman, and cubic correlation functions. In Section 6, the methods are compared for an example for which the true values of the sensitivity indices can be determined. The Bayesian methods, in particular, work well in estimating main effect and total effect sensitivity indices. Finally, Section 7 shows how to restrict the parameter space for the compactly supported Bohman and cubic correlation

functions so that (at least) a given proportion of the training data correlation entries are zero.

2 Global Sensitivity Indices

In this section, we give a careful description and definitions of global sensitivity indices, and provide a proof of a key property of the functions on which the indices are built. Let $Q = \{k_1, \ldots, k_s\} \subset \{1, 2, \ldots, d\}$ denote a subset of the input variables and let $\boldsymbol{x}_Q$ denote the vector $(x_{k_1}, \ldots, x_{k_s})$ where, for definiteness, it is assumed $1 \leq k_1 < k_2 < \cdots < k_s \leq d$. The vector of the remaining inputs will be denoted by $\boldsymbol{x}_{-Q}$ also arranged in lexicographical order of their input index. By rearranging the order of the entire set of input variables we write $\boldsymbol{x} = (\boldsymbol{x}_Q, \boldsymbol{x}_{-Q})$ in a slight abuse of notation.

One popular method of defining global sensitivity indices is in terms of the variability of the (weighted) average output $y(\boldsymbol{x})$ over $\boldsymbol{x} \in \mathcal{X} = \prod_{j=1}^{d}[l_j, u_j]$, (see Sobol´ (1990), Saltelli, Chan, and Scott (2000)). To simplify notation, the development below takes $[l_j, u_j] = [0, 1]$, for all $j = 1, \ldots, d$, so that $\mathcal{X} = [0, 1]^d$. The formulae can be extended to the more general hyper-rectangle case. Also for simplicity of notation, it is assumed that the weight function can be specified by a joint density function over $\mathcal{X} = [0, 1]^d$ having independent and identically distributed x_j components each with probability density function $g(x)$. For any subset $E \subseteq \{1, \ldots, d\}$ the notation $g(\boldsymbol{x}_E)$ denotes $\prod_{\ell \in E} g(x_\ell)$. It is a straightforward generalization to allow the weight function to have independent but not identically distributed components.

2.1 Uncorrected and corrected mean effect functions

Let

$$y_0 = \int y(\boldsymbol{x}) g(\boldsymbol{x}) \, d\boldsymbol{x} = E_g \left[y(\boldsymbol{X}) \right]$$

denote the overall (weighted) mean of $y(\boldsymbol{x})$, expressing the fact that $\boldsymbol{X} \sim g(\cdot)$. More generally, for any non-empty $Q = \{k_1, \ldots, k_s\} \subset \{1, 2, \ldots, d\}$, define the *uncorrected mean effect* (also known as the *joint effect function*) of the input vector $\boldsymbol{x}_Q$ on $y(\cdot)$ to be

$$u_Q(\boldsymbol{x}_Q) = \int y(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}) g(\boldsymbol{x}_{-Q}) d\boldsymbol{x}_{-Q} = E_g[y(\boldsymbol{X}) | \boldsymbol{X}_Q = \boldsymbol{x}_Q]. \tag{2.1}$$

Again, the notation makes clear that the function average can be viewed as an expectation with respect to subcomponents of $\boldsymbol{X}$. For example, when $Q = \{j\}$ for a given $j \in \{1, \ldots, d\}$, the uncorrected mean effect when X_j is held fixed at x_j is

$$u_j(x_j) = \int y(x_1, \ldots, x_d) \prod_{\ell \neq j} g(x_\ell) dx_\ell = E\left[y(\boldsymbol{X}) | X_j = x_j\right],$$

which is called the *main effect function* of input j associated with $y(\boldsymbol{x})$. Plots of the main effect functions $u_j(x_j)$ versus x_j, and plots of the joint effect functions $u_{j_1 j_2}(x_{j_1}, x_{j_2})$ versus pairs of inputs (x_{j_1}, x_{j_2}) can be used to provide a visual understanding of the change in the averaged $y(\boldsymbol{x})$ with respect to each single input or pairs of inputs (see, for example, Jones, Schonlau, and Welch (1998)).

In general, the joint effect function $u_Q(\boldsymbol{x}_Q)$ describes average changes in $y(\boldsymbol{x})$ on the same scale and in the same range as $y(\boldsymbol{x})$. The global sensitivity indices that will be defined shortly will be based on the *variances* of a centered and orthogonalized version of the $u_Q(\boldsymbol{X}_Q)$, where the variance is with respect to the $\boldsymbol{X}_Q$ input distribution.

Viewed with this goal in mind, the $u_Q(\boldsymbol{x}_Q)$ functions have an important defect that limits their usefulness in directly defining sensitivity indices. When viewed as functions of the random $\boldsymbol{X}_Q$ inputs, the mean effect functions corresponding to different Q will, in general, be correlated. Thus, Sobol´ (1990) and Sobol´ (1993) advocated the use of a functional analysis of variance (ANVOA) decomposition of $y(\boldsymbol{x})$ that modifies the uncorrected effect functions and produces uncorrelated and mean zero versions of these functions (see also Hoeffding (1948)). These modified functions are used to define the global sensitivity indices. In particular, Sobol´ (1993) used the decomposition

$$y(\boldsymbol{x}) = y_0 + \sum_{j=1}^{d} y_j(x_j) + \sum_{1 \leq j_1 < j_2 \leq d} y_{j_1, j_2}(x_{j_1}, x_{j_2}) + \cdots + y_{1,2,\ldots,d}(x_1, \ldots, x_d) \tag{2.2}$$

whose components satisfy the "zero mean property", meaning that for any $(j_1, \ldots, j_s)$,

$$\int y_{j_1,\ldots,j_s}(x_{j_1}, \ldots, x_{j_s}) g(x_{j_k})\, dx_{j_k} = 0 \qquad \text{for any } j_k,\ k = 1, \ldots, s\,, \tag{2.3}$$

and whose components are *pairwise orthogonal*, meaning that for any $(k_1, \ldots, k_s) \neq (j_1, \ldots, j_t)$,

$$\begin{aligned} &E_g\left[y_{k_1,\ldots,k_s}(X_{k_1}, \ldots, X_{k_s}) y_{j_1,\ldots,j_t}(X_{j_1}, \ldots, X_{j_t})\right] \\ &\qquad = \int y_{k_1,\ldots,k_s}(x_{k_1}, \ldots, x_{k_s}) y_{j_1,\ldots,j_t}(x_{j_1}, \ldots, x_{j_t}) g(\boldsymbol{x}_Q)\, d\boldsymbol{x}_Q = 0. \end{aligned} \tag{2.4}$$

where $Q = \{k_1, \ldots, k_s\} \cup \{j_1, \ldots, j_t\}$. The component terms of (2.2) are called *corrected (mean) effect functions* and are defined as follows. For $Q = \{j\}$ with $j \in \{1, \ldots, d\}$,

$$y_j(x_j) \equiv u_j(x_j) - \ y_0 \ = \ E_g\left[y\left(\boldsymbol{X}\right) \mid X_j = x_j\right] \ - \ E_g\left[y(\boldsymbol{X})\right] \ , \tag{2.5}$$

which is called the *corrected main effect function* of input x_j. For $Q \subseteq \{1, \ldots d\}$ having two or more elements, $y_Q(\boldsymbol{x}_Q)$ is defined recursively to be,

$$y_Q(\boldsymbol{x}_Q) = u_Q(\boldsymbol{x}_Q) - \sum_{E \subset Q} y_E(\boldsymbol{x}_E) - y_0, \tag{2.6}$$

where the sum is over the collection of all non-empty, *proper* subsets E of Q. For example, when $Q = \{j_1, j_2\}$ with $1 \leq j_1 < j_2 \leq d$,

$$\begin{aligned} y_{j_1 j_2}(x_{j_1}, x_{j_2}) &= u_{j_1 j_2}(x_{j_1}, x_{j_2}) \ - \ y_{j_1}(x_{j_1}) \ - \ y_{j_2}(x_{j_2}) - \ y_0 \\ &= u_{j_1 j_2}(x_{j_1}, x_{j_2}) \ - \ u_{j_1}(x_{j_1}) \ - \ u_{j_2}(x_{j_2}) + \ y_0 \end{aligned}$$

which is called the *corrected interaction effect function* of inputs x_{j_1} and x_{j_2}.

Once (2.3) has been established, it is straightforward to check that (2.4) holds for any $y_Q(\boldsymbol{x}_Q)$ term (2.6). However, the proof of (2.3) is more complicated and does not appear to be readily available in the literature. A new proof is provided in Lemma 2.1.

Lemma 2.1 *For $Q = \{j_1, \ldots, j_s\} \subseteq \{1, \ldots, d\}$,*

$$\int_{[0,1]} y_Q(\boldsymbol{x}_Q) g(x_{j_k}) dx_{j_k} = 0 \tag{2.7}$$

for any $j_k \in Q$.

Proof: The proof proceeds by induction on the number of elements in Q. First, from (2.1), (2.5) and the definition of y_0, (2.7) holds for any main effect function $y_j(x_j)$. Next, select a subset $Q \subseteq \{1, \ldots, d\}$ containing two or more elements, and assume that (2.7) holds for all proper subsets of $E \subset Q$. Focus on element $\ell \in Q$, and let $Q \backslash \ell$ denote the set difference of Q and ℓ, which is non-empty by definition of Q. Partition the set of non-empty subsets E of Q into the set $\mathcal{U}_+$ of subsets E that contain ℓ, and the set $\mathcal{U}_-$ of subsets E that do not contain ℓ; note that $Q \backslash \ell \in \mathcal{U}_-$. Then, by (2.6),

$$\int y_Q(\boldsymbol{x}_Q)\ g(x_\ell)dx_\ell = \int \left\{ u_Q(\boldsymbol{x}_Q) - \sum_{E\subset Q} y_E(\boldsymbol{x}_E) - y_0 \right\}\ g(x_\ell)\ dx_\ell$$

$$= \int \left\{ \int y(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q})\ g(\boldsymbol{x}_{-Q}) d\boldsymbol{x}_{-Q} \right\}\ g(x_\ell)\ dx_\ell$$

$$- \sum_{E\in\mathcal{U}_+} \int y_E(\boldsymbol{x}_E)\ g(x_\ell)\ dx_\ell - \sum_{E\in\mathcal{U}_-} y_E(\boldsymbol{x}_E) - y_0\,, \qquad (2.8)$$

using the fact that the third and fourth terms are constant with respect to integration over x_ℓ (since $\ell \notin E$ for $E \in \mathcal{U}_-$). Now, the second term in (2.8) is zero since (2.7) holds for all proper subsets of Q by assumption. Also, by (2.1), the first term is

$$\int u_Q(\boldsymbol{x}_Q)\ g(x_\ell)\ dx_\ell = \int\int y(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q})\ g(\boldsymbol{x}_{-Q})\ g(x_\ell)\ dx_Q\ dx_\ell = u_{Q\backslash\ell}(\boldsymbol{x}_{Q\backslash\ell})\,,$$

so that (2.8) becomes

$$\int y_Q(\boldsymbol{x}_Q)\ g(x_\ell)dx_\ell = u_{Q\backslash\ell}(\boldsymbol{x}_{Q\backslash\ell}) - 0 - \left(\sum_{E\in\mathcal{U}_-;E\neq Q\backslash\ell} y_E(\boldsymbol{x}_E) + y_{Q\backslash\ell}(\boldsymbol{x}_{Q\backslash\ell}) \right) - y_0\,,$$

which is zero by definition of $u_{Q\backslash\ell}(\boldsymbol{x}_{Q\backslash\ell})$ in (2.6).

Notice that Lemma 2.1 implies that $E_g\left[y_Q(\boldsymbol{x}_Q)\right] = 0$ for all $Q \subseteq \{1,\ldots,d\}$. In the next subsection, the corrected mean effect functions are used to define sensitivity indices.

2.2 Definitions of main effect and total effect sensitivity indices

We now define global sensitivity indices in terms of the variances of the corrected effect functions and, in the following subsection, calculation formulae using uncorrected mean effect functions will be given.

First, the *total variance* of $y(\boldsymbol{x})$ is defined to be

$$v = Var_g[y(\boldsymbol{X})] = \int y^2(\boldsymbol{x}) g(\boldsymbol{x}) d\boldsymbol{x} - y_0^2. \qquad (2.9)$$

For any $Q \subseteq \{1,\ldots d\}$, define

$$v_Q = \ Var_g[y_Q(\boldsymbol{X}_Q)] = \int y_Q^2(\boldsymbol{x}_Q) g(\boldsymbol{x}_Q)\ d\boldsymbol{x}_Q \qquad (2.10)$$

where we use the fact that $E_g\{y_Q(\boldsymbol{X}_Q)\} = 0$. So, for example,

$$v_j = Var_g\left(y_j(X_j)\right) = \int y_j^2(x_j)g(x_j)dx_j,$$

for any $j \in \{1 \ldots d\}$ and

$$v_{j_1 j_2} = Var_g\left(y_{j_1 j_2}(x_{j_1}, x_{j_2})\right) = \int y_{j_1 j_2}^2(x_{j_1}, x_{j_2})g(x_{j_1})g(x_{j_2})dx_{j_1}dx_{j_2},$$

for (j_1, j_2) satisfying $1 \leq j_1 < j_2 \leq d$.

Using (2.2) and (2.4), the variance of $y(\boldsymbol{x})$ can be partitioned as

$$v = \sum_{j=1}^{d} v_j + \sum_{1 \leq j_1 < j_2 \leq d} v_{j_1 j_2} + \cdots + v_{1,2,\ldots,d} \ . \tag{2.11}$$

The sensitivity of $y(\cdot)$ to inputs $x_{j_1}, \ldots, x_{j_s}$ is measured by the *sensitivity index*

$$S_{j_1,\ldots,j_s} \equiv v_{j_1,\ldots,j_s}/v. \tag{2.12}$$

In partiular, the quantities $S_1, \ldots, S_d$ are called *main effect sensitivity indices* and $S_{j_1 j_2}$ is a *two-factor sensitivity index*. By (2.11),

$$\sum_{j=1}^{d} S_j + \sum_{1 \leq j_1 < j_2 \leq d} S_{j_1 j_2} + \cdots + S_{1,2,\ldots,d} = 1.$$

The *total effect sensitivity index* of input x_j is defined to be the sum of *all* sensitivity indices involving the input x_j,

$$T_j = S_j + \sum_{k \neq j} S_{kj} + \cdots + S_{1,2,\ldots,d}. \tag{2.13}$$

For example, when there are $d = 3$ inputs, then $T_1 = S_1 + S_{12} + S_{13} + S_{123}$. Notice that by construction, $S_j \leq T_j$ for all $j \in \{1, \ldots, d\}$. If interactions involving x_j account for a large proportion of the variance v, then the difference between T_j and S_j will be large.

2.3 Calculation of main effect and total effect sensitivity indices

For calculation of main effect and total effect sensitivity indices, it is more efficient to calculate $\{S_j\}_{j=1}^d$ and $\{T_j\}_{j=1}^d$ in terms of the variances of the uncorrected effect functions which

are

$$v_Q^u = Var_g[u_Q(\boldsymbol{X}_Q)] = Var_g\left[E_g[y(\boldsymbol{X})|\boldsymbol{X}_Q]\right] \tag{2.14}$$

for nonempty $Q \subseteq \{1, \ldots d\}$. Since v_Q^u in (2.14) can be rewritten as

$$v_Q^u = Var_g[y(\boldsymbol{X})] - E_g\left[Var_g(y(\boldsymbol{X})|\ \boldsymbol{X}_Q)\right] = v - E_g\left[Var_g(y(\boldsymbol{X})|\ \boldsymbol{X}_Q)\right], \tag{2.15}$$

v_Q^u can be interpreted as the expected reduction in uncertainty in $y(\boldsymbol{X})$ due to observing $\boldsymbol{x}_Q$.

For the simple case $Q = \{j\}$, using (2.5),

$$v_j^u = Var_g[y_j(X_j) + y_0] = v_j\ , \tag{2.16}$$

so that the main effect S_j can be calculated in terms of the variance of the uncorrected main effect function; that is

$$S_j = v_j^u/v. \tag{2.17}$$

The total effect T_j can be computed in terms of the variances of uncorrected mean functions as follows. Observe from (2.6), (2.10) and (2.14) that

$$v_{-j}^u = Var_g[u_{-j}(\boldsymbol{X}_{-j})] = Var_g\left[\sum y_Q(\boldsymbol{X}_Q)\right] = \sum v_Q\,. \tag{2.18}$$

where the sum is over nonempty sets Q contained in $\{1, \ldots, d\} \setminus \{j\}$. In words, v_{-j}^u is the sum of all v_Q components that do *not involve* the subscript j in the variance decomposition (2.11). Thus, $v - v_{-j}^u$ is the sum of all v_Q components for which $j \in Q$, and so the total effect sensitivity index T_j in (2.13) can be expressed as

$$T_j = (v - v_{-j}^u)/v\ . \tag{2.19}$$

Results (2.17) and (2.19) imply that if only the *main effect* and *total effect* sensitivity indices $\{S_j\}_{j=1}^d$ and $\{T_j\}_{j=1}^d$ are to be estimated, then one need only estimate the variances of $2d$ uncorrected effect functions rather than the variances of $2^d - 1$ corrected effect functions specified by the definitions (2.12) and (2.13).

Sections 4 and 5 describe two general methods of estimating the variance v_Q^u, each using the Gaussian process underlying models. The first uses quadrature-based estimation, while the other uses Bayesian or empirical Bayesian process-based estimation. Before describing these methods and the new formulae needed for implementation of the latter, a technique will be described in Section 3 for designing experiments to obtain moment-based estimators of the numerator and denominator of S_j.

3 Moment-based Estimation of Global Main Effect Sensitivity Indices

In addition to the Morris (1991) design of Section 1 for estimating *local* sensitivity indices, experimental designs have been proposed to estimate main effect and total effect *global* sensitivity indices, $\{S_j\}_{j=1}^d$ and $\{T_j\}_{j=1}^d$. The designs rely on moment-based estimation of v, v_j^u, and v_{-j}^u, $j = 1, \ldots, d$ in (2.9), (2.16) and (2.18). Moment-based estimators use the simple idea that if $W_1, \ldots, W_n$ are independent and identically distributed random variables from a distribution having finite mean μ and finite variance σ^2, then their sample mean and sample variance are unbiased and consistent estimators of μ and σ^2, respectively.

Morris, Moore, and McKay (2008) described several methods designing a computer experiment to obtain moment-based estimators of the main effect sensitivity indices $\{S_j\}_{j=1}^d$. One method they advocate is the *permuted column sampling design*, introduced by McKay (1995), as follows. For $j = 1, \ldots, d$, let $\boldsymbol{u}_j$ be a vector of n values from the interval $[0, 1]$. We call the $n \times d$ matrix $\boldsymbol{M} = [\boldsymbol{u}_1 \cdots \boldsymbol{u}_d]$ the "base design". The values within the vector $\boldsymbol{u}_j$ may be identical to the columns of a space-filling Latin hypercube design using the mid-points of the intervals $(\ (i-1)/n,\ i/n\ ]$, or they may be different. Given an integer a, let $\pi_j^q(\boldsymbol{u}_j)$ denote the vector whose elements are a permutation of the elements of $\boldsymbol{u}_j$, $j = 1, \ldots, d$, $q = 1, \ldots, a$. Define the matrix $\boldsymbol{A}_q$ to be

$$\boldsymbol{A}_q = [\pi_1^q(\boldsymbol{u}_1)\ \pi_2^q(\boldsymbol{u}_2)\ \cdots\ \pi_d^q(\boldsymbol{u}_d)]\,, \quad q = 1, \ldots, a\,.$$

Letting $s^2(\boldsymbol{A}_q)$ denote the sample variance of the n outputs associated with inputs given by the rows of $\boldsymbol{A}_q$, then

$$\hat{v} = \frac{1}{a}\sum_{q=1}^{a} s^2(\boldsymbol{A}_q)\,. \tag{3.1}$$

is an estimate of v in (2.15).

Now fix an integer $j \in \{1, \ldots, d\}$ for the remainder of this section; to estimate v_j^u using the difference formula in (2.15) requires an estimate of $E_g\{Var_g(y(\boldsymbol{X})|X_j)\}$. The j^{th} column of each $\boldsymbol{A}_q$, $q = 1, \ldots a$, contains the elements of $\boldsymbol{u}_j$ in some permuted order. Let $\boldsymbol{u}_j = (x_{1j}, \ldots, x_{nj})^\top$, then for any fixed $r \in \{1, \ldots, n\}$, the sample variance $s^2(x_{rj})$ of the outputs corresponding to the rows in $\boldsymbol{A}_1, \ldots, \boldsymbol{A}_a$ having value x_{rj} as the j^{th} element is an estimate of $Var_g(y(\boldsymbol{X})|X_j = x_{rj})$. The average of $s^2(x_{1j}), \ldots, s^2(x_{nj})$ is an estimator of

$E_g\{Var_g(y(\boldsymbol{X})|X_j)\}$, so that v_j^u is estimated by

$$\hat{v}_j^u = \hat{v} - \frac{1}{n}\sum_{r=1}^{n} s^2(x_{rj}). \tag{3.2}$$

Morris et al. (2008) note that $\hat{v}_j^u$ is unbiased "if no two input values paired together in one array also were paired in another array" and they give a method of selecting permutations to achieve this. They illustrate their method for $n = d = a$, requiring $an = n^2$ code evaluations, although any n, a, d could be selected. Their method proceeds as follows. Select an orthogonal array $\text{OA}(na, d+1, n, 2)$ based on the n symbols $\{1, 2, \ldots, n\}$, na rows, $d+1$ columns and strength 2. Reorder the rows of the orthogonal array so that, in column 1, the first n rows contain symbol 1, the next n rows contain the symbol 2, and so on. Then columns 2 to $d+1$ of the orthogonal array are

$$[\boldsymbol{P}_1^\top, \boldsymbol{P}_2^\top, \ldots, \boldsymbol{P}_a^\top]^\top.$$

For $q \in \{1, \ldots, a\}$, the columns of $\boldsymbol{P}_q = [\pi_1^q \cdots \pi_d^q]$ are used to provide the permutations that are applied to the base design $\boldsymbol{M}$ to obtain the matrices $\boldsymbol{A}_q$ that give the input sites for the sample variance calculations above. Morris et al. (2008) also provide estimates of the variances of the permuted column S_j estimators.

In Section 6, we compare the estimates of the main effect sensitivity indices using permuted column sampling, with base design $\boldsymbol{M}$ selected to be a maximin Latin Hypercube Design, with those obtained via quadrature (Section 4) and Bayesian process based estimates (Section 5).

4 Quadrature-based Estimators of Global Sensitivity Indices

In this section, we describe quadrature-based estimators which do not require particular sampling designs but use predictors based on the Gaussian process model

$$Y(\boldsymbol{x}) = \boldsymbol{f}^\top(\boldsymbol{x})\boldsymbol{\beta} + Z(\boldsymbol{x}), \tag{4.1}$$

where $\boldsymbol{f}^\top(\boldsymbol{x})\boldsymbol{\beta}$ is a linear function of an unknown regression parameter vector $\boldsymbol{\beta}$, and $Z(\boldsymbol{x})$ is a zero-mean Gaussian process having variance σ^2. We illustrate the calculations of the quadrature-based estimators for the special case where $\boldsymbol{f}^\top(\boldsymbol{x})\boldsymbol{\beta} = \beta_0$ and $Z(\boldsymbol{x})$ is stationary

with separable correlation function

$$Cor(Z(\boldsymbol{x}_i), Z(\boldsymbol{x}_k)) = \prod_{j=1}^{d} R(x_{ij} - x_{kj} |\ \psi_j)\,, \tag{4.2}$$

where $R(\cdot|\ \psi_j)$ is known up to an unknown (vector of) parameter(s), ψ_j, associated with the j^{th} input.

One example of $R(h_j|\ \psi_j)$ is the one-dimensional Gaussian correlation function

$$R_G(h_j|\ \psi_j) = \exp\left[-\psi_j h_j^2\right] \tag{4.3}$$

which will be used later in the section to illustrate the quadrature-based estimation procedure. Other important correlations of the form (4.2) for which quadrature-based estimators can be explicitly derived are the Bohman and cubic correlation functions which will be discussed in Section 5 and the Supplementary Material.

An empirical best linear unbiased predictor (EBLUP) of $y(\boldsymbol{x}^*)$ based on (4.1) with training data $\{\boldsymbol{x}_i = (x_{i1}, \ldots, x_{id}), y(\boldsymbol{x}_i)\}_{i=1}^n$ has the form

$$\widehat{y}(\boldsymbol{x}^*) = d_0(\boldsymbol{x}^*) + \sum_{i=1}^{n} d_i \prod_{j=1}^{d} R(x_j^* - x_{ij} |\ \widehat{\psi}_j) \tag{4.4}$$

where $\widehat{\psi}_j$ is a REML (or other) estimate of the unknown correlation parameters ψ_j, $d_0(\boldsymbol{x}^*) = \boldsymbol{f}^\top(\boldsymbol{x}^*)\widehat{\boldsymbol{\beta}}$, with $\widehat{\boldsymbol{\beta}} = (\boldsymbol{F}^\top \boldsymbol{R}^{-1} \boldsymbol{F})^{-1} \boldsymbol{F}^\top \boldsymbol{R}^{-1} \boldsymbol{y}(\boldsymbol{x})$ the weighted least squares estimator of $\boldsymbol{\beta}$, and d_i is the i^{th} element of the vector $\boldsymbol{R}^{-1}(\boldsymbol{y}(\boldsymbol{x}) - \boldsymbol{F}\hat{\boldsymbol{\beta}})$ where $\boldsymbol{F} = [\boldsymbol{f}(\boldsymbol{x}_1), \ldots, \boldsymbol{f}(\boldsymbol{x}_n)]^\top$ and $\boldsymbol{R}$ is the matrix with $(i,k)^{th}$ element $\prod_{j=1}^{d} R(x_{ij} - x_{kj} |\ \widehat{\psi}_j)$. When $\boldsymbol{f}^\top(\boldsymbol{x})\boldsymbol{\beta} = \beta_0$,

$$d_0(\boldsymbol{x}^*) = d_0 = \widehat{\boldsymbol{\beta}}_0$$

with $\widehat{\boldsymbol{\beta}}_0 = (\mathbf{1}_n^\top \boldsymbol{R}^{-1} \boldsymbol{y}(\boldsymbol{x}))/(\mathbf{1}_n^\top \boldsymbol{R}^{-1} \mathbf{1}_n)$ and $\mathbf{1}_n$ is the $n \times 1$ column vector of ones.

The idea of quadrature-based estimation is to replace $y(\boldsymbol{x})$ in the variance expressions v, v_j^u, and v_{-j}^u of Section 2, $j = 1, \ldots, d$, by a predictor $\widehat{y}(\boldsymbol{x})$ and to integrate the associated expectations. A naïve form of this method estimates $u_Q(\boldsymbol{x}_Q)$ in (2.1) by

$$\widehat{u}_Q(\boldsymbol{x}_Q) = \int \widehat{y}(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}) \prod_{j \notin Q} g(x_j)\ dx_j = \sum_{\ell=1}^{N} \widehat{y}(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}^{(\ell)})\ w_\ell$$

where (i) $\widehat{y}(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}^{(\ell)})$ is an EBLUP of $y(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}^{(\ell)})$ as in (4.4); (ii) the sum is over the N user-selected points at which the function $\widehat{y}(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}^{(\ell)})$ is evaluated in the $(d - |Q|)$-dimensional

space over which the integration is being performed; (iii) the superscript ℓ denotes the ℓ^{th} such point, $(\boldsymbol{x}_Q, \boldsymbol{x}_{-Q}^{(\ell)})$, evaluated with weight w_ℓ; and (iv) the weights $\{w_\ell\}$ and points $\{\boldsymbol{x}_{-Q}^{(\ell)}\}$ depend on the selected quadrature method.

When $Z(\boldsymbol{x})$ has a separable correlation function of form (4.2), a more accurate method of estimating these variances uses the fact that $\widehat{y}(\boldsymbol{x})$ can be reduced to a product of one-dimensional integrals. In some cases these one-dimensional integrals can be integrated explicitly. To illustrate, consider estimation of the total variance, $v = E_g\left\{y^2\left(\boldsymbol{X}\right)\right\} - (y_0)^2$, in (2.9) when $Y(\boldsymbol{x})$ has mean β_0. Using (4.4), an estimate of the term y_0 is

$$d_0 + \sum_{i=1}^{n} d_i \; I^{(1)}(\boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) \, ,$$

where

$$I^{(1)}(\boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) = \prod_{j=1}^{d} \int R(x_j^* - x_{ij} | \; \widehat{\psi}_j) \; g(x_j^*) \; dx_j^* \tag{4.5}$$

and $I^{(1)}$ denotes a product of integrals, each over a single variable with integrand involving *one* $R(\cdot | \; \cdot)$ term. The first term of v is estimated by

$$\begin{aligned}
\widehat{E}_g\left[y^2\left(\boldsymbol{X}\right)\right] &= \int \left[d_0 + \sum_{i=1}^{n} d_i \; \prod_{j=1}^{d} R(x_j^* - x_{ij} \mid \widehat{\psi}_j) \right]^2 \; g(\boldsymbol{x}^*) \; d\boldsymbol{x}^* \\
&= \int \quad \Bigg[d_0^2 + \sum_{i=1}^{n} d_i^2 \; \prod_{j=1}^{d} R^2(x_j^* - x_{ij} \mid \widehat{\psi}_j) \\
&\qquad +2 \; d_0 \; \sum_{i=1}^{n} d_i \; \prod_{j=1}^{d} R(x_j^* - x_{ij} \mid \widehat{\psi}_j) \\
&\qquad + 2 \sum_{1 \le i < k \le n} d_i d_k \; \prod_{j=1}^{d} R(x_j^* - x_{ij} \mid \widehat{\psi}_j) R(x_j^* - x_{kj} \mid \widehat{\psi}_j) \Bigg] \; g(\boldsymbol{x}^*) \; d\boldsymbol{x}^* \, ,
\end{aligned} \tag{4.6}$$

and each term in (4.6) can be expressed as a product of one-dimensional integrals. For example, the third term can be written as

$$2 \; d_0 \; \sum_{i=1}^{n} d_i \; I^{(1)}(\boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) \, .$$

Similarly, the fourth term in (4.6) can be written as

$$2 \sum_{1 \le i < k \le n} d_i d_k \; I^{(2)}(\boldsymbol{x}_i, \boldsymbol{x}_k, \boldsymbol{\psi})$$

where

$$I^{(2)}(\boldsymbol{x}_i, \boldsymbol{x}_k, \boldsymbol{\psi}) = \prod_{j=1}^{d} \int \; R(x_j^* - x_{ij} \mid \widehat{\psi}_j) R(x_j^* - x_{kj} \mid \widehat{\psi}_j) \; g_j(x_j) \; dx_j \, . \tag{4.7}$$

and $I^{(2)}$ denotes a product of integrals, each over a single variable with integrand involving *two* $R(\cdot| \; \cdot)$ terms. Finally, an estimate of v is given by

$$\begin{aligned} \widehat{v} = \Bigg(& d_0^2 + \sum_{i=1}^{n} d_i^2 \; I^{(2)}(\boldsymbol{x}_i, \boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) + 2 \; d_0 \; \sum_{i=1}^{n} d_i \; I^{(1)}(\boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) \\ & + 2 \sum_{1 \le i < k \le n} d_i d_k \; I^{(2)}(\boldsymbol{x}_i, \boldsymbol{x}_k, \widehat{\boldsymbol{\psi}}) \Bigg) - \left(d_0 + \sum_{i=1}^{n} d_i \; I^{(1)}(\boldsymbol{x}_i, \widehat{\boldsymbol{\psi}}) \right)^2 . \end{aligned} \tag{4.8}$$

The Supplementary Material shows how the terms v_j^u and v_{-j}^u in (2.16) and (2.18) can be calculated using analagous methods.

Often the one-dimensional integrals in (4.5) can be expressed more simply. For example, for the Gaussian correlation (4.3) and uniform distribution $g(\boldsymbol{x})$ over $[0,1]^d$, $I^{(1)}(\boldsymbol{x}_i, \widehat{\psi})$ is

$$\begin{aligned} \prod_{j=1}^{d} \int_0^1 R\left(x_j^* - x_{ij} | \; \widehat{\psi}_j\right) \; dx_j^* &= \prod_{j=1}^{d} \int_0^1 exp\{-\psi_j (x_j^* - x_{ij})^2\} \; dx_j^* \\ &= \prod_{j=1}^{d} \frac{\sqrt{\pi}}{\sqrt{\psi_j}} \left\{ \Phi\left(\sqrt{2\psi_j}(1 - x_{ij})\right) - \Phi\left(\sqrt{2\psi_j}(0 - x_{ij})\right) \right\} \end{aligned}$$

where $\Phi(\cdot)$ denotes the cumulative distribution function of the standard normal distribution.

5 Process-based Estimation of Global Sensitivity Indices

This section presents Bayesian and plug-in Bayesian approaches for estimating sensitivity indices in the case where the *observed* output at input site $\boldsymbol{x} \in \mathcal{X}$ can be modeled as a draw, $y(\boldsymbol{x})$, from a (smooth) Gaussian stochastic process, $Y(\boldsymbol{x})$, possibly corrupted by additive noise, say numerical. The function $y(\boldsymbol{x})$ is regarded as the *true* output. In this section the process $Y(\boldsymbol{x})$ need not be stationary but is assumed to be separable with covariance

$$Cov_p[Y(\boldsymbol{x}_i), Y(\boldsymbol{x}_k)] = \sigma^2 R(\boldsymbol{x}_i, \boldsymbol{x}_k \mid \boldsymbol{\psi}) = \sigma^2 \prod_{j=1}^{d} R(x_{ij}, x_{kj} | \; \psi_j) \tag{5.1}$$

where σ^2 is the process variance and $R(\cdot, \cdot|\ \psi_j)$ is known up to an unknown (vector of) parameter(s) ψ_j. Here, and below, $Cov_p[\cdot, \cdot]$ and $E_p[\cdot]$ denote covariance and expectation with respect to the process $Y(\boldsymbol{x})$ to distinguish them from expectations $E_g[\cdot]$ with respect $\boldsymbol{X}$. As in Section 4, this approach allows estimation of sensitivity indices from runs based on an arbitrary design.

To simplify the expressions derived below, this section makes the following additional assumptions. First, not only has the input space been scaled to be $[0, 1]^d$, but the weight function $g(\cdot)$ is uniform on $[0, 1]$. Second, we take the process $Y(\boldsymbol{x})$ to have mean

$$\boldsymbol{f}^\top(\boldsymbol{x})\boldsymbol{\beta} = E_p\left[Y(\boldsymbol{x})\right] = \sum_{k_1=0}^{m_{k_1}} \cdots \sum_{k_d=0}^{m_{k_d}} \beta_{k_1 \ldots k_d} \prod_{j=1}^{d} x_j^{k_j}. \tag{5.2}$$

As Kaufman, Bingham, Habib, Heitmann, and Frieman (2010) demonstrate, a non-constant mean is essential when using compactly supported correlations to emulate computer simulator codes efficiently for large designs; the polynomial mean (5.2) is general enough to account for a wide variety of "large scale" trends. Third, while nothing in the calculations below requires that the process be stationary, the specific correlation functions used in the sample calculations all satisfy the stationary condition

$$R(x_{ij}, x_{kj}|\ \psi_j) = R(x_{ij} - x_{kj}|\ \psi_j).$$

Finally, to allow a greater breath of applications, it is assumed that the *observed output*, $z_{sim}(\boldsymbol{x})$, from the simulator runs is the true simulator output $y(\boldsymbol{x})$ plus noise, possibly numerical. The model for $z_{sim}(\boldsymbol{x})$ is

$$Z_{sim}(\boldsymbol{x}) = Y(\boldsymbol{x}) + \epsilon_{sim}(\boldsymbol{x}), \tag{5.3}$$

where $\epsilon_{sim}(\boldsymbol{x})$ is a white noise process with mean zero and variance σ_ϵ that is independent of $Y(\boldsymbol{x})$. The term $\epsilon_{sim}(\boldsymbol{x})$ can be thought of as a means of explicitly modeling non-deterministic behaviour of the computer output or of enhancing numerical stability in the estimation of the correlation parameters. For deterministic outputs, $\epsilon_{sim}(\boldsymbol{x})$ can be set to zero in the formulae below.

Assuming that evaluations are made at inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$, the $n \times 1$ vector of observed outputs is viewed as a realization of the stochastic process

$$\boldsymbol{Z}_{sim} = (Z_{sim}(\boldsymbol{x}_1), \ldots, Z_{sim}(\boldsymbol{x}_n))^\top$$

which has mean vector $\boldsymbol{F}\boldsymbol{\beta}$ with $\boldsymbol{F} = [\boldsymbol{f}(\boldsymbol{x}_1), \ldots, \boldsymbol{f}(\boldsymbol{x}_n)]^\top$ and covariance matrix

$$\boldsymbol{\Sigma}^Z_{sim} = \sigma^2 \boldsymbol{R} + \sigma^2_\epsilon \boldsymbol{I}_n = \sigma^2 \left(\boldsymbol{R} + a\boldsymbol{I}_n\right)$$

with $a = \sigma^2_\epsilon / \sigma^2$, where the $(i,k)^{th}$ element of the $n \times n$ matrix $\boldsymbol{R}$ is $R(\boldsymbol{x}_i, \boldsymbol{x}_k; \boldsymbol{\psi})$ and $\boldsymbol{I}$ is the $n \times n$ identity matrix.

5.1 Process-based estimators of sensitivity indices

The sensitivity indices (2.13) and (2.17) are defined in terms of the true simulator output $y(\boldsymbol{x})$. Bayesian estimation of these quantities replaces $y(\cdot)$ by the process $Y(\cdot)$ in the relevant definitions resulting, for example, in the random uncorrected effect function

$$V^u_Q = Var_g \left[E_g[Y(\boldsymbol{X})|\boldsymbol{X}_Q]\right]$$

for $Q \subseteq \{1, \ldots d\}$. A Bayesian estimator of v^u_Q is the posterior mean of V^u_Q given the observed code runs $\boldsymbol{z}_{sim}$; that is,

$$\widehat{v}^u_Q = E_P \left[V^u_Q |\ \boldsymbol{Z}_{sim} = \boldsymbol{z}_{sim}\right] \ . \tag{5.4}$$

where $E_P\left[\ \cdot \mid \boldsymbol{Z}_{sim}\right]$ denotes the conditional expectation with respect to the process $Y(\cdot)$ given $\boldsymbol{Z}_{sim}$. For Gaussian process models, the joint distribution of the integrated process, V^u_Q, and $\boldsymbol{Z}_{sim}$ is multivariate normal; this allows the posterior expected value (5.4) of the integrated process given the training data to be calculated explicitly.

A formula for (5.4) is presented in the following theorem. The proof of this result is rather long and technical and the details can be found in the Supplementary Material. The expression for (5.4) assumes that *all* Gaussian Process parameters are known. In the fully Bayesian approach to estimation, priors are placed on the unknown parameters and (5.4) is averaged over draws from the posterior distribution of parameters given $\boldsymbol{Z}_{sim}$. In the empirical Bayesian approach, estimates of the unknown parameters are plugged into the (5.4) formula. The notation in Theorem 1 is given in a style that facilitates function calls in a

computer program. In particular, it uses the following notation:

$$\begin{aligned}
\mathbf{S1}_k(x;\psi) &= \int_0^1 w^k R\left(w,x;\psi\right)\ dw, \quad k=0,1,2,\ldots,\\
\mathbf{S2}(x_1,x_2;\psi) &= \int_0^1 R(w,x_1;\psi)R(w,x_2;\psi)\ dw,\\
\mathbf{D}(\psi) &= \int_0^1\int_0^1 R(w,x;\psi)\ dx\ dw,\\
\mathbf{m1}(\boldsymbol{\beta}) &= \sum_{k_1=0}^{m_{k_1}}\cdots\sum_{k_d=0}^{m_{k_d}}\beta_{k_1\ldots k_d}\prod_{j=1}^{d}\left(k_j+1\right)^{-1},\\
\mathbf{m2}(\boldsymbol{\beta}) &= \sum_{k_1,\ldots k_d}\ \sum_{k_1',\ldots k_d'}\beta_{k_1,\ldots k_d}\beta_{k_1',\ldots k_d'}\\
&\qquad\times\left[\prod_{j\notin Q}\left(k_j+1\right)\left(k_j'+1\right)\right]^{-1}\left[\prod_{\ell\in Q}\left(k_\ell+k_\ell'+1\right)\right]^{-1}.
\end{aligned}$$

Theorem 1 *Assume that the true simulator output, $y(\boldsymbol{x})$ can be modeled by a stationary Gaussian process $Y(\cdot)$ with mean and covariance function of the form (5.2) and (5.1), respectively. Also assume that the observed output $\boldsymbol{z}_{sim}$ at the training data sites, is modeled by a process $Z_{sim}(\boldsymbol{x})$ satisfying (5.3). For a fixed $Q\subseteq\{1,\ldots d\}$,*

$$\begin{aligned}
\widehat{v}_Q^u &= E_P\left\{V_Q^u|\ \boldsymbol{Z}_{sim}=\boldsymbol{z}_{sim}\right\}\\
&=\left\{\sigma_Y^2\prod_{j\notin Q}\mathbf{D}(\psi_j)-trace\left[\left(\boldsymbol{\Sigma}_{sim}^Z\right)^{-1}\boldsymbol{C}\right]\right\}\\
&\quad+\left\{\mathbf{m2}(\boldsymbol{\beta})-\mathbf{m1}^2(\boldsymbol{\beta})+2\left(\boldsymbol{v}^\top-\mathbf{m1}(\boldsymbol{\beta})\boldsymbol{q}^\top\right)\left(\boldsymbol{\Sigma}_{sim}^Z\right)^{-1}\left(\boldsymbol{z}_{sim}-\boldsymbol{F}^\top\boldsymbol{\beta}\right)\right.\\
&\quad\left.+\left(\boldsymbol{z}_{sim}-\boldsymbol{F}^\top\boldsymbol{\beta}\right)^\top\left(\boldsymbol{\Sigma}_{sim}^Z\right)^{-1}\left(\boldsymbol{C}-\boldsymbol{q}\boldsymbol{q}^\top\right)\left(\boldsymbol{\Sigma}_{sim}^Z\right)^{-1}\left(\boldsymbol{z}_{sim}-\boldsymbol{F}^\top\boldsymbol{\beta}\right)\right\}\\
&\quad-\left\{\sigma_Y^2\prod_{j=1}^{d}\mathbf{D}(\psi_j)-trace\left[\left(\boldsymbol{\Sigma}_{sim}^Z\right)^{-1}\boldsymbol{q}\boldsymbol{q}^\top\right]\right\},
\end{aligned}\tag{5.5}$$

where $\boldsymbol{q}$ is the $n\times 1$ vector with i^{th} element

$$q_i=q(\boldsymbol{x}_i,\boldsymbol{\psi})=\sigma^2\prod_{j=1}^{d}\mathbf{S1}_0(x_{ij};\psi_j),\qquad 1\le i\le n,$$

$\boldsymbol{C}$ is the $n\times n$ matrix with $(i,k)^{th}$ element

$$C_{ik}=\sigma^4\prod_{j\notin Q}\mathbf{S1}_0(x_{ij};\psi_j)\ \mathbf{S1}_0(x_{kj};\psi_j)\prod_{j\in Q}\mathbf{S2}(x_{ij},x_{kj};\psi_j),\qquad 1\le i,k\le n\ ,$$

$\boldsymbol{v}$ *is the* $n \times 1$ *vector with* i^{th} *element*

$$\boldsymbol{v}(\boldsymbol{x}_i, \boldsymbol{\beta}, \boldsymbol{\psi}, \boldsymbol{\beta}) = \left[\sigma^2 \prod_{j \notin Q} \mathbf{S1}_0\left(x_{ij}; \psi_j\right)\right] \times \sum_{k_1=0}^{m_{k_1}} \cdots \sum_{k_d=0}^{m_{k_d}} \left\{\beta_{k_1 \ldots k_d} \prod_{j \notin Q} (k_j+1)^{-1} \prod_{\ell \in Q} \mathbf{S1}_{k_\ell}(x_{h\ell}; \psi_\ell)\right\}, \qquad 1 \le i \le n,$$

Proof. The proof of Theorem 1 involves three steps: (i) the derivation of the distribution of the process $U_Q(\boldsymbol{x}_Q) \equiv E_g[Y(\boldsymbol{X})|\boldsymbol{X}_Q = \boldsymbol{x}_Q]$; (ii) the determination of the conditional distribution of $[U_Q(\boldsymbol{x}_Q)|\ \boldsymbol{Z}_{sim}]$; and (iii) obtaining an expression for $E_P\left[Var_g\left(U_Q(\boldsymbol{x}_Q)\right)|\ \boldsymbol{Z}_{sim}\right]$. The details are given in the Supplementary Material.

The estimate $\hat{v}$ of the total variance v is given by (5.5) for $Q = \{1, \ldots, d\}$. The main effect sensitivity index S_j in (2.17) for the individual input x_j is estimated by

$$\widehat{S}_j = \widehat{v}_j^u / \widehat{v} \tag{5.6}$$

where $\widehat{v}_j^u$ is obtained from (5.5) with $Q = \{j\}$. The total effect sensitivity index is estimated by

$$\widehat{T}_j = (\widehat{v} - \widehat{v}_{-j}^u)/\widehat{v}, \tag{5.7}$$

where $\widehat{v}_{-j}^u$ is obtained from (5.5) with $Q = \{1, \ldots, i-1, i+1, \ldots, d\}$.

Given the model parameters, all components of $\widehat{v}_Q^u$ are specified above except the integrals $\mathbf{S1}_k$, $\mathbf{D}$, $\mathbf{S2}$, which depend on the user-selected correlation function $R(\cdot, \cdot|\ \psi)$. Formulas for these integrals are stated next for the Gaussian and Bohman correlation functions and, in the Supplementary Material, for the cubic correlation function $R(w, x|\ \psi) = R_C(w - x|\ \psi)$ for $\psi > 0$ where

$$R_C(h|\ \psi) = \begin{cases} 1 - 6\left(\frac{h}{\psi}\right)^2 + 6\left(\frac{|h|}{\psi}\right)^3, & |h| < \frac{\psi}{2}; \\ 2\left(1 - \frac{|h|}{\psi}\right)^3, & \frac{\psi}{2} \le |h| < \psi; \\ 0, & \psi \le |h|\ . \end{cases}$$

5.2 Formulae for the Gaussian correlation function

For the Gaussian correlation function, $R(w,x|\ \psi) = R_G(w-x|\ \psi)$ where

$$R_G(h|\ \psi) = \exp\left[-\psi h^2\right],$$

where $\psi > 0$. A formula for $\mathbf{S1}_k$ can be derived using results of Dhrymes (2005) for the moments of a truncated normal random variable. Application of this result gives

$$\begin{aligned}\mathbf{S1}_k(x;\psi) &= \int_0^1 w^k \exp[-\psi(w-x)^2]\ dw \\ &= \sqrt{\frac{\pi}{\psi}}\left\{\Phi\left(\sqrt{2\psi}(1-x)\right)\sum_{r=0}^{k}\binom{k}{r}x^{k-r}(2\psi)^{-r/2}I_r^{h_1}\right. \\ &\quad \left. - \Phi\left(-x\sqrt{2\psi}\right)\sum_{r=0}^{k}\binom{k}{r}\eta^{k-r}(2\psi)^{-r/2}I_r^{h_0}\right\} \qquad (5.8)\end{aligned}$$

where $h_0 = -x\sqrt{2\psi}$ and $h_1 = (1-x)\sqrt{2\psi}$, while I_r^h is defined recursively by $I_0^h = 1$, $I_1^h = -\phi(h)/\Phi(h)$, and for $r \in \{2,3,4,\ldots\}$ by

$$I_r^h = \frac{1}{\Phi(h)}\left[-h^{r-1}\phi(h) + (r-1)I_{r-2}^h\right], \qquad (5.9)$$

where $\phi(\cdot)$ denotes the probability density function (pdf) of the standard normal distribution. In particular, $\mathbf{S1}_0(x;\psi)$ becomes

$$\begin{aligned}\mathbf{S1}_0(x;\psi) &= \int_0^1 \exp\left[-\psi(w-x)^2\right]\ dw \\ &= \sqrt{\frac{\pi}{\psi}}\left[\Phi\left(\sqrt{2\psi}(1.0-x)\right) - \Phi\left(-x\sqrt{2\psi}\right)\right].\end{aligned}$$

Formulae for **S2** and **D** are

$$\begin{aligned}\mathbf{S2}(x_1,x_2;\psi) &= \int_0^1 \exp[-\psi(w-x_1)^2]\exp[-\psi(w-x_2)^2]\ dw \\ &= \exp\left[-\frac{1}{2}\psi(x_1-x_2)^2\right]\mathbf{S1}_0\left(\frac{x_1+x_2}{2};2\psi\right),\end{aligned}$$

$$\begin{aligned}\mathbf{D}(\psi) &= \int_0^1\int_0^1 \exp\left[-\psi(w-x)^2\right]\ dx\ dw \\ &= \frac{1}{\psi}\left[\sqrt{2\pi}\phi\left(\sqrt{2\psi}\right) - 1\right] + \sqrt{\frac{\pi}{\psi}}\left[2\Phi\left(\sqrt{2\psi}\right) - 1\right].\end{aligned}$$

5.3 Formulae using the Bohman correlation function

For the Bohman correlation function, $R(w,x|\ \psi) = R_B(w-x|\ \psi)$ where

$$R_B(h|\ \psi) = \begin{cases} \left(1-\frac{|h|}{\psi}\right)\cos\left(\frac{\pi|h|}{\psi}\right) + \frac{1}{\pi}\sin\left(\frac{\pi|h|}{\psi}\right), & |h| < \psi; \\ 0, & |h| \geq \psi \end{cases}$$

with $\psi > 0$. The integrals $\mathbf{S1}_0$, $\mathbf{S1}_k$, $\mathbf{S2}$, and $\mathbf{D}$ are as follows. Letting $l^* = l^*(x) = \min(\pi, x\pi/\psi)$ and $u^* = u^*(x) = \min(\pi, (1.0-x)\,\pi/\psi)$,

$$\begin{aligned} \mathbf{S1}_0(x;\psi) = & \frac{1}{u-l}\left\{\frac{4\psi}{\pi^2} - \frac{2\psi}{\pi^2}\cos(l^*(x)) - \frac{2\psi}{\pi^2}\cos(u^*(x))\right. \\ & \left. + \left\{\left(\frac{\psi}{\pi} - \frac{\psi\ l^*(x)}{\pi^2}\right)\sin(l^*(x)) + \left(\frac{\psi}{\pi} - \frac{\psi\ u^*(x)}{\pi^2}\right)\sin(u^*(x))\right\}\ . \end{aligned}$$

For the integral $\mathbf{S1}_k(x;\psi)$, let $l^* = \max(0, x-\psi)$ and $u^* = \min(1, x+\psi)$, then

$$\begin{aligned} \mathbf{S1}_k(x;\psi) &= \int_0^1 w^k R\,(w,x,;\psi)\ dw \\ &= \int_{l^*}^{x} w^k \left\{\left(1-\frac{x-w}{\psi}\right)\cos\left(\frac{\pi(x-w)}{\psi}\right) + \frac{1}{\pi}\sin\left(\frac{\pi(x-w)}{\psi}\right)\right\}\ dw \\ &\quad + \int_{x}^{u^*} w^k \left\{\left(1-\frac{w-x}{\psi}\right)\cos\left(\frac{\pi(w-x)}{\psi}\right) + \frac{1}{\pi}\sin\left(\frac{\pi(w-x)}{\psi}\right)\right\}\ dw \\ &= \mathbf{T}\,(x,-1,l^*,\eta) + \mathbf{T}\,(-x,+1,\eta,u^*)\,,\ \text{say}, \end{aligned}$$

where

$$
\begin{aligned}
\mathbf{T}\left(d,s,a,b\right) = & \int_a^b w^k \left\{ \left(1-\frac{d+sw}{\psi}\right)\cos\left(\frac{\pi(d+sw)}{\psi}\right) + \frac{1}{\pi}\sin\left(\frac{\pi(d+sw)}{\psi}\right)\right\}\, dw \\
= & \left(1-\frac{d}{\psi}\right)\cos\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+1}\mathbf{P1}\left(k,a',b'\right) \\
& -\left(1-\frac{d}{\psi}\right)\sin\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+1}\mathbf{P2}\left(k,a',b'\right) \\
& -\frac{s}{\psi}\cos\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+2}\mathbf{P1}\left(k+1,a',b'\right) \\
& +\frac{s}{\psi}\sin\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+2}\mathbf{P2}\left(k+1,a',b'\right) \\
& +\frac{1}{\pi}\sin\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+1}\mathbf{P1}\left(k,a',b'\right) \\
& +\frac{1}{\pi}\cos\left(\frac{d\pi}{\psi}\right)\left(\frac{\psi}{\pi s}\right)^{k+1}\mathbf{P2}\left(k,a',b'\right),
\end{aligned}
$$

after additional algebra, where $a' = sa\pi/\psi$, $a', b' = sb\pi/\psi$ and **P1** and **P2** are defined recursively as

$$
\begin{aligned}
& \mathbf{P1}\left(k,a',b'\right) \\
= & \begin{cases} \sin\left(b'\right) - \sin\left(a'\right), & k=0; \\ \left(b'\right)^k \sin\left(b'\right) - \left(a'\right)^k \sin\left(a'\right) - k\ \mathbf{P2}\left(k-1,a',b'\right), & k \geq 1, \end{cases}
\end{aligned}
$$

and

$$
\begin{aligned}
& \mathbf{P2}\left(k,a',b'\right) \\
= & \begin{cases} \cos\left(a'\right) - \cos\left(b'\right), & k=0; \\ \left(a'\right)^k \cos\left(a'\right) - \left(b'\right)^k \cos\left(b'\right) + k\ \mathbf{P1}\left(k-1,a',b'\right), & k \geq 1. \end{cases}
\end{aligned}
$$

The integral for $\mathbf{D}(\psi)$ is defined piecewise by

$$
\mathbf{D}(\psi) = \begin{cases} \frac{4\psi}{\pi^2} + \frac{2\psi^2}{\pi^2} - \frac{4\psi}{\pi^2}\left(\psi - 1.0\right), & 0 < \psi < 1.0 \\ \frac{4\psi}{\pi^2} + \frac{2\psi^2}{\pi^2}\left\{1 + \left(\frac{1.0-\psi}{\psi}\right)\cos\left(\frac{\pi}{\psi}\right) - \frac{3}{\pi}\sin\left(\frac{\pi}{\psi}\right)\right\}, & 1.0 \leq \psi. \end{cases}
$$

To calcuate the integral $\mathbf{S2}(x_1, x_2; \psi)$, the w regions of $[0,1]$ for which $R(w,x_1;\psi)R(w,x_2;\psi) \neq 0$ must be identified. These regions will depend on the relationship between $|x_1 - x_2|$ and ψ.

The following formulae assume, without loss of generality, that $x_1 < x_2$. There are different expressions for **S2** depending on whether $2\psi \leq |x_1 - x_2|$, $\psi \leq |x_1 - x_2| < 2\psi$, or $|x_1 - x_2| < \psi$. In the Supplementary Material, these integrals are simplified and shown to be as follows.

Case 1: For (x_1, x_2) satisfying $|x_1 - x_2| \geq 2\psi$, $R(w, x_1; \psi)R(w, x_2; \psi) = 0$ for all $w \in [0, 1]$; hence

$$\mathbf{S2}(x_1, x_2; \psi) = 0 \ .$$

Case 2: For (x_1, x_2) satisfying $\psi \leq |x_1 - x_2| < 2\psi$,

$$\begin{aligned}\mathbf{S2}(x_1, x_2; \psi) = &\int_{x_2-\psi}^{x_1+\psi} \left\{ \left(1 - \frac{w - x_1}{\psi}\right) \cos\left(\frac{\pi(w - x_1)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(w - x_1)}{\psi}\right) \right\} \\ &\times \left\{ \left(1 - \frac{(x_2 - w)}{\psi}\right) \cos\left(\frac{\pi(x_2 - w)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(x_2 - w)}{\psi}\right) \right\} \, dw \, .\end{aligned}$$

Case 3: For (x_1, x_2) satisfying $|x_1 - x_2| < \psi$, first let $l^* = \max(0, x_1 - \psi)$ and $u^* = \min(1, x_2 + \psi)$, then

$$\begin{aligned}\mathbf{S2}(x_1, x_2; \psi) = &\int_{l^*}^{x_1} \left\{ \left(1 - \frac{x_1 - w}{\psi}\right) \cos\left(\frac{\pi(x_1 - w)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(x_1 - w)}{\psi}\right) \right\} \\ &\times \left\{ \left(1 - \frac{(x_2 - w)}{\psi}\right) \cos\left(\frac{\pi(x_2 - w)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(x_2 - w)}{\psi}\right) \right\} \, dw \\ &+ \int_{x_1}^{x_2} \left\{ \left(1 - \frac{x - x_1}{\psi}\right) \cos\left(\frac{\pi(w - x_1)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(w - x_1)}{\psi}\right) \right\} \\ &\times \left\{ \left(1 - \frac{(x_2 - w)}{\psi}\right) \cos\left(\frac{\pi(x_2 - w)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(x_2 - w)}{\psi}\right) \right\} \, dw \\ &+ \int_{x_2}^{u^*} \left\{ \left(1 - \frac{w - x_1}{\psi}\right) \cos\left(\frac{\pi(w - x_1)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(w - x_1)}{\psi}\right) \right\} \\ &\times \left\{ \left(1 - \frac{w - x_2}{\psi}\right) \cos\left(\frac{\pi(w - x_2)}{\psi}\right) + \frac{1}{\pi} \sin\left(\frac{\pi(w - x_2)}{\psi}\right) \right\} \, dw \ .\end{aligned}$$

Table 6.1
Parameters, true main effect and total effect sensitivity indices for the Sobol-Levitan function (6.1).

j	1	2	3	4	5	6	7	8
b_j	3.2797	2.6467	2.0606	1.5258	1.0476	0.6340	0.2973	0.0638
S_j	0.2003	0.1370	0.0863	0.0487	0.0234	0.0087	0.0019	0.0001
T_j	0.5477	0.4342	0.3136	0.1985	0.1039	0.0406	0.0092	0.0004

6 An Example

To compare the results of applying the sensitivity analysis estimation methods described in Sections 3-5, we use a scaled version of function introduced in Sobol and Levitan (1999):

$$y(x_1, \ldots, x_d) = \exp\left(\sum_{j=1}^{d} b_j x_j\right) - I_d\,, \tag{6.1}$$

where $I_d = \prod_{j=1}^{d} \frac{e^{b_j}-1}{b_j}$. The theoretical main effect and total effect sensitivity indices are known for $y(\boldsymbol{x})$ (and are the same for any scaled version of $y(\boldsymbol{x})$). In particular, we used $d = 8$ inputs and a $\boldsymbol{b}$ vector that resulted in the $\{S_j\}_{j=1}^{d}$ and $\{T_j\}_{j=1}^{d}$ values shown in Table 6.1 for the Sobol/Levitan function scaled to have variance 100. This function has substantial interactions because the total of the main effect sensitivity indices is only 50% of the total $y(\boldsymbol{x})$ variance. A total of 64 function runs were used to estimate the sensitivity indices for each of the three estimation methods (permuted column sampling, quadrature-based, and plug-in Bayesian).

The permuted column sampling method was implemented using the permutations specified by the OA(64,9,8,2) design (from the website: *http://www.research.att.com/~njas/oadir*) applied to the maximin Latin Hypercube base design, $\boldsymbol{M}$, (*http://www.spacefillingdesigns.nl/*) scaled to their midpoints. Both the quadrature-based and plug-in Bayesian estimates of the main effect and total effect sensitivity indices were based on the 64 outputs of the Sobol-Levitan function evaluated at the rows of the 64×8 maximin design obtained from *http://www.spacefillingdesigns.nl/* and scaled to include endpoints; the minimum interpoint distance of this design is 0.9039. The quadrature-based estimates were computed using JMP software (JMP 2011) and the plug-in Bayesian estimators were computed using a MATLAB program written by the first author.

Table 6.2
Estimates and errors of the *main effect* sensitivity indices of the Sobol-Levitan function (6.1) with $\boldsymbol{b}$ listed in Table 6.1 based on $n = 64$ code runs using (1) Permuted column sampling (PermS); (2) quadrature-based estimation (Quad), and (3) plug-in (empirical) Bayesian Estimation (EmpB)

S_j	0.2003	0.1370	0.0863	0.0487	0.0234	0.0087	0.0019	0.0001
$\widehat{S}_j^{PermS}$	0.1118	0.1002	0.0514	0.0662	0.0047	0.0340	0.0385	0.0044
$\lvert\widehat{S}_j^{PermS} - S_j\rvert$	0.0885	0.0368	0.0349	0.0175	0.0187	0.0253	0.0366	0.0043
$\widehat{S}_j^{Quad}$	0.2528	0.2045	0.1098	0.0518	0.0206	0.0153	0.0070	0.0026
$\lvert\widehat{S}_j^{Quad} - S_j\rvert$	0.0525	0.0675	0.0235	0.0031	0.0028	0.0066	0.0051	0.0025
$\widehat{S}_j^{EmpB}$	0.2477	0.2004	0.1076	0.0510	0.0202	0.0153	0.0070	0.0026
$\lvert\widehat{S}_j^{EmpB} - S_j\rvert$	0.0474	0.0634	0.0213	0.0023	0.0032	0.0066	0.0051	0.0025

The estimates for the three methods are listed in Table 6.2, together with the absolute error of estimation. The quadrature and plug-in Bayesian estimators provide comparable estimates of all main effect sensitivity indices with respect to the absolute error of estimation. For all but S_2, the quadrature and plug-in estimators have smaller absolute error than the permuted column sampling estimator, and appear to be preferable methods.

Comparing these two methods further, we see in Table 6.3 that, for inputs with large total effect, i.e., those with $T_j > .10$, the plug-in Bayesian estimator has slightly smaller absolute error than the quadrature-based estimator, and also provides a slightly better estimator of the differences between the total and main effect sensitvity indices which are used to gauge the extent of the interaction.

We increased the number of runs to 81, using the orthogonal array $OA(81, 10, 9, 2)$ from the website above for the permuted column sampling. All methods provided better estimates, but the relative performance remained the same. Consequently, it appears that, on the whole, the Bayesian methodology preforms slightly better than the other two methods for estimation of main effect and total effect sensitivity indices.

Table 6.3
Estimates and errors of the *total* sensitivity indices of the Sobol-Levitan function (6.1) with $\boldsymbol{b}$ listed in Table 6.1 based on $n = 64$ code runs using quadrature-based estimation (Quad) and Empirical Bayesian Estimation (EmpB)

T_j	0.5477	0.4342	0.3136	0.1985	0.1039	0.0406	0.0092	0.0004
$\widehat{T}_j^{Quad}$	0.4744	0.4000	0.1971	0.1187	0.0379	0.03861	0.01199	0.0040
$\lvert\widehat{T}_j^{Quad} - T_j\rvert$	0.0733	0.0342	0.1165	0.0798	0.0660	0.0020	0.0028	0.0036
$\widehat{T}_j^{EmpB}$	0.4998	0.4262	0.2162	0.1329	0.0425	0.0474	0.0145	0.0049
$\lvert\widehat{T}_j^{EmpB} - T_j\rvert$	0.0479	0.0080	0.0974	0.0656	0.0614	0.0068	0.0053	0.0045

7 Summary and discussion

This paper reviews several experimental designs that have been proposed to allow the estimation of local and global sensitivity indices. It provides an overview of quadrature-based, empirical Bayesian, and permuted column moment-based estimators of global sensitivity indices. It introduces the detailed formulas required to compute plug-in Bayesian estimators of global sensitivity indices, which form the basis for fully Bayesian sensitivity index estimation for a broad class of regression plus stationary Gaussian process models using the Gaussian, cubic, or Bohman correlation functions.

It has been mentioned earlier that one motivation for using compactly supported correlation functions is that they can yield zero correlation; having a significant fraction of zero entries in the correlation matrix can make its inversion numerically more stable (see Barry and Pace (1997) and, in MATLAB, Gilbert, Moler, and Schreiber (1991)) and allows the inversion of larger training data sets. Kaufman et al. (2010) demonstrate that by use of a suitably rich regression mean with such a sparse correlation matrix, the predictive ability of the stochastic model is comparable to that prediction based on a model with Gaussian correlation function.

Kaufman et al. (2010) proposed using a compactly supported correlation function with parameters restricted to a portion of the parameter space that guarantees that at least a certain proportion of the correlation matrix values are zero. They suggest maximizing the likelihood

over the restricted parameter space

$$\Omega(K) = \left\{ \boldsymbol{\psi} \in \mathbb{R}^d \,:\, \psi_j \geq 0 \;\forall\; j \in \{1, \ldots, d\};\;\; \sum_{j=1}^{d} \psi_j \leq K \right\}, \tag{7.1}$$

where $K > 0$ is chosen so that at least a given proportion α of the $n(n-1)/2$ off diagonal elements of $\boldsymbol{\Sigma}^Z_{sim}$ are zero.

One method of selecting K to force at least a proportion α of zeroes among the off-diagonal elements of $\boldsymbol{\Sigma}^Z_{sim}$ is as follows. Calculate $d^1_{i,k} \equiv \sum_{j=1}^{d} |x_{ij} - x_{kj}|$ for each of the ${}^nC_2$ pairs $(\boldsymbol{x}_i, \boldsymbol{x}_k)$ with $1 \leq i < k \leq n$. Then, set K to be the $\lfloor {}^nC_2 \times \alpha \rfloor^{th}$ smallest value among the $d^1_{i,k}$'s where $\lfloor \cdot \rfloor$ denotes the integer part of ${}^nC_2 \times \alpha$. It follows that, for any $\boldsymbol{\psi} \in \Omega$, at most $\alpha 100\%$ of the off-diagonal elements of $\boldsymbol{\Sigma}^Z_{sim}$ are nonzero. To see that this is true for the Bohman and cubic correlation functions, first note that $R(\boldsymbol{x}_i, \boldsymbol{x}_k|\psi_j) = 0$ for either as long as $|x_{ij} - x_{kj}| \geq \psi_j$ for some $j \in \{1, \ldots d\}$. Now select any $(\boldsymbol{x}_i, \boldsymbol{x}_k)$ with $d^1_{i,k} \geq K$; there are at least $(1-\alpha) \times 100\%$ of these pairs among the $\binom{n}{2}$ pairings of rows. We show that

$$\prod_{j=1}^{d} R(x_{ij}, x_{kj}|\psi_j) = 0 \tag{7.2}$$

for any $\boldsymbol{\psi} \in \Omega(K)$ as follows. If the correlation in (7.2) is, instead, positive, then $|x_{ij} - x_{kj}| < \psi_j$ for all $j \in \{1, \ldots d\}$. Hence $d^1_{ik} \equiv \sum_{j=1}^{d} |x_{ij} - x_{kj}| < \sum_{j=1}^{d} \psi_j \leq K$ where the last inequality holds because $\boldsymbol{\psi} \in \Omega$. But this contradicts the assumption that $d^1_{i,k} \geq C$ and hence $|x_{ij} - x_{kj}| \geq \psi_j$ for some j and hence (7.2) holds.

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