VARIANCE COMPONENTS AND GENERALIZED SOBOL' INDICES *

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Abstract. This paper introduces generalized Sobol' indices, compares strategies for their estimation, and makes a systematic search for efficient estimators. Of particular interest are contrasts, sums of squares and indices of bilinear form which allow a reduced number of function evaluations compared to alternatives. The bilinear framework includes some efficient estimators from Saltelli (2002) and Mauntz (2002) as well as some new estimators for specific variance components and mean dimensions. This paper also provides a bias corrected version of the estimator of Janon et al. (2012) and extends the bias correction to generalized Sobol' indices. Some numerical comparisons are given.

1. Introduction. Computer simulations are now pervasive in engineering applications. The performance of an airplane, semiconductor, power dam, or automobile part are investigated computationally in addition to, and usually prior to, any laboratory experiments that may be carried out. These functions depend on numerous input variables, describing product dimensions, composition, features of the manufacturing process and details of how it will be used. Similar functions are used for models of more complex phenomena like climate or ecosystems. In all of these problems it is important to know which of the variables are most important, and then to quantify that importance. The important variables in one part of the input space may not be the same as those in another, and this has motivated the development of global sensitivity measures. Similarly, variables may act in concert to yield synergistic effects (also called interactions) so the importance of a subset of variables may not be the sum of individual variable importances. Sobol' indices, described in detail below, have been developed to quantify variable importance accounting for these issues. Saltelli et al. [2008] give an extensive introduction to Sobol' indices and related methods for investigating computer models.

Sobol' indices are certain sums of variance components in an ANOVA decomposition. This article reviews Sobol' indices, relates them to well known ideas in experimental design, particularly crossed random effects, and then generalizes them yielding some new quantities and some new estimates for previously studied quantities.

Adapting ANOVA methods from physical experiments to computer experiments brings important changes in both the costs and goals of the analysis. In physical experiments one may be interested in all components of variance, or at least all of the low order ones. In computer experiments, interest centers instead on sums of variance components. While the ANOVA for computer experiments is essentially the same as that for physical ones, the experimental designs are different.

Of particular interest are what are known as 'fixing methods' for estimation of Sobol' indices. These evaluate the function at two points. Those two points have identical random values for some of the input components (the ones that are 'fixed') but have independently sampled values for the other components. Sample variances and covariances of point pairs are then used to estimate the Sobol' indices. The methods are also known as pick-freeze methods.

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As a basic example, let f be a deterministic function on $[0,1]^5$. One kind of Sobol' index estimate takes a form like

$$\mathrm{Cov}\big(f(x_1,x_2,x_3,x_4,x_5), f(x_1,x_2,x_3,z_4,z_5)\big) \tag{1.1}$$

for $x_j \stackrel{\mathrm{iid}}{\sim} \mathbf{U}(0,1)$ independently of $z_j \stackrel{\mathrm{iid}}{\sim} \mathbf{U}(0,1)$. As we will see below, this index measures the sum of variance components over all subsets of the first three input variables. The natural design to estimate (1.1) consists of n pairs of function evaluations, which share the first 3 input values, and have independent draws in the last 2 inputs. In the language of statistical experimental design [Box et al., 1978] this corresponds to n independently generated $1 \times 1 \times 1 \times 2^{2-1}$ designs. The first three variables are at 1 level, while the last two are a fractional factorial. Each replicate uses different randomly chosen levels for the five variables.

An example of the second kind of Sobol' index is

$$\begin{aligned}&\frac{1}{2}\mathrm{Var}\big(f(x_1,x_2,x_3,x_4,x_5) - f(x_1,x_2,x_3,z_4,z_5)\big) \qquad (1.2)\\ &= \mathrm{Var}\big(f(x_1,x_2,x_3,x_4,x_5)\big) - \mathrm{Cov}\big(f(x_1,x_2,x_3,x_4,x_5), f(x_1,x_2,x_3,z_4,z_5)\big)\end{aligned}$$

The sampling design to estimate (1.2) is that same as that for (1.1), but the quantity estimated is now the sum of all variance components that involve any of the first three variables. We will see below that the difference between (1.1) and (1.2) is that the latter includes interactions between the first three and last two variables while the former excludes them.

The great convenience of Sobol's measures is that they can be directly estimated by integration, without explicitly estimating all of the necessary interaction effects, squaring them, integrating their squares and summing those integrated squared estimates. Sobol' provides a kind of tomography: integrals of cross-products of f reveal facts about the internal structure of f.

The main goal of this paper is to exhibit the entire space of linear combinations of cross-moments of function evaluations with some variables fixed and others independently sampled. Such a linear combination is a generalized Sobol' index, or GSI. Then, using this space of functions, we make a systematic search for estimators of interpretable quantities with desirable computational or statistical properties.

This systematic approach yields some new and useful estimators. Some have reduced cost compared to previously known ones. Some have reduced sampling variance. It also encompasses some earlier work. In particular, an efficient strategy to estimate all two factor interaction mean squares due to Saltelli [2002] appears as a special case.

Section 2 introduces some notation and reviews the ANOVA of $[0,1]^d$ and Sobol' indices. A compact notation is necessary to avoid cumbersome expressions with many indices. Section 3 defines the generalized Sobol' indices and gives an expression for their value. It also defines several special classes of GSI based on interpretability, computational efficiency, or statistical considerations. These are contrasts, squares, sums of squares and bilinear GSIs. Section 4 shows that many GSIs including the Sobol' index (1.1) cannot be estimated by unbiased sums of squares. Section 5 considers estimation of a specific variance component for a proper subset containing k of the variables. A direct approach requires 2^k function evaluations per Monte Carlo sample, while a bilinear estimate reduces the cost to $2^{\lfloor k/2\rfloor} + 2^{k-\lfloor k/2\rfloor}$. That section also introduces a bilinear estimate for the superset importance measure defined in

Section 2. Section 6 considers some GSIs for high dimensional problems. It includes a contrast GSI which estimates the mean square dimension of a function of d variables using only $d+1$ function evaluations per Monte Carlo trial as well as some estimators of the mean dimension in the truncation sense. Section 7 presents a bias correction for GSIs that are not contrasts. Section 8 makes some comparisons among alternative methods and Section 9 has conclusions.

Sobol' indices are based on the ANOVA of $[0,1]^d$, which is defined in reference to random variables uniformly distributed on $[0,1]^d$. Non-uniform distributions are naturally included via transformations. The probabilistic foundation makes it possible to include variables that take a fixed but unknown value, if we can specify an appropriate distribution capturing what is known about the value. The independence assumption is a very strong one and removing it is an active research area not addressed in this paper.

2. Background and notation. The analysis of variance originates with Fisher and Mackenzie [1923]. It partitions the variance of a quantity among all non-empty subsets of factors, defined on a finite Cartesian grid.

The ANOVA was generalized by Hoeffding [1948] to functions in $L^2[0,1]^d$ for integer $d \geqslant 1$. That generalization extends the one for factorial experimental designs in a natural way, and can be applied to L^2 functions on any tensor product domain. It is perhaps easier to see the ANOVA connection in Efron and Stein [1981]. For $d = \infty$, see Owen [1998].

The ANOVA of $L^2[0,1]^d$ is also attributed to Sobol' [1969]. For historical interest, we note that Sobol' used a different approach than Hoeffding. He represented f by an expansion in a complete orthonormal basis (tensor products of Haar functions) and gathered together terms corresponding to each subset of variables. That is, where Hoeffding has an analysis, Sobol' has a synthesis.

We use $\boldsymbol{x} = (x_1, x_2, \dots, x_d)$ to represent a typical point in $[0,1]^d$. The set of indices is $\mathcal{D} = \{1, 2, \dots, d\}$. We write $u \subset v$ to denote a proper subset, that is $u \subsetneq v$. For $u \subseteq \mathcal{D}$ we use $|u|$ to denote the cardinality of u, and either $-u$ or u^c (depending on typographical clarity) to represent the complementary set $\mathcal{D} - u$. The expression $u + v$ means $u \cup v$ where u and v are understood to be disjoint.

For $u = \{j_1, j_2, \dots, j_{|u|}\} \subseteq \mathcal{D}$, the point $\boldsymbol{x}_u \in [0,1]^{|u|}$ has components $(x_{j_1}, x_{j_2}, \dots, x_{j_{|u|}})$. The differential $\mathrm{d}\boldsymbol{x}_u$ is $\prod_{j\in u} \mathrm{d}x_j$.

The ANOVA decomposition represents $f(\boldsymbol{x})$ via

$$f(\boldsymbol{x}) = \sum_{u \subseteq \mathcal{D}} f_u(\boldsymbol{x})$$

where the functions f_u are defined recursively by

$$\begin{aligned} f_u(\boldsymbol{x}) &= \int_{[0,1]^{d-|u|}} \Bigl(f(\boldsymbol{x}) - \sum_{v \subset u} f_v(\boldsymbol{x}) \Bigr) \, \mathrm{d}\boldsymbol{x}_{-u} \\ &= \int_{[0,1]^{d-|u|}} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}_{-u} - \sum_{v \subset u} f_v(\boldsymbol{x}). \end{aligned}$$

In statistical language, u is a set of factors and f_u is the corresponding effect. We get f_u by subtracting sub-effects of f_u from f and then averaging the residual over x_j for all $j \notin u$. The singletons $f_{\{j\}}$ are known as main effects, and when $|u| > 1$, then f_u is known as the interaction among all of the x_j for $j \in u$. The ANOVA decomposition gives f as a constant $f_\varnothing(\boldsymbol{x}) = \mu$ plus a sum of $2^d - 1$ uncorrelated random effects $f_u(\boldsymbol{x})$ for $|u| > 0$.

From usual conventions, $f_\varnothing(\boldsymbol{x}) = \mu \equiv \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ for all $\boldsymbol{x} \in [0,1]^d$. The effect f_u only depends on x_j for those $j \in u$. For $f \in L^2[0,1]^d$, these functions satisfy $\int_0^1 f_u(\boldsymbol{x})\,\mathrm{d}x_j = 0$, when $j \in u$ (proved by induction on $|u|$), from which it follows that $\int f_u(\boldsymbol{x}) f_v(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 0$, for $u \neq v$. The ANOVA identity is $\sigma^2 = \sum_u \sigma_u^2$ where $\sigma^2 = \int (f(\boldsymbol{x}) - \mu)^2\,\mathrm{d}\boldsymbol{x}$, $\sigma_\varnothing^2 = 0$ and $\sigma_u^2 = \int f_u(\boldsymbol{x})^2\,\mathrm{d}\boldsymbol{x}$ is the variance component for $u \neq \varnothing$.

We will need the following quantities.

DEFINITION 2.1. *For integer $d \geqslant 1$, let u and v be subsets of $\mathcal{D} = \{1, \dots, d\}$. Then the sets* $\mathrm{XOR}(u, v)$ *and* $\mathrm{NXOR}(u, v)$ *are*

$$\begin{aligned} \mathrm{XOR}(u,v) &= u \cup v - u \cap v \\ \mathrm{NXOR}(u,v) &= (u \cap v) + (u^c \cap v^c). \end{aligned}$$

These are the exclusive-or of u and v and its complement, respectively.

2.1. Sobol' indices. This section introduces the Sobol' indices that we generalize, and mentions some of the methods for their estimation.

There are various ways that one might define the importance of a variable x_j. The importance of variable $j \in \{1, \dots, d\}$ is due in part to $\sigma_{\{j\}}^2$, but also due to σ_u^2 for other sets u with $j \in u$. More generally, we may be interested in the importance of $\boldsymbol{x}_u$ for a subset u of the variables.

Sobol' [1993] introduced two measures of variable subset importance, which we denote

$$\underline{\tau}_u^2 = \sum_{v \subseteq u} \sigma_v^2, \quad \text{and} \quad \overline{\tau}_u^2 = \sum_{v \cap u \neq \varnothing} \sigma_v^2.$$

These are called global sensitivity indices, to distinguish them from local methods based on partial derivatives. These Sobol' indices satisfy $\underline{\tau}_u^2 \leqslant \overline{\tau}_u^2$ and $\underline{\tau}_u^2 + \overline{\tau}_{-u}^2 = \sigma^2$. The larger one, $\overline{\tau}_u^2$ is called the ***total*** sensitivity index. The smaller one is often called the ***closed*** sensitivity index.

The closed index is the sum of the variance components for u and all of its subsets. One interpretation is that $\underline{\tau}_u^2 = \mathrm{Var}(\mu_u(\boldsymbol{x}))$ where $\mu_u(\boldsymbol{x}) = \mathbb{E}(f(\boldsymbol{x}) \mid \boldsymbol{x}_u)$.

The total index counts every ANOVA component that touches the set u in any way. If $\underline{\tau}_u^2$ is large then the subset u is clearly important. If $\overline{\tau}_u^2$ is small, then the subset u is not important and Sobol et al. [2007] investigate the effects of fixing such $\boldsymbol{x}_u$ at some specific values. The second measure includes interactions between $\boldsymbol{x}_u$ and $\boldsymbol{x}_{-u}$ while the first measure does not.

Sobol' usually normalizes these quantities, yielding global sensitivity indices $\underline{\tau}_u^2/\sigma^2$ and $\overline{\tau}_u^2/\sigma^2$. In this paper we work mostly with unnormalized versions.

Sobol's original work was published in Sobol' [1990] before being translated in Sobol' [1993]. Ishigami and Homma [1990] independently considered computation of $\underline{\tau}_{\{j\}}^2$.

To estimate Sobol' indices, one pairs the point $\boldsymbol{x}$ with a hybrid point $\boldsymbol{y}$ that shares some but not all of the components of $\boldsymbol{x}$. We denote the hybrid point by $\boldsymbol{y} = \boldsymbol{x}_u{:}\boldsymbol{z}_{-u}$ where $y_j = x_j$ for $j \in u$ and $y_u = z_j$ for $j \notin u$.

From the ANOVA properties one can show directly that

$$\int_{[0,1]^{2d-|u|}} f(\boldsymbol{x}) f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}_{-u} = \sum_v \int_{[0,1]^{2d-|u|}} f_v(\boldsymbol{x}) f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}_{-u}$$

$$= \mu^2 + \underline{\tau}_u^2.$$

This is also a special case of Theorem 3.1 below. As a result $\underline{\tau}_u^2 = \mathrm{Cov}(f(\boldsymbol{x}), f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}))$ and so this Sobol index takes the covariance form described at (1.1). Plugging in sample moments for the population ones yields

$$\widehat{\underline{\tau}}_u^2 = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_i) f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}) - \hat{\mu}^2, \tag{2.1}$$

for $\boldsymbol{x}_i, \boldsymbol{z}_i \overset{\text{iid}}{\sim} \mathbf{U}(0,1)^d$, where $\hat{\mu} = (1/n)\sum_{i=1}^n f(\boldsymbol{x}_i)$. It is even better to use $\hat{\mu} = (1/n)\sum_{i=1}^n (f(\boldsymbol{x}_i) + f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}))/2$ instead, as shown by Janon et al. [2012].

Similarly as shown by Sobol' [1990],

$$\overline{\tau}_u^2 = \frac{1}{2}\int_{[0,1]^{d+|u|}} (f(\boldsymbol{x}) - f(\boldsymbol{x}_{-u}{:}\boldsymbol{z}_u))^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}_u,$$

generalizing the mean square expression (1.2), and leading to the estimate

$$\widehat{\overline{\tau}}_u^2 = \frac{1}{2n}\sum_{i=1}^n (f(\boldsymbol{x}_i) - f(\boldsymbol{x}_{i,-u}{:}\boldsymbol{z}_{i,u}))^2,$$

for $\boldsymbol{x}_i, \boldsymbol{z}_i \overset{\text{iid}}{\sim} \mathbf{U}(0,1)^d$.

The estimate $\widehat{\overline{\tau}}_u^2$ is unbiased for $\overline{\tau}_u^2$ but $\widehat{\underline{\tau}}_u^2$ above is not unbiased for $\underline{\tau}_u^2$. It has a bias equal to $-\mathrm{Var}(\hat{\mu})$. If $\int |f(\boldsymbol{x})|^4 \,\mathrm{d}\boldsymbol{x} < \infty$ then this bias is asymptotically negligible, but in cases where $\underline{\tau}_u^2$ is small, the bias may be important.

Mauntz [2002] and Kucherenko et al. [2011] use an estimator for $\underline{\tau}_u^2$ derived as a sample version of the identity

$$\underline{\tau}_u^2 = \iint f(\boldsymbol{x})(f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) - f(\boldsymbol{z}))\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}. \tag{2.2}$$

Saltelli [2002] also mentions this estimator. Here and below, integrals are by default over $\boldsymbol{x} \in [0,1]^d$ and/or $\boldsymbol{z} \in [0,1]^d$ even though some components x_j or z_j may not be required. An estimator based on (2.2) with $\boldsymbol{x}_i, \boldsymbol{z}_i \overset{\text{iid}}{\sim} \mathbf{U}(0,1)^d$ is unbiased for $\underline{\tau}_u^2$. Proposition 7.1 in Section 7 gives an unbiased variant on the estimator of (2.1) using the same function evaluations.

The utility of these estimates depends on both their costs and their variances. Given a list of L sets u of interest (such as all of the singletons) we can estimate all of their $\underline{\tau}_u^2$ at cost $(L+2)n$ using (2.2) or at cost $(L+1)n$ using (2.1). Thus if we only want one index, then (2.1) is cheaper but if we want many, then the costs are nearly equal. Formula (2.2) has a further cost advantage in that we can get $\underline{\tau}_{-u}^2$ (and hence $\overline{\tau}_u^2$) for each of the L indices of interest without making further function evaluations. We simply reverse the roles of $f(\boldsymbol{x})$ and $f(\boldsymbol{z})$ in the right side of (2.2). This idea is commonly used to get both $\underline{\tau}_{\{j\}}^2$ and $\overline{\tau}_{\{j\}}^2$ for $j = 1, \dots, d$.

There are $2^d - 1$ variance components σ_u^2 as well as $2^d - 1$ Sobol' indices $\underline{\tau}_u^2$ and $\overline{\tau}_u^2$ of each type. We can recover any desired σ_u^2 as a linear combination of $\underline{\tau}_v^2$. For example $\sigma_{\{1,2,3\}}^2 = \underline{\tau}_{\{1,2,3\}}^2 - \underline{\tau}_{\{1,2\}}^2 - \underline{\tau}_{\{1,3\}}^2 - \underline{\tau}_{\{2,3\}}^2 + \underline{\tau}_{\{1\}}^2 + \underline{\tau}_{\{2\}}^2 + \underline{\tau}_{\{3\}}^2$. More generally, we have the Moebius-type relation

$$\sigma_u^2 = \sum_{v \subseteq u} (-1)^{|u-v|} \underline{\tau}_v^2. \tag{2.3}$$

Because f is defined on a unit cube and can be computed at any desired point, methods other than simple Monte Carlo can be applied. Quasi-Monte Carlo (QMC) sampling (see Niederreiter [1992]) can be used instead of plain Monte Carlo, and Sobol' [2001] reports that QMC is more effective. For functions f that are very expensive, a Bayesian numerical analysis approach [Oakley and O'Hagan, 2004] based on a Gaussian process model for f is an attractive way to compute Sobol' indices.

2.2. Related indices. Another measure of the importance of $\boldsymbol{x}_u$ is the superset importance measure

$$\Upsilon_u^2 = \sum_{v \supseteq u} \sigma_v^2 \tag{2.4}$$

used by Hooker [2004] to quantify the effect of dropping all interactions containing the set u of variables from a black box function.

Sums of ANOVA components are also used in quasi-Monte Carlo sampling. QMC is often observed to be very effective on integrands f that are dominated by their low order ANOVA components and hence have low effective dimension [Lemieux, 2009, Chapter 6.3]. Two versions of f that are equivalent in Monte Carlo sampling may behave quite differently in QMC. For example the basis used to sample Brownian paths has been seen to affect the accuracy of QMC integrals [Caflisch et al., 1997; Acworth et al., 1997; Imai and Tan, 2002].

The function f has effective dimension s in the superposition sense [Caflisch et al., 1997], if $\sum_{|u|\leqslant s} \sigma_u^2 \geqslant (1-\epsilon)\sigma^2$. Typically $\epsilon = 0.01$ is used as a default. Similarly, f has effective dimension s in the truncation sense [Caflisch et al., 1997], if $\sum_{u\subseteq\{1,2,\dots,s\}} \sigma_u^2 = \underline{\tau}^2_{\{1,2,\dots,s\}} \geqslant (1-\epsilon)\sigma^2$.

An alternative to the effective dimension is the mean dimension (in the superposition sense) defined as $\sum_u |u|\sigma_u^2/\sigma^2$. This is the mean cardinality of a random set U chosen with probability proportional to σ_u^2 [Owen, 2003]. The mean dimension offers better resolution than effective dimension. For instance, two functions having identical effective dimension 2 might have different mean dimensions, say 1.03 and 1.05. It is also much easier to estimate the mean dimension than the effective dimension [Liu and Owen, 2006], because the mean dimension is a linear combination of variance components. Similarly one can estimate a mean square dimension $\sum_u |u|^2\sigma_u^2/\sigma^2$:

THEOREM 2.2.

$$\sum_{j=1}^d \overline{\tau}^2_{\{j\}} = \sum_u |u|\sigma_u^2 \tag{2.5}$$

$$\sum_{j=1}^d \sum_{k\neq j} \overline{\tau}^2_{\{j,k\}} = 2(d-1)\sum_u |u|\sigma_u^2 - \sum_u |u|^2\sigma_u^2 \tag{2.6}$$

Proof. This follows from Theorem 2 of Liu and Owen [2006]. □

3. Generalized Sobol' indices. Here we consider a general family of quadratic indices similar to those of Sobol'. The general form of these indices is

$$\sum_{u\subseteq\mathcal{D}} \sum_{v\subseteq\mathcal{D}} \Omega_{uv} \iint f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z} \tag{3.1}$$

for coefficients Ω_{uv}. If we think of $f(\boldsymbol{x})$ as being the standard evaluation, then the generalized Sobol' indices (3.1) are linear combinations of all possible second order moments of f based on fixing two subsets, u and v, of input variables.

A matrix representation of (3.1) will be useful below. First we introduce the Sobol' matrix $\Theta \in \mathbb{R}^{2^d\times 2^d}$. This matrix is indexed by subsets u and v, that is, $(\Theta_{uv})_{u,v\in\{\varnothing,\{1\},\{2\},\dots,\{d\},\{1,2\},\{1,3\},\dots,\{1,2,\dots,d\}\}}$, with entries

$$\Theta_{uv} = \iint f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}.$$

Now (3.1) is the matrix inner product $\mathrm{tr}(\Omega^{\mathsf{T}}\Theta)$ for the matrix Ω. Here and below, we use matrices and vectors indexed by the 2^d subsets of $\mathcal{D}$. The order in which subsets appear is not material; any consistent ordering is acceptable.

The Sobol' matrix is symmetric. It also satisfies $\Theta_{uv} = \Theta_{u^cv^c}$. Theorem 3.1 gives the general form of a Sobol' matrix entry.

THEOREM 3.1. *Let $f \in L^2[0,1]^d$ for $d \geqslant 1$, with mean $\mu = \int f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ and variance components σ_u^2 for $u \subseteq \mathcal{D}$. Let $u, v \subseteq \mathcal{D}$. Then the uv entry of the Sobol' matrix is*

$$\Theta_{uv} = \mu^2 + \underline{\tau}^2_{\mathrm{NXOR}(u,v)}.$$

Proof. First,

$$\begin{aligned}\Theta_{uv} &= \iint f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}\\ &= \sum_{w\subseteq\mathcal{D}}\sum_{w'\subseteq\mathcal{D}}\iint f_w(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f_{w'}(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}\\ &= \sum_{w\subseteq\mathcal{D}}\iint f_w(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f_w(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z},\end{aligned}$$

because if $w \neq w'$, then there is an index $j \in \mathrm{XOR}(w, w')$, for which either the integral over x_j or the integral over z_j of $f_w f_{w'}$ above vanishes.

Next, suppose that w is not a subset of $\mathrm{NXOR}(u, v)$. Then there is an index $j \in \mathrm{XOR}(u, v) \cap w$. If $j \in w \cap u \cap v^c$, then the integral over x_j vanishes, while if $j \in w \cap v \cap u^c$, then the integral over z_j vanishes. Therefore

$$\begin{aligned}\Theta_{uv} &= \sum_{w\subseteq\mathrm{NXOR}(u,v)}\iint f_w(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f_w(\boldsymbol{z}_v{:}\boldsymbol{x}_{-v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}\\ &= \sum_{w\subseteq\mathrm{NXOR}(u,v)}\int f_w(\boldsymbol{x})^2\,\mathrm{d}\boldsymbol{x}\\ &= \mu^2 + \underline{\tau}^2_{\mathrm{NXOR}(u,v)}.\end{aligned}$$

□

3.1. Special GSIs. Equation (3.1) describes a 2^{2d} dimensional family of linear combinations of pairwise function products. There are only 2^d-1 ANOVA components to estimate. Accordingly we are interested in special cases of (3.1) with desirable properties.

A GSI is a ***contrast*** if $\sum_u \sum_v \Omega_{uv} = 0$. Contrasts are unaffected by the value of the mean μ, and so they lead to unbiased estimators of linear combinations of variance components. GSIs that are not contrasts contain a term $\mu^2 \sum_u \sum_v \Omega_{uv}$ and require us to subtract an estimate $\hat{\mu}^2 \sum_u \sum_v \Omega_{uv}$ in order to estimate $\sum_u \sum_v \Omega_{uv} \underline{\tau}^2_{\mathrm{NXOR}(u,v)}$ as in Section 7.

A generalized Sobol' index is a ***square*** if it takes the form

$$\iint \Bigl(\sum_u \lambda_u f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) \Bigr)^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}.$$

Squares and sums of squares have the advantage that they are non-negative and hence avoid the problems associated with negative sample variance components. A square GSI can be written compactly as $\mathrm{tr}(\lambda\lambda^{\mathsf{T}}\Theta) = \lambda^{\mathsf{T}}\Theta\lambda$ where λ is a vector of 2^d coefficients. If λ_u is sparse (mostly zeros) then a square index is inexpensive to compute.

A generalized Sobol' index is ***bilinear*** if it takes the form

$$\iint \Bigl(\sum_u \lambda_u f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) \Bigr)\Bigl(\sum_v \gamma_v f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v}) \Bigr) \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}.$$

Bilinear estimates have the advantage of being rapidly computable. If there are $\|\lambda\|_0$ nonzero elements in λ and $\|\gamma\|_0$ nonzero elements in γ then the integrand in a bilinear generalized Sobol' index can be computed with at most $\|\gamma\|_0 + \|\lambda\|_0$ function calls and sometimes fewer (see Section 3.3) even though it combines values from $\|\gamma\|_0 \times \|\lambda\|_0$ function pairs. We can write the bilinear GSI as $\mathrm{tr}(\lambda\gamma^{\mathsf{T}}\Theta) = \gamma^{\mathsf{T}}\Theta\lambda$. The sum of a small number of bilinear GSIs is a low rank GSI.

A GSI is ***simple*** if it is written as a linear combination of entries in just one row or just one column of Θ, such as

$$\iint \sum_u \lambda_u f(\boldsymbol{x}) f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}.$$

It is convenient if the chosen row or column corresponds to u or v equal to $\varnothing$ or $\mathcal{D}$. Any linear combination $\sum_u \delta_u(\mu^2 + \underline{\tau}^2_u)$ of variance components and μ^2 can be written as a simple GSI taking $\lambda_u = \delta_u$. There are computational advantages to some non-simple representations.

3.2. Sample GSIs. To estimate a GSI we take pairs $(\boldsymbol{x}_i, \boldsymbol{z}_i) \overset{\mathrm{iid}}{\sim} \mathbf{U}(0,1)^{2d}$ for $i = 1, \dots, n$ and compute $\mathrm{tr}(\Omega^{\mathsf{T}}\widehat{\Theta})$ where

$$\widehat{\Theta}_{uv} = \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}) f(\boldsymbol{x}_{i,v}{:}\boldsymbol{z}_{i,-v}).$$

We can derive a matrix expression for the estimator by introducing the vectors

$$F_i \equiv F(\boldsymbol{x}_i, \boldsymbol{z}_i) = \bigl(f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u})\bigr)_{u \subseteq \mathcal{D}} \in \mathbb{R}^{2^d \times 1},$$

for $i = 1, \dots, n$ and the matrix

$$\mathbf{F} = \begin{pmatrix} F_1 & F_2 & \cdots & F_n \end{pmatrix}^{\mathsf{T}} \in \mathbb{R}^{n \times 2^d}.$$

The vectors F_i have covariance $\Theta - \mu^2\, 1_{2^d\times 2^d}$. Then

$$\widehat{\Theta} = \frac{1}{n}\sum_{i=1}^n F_iF_i^\mathsf{T} = \frac{1}{n}\mathbf{F}^\mathsf{T}\mathbf{F},$$

and the sample GSI is

$$\mathrm{tr}(\Omega^\mathsf{T}\widehat{\Theta}) = \mathrm{tr}(\widehat{\Theta}^\mathsf{T}\Omega) = \frac{1}{n}\mathrm{tr}(\mathbf{F}^\mathsf{T}\mathbf{F}\Omega) = \frac{1}{n}\mathrm{tr}(\mathbf{F}\Omega\mathbf{F}^\mathsf{T}).$$

3.3. Cost per $(\boldsymbol{x},\boldsymbol{z})$ pair. We suppose that the cost of computing a sample GSI is dominated by the number of function evaluations required. If the GSI requires $C(\Omega)$ (defined below) distinct function evaluations per pair $(\boldsymbol{x}_i,\boldsymbol{z}_i)$ for $i=1,\dots,n$, then the cost of the sample GSI is proportional to $nC(\Omega)$.

If the row Ω_{uv} for given u and all values of v is not entirely zero then we need the value $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})$. Let

$$C_{u\bullet}(\Omega) = \begin{cases} 1, & \exists v\subseteq\mathcal{D} \quad \text{with} \quad \Omega_{uv}\ne 0\\ 0, & \text{else}\end{cases}$$

indicate whether $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})$ is needed as the 'left side' of a product $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})$. Next, let $C_{u\bullet}(\Omega^\mathsf{T})$ indicate whether $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})$ is ever needed as the 'right side' of such a product. The number of function evaluations required for the GSI $\mathrm{tr}(\Omega^\mathsf{T}\Theta)$ is:

$$C(\Omega) = \sum_{u\subseteq\mathcal{D}}\Bigl(C_{u\bullet}(\Omega) + C_{u\bullet}(\Omega^\mathsf{T}) - C_{u\bullet}(\Omega)C_{u\bullet}(\Omega^\mathsf{T})\Bigr). \tag{3.2}$$

We count the number of rows of Ω for which $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})$ is needed, add the number of columns and then subtract the number of double counted sets u.

For example, suppose we take $\Omega_{\{1\},\{1\}} = \Omega_{\{2\},\{2\}} = 1/2$ and $\Omega_{\{1\},\{2\}} = -1$ and all other $\Omega_{u,v}=0$. Then

$$\mathrm{tr}(\Omega^\mathsf{T}\Theta) = \frac{1}{2}\underline{\tau}^2_{\mathrm{NXOR}(\{1\},\{1\})} + \frac{1}{2}\underline{\tau}^2_{\mathrm{NXOR}(\{2\},\{2\})} - \underline{\tau}^2_{\mathrm{NXOR}(\{1\},\{2\})} = \sigma^2_{\{1,2\}}$$

after some algebra. Notice that, as here, Ω need not be symmetric. First $C_{\{1\}\bullet}(\Omega) = C_{\{2\}\bullet}(\Omega) = 1$ because both rows $u=\{1\}$ and $u=\{2\}$ are needed. All other $C_{u\bullet}(\Omega) = 0$. Similarly $C_{\{1\}\bullet}(\Omega^\mathsf{T}) = C_{\{2\}\bullet}(\Omega^\mathsf{T}) = 1$ because both columns $u=\{1\}$ and $\{2\}$ of Ω contain nonzero entries and all other $C_{u\bullet}(\Omega^\mathsf{T})=0$. It follows that $C_{u\bullet}(\Omega)+C_{u\bullet}(\Omega^\mathsf{T})-C_{u\bullet}(\Omega)C_{u\bullet}(\Omega^\mathsf{T})$ is 1 for $u=\{1\}$ or $\{2\}$ and is otherwise 0. Now equation (3.2) gives $C(\Omega)=2$, even though Ω has 3 nonzero entries. To verify that the cost is 2 per $(\boldsymbol{x},\boldsymbol{z})$ pair, we may write the estimator $\mathrm{tr}(\Omega^\mathsf{T}\widehat{\Theta})$ as

$$\frac{1}{n}\sum_{i=1}^n\biggl(\frac{1}{2}f(\boldsymbol{x}_{i,\{1\}}{:}\boldsymbol{z}_{i,-\{1\}})^2 + \frac{1}{2}f(\boldsymbol{x}_{i,\{2\}}{:}\boldsymbol{z}_{i,-\{2\}})^2 - f(\boldsymbol{x}_{i,\{1\}}{:}\boldsymbol{z}_{i,-\{1\}})f(\boldsymbol{x}_{i,\{2\}}{:}\boldsymbol{z}_{i,-\{2\}})\biggr)$$

and see that the two function evaluations needed are $f(\boldsymbol{x}_{i,\{1\}}{:}\boldsymbol{z}_{i,-\{1\}})$ and $f(\boldsymbol{x}_{i,\{2\}}{:}\boldsymbol{z}_{i,-\{2\}})$.

The preceding example is a contrast, and so it was not necessary to subtract $\hat{\mu}^2$ from any of the terms. For non-contrasts, the estimate $\hat{\mu}$ can be constructed by averaging all nC function evaluations $f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u})$ that are computed. No additional function evaluations are required for $\hat{\mu}$.

4. Squares and sums of squares. A square or sum of squares yields a nonnegative estimate. An unbiased and nonnegative estimate is especially valuable. When the true GSI is zero, an unbiased nonnegative estimate will always return exactly zero as Fruth et al. [2012] remark. The Sobol' index $\overline{\tau}_u^2$ is of square form, but $\underline{\tau}_u^2$ is not. Theorem 2.2 leads to a sum of squares for $\sum_u |u|\sigma_u^2$.

Liu and Owen [2006] express the superset importance measure as a square:

$$\Upsilon_u^2 = \frac{1}{2^{|u|}} \iint \Bigl|\sum_{v\subseteq u} (-1)^{|u-v|} f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v})\Bigr|^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}. \tag{4.1}$$

Fruth et al. [2012] find that a sample version of (4.1) is the best among four estimators of Υ_u^2.

In classical crossed mixed effects models [Montgomery, 1998] every ANOVA expected mean square has a contribution from the highest order variance component, typically containing measurement error. A similar phenomenon applies for Sobol' indices. In particular, no square GSI or sum of squares will yield $\underline{\tau}_u^2$ for $|u| < d$, as the next proposition shows.

PROPOSITION 4.1. *The coefficient of $\sigma_{\mathcal{D}}^2$ in $\sum_{r=1}^R \iint (\sum_u \lambda_{r,u} f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}))^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}$ is $\sum_{r=1}^R \sum_u \lambda_{r,u}^2$.*

Proof. It is enough to show this for $R = 1$ with $\lambda_{1,u} = \lambda_u$. First,

$$\iint (\sum_u \lambda_u f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}))^2 \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z} = \lambda^{\mathsf{T}}\Theta\lambda. \tag{4.2}$$

Next, the only elements of Θ containing $\sigma_{\mathcal{D}}^2$ are the diagonal ones, equal to σ^2. Therefore the coefficient of $\sigma_{\mathcal{D}}^2$ in (4.2) is $\sum_u \lambda_u^2$. ◻

For a square or sum of squares to be free of $\sigma_{\mathcal{D}}^2$ it is necessary to have $\sum_{r=1}^R \sum_u \lambda_{r,u}^2 = 0$. That in turn requires all the $\lambda_{r,u}$ to vanish, leading to the degenerate case $\Omega = 0$. As a result, we cannot get an unbiased sum of squares for any GSI that does not include $\sigma_{\mathcal{D}}^2$. In particular, we have the following corollary.

COROLLARY 4.2. *If $|u| < d$ then no sum of squares GSI can yield an unbiased estimate of $\underline{\tau}_u^2$.*

5. Specific variance components. For any $w \subseteq \mathcal{D}$ the variance component for w is given in (2.3) as an alternating sum of $2^{|w|}$ Sobol' indices. It can thus be estimated by a simple GSI,

$$f(\boldsymbol{x}) \sum_{v\subseteq w} \lambda_v f(\boldsymbol{x}_v{:}\boldsymbol{z}_{-v}) \tag{5.1}$$

where $\lambda_v = (-1)^{|w-v|}$. The cost of this simple GSI is $C = 2^{|w|} + 1_{|w|<d}$. If $w = \mathcal{D}$, then $f(\boldsymbol{x})$ appears twice, but otherwise it is only used once.

This GSI can also be estimated by some bilinear GSIs using fewer function evaluations as we show here. Because it is an alternating sum, there is the possibility of writing it as the product of two smaller alternating sums, as described below.

We begin by noting that for $u, v \subseteq w$,

$$\mathrm{NXOR}(u, v + w^c) = (\mathrm{XOR}(u, v) + w^c)^c = \mathrm{NXOR}(u, v) \cap w$$

and so

$$\Theta_{u,v+w^c} = \mu^2 + \underline{\tau}^2_{\mathrm{NXOR}(u,v)\cap w}$$

does not involve any of the variables x_j for $j \notin w$. Note especially that $\mathrm{NXOR}(u, v)$ itself contains all of w^c and is *not* helpful in estimating σ_w^2 when $|w| < d$.

We develop the method by first getting an expression for σ_w^2 with $w = \{1, 2, 3\}$. Then we give Theorem 5.1 below for the general case. Let u be any subset of $\{1\}$, that is $u = \varnothing$ or $u = \{1\}$. Let v be any of the eight subsets of w. Then we can work out a 2×8 submatrix of the Sobol' matrix with entries $\mathrm{NXOR}(u, v + w^c)$,

$$\begin{array}{c|cccccccc} \mathrm{NXOR}(u,v{+}w^c) & \varnothing & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ \hline \varnothing & 123 & 23 & 13 & 12 & 3 & 2 & 1 & \varnothing \\ 1 & 23 & 123 & 3 & 2 & 13 & 12 & \varnothing & 1 \end{array} \tag{5.2}$$

where we omit braces and commas from the set notation.

We want $\sigma_w^2 = \Theta_{\{1,2,3\}} - \Theta_{\{1,2\}} - \Theta_{\{1,3\}} - \Theta_{\{2,3\}} + \Theta_{\{1\}} + \Theta_{\{2\}} + \Theta_{\{3\}} - \Theta_{\varnothing}$. This is the componentwise inner product of the matrix Θ indexed by (5.2) with coefficients given by

$$\begin{array}{c|cccccccc} & \varnothing & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ \hline \varnothing & 1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 1 & 1 & 0 & 0 & -1 & 0 \end{array}. \tag{5.3}$$

There are other matrices of coefficients that would also yield σ_w^2 but the one in (5.3) has zeros in every column containing a 1 in its index and this proves useful below.

The coefficients in (5.3) form a rank one matrix. If we construct an entire $2^d \times 2^d$ Sobol' matrix matching those entries and take all other entries to be zero, the result remains of rank 1. It follows now that we can use a non-simple bilinear GSI, $\lambda^{\mathsf{T}}\Theta\gamma$, where λ and γ are given by

$$\begin{array}{c|cccccccc} & \varnothing & 1 & 2 & 3 & 12 & 13 & 23 & 123 \\ \hline \lambda_u & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \gamma_v & 1 & 0 & -1 & -1 & 0 & 0 & 1 & 0 \end{array} \tag{5.4}$$

with u and $v - w^c$ given along the top labels in (5.4) while the remaining $2^d - 8$ elements of λ and γ are all zero. Specifically, the expected value of

$$\sum_{u \subseteq \{1\}} \sum_{v \subseteq \{2,3\}} (-1)^{|u|+|v|} f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) f(\boldsymbol{x}_{v+w^c}{:}\boldsymbol{z}_{w-v}) \tag{5.5}$$

is $\sigma^2_{\{1,2,3\}}$. While equation (5.1) for $w = \{1, 2, 3\}$ requires 9 function evaluations per $(\boldsymbol{x}, \boldsymbol{z})$ pair, equation (5.5) only requires 6 function evaluations. For $|w| < d$, the $u = \varnothing$ and $v = \varnothing$ evaluations are different due to the presence of w^c, so no evaluations are common to both the λ and γ expressions. There are also two variants of (5.4) that single out variables 2 and 3 respectively, analogously to the way that (5.5) treats variable 1. Theorem 5.1 generalizes the example above.

THEOREM 5.1. *Let w be a nonempty subset of $\mathcal{D}$ for $d \geqslant 1$. Let $f \in L^2[0, 1]^d$. Choose $w_1 \subseteq w$ and put $w_2 = w - w_1$. Then*

$$\sigma_w^2 = \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \iint f(\boldsymbol{x}_{u_1}{:}\boldsymbol{z}_{-u_1}) f(\boldsymbol{x}_{u_2+w^c}{:}\boldsymbol{z}_{w-u_2}) \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{z}. \tag{5.6}$$

Proof. Because the right hand side of (5.6) is a contrast, we can assume that $\mu = 0$. Then $\mathrm{NXOR}(u_1, u_2 + w^c) = \mathrm{NXOR}(u_1, u_2) \cap w = w - (u_1 + u_2)$. Therefore

$$\sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \Theta_{u_1, u_2 + w^c} = \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \underline{\tau}^2_{w-(u_1+u_2)}$$
$$= \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|w_1-u_1|+|w_2-u_2|} \underline{\tau}^2_{u_1+u_2}$$

after a change of variable from u_j to $w_j - u_j$ for $j = 1, 2$. We may write the above as

$$\sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|w_1-u_1|+|w_2-u_2|} \sum_{v \subseteq u_1+u_2} \sigma^2_v. \tag{5.7}$$

Consider the set $v \subseteq \mathcal{D}$. The coefficient of σ^2_v in (5.7) is 0 if $v \cap w^c \neq \varnothing$. Otherwise, we may write $v = v_1 + v_2$ where $v_j \subseteq w_j$, $j = 1, 2$. Then the coefficient of σ^2_v in (5.7) is

$$\sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|w_1-u_1|+|w_2-u_2|} 1_{v \subseteq u_1+u_2}$$
$$= \sum_{u_1 : v_1 \subseteq u_1 \subseteq w_1} (-1)^{|w_1-u_1|} \sum_{u_2 : v_2 \subseteq u_2 \subseteq w_2} (-1)^{|w_2-u_2|}.$$

These alternating sums over u_j with $v_j \subseteq u_j \subseteq w_j$ equal 1 if $v_j = w_j$ but otherwise they are zero. Therefore the coefficient of σ^2_v in (5.7) is 1 if $v = w$ and is 0 otherwise. ∎

In general, bilinear GSIs let us estimate σ^2_w using $2^k + 2^{|w|-k}$ function evaluations per $(\boldsymbol{x}, \boldsymbol{z})$ pair for integer $1 \leqslant k < |w|$ instead of the $2^{|w|}$ evaluations that a simple GSI requires.

We can use Theorem 5.1 to get a bilinear (but not square) estimator of $\sigma^2_{\mathcal{D}} = \Upsilon^2_{\mathcal{D}}$. A similar argument to that in Theorem 5.1 yields a bilinear estimator of superset importance Υ^2_w for a general set w.

THEOREM 5.2. *Let w be a nonempty subset of $\mathcal{D}$ for $d \geqslant 1$. Let $f \in L^2[0,1]^d$. Choose $w_1 \subseteq w$ and put $w_2 = w - w_1$. Then*

$$\Upsilon^2_w = \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \Theta_{w^c+u_1, w^c+u_2}. \tag{5.8}$$

Proof. Because $w \neq \varnothing$, the estimate is a contrast and so we may suppose $\mu = 0$. For disjoint $u_1, u_2 \subseteq w$, $\mathrm{NXOR}(w^c + u_1, w^c + u_2) = \mathcal{D} - u_1 - u_2$, and so the right side of (5.8) equals

$$\sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \underline{\tau}^2_{\mathcal{D}-u_1-u_2} = \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} \sum_{v \subseteq \mathcal{D}-u_1-u_2} \sigma^2_v$$
$$= \sum_v \sigma^2_v \sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} 1_{v \subseteq \mathcal{D}-u_1-u_2}.$$

Now write $v = (v \cap w^c) + v_1 + v_2$ with $v_j \subseteq w_j$, $j = 1, 2$. The coefficient of σ^2_v is

$$\sum_{u_1 \subseteq w_1} \sum_{u_2 \subseteq w_2} (-1)^{|u_1|+|u_2|} 1_{u_1 \cap v_1 = \varnothing} 1_{u_2 \cap v_2 = \varnothing}.$$

Now

$$\sum_{u_1\subseteq w_1}(-1)^{|u_1|}1_{u_1\cap v_1=\varnothing}=\sum_{u_1\subseteq w_1-v_1}(-1)^{|u_1|}$$

which vanishes unless $w_1=v_1$ and otherwise equals 1. Therefore the coefficient of σ_v^2 is 1 if $v\supseteq w$ and is 0 otherwise. □

The cost of the estimator (5.8) is $C=2^{|w_1|}+2^{|w_2|}-1$, because the evaluation $f(\boldsymbol{x}_{w^c}{:}\boldsymbol{z}_w)$ can be used for both $u_1=\varnothing$ and $u_2=\varnothing$.

6. GSIs with cost $O(d)$.

Some problems, like computing mean dimension, can be solved with $O(d)$ different integrals instead of the $O(2^d)$ required to estimate all ANOVA components. In this section we enumerate what can be estimated by certain GSIs based on only $O(d)$ carefully chosen function evaluations per $(\boldsymbol{x}_i,\boldsymbol{z}_i)$ pair.

6.1. Cardinality restricted GSIs.

One way to reduce function evaluations to $O(d)$ is to consider only subsets u and v with cardinality 0, 1, $d-1$, or d. We suppose that $d>2$ (so that no set has cardinality equal to two of 0, 1, $d-1$ and d) and that j and k are distinct elements of $\mathcal{D}$. Letting j and k substitute for $\{j\}$ and $\{k\}$ respectively we can enumerate $\mathrm{NXOR}(u,v)$ for all of these subsets as follows,

$$\begin{array}{c} \text{NXOR} \\ \varnothing \\ j \\ -j \\ \mathcal{D} \end{array}\begin{array}{c} \begin{array}{cccccc} \varnothing & j & k & -j & -k & \mathcal{D} \end{array} \\ \left[\begin{array}{cccccc} \mathcal{D} & -j & -k & j & k & \varnothing \\ -j & \mathcal{D} & -\{j,k\} & \varnothing & \{j,k\} & j \\ j & \varnothing & \{j,k\} & \mathcal{D} & -\{j,k\} & -j \\ \varnothing & j & k & -j & -k & \mathcal{D} \end{array}\right] \end{array},$$

and hence the accessible elements of the Sobol' matrix are:

$$\begin{array}{c} \Theta_{uv}-\mu^2 \\ \varnothing \\ j \\ -j \\ \mathcal{D} \end{array}\begin{array}{c} \begin{array}{cccccc} \varnothing & j & k & -j & -k & \mathcal{D} \end{array} \\ \left[\begin{array}{cccccc} \sigma^2 & \underline{\tau}^2_{-j} & \underline{\tau}^2_{-k} & \underline{\tau}^2_{j} & \underline{\tau}^2_{k} & 0 \\ \underline{\tau}^2_{-j} & \sigma^2 & \underline{\tau}^2_{-\{j,k\}} & 0 & \underline{\tau}^2_{\{j,k\}} & \underline{\tau}^2_{j} \\ \underline{\tau}^2_{j} & 0 & \underline{\tau}^2_{\{j,k\}} & \sigma^2 & \underline{\tau}^2_{-\{j,k\}} & \underline{\tau}^2_{-j} \\ 0 & \underline{\tau}^2_{j} & \underline{\tau}^2_{k} & \underline{\tau}^2_{-j} & \underline{\tau}^2_{-k} & \sigma^2 \end{array}\right] \end{array}. \tag{6.1}$$

Using (6.1) we can estimate $\sum_{j=1}^d(\sigma^2-\underline{\tau}^2_{-\{j\}})=\sum_{j=1}^d\overline{\tau}^2_{\{j\}}=\sum_u|u|\sigma_u^2$, by

$$\sum_{j=1}^d f(\boldsymbol{x})\bigl(f(\boldsymbol{x})-f(\boldsymbol{x}_{-\{j\}}{:}\boldsymbol{z}_{\{j\}})\bigr),$$

at cost $C=d+1$. Similarly

$$\sum_{j=1}^d f(\boldsymbol{x})(f(\boldsymbol{x}_{\{j\}}{:}\boldsymbol{z}_{-\{j\}})-f(\boldsymbol{z}))$$

provides an unbiased GSI estimator of $\sum_{j=1}^d\underline{\tau}^2_{\{j\}}=\sum_{j=1}^d\sigma^2_{\{j\}}=\sum_{|u|=1}\sigma_u^2$. The cost is $C=d+2$.

More interestingly, it is possible to compute all $d(d-1)/2$ indices $\overline{\tau}^2_{\{j,k\}}$ along with all $\underline{\tau}^2_{\{j\}}$ and $\overline{\tau}^2_{\{j\}}$ for $j=1,\dots,d$, at total cost $C=d+2$ as was first shown by Saltelli [2002, Theorem 1]. Given $C=2d+2$ evaluations one can also compute all of the $\underline{\tau}^2_{\{j,k\}}$ indices by pairing up $u=\{j\}$ and $v=-\{k\}$ [Saltelli, 2002, Theorem 2].

For the remainder of this section we present some contrast estimators. The estimate

$$\frac{1}{2n}\sum_{j=1}^{d}\bigl(f(\boldsymbol{x})-f(\boldsymbol{x}_{\{-j\}}{:}\boldsymbol{z}_{\{j\}})\bigr)^2.$$

is both a contrast and a sum of squares. It has expected value $\sum_u |u|\sigma_u^2$ and cost $C=d+1$.

The total of second order interactions can be estimated with a contrast at cost $C=2d+2$. Taking

$$\lambda_u=\begin{cases}1, & |u|=1\\ -d, & |u|=0\\ 0, & \text{else,}\end{cases}\quad\text{and}\quad \gamma_v=\begin{cases}1, & |v|=d-1\\ -(d-2), & |v|=d\\ 0, & \text{else}\end{cases}$$

we get a contrast with

$$\begin{aligned}\lambda^{\mathsf{T}}\Theta\gamma&=\sum_{j=1}^{d}\sum_{k=1}^{d}\underline{\tau}^2_{\{j,k\}}1_{j\ne k}-d\sum_{k=1}^{d}\underline{\tau}^2_{\{k\}}-(d-2)\sum_{j=1}^{d}\underline{\tau}^2_{\{j\}}\\&=2\sum_{|u|=2}\underline{\tau}^2_u-(2d-2)\sum_{|u|=1}\underline{\tau}^2_u=2\sum_{|u|=2}\sigma_u^2.\end{aligned}$$

Thus $\lambda^{\mathsf{T}}\widehat{\Theta}\gamma/2$ estimates $\sum_{|u|=2}\sigma_u^2$, at cost $C=2d+2$.

Next, taking

$$\lambda_u=\begin{cases}1, & |u|=1\\ -d, & |u|=0\\ 0, & \text{else,}\end{cases}\quad\text{and}\quad \gamma_v=\begin{cases}1, & |v|=1\\ -(d-2), & |v|=0\\ 0, & \text{else}\end{cases}$$

we get a contrast with

$$\begin{aligned}\lambda^{\mathsf{T}}\Theta\gamma&=\sum_{j=1}^{d}\sum_{k=1}^{d}\underline{\tau}^2_{-\{j,k\}}1_{j\ne k}+\sum_{j=1}^{d}\sigma^2-d\sum_{k=1}^{d}\underline{\tau}^2_{-\{k\}}-(d-2)\sum_{j=1}^{d}\underline{\tau}^2_{-\{j\}}+d(d-2)\sigma^2\\&=d^2\sigma^2-\sum_{j=1}^{d}\sum_{k=1}^{d}\overline{\tau}^2_{\{j,k\}}1_{j\ne k}-2d(d-1)\sigma^2+2(d-1)\sum_{j=1}^{d}\overline{\tau}^2_{\{j\}}+d(d-2)\sigma^2\\&=2(d-1)\sum_{j=1}^{d}\overline{\tau}^2_{\{j\}}-\sum_{j=1}^{d}\sum_{k=1}^{d}\overline{\tau}^2_{\{j,k\}}1_{j\ne k}=\sum_u |u|^2\sigma_u^2,\end{aligned}$$

using Theorem 2.2. Therefore $\mathbb{E}\bigl(\lambda^{\mathsf{T}}\widehat{\Theta}\gamma\bigr)=\sum_u |u|^2\sigma_u^2$, at cost $C=d+1$ because only sets u with $|u|=1$ and $|u|=0$ are used.

6.2. Consecutive index GSIs. A second way to reduce function evaluations to $O(d)$ is to consider only subsets u and v of the form $\{1,2,\dots,j\}$ and $\{j+1,\dots,d\}$. We write these as $(0,j]$ and $(j,d]$ respectively. If $f(\boldsymbol{x})$ is the result of a process evolving in discrete time then $(0,j]$ represents the effects of inputs up to time j and $(j,d]$ represents those after time j. A small value of $\overline{\tau}^2_{(0,j]}$ then means that the first j

inputs are nearly forgotten while a large value for $\underline{\tau}^2_{(0,j]}$ means the initial conditions have a lasting effect.

We suppose for $d \geqslant 2$ that $1 \leqslant j < k \leqslant d$. Once again, we can enumerate $\mathrm{NXOR}(u, v)$ for all of the subsets of interest:

$$
\begin{array}{c} \text{NXOR} \\ \varnothing \\ (0,j] \\ (j,d] \\ \mathcal{D} \end{array}
\begin{array}{c}
\begin{array}{cccccc} \varnothing & (0,j] & (0,k] & (j,d] & (k,d] & \mathcal{D} \end{array} \\
\left[\begin{array}{cccccc}
\mathcal{D} & (j,d] & (k,d] & (0,j] & (0,k] & \varnothing \\
(j,d] & \mathcal{D} & -(j,k] & \varnothing & (j,k] & (0,j] \\
(0,j] & \varnothing & (j,k] & \mathcal{D} & -(j,k] & (j,d] \\
\varnothing & (0,j] & (0,k] & (j,d] & (k,d] & \mathcal{D}
\end{array}\right]
\end{array}, \tag{6.2}
$$

and hence the accessible elements of the Sobol' matrix are $\mu^2 + \underline{\tau}^2_u$ for the sets u in the array above.

The same strategies used on singletons and their complements can be applied to consecutive indices. They yield interesting quantities related to mean dimension in the truncation sense. To describe them, we write $\lfloor u \rfloor = \min\{j \mid j \in u\}$ and $\lceil u \rceil = \max\{j \mid j \in u\}$ for the least and greatest indices in the non-empty set u.

PROPOSITION 6.1. *Let $f \in L^2[0,1]^d$ have variance components σ^2_u. Then*

$$
\sum_{j=1}^{d-1} \bigl(\Theta_{(0,j],\mathcal{D}} - \Theta_{\varnothing,\mathcal{D}}\bigr) = \sum_{u \subseteq \mathcal{D}} (d - \lceil u \rceil)\sigma^2_u, \quad \textit{and,}
$$

$$
\sum_{j=1}^{d-1} \bigl(\Theta_{(j,d],\mathcal{D}} - \Theta_{\varnothing,\mathcal{D}}\bigr) = \sum_{u \subseteq \mathcal{D}} (\lfloor u \rfloor - 1)\sigma^2_u.
$$

Proof. Since these are contrasts, we may suppose that $\mu = 0$. Then, using (6.2)

$$
\sum_{j=1}^{d-1} \Theta_{(0,j],\mathcal{D}} = \sum_{j=1}^{d-1} \underline{\tau}^2_{(0,j]} = (d-1)\sigma^2 - \sum_{j=1}^{d-1} \overline{\tau}^2_{(j,d]}.
$$

Next, $\Theta_{\varnothing,\mathcal{D}} = 0$, and

$$
\sum_{j=1}^{d-1} \overline{\tau}^2_{(j,d]} = \sum_{u \subseteq \mathcal{D}} \sigma^2_u \sum_{j=1}^{d-1} 1_{\{j+1,\dots,d\} \cap u \neq \varnothing} = \sum_{u \subseteq \mathcal{D}} (\lceil u \rceil - 1)\sigma^2_u.
$$

Combining these yields the first result. The second is similar. ∎

Using Proposition 6.1 we can obtain an estimate of $\sum_u \lceil u \rceil \sigma^2_u / \sigma^2$, the mean dimension of f in the truncation sense. We also obtain a contrast

$$
\sum_{j=1}^{d-1} (\Theta_{\mathcal{D},\mathcal{D}} - \Theta_{(0,j],\mathcal{D}} - \Theta_{(j,d],\mathcal{D}} + 2\Theta_{\varnothing,\mathcal{D}}) = \sum_u (\lceil u \rceil - \lfloor u \rfloor)\sigma^2_u
$$

which measures the extent to which indices at distant time lags contribute important interactions.

We can also construct GSIs based on pairs of segments. For example,

$$
\begin{aligned}
\sum_{j=0}^{d-1} \sum_{k=j+1}^{d} \Theta_{(0,j],(k,d]} - \frac{d(d-1)}{2}\mu^2 &= \sum_u \sigma^2_u \sum_{j=0}^{d-1} \sum_{k=j+1}^{d} 1_{u \subseteq (j,k]} \\
&= \sum_u \sigma^2_u \lfloor u \rfloor \bigl(d - \lceil u \rceil + 1\bigr).
\end{aligned}
$$

7. Bias corrected GSIs. When we are interested in estimating a linear combination of variance components, then the corresponding GSI is a contrast. To see this, note that a linear combination of variance components σ_u^2 is also a linear combination of $\underline{\tau}_u^2$ by the Moebius relation (2.3). The coefficient of μ^2 in the GSI is $\sum_u \sum_v \Omega_{uv}$ which must be zero (yielding a contrast) if our target is a linear combination of $\underline{\tau}_u^2$. Sometimes an unbiased estimate of a contrast contrast uses more function evaluations per $(\boldsymbol{x}_i, \boldsymbol{z}_i)$ pair than a corresponding biased estimator does. For instance the unbiased estimator (2.2) of $\underline{\tau}_u^2$ requires three function evaluations per pair compared to the two required by the biased estimator of Janon et al. [2012].

Proposition 7.1 supplies a bias-corrected version of Janon et al.'s (2011) estimator of $\underline{\tau}_u^2$ using only two function evaluations per $(\boldsymbol{x}_i, \boldsymbol{z}_i)$ pair.

PROPOSITION 7.1. *Let $f \in L^2[0,1]^d$ and suppose that $\boldsymbol{x}_i, \boldsymbol{z}_i \overset{\text{iid}}{\sim} \mathbf{U}(0,1)^d$ for $i = 1, \dots, n$ where $n \geqslant 2$. Let $\boldsymbol{y}_i = \boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}$ and define*

$$\hat\mu = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_i), \qquad \hat\mu' = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{y}_i),$$

$$s^2 = \frac{1}{n-1}\sum_{i=1}^n (f(\boldsymbol{x}_i)-\hat\mu)^2, \quad \text{and} \qquad {s'}^2 = \frac{1}{n-1}\sum_{i=1}^n (f(\boldsymbol{y}_i)-\hat\mu')^2.$$

Then $\mathbb{E}\bigl(\widetilde{\underline{\tau}}_u^2\bigr) = \underline{\tau}_u^2$ where

$$\widetilde{\underline{\tau}}_u^2 = \frac{2n}{2n-1}\biggl(\frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_i)f(\boldsymbol{y}_i) - \Bigl(\frac{\hat\mu+\hat\mu'}{2}\Bigr)^2 + \frac{s^2+{s'}^2}{4n}\biggr)$$

Proof. First $\mathbb{E}(f(\boldsymbol{x}_i)f(\boldsymbol{y}_i)) = \mu^2 + \underline{\tau}_u^2$. Next

$$\begin{aligned}\mathbb{E}((\hat\mu+\hat\mu')^2) &= 4\mu^2 + \mathrm{Var}(\hat\mu) + \mathrm{Var}(\hat\mu') + 2\mathrm{Cov}(\hat\mu,\hat\mu') \\ &= 4\mu^2 + 2\frac{\sigma^2}{n} + 2\frac{\underline{\tau}_u^2}{n}.\end{aligned}$$

Finally $\mathbb{E}(s^2) = \mathbb{E}({s'}^2) = \sigma^2$. Putting these together yields the result. □

More generally, suppose that $\mathbb{E}\bigl(\mathrm{tr}(\Omega^{\mathsf{T}}\widehat{\Theta})\bigr)$ contains a contribution of $\mu^2\mathbf{1}^{\mathsf{T}}\Omega\mathbf{1}$ which is nonzero if Ω is not a contrast. Then a bias correction is available for $\mathrm{tr}(\Omega^{\mathsf{T}}\Theta)$. We may take the bias correction from Proposition 7.1 and apply it term by term as Proposition 7.2 shows.

PROPOSITION 7.2. *Let $f \in L^2[0,1]^d$ and suppose that $\boldsymbol{x}_i, \boldsymbol{z}_i \overset{\text{iid}}{\sim} \mathbf{U}(0,1)^d$ for $i = 1, \dots, n$ for $n \geqslant 2$. For $u \subseteq \mathcal{D}$ define*

$$\hat\mu_u = \frac{1}{n}\sum_{i=1}^n f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}), \quad \text{and} \quad s_u^2 = \frac{1}{n-1}\sum_{i=1}^n (f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u}) - \hat\mu_u)^2.$$

Then

$$\frac{2n}{2n-1}\sum_u\sum_v \Omega_{uv}\Bigl(\widehat{\Theta}_{uv} - \Bigl(\frac{\hat\mu_u+\hat\mu_v}{2}\Bigr)^2 + \frac{s_u^2+{s_v}^2}{4n}\Bigr) \tag{7.1}$$

is an unbiased estimate of $\sum_u\sum_v \Omega_{uv}(\Theta_{uv}-\mu^2)$.

Proof. This follows by applying Proposition 7.1 term by term. □

The computational burden for the unbiased estimator in Proposition 7.2 is not much greater than that for the possibly biased estimator $\mathrm{tr}(\Omega^\mathsf{T}\widehat{\Theta})$. It requires no additional function evaluations. The quantities $\hat\mu_u$ and s_u^2 need only be computed for sets $u \subseteq \mathcal{D}$ for which Ω_{uv} or Ω_{vu} is nonzero for some v. If Ω is a sum of bilinear estimators then the $-\sum_u\sum_v \Omega_{uv}\hat\mu_u\hat\mu_v/2$ cross terms also have that property.

The bias correction in estimator (7.1) complicates calculation of confidence intervals for $\mathrm{tr}(\Omega^\mathsf{T}\Theta)$. Jackknife or bootstrap methods will work but confidence intervals for contrasts are much simpler because the estimators are simple averages.

8. Comparisons. There is a 2^{2d}–dimensional space of GSIs but only a 2^d-1–dimensional space of linear combinations of variance components to estimate. As a result there is more than one way to estimate a desired linear combination of variance components.

As a case in point the Sobol' index $\underline{\tau}_u^2$ can be estimated by either the original method or by the contrast (2.2). Janon et al. [2012] prove that their estimate of $\hat\mu$ improves on the simpler one and establish asymptotic efficiency for their estimator within a class of methods based on exchangeability, but that class does not include the contrast. Similarly, inspecting the Sobol' matrix yields at least four ways to estimate the variance component $\sigma^2_{\{1,2,3\}}$, and superset importance can be estimated via a square or a bilinear term.

Here we consider some theoretical aspects of the comparison, but they do not lead to unambiguous choices. Next we consider a small set of empirical investigations.

8.1. Minimum variance estimation. Ideally we would like to choose Ω to minimize the variance of the sample GSI. But the variance of a GSI depends on fourth moments of ANOVA contributions which are ordinarily unknown and harder to estimate than the variance components themselves.

The same issue comes up in the estimation of variance components, where MINQE (minimum norm quadratic estimation) estimators were proposed in a series of papers by C. R. Rao in the 1970s. For a comprehensive treatment see Rao and Kleffe [1988] who present MINQUE and MINQIE versions using unbiasedness or invariance as constraints. The idea in MINQUE estimation is to minimize a convenient quadratic norm as a proxy for the variance of the estimator.

The GSI context involves variance components for crossed random effects models with interactions of all orders. Even the two way crossed random effects model with an interaction is complicated enough that no closed form estimator appears to be known for that case. See Kleffe [1980].

We can however generalize the idea behind MINQE estimators to the GSI setting. Writing

$$\mathrm{Var}(\mathrm{tr}(\Omega^\mathsf{T}\widehat{\Theta})) = \sum_{u\subseteq\mathcal{D}}\sum_{v\subseteq\mathcal{D}}\sum_{u'\subseteq\mathcal{D}}\sum_{v'\subseteq\mathcal{D}} \Omega_{uv}\Omega_{u'v'}\mathrm{Cov}\bigl(\widehat{\Theta}_{uv},\widehat{\Theta}_{u'v'}\bigr)$$

we can obtain the upper bound

$$\mathrm{Var}(\mathrm{tr}(\Omega^\mathsf{T}\widehat{\Theta})) \leqslant \biggl(\sum_{u\subseteq\mathcal{D}}\sum_{v\subseteq\mathcal{D}}|\Omega_{uv}|\biggr)^2 \max_{u,v}\mathrm{Var}\bigl(\widehat{\Theta}_{uv}\bigr),$$

leading to a proxy measure

$$V(\Omega) = \biggl(\sum_{u\subseteq\mathcal{D}}\sum_{v\subseteq\mathcal{D}}|\Omega_{uv}|\biggr)^2. \tag{8.1}$$

Using the proxy for variance suggests choosing the estimator which minimizes $C(\Omega)\times V(\Omega)$. The contrast estimator (2.2) of $\underline{\tau}_u^2$ has $C(\Omega)\times V(\Omega) = 3\times(1+1)^2 = 12$ while the original Sobol' estimator has $C(\Omega)\times V(\Omega) = 2\times 1 = 2$. An estimator for $\sigma^2_{\{1,2,3\}}$ based on (5.1) has $V(\Omega) = 8^2 = 64$, the same as one based on (5.5). The former has cost $C(\Omega) = 9$, while the latter costs $C(\Omega) = 6$. As a result, the proxy arguments support the original Sobol' estimator and the alternative estimator (5.4) for $\sigma^2_{\{1,2,3\}}$. This proxy is very crude. For example it does not take account of alternating signs among the Ω_{uv} and these are empirically seen to be important in the numerical examples of this section.

8.2. Test cases. To compare some estimators we use test functions of product form:

$$f(\boldsymbol{x}) = \prod_{j=1}^d (\mu_j + \tau_j g_j(x_j)) \tag{8.2}$$

where each g_j satisfies

$$\int_0^1 g(x)\,\mathrm{d}x = 0, \quad \int_0^1 g(x)^2\,\mathrm{d}x = 0, \quad \text{and} \quad \int_0^1 g(x)^4\,\mathrm{d}x < \infty.$$

The third condition ensures that all GSIs have finite variance, while the first two allow us to write the variance components of f as

$$\sigma_u^2 = \begin{cases} \prod_{j\in u}\tau_j^2 \times \prod_{j\notin u}\mu_j^2, & |u|>0\\ 0, & \text{else,}\end{cases}$$

along with $\mu = \prod_{j=1}^d \mu_j$.

We will compare Monte Carlo estimates and so smoothness or otherwise of $g_j(\cdot)$ plays no role. Only μ_j, τ_j and the third and fourth moments of g play a role. Monte Carlo estimation is suitable when f is inexpensive to evaluate, like surrogate functions in computer experiments. For our examples we take $g_j(x) = \sqrt{12}(x-1/2)$ for all j.

For an example function of non-product form, we take the minimum,

$$f(\boldsymbol{x}) = \min_{1\leqslant j\leqslant d} x_j.$$

Liu and Owen [2006] show that

$$\underline{\tau}_u^2 = \frac{|u|}{(d+1)^2(2d-|u|+2)},$$

for this function. Taking $u = \mathcal{D}$ gives $\sigma^2 = d(d+1)^{-2}(d+2)^{-1}$.

8.3. Estimation of $\sigma^2_{\{1,2,3\}}$. We considered both simple and bilinear estimators of $\sigma^2_{\{1,2,3\}}$ in Section 5. The simple estimator requires 9 function evaluations per $(\boldsymbol{x},\boldsymbol{z})$ pair, while three different bilinear ones each require only 6.

For a function of product form, all four of these estimators yield the same answer for any specific set of $(\boldsymbol{x}_i,\boldsymbol{z}_i)$ pairs. As a result the bilinear formulas dominate the simple one for product functions.

For the minimum function, with $d=5$ we find that by symmetry,

$$\sigma^2_{\{1,2,3\}} = \underline{\tau}^2_{\{1,2,3\}} - 3\underline{\tau}^2_{\{1,2\}} + 3\underline{\tau}^2_{\{1\}} = \frac{1}{5940} \doteq 1.68\times 10^{-4}.$$

TABLE 8.1

Estimated mean and corresponding standard error for three estimators of $\sigma^2_{\{1,2,3\}}$ for $f(\boldsymbol{x}) = \min_{1\leqslant j\leqslant 5} x_j$ when $\boldsymbol{x} \sim \mathbf{U}(0,1)^5$. The Bilin.{1} estimator is from equation (5.5), and the other Bilinear estimators are defined analogously.

Estimator	Simple	Bilin.{1}	Bilin.{2}	Bilin.{3}
Mean	1.74×10^{-4}	1.72×10^{-4}	1.68×10^{-4}	1.70×10^{-4}
Standard error	1.05×10^{-5}	5.69×10^{-6}	5.71×10^{-6}	5.67×10^{-6}

Because we are interested in comparing the variance of estimators of a variance, a larger sample is warranted than if we were simply estimating a variance component. Based on 1,000,000 function evaluations we find the estimated means and standard errors are given in Table 8.1. We see that the bilinear estimators give about half the standard error of the simple estimator, corresponding to about $(1.05/.571)^2 \times 9/6 \doteq 5.1$ times the statistical efficiency.

8.4. Estimation of $\underline{\tau}^2_{\{1,2\}}$. We consider two estimators of $\underline{\tau}^2_u$. The estimator (2.2) is a bilinear contrast, averaging $f(\boldsymbol{x})(f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) - f(\boldsymbol{z}))$. The estimator (2.1) using the estimator of $\hat{\mu}$ from Janon et al. [2012] is a modification of Sobol's original simple estimator based on averaging $f(\boldsymbol{x})f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u})$. The bias correction of Section 7 makes an asymptotically negligible difference, so we do not consider it here.

Both estimators make an adjustment to compensate for the bias μ^2. Estimator (2.1) subtracts an estimate $\hat{\mu}^2$ based on combining all $2n$ function evaluations, the square of the most natural way to estimate μ from the available data. Estimator (2.2) subtracts $(1/n^2)\sum_i\sum_{i'} f(\boldsymbol{x}_i)f(\boldsymbol{x}_{i,u}{:}\boldsymbol{z}_{i,-u})$, which may be advantageous when the difference $f(\boldsymbol{x}_u{:}\boldsymbol{z}_{-u}) - f(\boldsymbol{z})$ involves considerable cancellation, as it might if $\boldsymbol{x}_u$ is unimportant. Thus we might expect (2.2) to be better when $\underline{\tau}^2_u$ is small. We compare the estimators on a product function, looking at $\underline{\tau}^2_u$ for three subsets u of size 2 and varying importance.

For the product function with $d = 6$, $\tau = (1, 1, 1/2, 1/2, 1/4, 1/4)$, all $\mu_j = 1$ for $j = 1, \dots, 6$, and $g_j(x_j) = \sqrt{12}(x_j - 1/2)$, we may compute $\underline{\tau}^2_{\{1,2\}} = 3 \doteq 0.50\sigma^2$, $\underline{\tau}^2_{\{3,4\}} \doteq 1.56 \doteq 0.093\sigma^2$, and $\underline{\tau}^2_{\{5,6\}} \doteq 0.13 \doteq 0.021\sigma^2$.

Results from $R = 10{,}000$ trials with $n = 10{,}000$ $(\boldsymbol{x}_i, \boldsymbol{z}_i)$ pairs each, are shown in Table 8.2. Because the contrast estimator is unbiased and the other estimator has only a tiny bias we may compare these estimators by their standard deviations. The contrast estimator comes out well ahead for the small quantity $\underline{\tau}^2_{\{5,6\}}$ and roughly equal otherwise. Sobol et al. [2007] also report superiority of the contrast estimator on a small $\underline{\tau}^2_u$.

In the event that we only wanted one index the simple estimator has only 2/3 the cost of the contrast and then it has greater efficiency than the contrast for $\underline{\tau}^2_{\{1,2\}}$ but not for $\underline{\tau}^2_{\{5,6\}}$. Neither estimator is always more efficient than the other, hence no proxy based solely on Ω can reliably predict which of these is better for a specific problem. In more usual circumstances we compute many sensitivity indices and then the simple estimator has no cost advantage.

The bias correction from Section 7 makes little difference here because for $n = 10{,}000$ there is very little bias to correct. It does make a difference when $n = 100$ (data not shown) but at such small sample sizes the standard deviation of $\hat{\underline{\tau}}^2_u$ can be comparable to or larger than $\underline{\tau}^2_u$ itself for this function.

TABLE 8.2

This table compares a simple estimator versus a contrast for $\underline{\tau}_u^2$ with $n = 10{,}000$. The sets compared are $u = \{1,2\}$, $\{3,4\}$, and $\{5,6\}$ and f is the product function described in the text. The rows give the true values of $\underline{\tau}_u^2$, and for 10,000 replicates, the (rounded) sample values of their average, bias, standard deviation and proportion negative.

$n = 1000$	$\{1,2\}$		$\{3,4\}$		$\{5,6\}$	
	Cont.	Simp.	Cont.	Simp.	Cont.	Simp.
True	3.0000	3.0000	0.5625	0.5625	0.1289	0.1289
Avg.	3.0002	3.0002	0.5624	0.5628	0.1291	0.1294
Bias	0.0002	0.0002	−0.0005	0.0003	0.0002	0.0005
S.Dev	0.1325	0.1186	0.0800	0.0998	0.0378	0.0737
Neg	–	–	–	–	0.0001	0.0336

TABLE 8.3

Standard errors for estimation of Υ_w^2 by the bilinear estimate and a square as described in the text. The estimated standard errors based on $n = 1{,}000{,}000$ replicates are 10^{-3} times the values shown. The relative efficiency of the square is 7/16 times the squared ratio of standard deviations.

	$\{1,2,3,4\}$	$\{5,6,7,8\}$
Bilinear	35.07	4.019
Square	6.04	0.051
Efficiency	14.7	2,710

8.5. Estimation of $\Upsilon^2_{\{1,2,3,4\}}$. Here we compare two estimates of $\Upsilon^2_{\{1,2,3,4\}}$, the square (4.1) and the bilinear estimator (5.8) from Theorem 5.2. For a product function, $\Upsilon_w^2 = \prod_{j\in w}\tau_j^2\prod_{j\notin w}(\mu_j^2+\tau_j^2)$. Squares have an advantage estimating small GSIs so we consider one small and one large (for a four way interaction) Υ^2.

For $d = 8$, $\tau = c(4,4,3,3,2,2,1,1)/4$ and all $\mu_j = 1$ we find that $\Upsilon^2_{\{1,2,3,4\}} \doteq 0.558 \doteq 0.0334\sigma^2$ and $\Upsilon^2_{\{5,6,7,8\}} \doteq 0.00238 \doteq 0.000147\sigma^2$. The bilinear estimate (5.8) based on $w_1 = \{1,2\}$ and $w_2 = \{3,4\}$ for $\Upsilon_{\{1,2,3,4\}}$ (respectively $w_1 = \{5,6\}$ and $w_2 = \{7,8\}$ for $\Upsilon_{\{5,6,7,8\}}$) requires $C = 7$ function evaluations, while the square (4.1) requires $C = 16$. From Table 8.3 we see that the square has an advantage that more than compensates for using a larger number of function evaluations and the advantage is overwhelming for the smaller effect.

The outlook for the bilinear estimator of Υ_w^2 is pessimistic when $|w|$ is very large. Its cost advantage grows with $|w|$; for $|w| = 20$ it has cost 1023 compared to 2^{20} for the square. But Υ_w^2 for such a large w will often be so small that the variance advantage from using a square will be extreme.

9. Conclusions. This paper has generalized Sobol' indices to estimators of arbitrary linear combinations of variance components. Sometimes there are multiple ways to estimate a generalized Sobol' index with important efficiency differences. Square GSIs where available are very effective. When no square or sum of squares is available a bilinear or low rank GSI can at least save some function evaluations. Contrasts are simpler to work than other GSIs, because they do not require bias corrections.

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