



Estimating Sobol sensitivity indices using correlations

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ABSTRACT

Sensitivity analysis is a crucial tool in the development and evaluation of complex mathematical models. Sobol's method is a variance-based global sensitivity analysis technique that has been applied to computational models to assess the relative importance of input parameters on the output. This paper introduces new notation that describes the Sobol indices in terms of the Pearson correlation of outputs from pairs of runs, and introduces correction terms to remove some of the spurious correlation. A variety of estimation techniques are compared for accuracy and precision using the *G* function as a test case.

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1. Introduction

Sobol's method is a global sensitivity analysis (SA) technique which determines the contribution of each input (or group of inputs) to the variance of the output. The usual Sobol sensitivity indices include the main and total effects for each input, but the method can also provide specific interaction terms, if desired. Sobol's method was originally presented in Russian by Sobol' (1990); the article was reprinted in English in Sobol', (1993). The method is notable because it works well without simplifying approximations, even for models with very large numbers of random variables. The method is superior to traditional sensitivity methods (such as local methods that examine parameters one at a time) when considering cases where the assumption of linearity is invalid (Saltelli and Annoni, 2010), and has been shown to be robust (Yang, 2011). Sobol's method has been applied successfully to complex environmental models to identify critical input parameters and major sources of uncertainty (e.g., Nossent et al., 2011; Vezzaro and Mikkelsen, 2012; Confalonieri et al., 2010; Estrada and Diaz, 2010). In addition, the method has been used as a basis for multiple criteria analyses (Annoni et al., 2011).

In this paper, new formulations of Sobol indices in terms of Pearson correlation coefficients are presented. These formulations suggest the inclusion of “correction terms” that remove some

spurious correlation. Such correction terms are presented, and multiple estimation methods are compared for precision, accuracy, and efficiency, using the *G* function as a test case. The *G* function has the advantage that the theoretical values for all the sensitivity indices are known, so the accuracy of various estimation techniques can be evaluated.

2. Theory

2.1. Variance decomposition, main effects, total effects, and interaction terms

Many SA methods are based on an analysis of the variance of the model output (Chan et al., 2000); the theoretical basis of several of these methods is variance decomposition. Such techniques include Fourier Amplitude Sensitivity Test (FAST; Cukier et al., 1973, 1978; Saltelli et al., 1999), High Dimensional Model Representation (HDMR; Rabitz and Alis, 1999), random balance designs (Tarantola et al., 2006a), and traditional ANOVA methods. In variance decomposition, the model output variance is represented as a sum of $(2^J - 1)$ partial variances. Here, *J* is the number of random samples needed per model iteration. While *J* is often called “the number of inputs”, this is not necessarily the same as the number of modeling input variables, because some models (typically ones with either spatial or temporal variation) may draw multiple samples for the same modeling variable on each iteration.

The Sobol sensitivity indices are ratios of partial variances to total variance, and for independent variables satisfy the relationship

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$$1 = \sum_i S_i + \sum_i \sum_{j>i} S_{ij} + \sum_i \sum_{j>i} \sum_{k>j} S_{ijk} + \dots \quad (1)$$

None of the sensitivity indices in (1) may be negative; therefore none may exceed one. For any input j , S_j is called its *first-order* or *main effect sensitivity index*. S_j represents the sensitivity of the output to changes in input j alone. Indices in (1) with multiple subscripts are called *interaction terms*. Subscript order is not relevant for interaction terms, so by convention numerical order is used. Methods for evaluating specific interaction terms are discussed later.

The *total effect index* T_j for a given input j is defined as the sum of all terms in (1) that contain the subscript j . The total effect places an upper bound on the importance of a given input by crediting the full effect of all relevant interactions to the given input. For any input j , $T_j \geq S_j$ since the interaction terms may not be negative. As shown below, any total effect may be easily calculated without having to evaluate the interaction terms separately, which becomes crucial when J is large. Total effects may also be defined for multiple inputs: T_{jk} is the sum of all terms in (1) that contain either j or k (or both) as subscripts.

Total effects were discussed by Homma and Saltelli (1996), who used the symbol S_{Tj} , while Saltelli (2002) used S_j^T . The symbol T_j used here is equivalent but orthographically simpler. The sum of S_j over all inputs j cannot exceed one, and does not equal one unless all the interaction terms are zero. By contrast, the sum of T_j over all j is never less than one, and equals one only if all interaction terms are zero, because this sum includes every main effect once and every interaction term multiple times.

The number of sensitivity indices quickly becomes unmanageable as the number of inputs increases, a phenomenon called the *dimensionality curse*. For example, even with $J = 50$ there are too many indices (more than 10^{15}) for practical evaluation. Many models easily exceed this number, especially if each iteration requires spatial or temporal vectors of random samples for a given modeling variable. For example, Sobol analysis has been coded into the U.S. Environmental Protection Agency's SHEDS-Multimedia stochastic human exposure model (Isaacs et al., 2010; Glen et al., 2010), hereafter called "SHEDS". In SHEDS, one iteration produces a time series of exposure for one simulated person. There are roughly 100 modeling input variables but around 45,000 random samples per iteration are required, due to the many time series vectors. From a practical standpoint, use of the variance decomposition requires either dropping most of the terms, or else grouping them to permit the collective evaluation of whole groups rather than single inputs. Dropping terms without evaluating them may be dangerous, as it is unknown whether they are truly small enough to neglect. Sobol's method does not drop terms but can reduce the number of terms to be evaluated using grouping of inputs (see next section). Grouping does not modify either the model or the independence of its inputs in any way, and may be applied to terms of any size.

2.2. Groups of inputs, classes, and collective sensitivity indices

An extremely important result from Sobol' (1990) is that the same method applies when the subscripts in (1) represent groups of inputs. The analyst may arbitrarily partition the inputs into a set of disjoint groups, and Equation (1) remains valid as long as the groups are independent. Inputs in the same group do not need to be independent. Grouping limits the number of model runs that are necessary by only assessing the combined influence of all inputs in each group. Groups may contain any number of inputs without restriction. One group could have a single input while another has thousands, which is common in SHEDS. From this point on grouping is assumed, and the symbols S_j and T_j are taken to represent the main and total effects for a group j .

Sobol' (1990) also introduced a second level of grouping, in which each user-specified input group is assigned to one of two *classes* in each model run. Each class k has a collective sensitivity index C_k , equal to the sum of all sensitivity indices in (1) with subscripts belonging entirely to k . The most useful class division is to assign one group j to one class (with $C_j = S_j$), and all other input groups to the $-j$ class. The collective index C_{-j} equals the sum of all terms in (1) that do not contain j . Since every term in (1) is either in T_j or C_{-j} (but not both), then for any group j ,

$$T_j + C_{-j} = 1 \quad (2)$$

This leads directly to Theorem 2, below. In the limit of large N , C_j and C_{-j} are simply the Pearson correlation coefficients between the output vectors from pairs of model runs, as noted previously by Sobol' (1996), Sobol' and Levitan (1999). These results are summarized as:

Theorem 1. For any input group j , the main effect S_j equals the expectation value of the correlation coefficient C_j of the output vectors from two model runs in which the realizations of all inputs in j are common to both runs, while all other inputs use independent samples in the two runs.

Theorem 2. For any input group j , the total effect T_j equals one minus the expectation value of the correlation coefficient C_{-j} of the output from two model runs which use independently sampled values for inputs in j , but use the same realizations in both runs for all other inputs.

These theorems form the basis for numerically estimating all the sensitivity indices for the J input groups. Specifically, by systematically varying the classes so that each input group j is isolated in turn, a relatively small set of model runs provide all C_j and C_{-j} , and thus all the main and total effects. The details are given in the next section.

2.3. Practical methods for evaluating the sensitivity indices

For simple enough models, the sensitivity indices may be derived analytically by integrating the output function over selected input axes. But for most models it is necessary to numerically estimate the indices, and explicit formulas were refined over a series of papers. Sobol' (1990) stopped after presenting the equivalent of Theorem 1. Saltelli et al. (1993) gave a formula for the main effects only. Homma and Saltelli (1996) introduced total effects. Saltelli (2002) offered an approach for obtaining double estimates of all main and total effect indices, as well as all the second-order indices. Tarantola et al. (2006b), and Lilburne and Tarantola (2009), presented formulas that average eight estimates for each S_j and four estimates for each T_j . Sobol' et al. (2007) provided a theoretical justification for using the cross product $\sum f_0 f'_0$ for the square of the mean when calculating variances and covariances. Saltelli et al. (2010) concluded that Jansen's formula (Jansen, 1999) was best for estimating total effects.

In the following discussion, capitalized symbols represent properties of the model itself, while numerical estimates of these quantities are represented by corresponding lower-case letters (which includes ρ). Equations relating capitalized quantities are exact relationships between properties, while equations relating lower-case letters may be seen as definitions. This paper explicitly uses correlations to estimate the sensitivity indices, which are more straightforward than the integral-based formula presented in the above papers. Without requiring additional model runs, certain methods include correction terms for spurious correlation, which improve the estimates.

The numerical estimation methods examined here all use variations of the following scheme of Sobol' (1990). First, randomly generate two sets of N sample values (or realizations) for each input variable. Here, these are called the *unprimed* and *primed* sets (or u_j and u'_j) due to the symbolism used for them, although the names

sample and resample are more common in the literature. The symbol u emphasizes that these are random samples from a unit uniform or $U(0,1)$ distribution. Random samples are used here, although Sobol' (1994, 2001) has suggested using quasi-random samples that are more regularly distributed than true random numbers.

All first-order main and total effects can be evaluated using a set of $J + 2$ different model runs. Each run consists of N iterations (with N selected by the analyst); higher N gives estimates with less error but take more computational time to produce. One of these runs uses u_j for all groups, while another uses u'_j for all groups. For the remaining J runs, class j uses the u'_j samples while class $-j$ uses the u_j samples, where j loops over the J variable groups. However, double (and thus more accurate) estimates can be calculated by using $2J + 2$ runs (Saltelli, 2002). These require another J runs in which class j uses the u_j samples while the $-j$ class uses the u'_j samples. This design is called "radial sampling" in Saltelli et al. (2010), where it is preferred to the "winding stairs" design. Furthermore, the choice of just two base sets of random samples (the primed and unprimed), instead of more, is also recommended by Saltelli et al. (2010).

Let f symbolize the vector of model output (containing one element per iteration) from a given run. Indicate the samples used for the $-j$ class by the presence or absence of a prime. Use a subscript to indicate which group j forms the other class. When class j is empty, use a subscript zero for clarity. As examples, f_j is the output from the run that used u'_j for input group j and u_j for all other variables, and f'_0 is the output from the run using u'_j for all inputs. A second subscript may be added to indicate a specific iteration number (as in f_{jn}), if needed. The set of vectors (f_0, f'_0, f_j, f'_j) , with j running over all J groups, captures the full output from all $2J + 2$ model runs.

The Pearson correlation coefficient between the pair of vectors f'_j and f_k may be defined as

$$\rho''_{jk} = \left(\frac{1}{N} \right) \sum_{n=1}^N \frac{(f'_{jn} - m'_j)(f_{kn} - m'_k)}{\sqrt{v'_j v'_k}} \quad (3)$$

Here m and v represent the mean and variance of the output vectors, respectively. Various estimates of the mean and variance may be used in place of the ones above, and the divisor N is usually replaced by $(N - 1)$ when the mean and variance are estimated from the same data. Several of these alternatives are examined in the Methods and Results sections. By varying the choice of output vectors, such correlations may be generated for all pairs of model runs. In this notation, the first superscript and subscript pair on ρ apply to one model run, while the second pair apply to the other run. Correlation does not depend on run order, so for clarity, list the primed run first (for example, ρ'_{kj} in preference to ρ'_{jk}) when both types are present.

An alternative to using Equation (3) directly is to first define a set g of standardized model output vectors:

$$g_{jn} = (f_{jn} - m_j) / \sqrt{v_j} \quad (4)$$

Use the uncorrected variance, so each g vector has mean zero and sum of squares equal to N . With this notation the correlation coefficients take on a simple form. For example:

$$\rho'_{jk} = \sum g'_j g_k / N \quad (5)$$

The summation is over the model iterations, from $n = 1$ to N , which will usually be suppressed to avoid clutter. In (4), each run is standardized independently, using just its own results. When using (3), the results may be pooled across runs to obtain better estimates of the true mean and variance, variations of which are tested in the Methods and Results sections, below.

By Theorem 1, both ρ'_{j0} and ρ'_{0j} are estimates of S_j . While these are not fully independent, the mean of the two provides a better estimate than either one alone. Hence, given the full set of $2J + 2$ runs, an improved estimate of S_j is

$$S_j = C_j \cong (\rho'_{j0} + \rho'_{0j}) / 2 = \frac{1}{2N} \sum (g'_j g_0 + g'_0 g_j) \quad (6)$$

Here the symbol " \cong " means "may be approximated by" and is used when an exact property of the model is being estimated. While (6) uses the standardized forms, these may be replaced by the "raw" forms of Equation (3), as in Saltelli (2002). The total effects require estimates for C_{-j} , for which there are two such pairs: g_0 with g_j , and g'_0 with g'_j ,

$$T_j = 1 - C_{-j} \cong 1 - (\rho_{j0} + \rho''_{0j}) / 2 = 1 - \frac{1}{2N} \sum (g_j g_0 + g'_0 g'_j) \quad (7)$$

Even better performance may be obtained by adding correction terms to these formulas, as discussed in the next section.

2.4. Spurious correlation and new correction terms

Two vectors of length N of independent random samples have an expected correlation of zero, but in practice may have some small *spurious* correlation. For all inputs, the u_j and u'_j vectors are sampled from $U(0,1)$ and the distribution of spurious correlation has mean zero and variance of $(N - 1)^{-1}$. Two model runs with spurious correlation in their input vectors will also have some in their output vectors, producing errors in the estimates of the sensitivity indices (since these are based on measured output correlations). This can be reduced to any desired level by making N sufficiently large, but at a computational burden. Generally, one wants the best available estimates of the sensitivity indices obtainable with a given number of model evaluations.

Consider the sample correlation $p_0 = \rho'_{00}$ between the outputs from the "all primed" run and the "all unprimed" run. This correlation is entirely spurious, but these runs use almost the same input realizations as those used to determine ρ'_{j0} ; only the samples for input j are different in one run, and there are no differences in the other run. Unless input j dominates the model, most of the spurious correlation ρ'_{00} will be shared with ρ'_{j0} . Another all-spurious correlation with similar properties is ρ'_{jj} . Define a vector p_j as

$$p_j = (\rho'_{00} + \rho'_{jj}) / 2 = \frac{1}{2N} \sum (g'_0 g_0 + g'_j g_j) \quad (8)$$

The expectation value of p_j is zero, but any realization will generally be non-zero. Another possible estimate of the index S_j is

$$S_j \cong c_j - p_j = \frac{1}{2N} \sum (g'_j g_0 + g'_0 g_j - g'_0 g_0 - g'_j g_j) \quad (9)$$

As shown below, formula (9) is better than formula (6) when $t_j < 1/2$ (or equivalently, $c_{-j} > 1/2$), whereas formula (6) is better otherwise. The corresponding formula for the total effects is

$$T_j \cong 1 - c_{-j} + p_j = 1 - \frac{1}{2N} \sum (g_j g_0 + g'_0 g'_j - g'_0 g_0 - g'_j g_j) \quad (10)$$

This formula improves on Equation (7) whenever $c_j > 1/2$. While it is possible to switch from one form to the other abruptly at one-half, another option is a smooth transition, as examined in the Methods section below.

A measured output correlation such as $1/N \sum g'_j g_j$ can be seen as a sum of three parts: a true correlation that arises from repeating

the inputs in group j , a spurious correlation arising from the inputs in $-j$, and a spurious correlation due to the interaction of j with $-j$. The expression $1/N \sum g'_0 g_0$ is also a sum of three parts: the spurious correlation in $-j$, spurious correlation in j , and finally an interaction between j and $-j$. The expected variance in $1/N \sum g'_0 g_0$ is the sum of these three, which are proportional to their relative contributions to the overall model variance; namely, S_j , S_{-j} , and $S_{j,-j}$. The expected amount of spurious correlation in $1/N \sum g'_0 g_j$ is proportional to $S_{-j} + S_{j,-j}$.

The spurious correlation from $-j$ is exactly the same in both $1/N \sum g'_0 g_j$ and $1/N \sum g'_0 g_0$ since the input realizations are the same, so subtraction of the two expressions removes this term. The expected amount of spurious correlation in $1/N \sum (g'_0 g_j - g'_0 g_0)$ is proportional to $S_j + 2S_{j,-j}$. The factor 2 appears because both $g'_0 g_j$ and $g'_0 g_0$ contribute separate realizations of the interaction term. The latter expression is expected to be smaller when $S_j + S_{j,-j} < S_{-j}$, or equivalently, $T_j < 1/2$.

A similar calculation for the total effects shows that the expected amount of spurious correlation in $1/N \sum g_0 g_j$ is proportional to $S_j + S_{j,-j}$, while that in $1/N \sum (g_0 g_j - g'_0 g_0)$ is proportional to $S_{-j} + 2S_{j,-j}$.

The latter is smaller provided $S_{-j} + S_{j,-j} < S_j$, or $S_j > 1/2$. The same results are obtained if $g'_j g_j$ is substituted for $g'_0 g_0$, or if primed and unprimed superscripts are swapped on $g_0 g_j$ or $g'_0 g_j$.

2.5. Evaluation of higher-order sensitivity indices

Saltelli (2002) pointed out that the same $2J + 2$ model runs which provide double estimates for the first-order effects may be used to obtain double estimates of all the second-order effects. These are based on the sample correlations

$$c_{jk} = (\rho'_{jk} + \rho'_{kj})/2 = \frac{1}{2N} \sum (g'_j g_k + g'_k g_j) \quad (11)$$

$$c_{-jk} = (\rho_{jk} + \rho''_{kj})/2 = \frac{1}{2N} \sum (g_j g_k + g'_k g'_j) \quad (12)$$

Then

$$S_{jk} = c_{jk} - S_j - S_k \quad (13)$$

$$T_{jk} = 1 - C_{-jk} \quad (14)$$

Define the estimates s_{jk} and t_{jk} as $s_{jk} = c_{jk} - S_j - S_k$, and $t_{jk} = 1 - c_{-jk}$, respectively. The former may involve subtraction of near-equal quantities and may lead to substantial error, especially when s_{jk} is much smaller than the main effects. For this reason correction factors are important, especially for the first-order indices. Sensitivity indices beyond second-order would require more than the standard $2J + 2$ model runs, but if they were calculated the problem of near-total cancellation might become even more acute. To correct c_{jk} , note that the spurious correlation

$$p_{jk} = (\rho'_{jj} + \rho'_{kk})/2 = \frac{1}{2N} \sum (g'_j g_j + g'_k g_k) \quad (15)$$

shares all its input realizations with c_{jk} , except for inputs j and k . Provided that $c_{-jk} > 1/2$, it is expected that $(c_{jk} - p_{jk})$ will provide a better estimate of C_{jk} than does c_{jk} alone.

3. Methods

Computing the Sobol indices numerically requires evaluating the Pearson correlation coefficients between the output vectors from pairs of model runs. There are multiple variations on either Equation (3) which uses the "raw" model output, or on Equation (5) which uses standardized output. We present equations for a total of 12 previously published and new methods in this section. These equations are evaluated using the "G function" (Davis and Rabinowitz, 1984).

3.1. Definition of the various formulas for the Sobol indices

The twelve methods, labeled A₁–A₃ through D₁–D₃, are summarized in Table 1. As noted below, some have been previously recommended by other authors, and some are new. The equations are formulated in terms of different estimates for the means, variances, covariances, and correlations of the output vectors of the model runs.

The mean of the model output and the square of the mean can be calculated using any of the following equations. The subscript j may range from 0 to J . Also, the variable on the left side of each equation may be primed, in which case each unprimed f on the right becomes primed, and vice versa.

$$m_j = \frac{1}{N} \sum f_j \quad (16)$$

$$m_{xj}^2 = \frac{1}{N} \sum f_j f'_j \quad (17)$$

$$m_{ij}^2 = \frac{1}{2} (m_0^2 + m_j^2) \quad (18)$$

Note that the primed and unprimed versions of m_{xj}^2 are identical. While other estimates of the mean may be created, they have not been found to improve the estimates of the sensitivity indices. The equations for the covariance factors (u) and variance (v) of the model output vectors are:

$$u_j = \frac{1}{N} \sum f'_0 f_j \quad (19)$$

$$u_{-j} = \frac{1}{N} \sum f_0 f_j \quad (20)$$

$$v_j = \frac{1}{N} \sum f_j^2 - m_j^2 \quad (21)$$

$$v_{xj} = \frac{1}{N} \sum f_j^2 - m_{x0}^2 \quad (22)$$

$$v_{sj} = \frac{1}{2} (v'_{x0} + v_{xj}) \quad (23)$$

$$v_{ij} = \frac{1}{2} (v_0 + v_j) \quad (24)$$

Finally, various estimates of the correlation between standardized model outputs (g_0, g'_0, g_j , or g'_j) can be formulated, where c_s indicates an estimate based on single paired runs, c_d indicates a double estimate, p indicates the spurious correlation between runs, and c_a indicates correlation estimates partly adjusted for spurious correlation:

$$c_{sj} = \frac{1}{N} \sum g'_0 g_j \quad (25)$$

$$c_{s-j} = \frac{1}{N} \sum g_0 g_j \quad (26)$$

$$c_{dj} = \frac{1}{2N} \sum (g'_0 g_j + g_0 g'_j) \quad (27)$$

$$c_{d-j} = \frac{1}{2N} \sum (g_0 g_j + g'_0 g'_j) \quad (28)$$

$$p_0 = \frac{1}{N} \sum g_0 g'_0 \quad (29)$$

$$p_j = \frac{1}{2N} \sum (g_0 g'_0 + g_j g'_j) \quad (30)$$

$$c_{aj} = \frac{c_{dj} - p_j c_{d-j}}{1 - p_j^2} \quad (31)$$

$$c_{a-j} = \frac{c_{d-j} - p_j c_{dj}}{1 - p_j^2} \quad (32)$$

The equations in Table 1 also include two special functions. $H(x)$ is the Heavyside or unit step function

$$H(x) = 0, \text{ for } x < 0, \text{ and } H(x) = 1, \text{ for } x > 0 \quad (33)$$

and $R(x)$ is the following ramp function:

$$R(x) = 0 \text{ for } x < \frac{1}{6}, R(x) = 1 \text{ for } x > \frac{5}{6} \quad (34)$$

where $R(x)$ varies linearly between (1/6,0) and (5/6,1).

Table 1

The twelve methods used to estimate the sensitivity indices. Definitions of the m (mean), v (variance), u (covariance factor), c (correlation), p (spurious correlation) terms and the H and R functions are given in Equations 16–34.

Method	Main effect, s_j	Total effect, t_j	Notes
A ₁	$\frac{u_j - m_0^2}{v_0}$	$1 - \frac{u_{-j} - m_0^2}{v_0}$	These are the most basic equations for estimating the indices.
A ₂	$\frac{u_j - m_{x0}^2}{v_{x0}}$	$1 - \frac{u_{-j} - m_0^2}{v_{tj}}$	The m_{x0}^2 term for s_j was recommended by Saltelli (2002) and by Sobol' et al. (2007).
A ₃	$\frac{u_j - m_{x0}^2}{v_{sj}}$	$1 - \frac{u_{-j} - m_{tj}^2}{v_{tj}}$	The t_j formula is from Jansen (1999), and recommended by Saltelli et al. (2010).
B ₁	$c_{sj} - p_0 H\left(c_{s-j} - \frac{1}{2}\right)$	$1 - c_{s-j} + p_0 H\left(c_{sj} - \frac{1}{2}\right)$	For s_j the spurious correlation is subtracted only when $c_{s-j} > 1/2$. For t_j the roles of c_{sj} and c_{s-j} are reversed.
B ₂	$c_{sj} - p_0 R\left(c_{s-j} - \frac{1}{2}\right)$	$1 - c_{s-j} + p_0 R\left(c_{sj} - \frac{1}{2}\right)$	These ramp function formulas are new in this paper.
B ₃	$\frac{c_{sj} - p_0 c_{s-j}}{1 - p_0^2}$	$1 - \frac{c_{s-j} - p_0 c_{sj}}{1 - p_0^2}$	These formulas are presented here for the first time.
C ₁	$\frac{u_j - m_0^2}{2v_0} + \frac{u'_j - m_0^2}{2v_0}$	$1 - \frac{u_{-j} - m_0^2}{2v_0} - \frac{u'_{-j} - m_0^2}{2v_0}$	These are averages of two estimates each, formed by interchanging the primed and unprimed quantities in the A ₁ formulas.
C ₂	$\frac{u_j - m_{x0}^2}{2v_{sj}} + \frac{u'_j - m_{x0}^2}{2v'_{sj}}$	$1 - \frac{u_{-j} - m_{tj}^2}{2v_{tj}} - \frac{u'_{-j} - m_{tj}^2}{2v'_{tj}}$	These formulas average the primed and unprimed versions of A ₃ .
C ₃	$\frac{u_j - m_{x0}^2}{8v_{x0}} + \frac{u'_j - m_{x0}^2}{8v'_{x0}} + \frac{u_j - m_{xj}^2}{8v_{xj}} + \frac{u'_j - m_{xj}^2}{8v'_{xj}}$	$1 - \frac{u_{-j} - m_{x0}^2}{4v_{x0}} - \frac{u'_{-j} - m_{x0}^2}{4v'_{x0}} - \frac{u_{-j} - m_{xj}^2}{4v_{xj}} - \frac{u'_{-j} - m_{xj}^2}{4v'_{xj}}$	These formulas are from Lilburne and Tarantola (2009), and are found to be the best of the methods using the raw data.
D ₁	$c_{dj} - p_j H\left(c_{d-j} - \frac{1}{2}\right)$	$1 - c_{d-j} + p_j H\left(c_{dj} - \frac{1}{2}\right)$	SHEDS-Multimedia version 4 has used these formulas since 2008 (Glen et al., 2010).
D ₂	$c_{dj} - p_j R\left(c_{d-j} - \frac{1}{2}\right)$	$1 - c_{d-j} + p_j R\left(c_{dj} - \frac{1}{2}\right)$	The ramp function provides a small improvement over method D ₁ .
D ₃	$c_{dj} - p_j \frac{c_{a-j}}{1 - c_{aj}c_{a-j}}$	$1 - c_{d-j} + p_j \frac{c_{aj}}{1 - c_{aj}c_{a-j}}$	These new formulas provide the best results found so far as measured by mean absolute deviation.

Method A₁ is the most basic of all, and is essentially the method suggested in Sobol' (1990) (although that paper did not discuss total effects). For method A₁, the choices for the mean were restricted to m_0 or m'_0 , and the variance to v_0 or v'_0 . It was found empirically that the primed versions provide the best estimates for the main effects, while the unprimed versions are best for the total effects. This is reasonable, since the estimate u_j uses the primed run f'_0 , while u_{-j} uses the unprimed run f_0 .

Method A₂ uses m_{x0}^2 in estimating the main effect, which was justified theoretically by Sobol' et al. (2007) as being superior to A₁. The total effects use an average of two variances (empirically, those of the runs used to calculate u_{-j} perform best). Method A₃ extends variance averaging to the main effect, and uses the Jansen estimator for the total effect, as recommended by Saltelli et al. (2010). This estimator (Jansen, 1999) may be more recognizable as $t_j = 1/2N \sum (f_0 - f_j)^2$. This is rewritten in the form common to Table 1 by expanding the square to obtain $t_j = 1/2v(v_0 + m_0^2 + v_j + m_j^2) - u_{-j}/v$.

Taking $v = v_{tj} = 1/2(v_0 + v_j)$, then $t_j = 1 - (u_{-j} - m_{tj}^2)/v_{tj}$.

Methods B₁–B₃ produce single estimates for each index using $J + 2$ runs and standardized output. The first two differ only in the spurious correlation adjustment. Method B₃ attempts to account for the spurious correlation that p_j shares with c_j or c_{-j} , which effectively produces a p_j^2 term.

Methods C₁–C₃ use $2J + 2$ model runs to produce double estimates, using the raw output data. Method C₁ is analogous to A₁. Method C₂ corresponds to A₃ (not A₂). Method C₃ uses the Lilburne and Tarantola (2009) formulas which extend the concept of “double estimates” further by using more combinations of the mean and variance estimates.

Methods D₁–D₃ are the double-estimate analogs of B₁–B₃. Formula D₁ has been used in SHEDS (Glen et al., 2010) since 2008. Formulas D₂ and D₃ are presented here for the first time.

3.2. Comparison of numerical estimation methods using the G function

The G function (Davis and Rabinowitz, 1984) has been used previously to test both the accuracy and precision of various numerical estimation methods (Sobol', 1990; Saltelli and Sobol', 1995; Archer et al., 1997). The G function is the product of J inputs, each transformed from a unit uniform u_j . The general G function is

$$G = \prod_{j=1}^J \frac{(|4u_j - 2| + a_j)}{1 + a_j} \quad (35)$$

We follow the choice of Saltelli (2002) with $J = 6$ and $a_j = (0, .5, 3, 9, 99, 99)$. Factors with smaller a_j have greater range and contribute more variance. The sensitivity indices can be derived directly by integration, which allows comparison with numerical estimates. The mean value of G is one, as is the mean value of each of the J factors.

The model was run $2J + 2 = 14$ times with $N = 200,000$, and the same output was processed using the 12 method variations in Table 1. The single-estimate methods required just 8 of the 14 model runs. This entire process was repeated 50,000 times with different random numbers, to determine (1) the reproducibility or precision of each estimate, and (2) whether there was any bias in the estimates. Repeating the entire analysis to obtain the scatter in the estimates is a well-known technique called *bootstrapping*; this has been used previously with Sobol's method (Archer et al., 1997; Mokhtari et al., 2006). The terminology suggested here is that this analysis consists of 50,000 bootstrap sets of $N = 200,000$ iterations each. These numbers are quite large, but the model is extremely simple to evaluate and the stochastic variation in the results is thereby reduced to a level where small differences between the methods can be discerned. As a more practical example, method D₃ from this analysis was re-run on the same G function using just 10 sets of $N = 1000$ each. These smaller numbers still provided reasonable estimates of the indices, although in general with small N there is a risk of leaving significant portions of the input hypercube unsampled. The minimum N needed to properly characterize the model output surface will depend on the regularity and smoothness of that surface, and general guidelines cannot be given.

4. Results

Summary statistics from all the test runs are presented in Table 2. The prefix ‘avg’ indicates that the reported statistics are averaged across the 12 first-order indices (6 main and 6 total effects). E_{mad} is the mean absolute deviation of the 50,000 estimates from the theoretical value, E_{std} is the standard deviation of the estimates, S_{err} is the standard error in the mean, and A_{err} is the absolute deviation of the overall mean from the theoretical value.

The standardized methods B₁–B₃ score better than methods A₁–A₃. Methods B₂ and B₃ have the smallest mean absolute

Table 2

Various average error measurements are provided for the sensitivity indices for the G function, using 50,000 bootstrap sets, each of $N = 200,000$ iterations. E_{mad} is the mean absolute deviation of the 50,000 estimates from the theoretical value. E_{std} is the standard deviation of the estimates, S_{err} is the standard error in the mean, and A_{err} is the absolute deviation of the mean from the theoretical value. The prefix 'avg' indicates that the reported statistics are averaged across the 12 first-order indices (6 main and 6 total effects). Each statistic has a multiplier at the top of the column; for example, avg E_{mad} for method A_1 is 2600×10^{-6} , or .0026.

Method	Output type	Required # of runs	avg $E_{\text{mad}} \times 10^{-6}$	avg $E_{\text{std}} \times 10^{-6}$	avg $S_{\text{err}} \times 10^{-8}$	avg $A_{\text{err}} \times 10^{-8}$
A_1	Raw	8	2600	3250	1450	1520
A_2	Raw	8	1090	1370	613	653
A_3	Raw	8	677	848	379	502
B_1	Standardized	8	549	688	308	250
B_2	Standardized	8	520	652	292	351
B_3	Standardized	8	522	654	292	368
C_1	Raw	14	1300	1630	730	1260
C_2	Raw	14	400	501	224	346
C_3	Raw	14	340	426	190	402
D_1	Standardized	14	354	444	198	121
D_2	Standardized	14	339	425	190	316
D_3	Standardized	14	335	419	187	314

deviations among the single-estimate methods. This statistic is preferred by Saltelli et al. (2010), and is a combination of both accuracy and precision. These methods also have the greatest precision (that is, the smallest standard deviation and smallest standard error), but have somewhat less accuracy than method B_1 (as seen in avg A_{err}).

Among the raw data methods using 14 runs, method C_3 performs best. The standardized methods D_1 – D_3 all score similarly and are as good as C_3 . Methods D_2 and D_3 have slightly greater precision but less accuracy than method D_1 . By a small margin, method D_3 had the smallest mean absolute deviation among all methods tested.

Table 3 shows all 42 first and second-order indices using method D_3 with $N = 200,000$. Also included in Table 3 are the spurious correlations p_1 through p_6 . The theoretical values and the mean estimates are presented to either six significant digits or eight decimal places, whichever is fewer. Four additional statistics are presented. The first two (the error in the mean estimate and its standard error) would be expected to improve if more sets were run. By contrast, the standard deviation and the mean absolute difference would not improve with more sets; these depend only on the number of iterations N per run.

The standard deviation measures the scatter in the 50,000 estimates for each index. The largest standard deviations were for the largest indices. It is shown in the Appendix that the theoretical standard deviation of p_j is $\sqrt{(1 - S_j + S_j T_j)/N}$. Note that all 42 sensitivity indices have smaller standard deviations than do these spurious correlations. Without the correction terms, the scatter in each index would be closer to that of the p_j , which measure the random noise in the system.

All of the first and second-order sensitivity indices are estimated quite well, with the largest error being just .0000122 (in S_1). Even the very smallest indices are remarkably accurate, being estimated correctly to nine decimal places in some cases. The smallest index S_{56} has a very small but negative estimated mean, which is not significantly different from zero. The largest index T_{12} is correctly estimated to within one part per million. In general, indices close to $\frac{1}{2}$ are the least reliably estimated.

Table 4 presents the same information as Table 3, except the sample size N was reduced to 1000, and the number of bootstrap sets reduced to just 10. These are more practical values for complicated models that take significant time to run. Nevertheless, the indices are estimated fairly well. The largest errors were .011 for T_1 , T_{15} , and T_{16} . The small first-order indices are estimated quite well, as are all the second-order total effects. The second-order main effects are less reliable, because of the subtractions of comparably-sized terms in

Equation (13). This is due to stochastic noise, which can easily be reduced by using larger N (or more sets), as was seen in Table 3.

5. Discussion

5.1. Bootstrapping

For Table 3, the full analysis of $2J + 2$ model runs was performed $M = 50,000$ with different random samples, with each of these sets producing $N = 200,000$ samples of model output. For all practical purposes, the mean of M sets (each producing N estimates) provides the same precision as one set producing $(M \cdot N)$ estimates. However, the former approach has two advantages: first, one can calculate not only the mean value for each index, but also the standard error of the mean. Second, breaking the problem into a series of smaller problems requires smaller vectors and less computer memory. For example, the above tests were run on a standard personal computer, but producing one set of ten billion estimates was not feasible. Even when possible, very long vectors are less efficient since the processing speed does not scale linearly beyond a certain size, due to the need to utilize virtual memory.

5.2. Number of model iterations N

In most practical cases the sensitivity indices will only need to be evaluated correctly to two decimal places or so, allowing relatively small M and N to be used. Table 4 gives estimates of the G -function indices obtained when cutting back the total number of iterations $(M \cdot N)$ from ten billion to ten thousand. These estimates would be sufficient for most purposes. Models with more complicated output surfaces might require larger N , but even for relatively complicated Monte Carlo models, it should be possible to achieve several thousand iterations.

The $2J + 2$ run scheme of Saltelli (2002) requires less than half the N to obtain the precision of the $J + 2$ run approach, using either the raw or standardized output. Hence, the double estimate methods should be preferred when using random inputs. However, Saltelli et al. (2010) point out that the second set of estimates are less precise than the first when quasi-random inputs are used, so they prefer single-estimate methods in that case.

5.3. Use of quasi-random inputs

Several papers, including Sobol' (1994, 2001) and Saltelli et al. (2010), state that the use of quasi-random inputs produces faster convergence to the correct indices than does the use of true random

Table 3Sensitivity indices estimated using method D₃, with 50,000 sets of model runs with $N = 200,000$ each. The notation “E- n ” stands for “ $\times 10^{-n}$ ”.

Index	Theoretical value	Mean estimate	Error in mean estimate	Std. error of mean	Standard deviation	Mean absolute difference
S ₁	.586781	.586769	−1.22 E-5	5.34 E-6	1.20 E-3	9.55 E-4
S ₂	.260792	.260797	5.15 E-6	4.68 E-6	1.05 E-3	8.36 E-4
S ₃	.0366738	.0366748	9.55 E-7	8.46 E-7	1.89 E-4	1.51 E-4
S ₄	.00586781	.00586795	1.34 E-7	1.39 E-7	3.11 E-5	2.48 E-5
S ₅	.00005868	.00005868	2.01 E-9	1.40 E-9	3.13 E-7	2.49 E-7
S ₆	.00005868	.00005868	−2.21 E-10	1.40 E-9	3.12 E-7	2.49 E-7
T ₁	.690086	.690076	−1.03 E-5	5.29 E-6	1.18 E-3	9.45 E-4
T ₂	.356173	.356181	7.36 E-6	5.00 E-6	1.12 E-3	8.92 E-4
T ₃	.0563335	.0563350	1.45 E-6	1.02 E-6	2.27 E-4	1.81 E-4
T ₄	.00917058	.00917077	1.92 E-7	1.71 E-7	3.82 E-5	3.05 E-5
T ₅	.00009201	.00009201	3.04 E-9	1.72 E-9	3.85 E-7	3.06 E-8
T ₆	.00009201	.00009201	−1.43 E-10	1.72 E-9	3.84 E-7	3.06 E-8
S ₁₂	.0869305	.0869354	4.84 E-6	2.85 E-6	6.36 E-4	5.07 E-4
S ₁₃	.0122246	.0122281	3.53 E-6	2.25 E-6	5.03 E-4	4.02 E-4
S ₁₄	.00195594	.00195640	4.66 E-7	9.91 E-7	2.22 E-4	1.77 E-4
S ₁₅	.00001956	.00001969	1.32 E-7	1.01 E-7	2.25 E-5	1.80 E-5
S ₁₆	.00001956	.00001954	−2.17 E-8	1.01 E-7	2.25 E-5	1.80 E-5
S ₂₃	.00543316	.00543023	−2.93 E-6	2.09 E-6	4.68 E-4	3.74 E-4
S ₂₄	.00086931	.00086936	5.24 E-8	8.82 E-7	1.97 E-4	1.57 E-4
S ₂₅	.00000869	.00000857	−1.23 E-7	8.91 E-8	1.99 E-5	1.59 E-5
S ₂₆	.00000869	.00000871	1.62 E-8	8.93 E-8	2.00 E-5	1.59 E-5
S ₃₄	.00012225	.00012194	−3.05 E-7	4.34 E-7	9.70 E-5	7.75 E-5
S ₃₅	.00000122	.00000125	2.27 E-8	4.38 E-8	9.79 E-6	7.82 E-6
S ₃₆	.00000122	.00000125	2.59 E-8	4.39 E-8	9.82 E-6	7.83 E-6
S ₄₅	.00000020	.00000019	−6.81 E-9	1.82 E-8	4.08 E-6	3.25 E-6
S ₄₆	.00000020	.00000017	−2.97 E-8	1.83 E-8	4.10 E-6	3.28 E-6
S ₅₆	2.0 E-9	−3.09 E-10	−2.26 E-9	1.84 E-9	4.12 E-7	3.29 E-7
T ₁₂	.957216	.957215	−8.64 E-7	1.01 E-6	2.25 E-4	1.80 E-4
T ₁₃	.732336	.732331	−5.22 E-6	4.75 E-6	1.06 E-3	8.49 E-4
T ₁₄	.696964	.696954	−9.35 E-6	5.20 E-6	1.16 E-3	9.29 E-4
T ₁₅	.690155	.690145	−1.01 E-5	5.29 E-6	1.18 E-3	9.45 E-4
T ₁₆	.690155	.690145	−1.03 E-5	5.29 E-6	1.18 E-3	9.45 E-4
T ₂₃	.405238	.405244	5.97 E-6	5.29 E-6	1.18 E-3	9.47 E-4
T ₂₄	.364161	.364168	7.47 E-6	5.06 E-6	1.13 E-3	9.02 E-4
T ₂₅	.356254	.356261	7.22 E-6	5.00 E-6	1.12 E-3	8.92 E-4
T ₂₆	.356254	.356261	7.36 E-6	5.00 E-6	1.12 E-3	8.92 E-4
T ₃₄	.0653170	.0653180	1.00 E-6	1.20 E-6	2.69 E-4	2.14 E-4
T ₃₅	.0564237	.0564251	1.46 E-6	1.02 E-6	2.28 E-4	1.82 E-4
T ₃₆	.0564237	.0564252	1.49 E-6	1.02 E-6	2.28 E-4	1.82 E-4
T ₄₅	.00926228	.00926248	1.96 E-7	1.73 E-7	3.87 E-5	3.09 E-5
T ₄₆	.00926228	.00926243	1.50 E-7	1.73 E-7	3.86 E-5	3.08 E-5
T ₅₆	.00018401	.00018401	−1.34 E-10	3.72 E-9	8.32 E-7	6.63 E-8
P ₁	0	.0000156	1.56 E-5	9.02 E-6	2.02 E-3	1.61 E-3
P ₂	0	.0000177	1.77 E-5	9.10 E-6	2.03 E-3	1.62 E-3
P ₃	0	.0000219	2.19 E-5	9.78 E-6	2.18 E-3	1.74 E-3
P ₄	0	.0000187	1.87 E-5	9.93 E-6	2.22 E-3	1.77 E-3
P ₅	0	.0000195	1.95 E-5	9.96 E-6	2.23 E-3	1.77 E-3
P ₆	0	.0000194	1.94 E-5	9.96 E-6	2.23 E-3	1.77 E-3

numbers. For the methods comparison in Table 2, the use of quasi-random numbers would benefit the single-estimate methods more than the double estimate methods, because the performance degrades when the primed and unprimed inputs are interchanged (Saltelli et al., 2010). The single-estimate standardized methods B₁–B₃ performed better than any of the raw data single-estimate methods, and might therefore be preferred when using quasi-random numbers.

The use of quasi-random numbers in models like SHEDS (Isaacs et al., 2010; Glen et al., 2010) is problematic when the number of required inputs is large (SHEDS requires about 45,000 per iteration). Each input occupies one column of the quasi-random matrix (each row is a model iteration), and the columns further to the right are less well uniformly distributed (Saltelli et al., 2010). In addition, SHEDS analysis typically involves various subgroupings of the model output into specific population cohorts. With quasi-random numbers these subgroups would technically no longer be representative samples because the inputs used by them would not exactly be equidistributed in the allowed space. With larger N this problem would diminish, but SHEDS runs are fairly slow (about

$N = 5$ to 10 per minute, depending on model settings), so runs of more than several thousand are impractical.

5.4. Limits as the indices approach zero or one

It can be disconcerting to obtain estimates that are negative or above one, which are not possible values for the true indices. This is relatively infrequent when using method D₃. Method D₃ works well even for first-order indices close to zero. Even with just $N = 1000$ iterations, every estimate of S_5 and S_6 was between .0000531 and .0000673, not far from the theoretical value of .0000587. Using standardized output, the estimates $s_j = c_j - p_j$ and $t_j = 1 - c_{-j}$ both approach zero when the true indices approach zero. Conversely, the estimates $s_j = c_j$ and $t_j = 1 - c_{-j} + p_j$ both approach one when the true indices approach one.

5.5. Use of raw versus standardized output

Methods B₁–B₃ and D₁–D₃ use standardized model output and were initially included because modelers sometimes use this

Table 4Sensitivity indices estimated using method D₃, with 10 sets of model runs with $N = 1000$ each. The notation “E- n ” stands for “ $\times 10^{-n}$ ”.

Index	Theoretical value	Mean estimate	Error in mean estimate	Std. error of mean	Standard deviation	Mean absolute difference
S ₁	.587	.593	6.4 E-3	3.3 E-3	1.0 E-2	9.8 E-3
S ₂	.261	.257	−3.8 E-3	4.8 E-3	1.5 E-2	1.3 E-2
S ₃	.0367	.0368	1.3 E-4	8.4 E-4	2.7 E-3	2.2 E-3
S ₄	.00587	.00589	1.8 E-5	1.3 E-4	4.2 E-4	3.2 E-4
S ₅	.0000587	.0000593	6.1 E-7	1.5 E-6	4.6 E-6	3.9 E-6
S ₆	.0000587	.0000604	1.7 E-6	9.7 E-7	3.1 E-6	2.7 E-6
T ₁	.690	.701	1.0 E-2	3.2 E-3	1.0 E-2	1.3 E-2
T ₂	.356	.354	−2.1 E-3	4.4 E-3	1.4 E-2	1.2 E-2
T ₃	.0563	.0566	2.5 E-4	1.0 E-3	3.2 E-3	2.6 E-3
T ₄	.00917	.00932	1.5 E-4	1.7 E-4	5.5 E-4	4.8 E-4
T ₅	.0000920	.0000926	5.9 E-7	2.0 E-6	6.5 E-6	5.4 E-6
T ₆	.0000920	.0000950	3.0 E-6	1.3 E-6	4.1 E-6	3.7 E-6
S ₁₂	.0869	.0850	−1.9 E-3	3.8 E-3	1.2 E-2	1.1 E-2
S ₁₃	.0122	.0076	−4.6 E-3	3.0 E-3	9.5 E-3	8.2 E-3
S ₁₄	.00196	.00066	−1.3 E-3	8.1 E-4	2.6 E-3	2.4 E-3
S ₁₅	.0000196	−2.6E-5	−4.6 E-5	8.8 E-5	2.8 E-4	2.4 E-4
S ₁₆	.0000196	−2.9E-5	−4.9 E-5	9.1 E-5	2.9 E-4	2.4 E-4
S ₂₃	.00543	.00928	3.9 E-3	2.4 E-3	7.7 E-3	6.3 E-3
S ₂₄	.000869	.001987	1.1 E-3	1.0 E-3	3.2 E-3	2.8 E-3
S ₂₅	.0000087	.0000189	1.0 E-5	7.7 E-5	2.4 E-4	1.8 E-4
S ₂₆	.0000087	.0001468	1.4 E-4	5.1 E-5	1.6 E-4	1.8 E-4
S ₃₄	.000122	.000066	−5.7 E-5	3.5 E-4	1.1 E-3	8.9 E-4
S ₃₅	.0000012	.0000039	2.7 E-6	5.4 E-5	1.7 E-4	1.3 E-4
S ₃₆	.0000012	−6.7E-5	−6.8 E-5	4.8 E-5	1.8 E-4	1.3 E-4
S ₄₅	.0000002	−1.3E-5	−1.3 E-5	1.7 E-5	5.5 E-5	4.8 E-5
S ₄₆	.0000002	−2.4E-6	−2.6 E-6	1.2 E-5	3.8 E-5	3.1 E-5
S ₅₆	2 E-9	2.1 E-7	2.1 E-7	2.6 E-6	8.3 E-6	7.2 E-6
T ₁₂	.957	.958	4.8 E-4	8.0 E-4	2.5 E-3	1.6 E-3
T ₁₃	.732	.738	5.3 E-3	5.2 E-3	1.7 E-2	1.5 E-2
T ₁₄	.697	.706	9.1 E-3	3.3 E-3	1.0 E-2	1.2 E-2
T ₁₅	.690	.701	1.0 E-2	3.2 E-3	1.0 E-2	1.3 E-2
T ₁₆	.690	.701	1.0 E-2	3.2 E-3	1.0 E-2	1.3 E-2
T ₂₃	.405	.407	2.1 E-3	5.9 E-3	1.9 E-2	1.6 E-2
T ₂₄	.364	.363	−7.1 E-4	4.7 E-3	1.5 E-2	1.3 E-2
T ₂₅	.356	.354	−2.0 E-3	4.4 E-3	1.4 E-2	1.2 E-2
T ₂₆	.356	.354	−1.9 E-3	4.4 E-3	1.4 E-2	1.2 E-2
T ₃₄	.0653	.0659	5.4 E-4	1.2 E-3	3.7 E-3	2.8 E-3
T ₃₅	.0564	.0567	2.3 E-4	9.9 E-4	3.1 E-3	2.6 E-3
T ₃₆	.0564	.0566	1.8 E-4	1.0 E-3	3.2 E-3	2.7 E-3
T ₄₅	.00926	.00940	1.4 E-4	1.8 E-4	5.6 E-4	4.9 E-4
T ₄₆	.00926	.00941	1.4 E-4	1.8 E-4	5.8 E-4	4.9 E-4
T ₅₆	.000184	.000187	3.0 E-6	4.9 E-6	1.5 E-5	1.1 E-5
P ₁	0	−.0026	−2.6 E-3	8.8 E-3	2.8 E-2	2.3 E-2
P ₂	0	−.0046	−4.6 E-3	9.2 E-3	2.9 E-2	2.5 E-2
P ₃	0	.0003	2.6 E-4	8.9 E-3	2.8 E-2	2.1 E-2
P ₄	0	.0023	2.3 E-3	1.1 E-2	3.3 E-2	2.6 E-2
P ₅	0	.0026	2.6 E-3	1.1 E-2	3.4 E-2	2.6 E-2
P ₆	0	.0025	2.5 E-3	1.1 E-2	3.3 E-2	2.6 E-2

practice. The standardization process destroys some information, and any formula utilizing standardized output can also be written in terms of raw output, by replacing each g with Equation (4). Hence, formulas using the raw output can always be created that equal or exceed the performance of formulas that use standardized output.

The use of standardized output may result in simpler-appearing formulas, and has the benefit of focusing on the direct evaluation of correlations. The raw data methods tend to focus on separately evaluating covariances and variance, and then taking ratios. These estimates are not independent, being derived from the same model runs. The standardization process simplifies the determination of the spurious correlation term. However, p_j only approximates the actual spurious correlation in each index, so methods D₁–D₃ might still be improved. Ultimately, a raw data method may be found that outperforms all the standardized methods.

5.6. Higher-order indices

When evaluating second-order (and higher) indices, the methods using standardized output provide clear guidance. For example, to

obtain s_{12} and t_{12} using method D₁, first calculate $c_{12} = 1/2N \sum (g_1 g_2' + g_2 g_1')$ and $c_{-12} = 1/2N \sum (g_1 g_2 + g_2' g_1')$. Then $s_{12} = c_{12} - p_{12}H(c_{-12} - 1/2) - s_1 - s_2$ and $t_{12} = 1 - c_{-12} + p_{12}H(c_{12} - 1/2)$. By contrast, the optimal formulas for raw data methods may not always be clear. For example, the proper combinations of means and variances for method C₃ may not be obvious for second order indices. For total effects, the generalization of Jansen's formula given by Equation (20) in Saltelli et al. (2010) seems reasonable, but comparison testing of estimates of second-order indices is beyond the scope of this paper.

The $2J + 2$ model run scheme allows evaluation of all possible sensitivity indices for models with $J = 5$ or fewer groups of inputs. For $J > 5$ the evaluation of specific higher-order interaction terms will generally require additional model runs. For example, to find S_{abc} , place inputs a , b , and c into a separate class by assigning them their primed sample vectors, while assigning the unprimed vectors to all other inputs. The collective index for this class is $C_{abc} = S_a + S_b + S_c + S_{ab} + S_{ac} + S_{bc} + S_{abc}$. This equals the correlation between the output vectors from the run with the above class assignments and the run with all inputs in the primed

class. Subtracting the appropriate first and second-order indices leaves S_{abc} .

Even without additional runs the size of higher-order indices can be bounded. Clearly, any interaction term involving j cannot be larger than the difference $(T_j - S_j)$. Even stricter bounds are possible. For example, S_{135} cannot be larger than the minimum of $(T_1 - S_1 - S_{13} - S_{15})$, $(T_3 - S_3 - S_{13} - S_{35})$, and $(T_5 - S_5 - S_{15} - S_{35})$, all of which may be estimated using the standard set of $2J + 2$ model runs.

5.7. Use of available information

Given $2J + 2$ model runs, there are $(J + 1)(2J + 1)$ distinct pairs of output vectors, and each pair has a sample correlation. Of these, $J + 1$ measure spurious correlations, leaving $2(J^2 + J)$ others. For both main and total effects, there are J first-order and $J(J - 1)/2$ second-order indices, or $J^2 + J$ together. With two pairs of outputs used to estimate each index, all the non-spurious correlations are utilized. Methods D₁–D₃ use the $J + 1$ spurious correlations to improve the other estimates. Since all possible pairs of output are utilized, it is unlikely that another evaluation system using the standardized output would be much more efficient for evaluating all the first and second-order indices.

5.8. Extension to more complicated models

While these methods have been tested on other simple functions, it would be useful to compare the various numerical evaluation formulas from Table 2 on more irregular functions than the G-function. This would require functions that can still have their sensitivity indices computed by direct integration, to allow the accuracy of the methods to be determined. However, the concept of subtracting an estimate of the spurious correlation from the estimate of the sensitivity index appears to be general and should not depend on the choice of model.

6. Conclusion

Sobol's method of sensitivity analysis is well suited to high-dimensional stochastic computer models, and has been successfully implemented in SHEDS. The methods presented herein provide a simple correlation-based numerical approach to calculating the estimates and reducing errors associated with spurious correlation. The use of $2J + 2$ model runs to obtain double estimates provides good estimates of all the first and second-order main and total effect indices. The method is easy to implement, and provides a framework for iterative examination of groups of inputs in complicated stochastic models. Sobol's method can aid in the identification of key input distributions in SHEDS and other EPA human exposure models, and thus inform data analysis or data collection prioritization decisions.

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Appendix. Variance in the double estimate of spurious correlation

The double estimate of the spurious correlation p_j is $(\rho'_{jj} + \rho'_{00}) / 2$. While the variance of ρ'_{jj} and ρ'_{00} are both $1/N$, the variance of the average differs because the two are not independent. In general, $\text{Var}(x) = E(x^2) - E(x)^2$. For p_j , the expectation value $E(p_j) = 0$ and the variance is $\text{Var}(p_j) = \frac{1}{4}E(\rho'^2_{jj} + 2\rho'_{jj}\rho'_{00} + \rho'^2_{00}) = \frac{1}{2N} + \frac{1}{2}E(\rho'_{jj}\rho'_{00})$

Since $\rho'_{jj} = \frac{1}{N} \sum g'_j g_j$ and $\rho'_{00} = \frac{1}{N} \sum g'_0 g_0$, then $\rho'_{jj}\rho'_{00} = \frac{1}{N^2} \sum_i \sum_k g'_j g_{ji} g'_{0k} g_{0k}$. Explicit summation indices have been added for clarity. When $k \neq i$ the two summations may be separated and both have expected values of zero. The remaining case for $k = i$ is $E(\rho'_{jj}\rho'_{00}) = \frac{1}{N^2} E\left[\sum_i g'_j g_{ji} g'_{0i} g_{0i}\right] = \frac{1}{N} E(g'_j g_j g'_0 g_0)$

While this formula applies to any model, the last expression is difficult to evaluate in general. However, the G-function has a special property that each partial variance equals the product of the first-order partial variances with the same set of indices. This property extends to the h functions in the decomposition of the output as described in Sobol' (1990):

$$f = h_0 + \sum_i h_i(u_i) + \sum_i \sum_{j>i} h_{ij}(u_i, u_j) + \sum_i \sum_{j>i} \times \sum_{k>j} h_{ijk}(u_i, u_j, u_k) + \dots$$

The arguments are all random numbers sampled uniformly between zero and one. These are suppressed from here on, as the subscripts on each h indicate the relevant arguments. For the G-function, $h_{jk} = h_j h_k$, $h_{ijk} = h_i h_j h_k$, $V_{jk} = V_j V_k$, $V_{ijk} = V_i V_j V_k$, and so on. It is easily demonstrated that this property is unaffected by grouping, for both the h functions and the partial variances. For any G-function, divide the inputs into two groups: one contains only input j , and the other group $-j$ contains all other inputs. The output is decomposed as

$$f = h_0 + h_j + h_{-j} + h_{j,-j} = h_0 + h_j + h_{-j} + h_j h_{-j}$$

Let V be the variance of this particular choice of G-function. The output standardized to mean zero and variance one is $g = (h_j + h_{-j} + h_j h_{-j})/V$. There are four possible model runs using given realizations in the Sobol method: groups j and $-j$ may be either primed or unprimed, independently. Indicate the choice by appending a prime (or not) to each h . The four specific realization vectors are

$$g_0 = (h_j + h_{-j} + h_j h_{-j})/\sqrt{V}$$

$$g'_0 = (h'_j + h'_{-j} + h'_j h'_{-j})/\sqrt{V}$$

$$g_j = (h'_j + h_{-j} + h'_j h_{-j})/\sqrt{V}$$

$$g'_j = (h_j + h'_{-j} + h_j h'_{-j})/\sqrt{V}$$

The expectation values of various combinations of h terms are found by integrating over the appropriate inputs from zero to one. Each h function has mean zero and the integral of h^2 is the corresponding partial variance. Expand the product of the four g terms listed above and keep only terms containing no first powers of any h (since those integrate to zero). Thus,

$$V^2 E(g'_j g_j g'_0 g_0) = \int h_j^2 h_j^2 + \int h_j^2 h_j^2 h_{-j}^2 + \int h_j^2 h_j^2 h_{-j}^2 \\ + \int h_{-j}^2 h_{-j}^2 + \int h_j^2 h_{-j}^2 h_{-j}^2 + \int h_j^2 h_{-j}^2 h_{-j}^2 \\ + \int h_j^2 h_j^2 h_{-j}^2 h_{-j}^2$$

The above integral signs represent the entire input space, both primed and unprimed. The four cases $j, j', -j$, and $-j'$ use independent random samples, so the integrals may be separated. Note that $\int h_j^2 dj = \int h_j^2 dj' = VS_j$, and $\int h_{-j}^2 d(-j) = \int h_{-j}^2 d(-j') = VS_{-j}$. Hence,

$$V^2 E(g'_j g_j g'_0 g_0) = V^2 S_j^2 + V^3 S_j^2 S_{-j} + V^3 S_j^2 S_{-j} + V^2 S_{-j}^2 + V^3 S_j S_{-j}^2 \\ + V^3 S_j S_{-j}^2 + V^4 S_j^2 S_{-j}^2$$

For the two-group model as a whole,

$$1 = S_j + S_{-j} + S_{j,-j}$$

The interaction term is $S_{j,-j} = \int h_j^2 h_{-j}^2 = V^2 S_j S_{-j}$. Hence, $1 = S_j + S_{-j} + VS_j S_{-j}$, and

$$S_{-j} = \frac{1 - S_j}{1 + VS_j}$$

Substituting this into the above equation for $E(g'_j g_j g'_0 g_0)$ produces (after some algebra)

$$E(g'_j g_j g'_0 g_0) = 1 - 2S_j \left(\frac{1 - S_j}{1 + VS_j} \right) = 1 - 2S_j S_{-j}$$

The total effect index for j is $T_j = S_j + S_{j,-j} = 1 - S_{-j}$. Hence,

$$E(g'_j g_j g'_0 g_0) = 1 - 2S_j(1 - T_j) = 1 - 2S_j + 2S_j T_j$$

Therefore, the variance of p_j is

$$\text{Var}(p_j) = \frac{1}{2N} + \frac{1}{2N} E(g'_j g_j g'_0 g_0) = \frac{1 - S_j + S_j T_j}{N}$$

Neither S_j nor T_j is affected by regrouping the inputs in $-j$, so this formula applies to input j in the ungrouped G -function as well. This derivation may be applied to any choice of j . The contribution $(-S_j + S_j T_j)$ is never positive and results in less overall variance than for either ρ'_{jj} or ρ'_{00} alone, unless $S_j = 0$ or $T_j = 1$. This result applies to any model for which the partial variance relation ($V_{jk} = V_j V_k$) holds for all combinations of indices, which includes the entire family of G -functions.

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