# VARIANCE-BASED GLOBAL SENSITIVITY ANALYSIS VIA SPARSE-GRID INTERPOLATION AND CUBATURE

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Abstract. We use sparse grid interpolation and cubature methods of Smolyak together with combinatorial analysis to give a computationally efficient method for computing the global sensitivity values of Sobol'. This method allows for approximation of all main effect and total effect values from evaluation of $f$ on a single set of sparse grids. We discuss convergence of this method, apply it to several test cases and compare to existing methods. As a result which may be of independent interest, we give a formula that generalizes the standard discrete orthogonality formula for Chebyshev polynomials evaluated at their extrema. We use this to recover an explicit formula for evaluating a Lagrange basis interpolating polynomial associated with the Chebyshev extrema.

## 1. Introduction

The growing popularity of computational models in various fields of science, engineering, and econometrics has led to a corresponding growth in interest in methods to understand parameter space. For instance, a typical model of the electrophysiology of a single cardiac cell may depend on dozens of parameters, many of which are not well constrained by existing data and many of which affect the output in nonlinear and nonintuitive ways. Moreover, in general there are no experimental techniques to measure many of these parameters. Rather, the parameters must be inferred from measurements of some observable quantity; this approach often leads to an ill-posed or ill-conditioned inverse problem.

A common task in developing a model is to find a set of parameters so that the model output is in close agreement with some data set. In simplest form, we may assume that the notion of close agreement is captured by some cost function, $C(p)$, which depends on the parameters $p = (p_1, \dots, p_n)$. Often, $C(p)$ is a sum of squared differences between model output and experimental data at specified times and/or positions. Such parameter selection is a difficult task when the dimensionality of the parameter space is large and the dependence of $C$ on $p$ is nonlinear. Hence, the development of efficient tools for reducing the size of the search space is vital.

Local sensitivity analysis, which computes partial derivatives $\partial C/\partial p_j$, may be used to determine which parameters are relatively more important

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than others at a single point in parameter space. In contrast, global sensitivity analysis (GSA) seeks a measure of relative importance over the entire parameter space. One approach to GSA is variance based. With an appropriate measure, we may regard parameter space as a probability space and $C$ as a random variable on this space. The sensitivity of $C$ to a given parameter $p_j$ is then

$$\frac{\mathrm{Var}_{p_j}(E[C|p_j])}{\mathrm{Var}(C)},$$

where $E[C|p_j]$ is the expected value obtained by fixing a given value of $p_j$ and integrating over the remaining variables, and $\mathrm{Var}_{p_j}$ is the variance as a function of $p_j$ only. As noted by Saltelli, et al., (see [5] and the references therein), this quantity has appeared in various formulations in many places in the literature.

Sobol' [8] provides a particularly appealing formulation of this quantity as a special case of a more general approach to GSA for arbitrary subsets of parameters. The measure above, which is meant to capture the effect of the single parameter $p_j$, is often called the *Main effect* due to $p_j$. By considering other subsets containing $p_j$, the sensitivity values of Sobol' can be used to identify interaction effects between multiple variables. For instance, by considering the sum of all sensitivity values in which $p_j$ takes part, we obtain what is often called the *Total effect* due to $p_j$. Sobol' [8] describes a method for evaluating the main effect values using Monte Carlo or quasi-Monte Carlo methods. Saltelli, et al. [5] give a Fourier analysis based method for computing both the main and total effects. This is often called the Extended FAST method.

For a detailed discussion of many approaches to sensitivity analysis as well as a discussion of the Extended FAST method and many additional references, see [7]. For other approaches to improve the efficiency of computing sensitivity values, see [2], [3], [6], [9], and references therein. In particular, [2] uses an approach related to ours but based on polynomial chaos (expansion of a function in terms of an orthogonal set of polynomials) with a cubature rule used to determine the polynomial expansion. This approach uses the orthogonality of the basis polynomials to produce an elegant formula for the sensitivity coefficients. Our method is more closely related to ideas of stochastic collocation (see e.g., [11]), in which function values are used to determine an interpolating polynomial, which is then used to approximate the integrals defining the sensitivity values.

In this paper we review the Sobol' decomposition and interpolation and quadrature with Chebyshev polynomials, then give computationally efficient methods for calculating the main effect and total effect sensitivity values using sparse grid interpolation and cubature. Some advantages of our approach over Monte Carlo methods are a faster rate of convergence as the number of function evaluations increases (at least for differentiable functions) and the fact that once the cost function has been evaluated at a given set of predetermined points, then any of the sensitivity values may be approximated without further function evaluations. Some advantages of our method over Extended FAST are greater accuracy and faster, provable convergence rates for differentiable functions, the fact that there are no choices required to tune the algorithm to a given application, and the fact that our use of nested sparse grids means that the evaluations at a given level of accuracy may be reused as part of a larger sparse grid in order to improve accuracy. Here we focus on the main effect and total effect values, but our approach may be applied in principle to any of the sensitivity values. We discuss rates of convergence and numerical results in several test cases below.

As a result which may be of independent interest, we give a formula that generalizes the standard discrete orthogonality formula for Chebyshev polynomials evaluated at their extrema (Proposition 4.3). We use this to recover an explicit formula for evaluating a Lagrange basis interpolating polynomial associated with the Chebyshev extrema (Corollary 4.4). This latter formula may be derived from Lemma 6.4 of [4], but perhaps deserves greater attention since it allows for evaluation at any point in the interval $[-1, 1]$ and has computational cost $O(1)$, independent of the degree of the interpolating polynomial.

In Section 2, we review the orthogonal decomposition of Sobol'. In Section 3, we use this decomposition to define the main and total effect sensitivity values and then prove an integral formula (Proposition 3.2) that may be seen as a generalization of Parseval's Theorem for this decomposition. This proposition also allows us to derive formulas for the desired sensitivity values. In Section 4, we review Chebyshev interpolation and the associated quadrature method of Clenshaw-Curtis, then state and derive a closed-form formula for the value at any point in $[-1, 1]$ of the Lagrange interpolating polynomial associated with the Chebyshev extrema (Corollary 4.4). In Section 5, we review the ideas of sparse grid interpolation and cubature, and in Section 6, we apply these ideas in two different ways to approximate the main and total effect sensitivity values. Finally, in Section 7, we apply our method to several test functions and compare to quasi-Monte Carlo and Extended FAST.

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## 2. Orthogonal decomposition

Here we review the key ideas of [8] with somewhat different notation and give modified proofs of some of the main results of that paper. Also, we use the interval $[-1, 1]$ for our calculation instead of the original $[0, 1]$ in order to mesh more easily with techniques of sparse grid cubature.

Let $K = [-1, 1]$ and $f : K^n \to \mathbb{R}$. Let $x$ denote coordinates on $K^n$. Let $\alpha$ denote a multi-index in $\{0, 1\}^n$, let $\alpha_j$ denote the $j$th entry in $\alpha$, let $\mathbf{1}$

denote the multi-index with each entry equal to 1, let $\mathbf{0}$ denote the multi-index with each entry equal to 0, and let $\mathbf{1}^j$ denote the multi-index such that $\mathbf{1}^j_k = \delta_{jk}$. Also, let $\alpha' = \mathbf{1} - \alpha$ and $|\alpha| = \sum_j \alpha_j$. Define a partial order on such multi-indices by $\alpha \leq \beta$ if $\alpha_j \leq \beta_j$ for all $j$, with the obvious notion of equality. With this order, the set of $\gamma$ satisfying $\alpha \leq \gamma \leq \beta$ is exactly the set of $\gamma$ with $\alpha_j \leq \gamma_j \leq \beta_j$ for all $j$. Finally, for purposes of integration, let $d\mu_j = dx_j/2$ be normalized Lebesgue measure, let $d\mu = d\mu_1 \cdots d\mu_n$, and for a multi-index $\alpha = \sum_{j=1}^k \mathbf{1}^{i_j}$, let $d\mu_\alpha = d\mu_{i_1} \cdots d\mu_{i_k}$.

For the method of Sobol', we assume that $f$ is $L^2$ integrable on $K^n$ and look for a functional decomposition

$$f = \sum_{\mathbf{0} \leq \alpha \leq \mathbf{1}} f_\alpha \tag{1}$$

satisfying

(A) $f_\alpha$ is independent of $x_j$ if $\alpha_j = 0$.
(B) $\int_K f_\alpha(x) d\mu_j = 0$ if $\alpha_j = 1$.
(C) $\int_{K^n} f_\alpha f_\beta d\mu = 0$ if $\alpha \neq \beta$

We show below that this decomposition is achieved via the formula

$$f_\alpha(x) = \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} - \sum_{\mathbf{0} \leq \beta < \alpha} f_\beta(x). \tag{2}$$

Here we make the convention that $\int_{K^0} f(x) d\mu_{\mathbf{1}'} = f(x)$. Note also that $f_{\mathbf{0}}(x) = \int_{K^n} f(x) d\mu$ is a constant function with value equal to the expected value of $f$ in $K^n$, assuming uniform distribution in each variable. From now on we use $f_0$ for this expected value. The formula in (2) agrees with the definition given in [8], although the presentation is more explicit here.

**Proposition 2.1.** *With $f_\alpha$ as in* (2)*, the decomposition* (1) *holds, and statements (A), (B), and (C) are true.*

*Proof.* We show first that $f = \sum_{0 \leq \alpha \leq \mathbf{1}} f_\alpha$. By definition of $f_{\mathbf{1}}$, we have

$$\begin{aligned} \sum_{\mathbf{0} \leq \alpha \leq \mathbf{1}} f_\alpha &= f_{\mathbf{1}} + \sum_{\mathbf{0} \leq \alpha < \mathbf{1}} f_\alpha \\ &= (f - \sum_{\mathbf{0} \leq \alpha < \mathbf{1}} f_\alpha) + \sum_{\mathbf{0} \leq \alpha < \mathbf{1}} f_\alpha \\ &= f \end{aligned}$$

To prove statement (A), we induct on $|\alpha|$. Note that $f_0$ is constant, hence independent of all $x_j$. Also, if $\alpha_j = 0$ for some $\alpha \neq \mathbf{0}$, then $\beta_j = 0$ for all $\beta < \alpha$, and hence $f_\beta(x)$ is independent of $x_j$ by induction. Moreover, in this case, $\alpha'$ has $\alpha'_j = 1$, so $\int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'}$ is independent of $x_j$. Using this with the definition of $f_\alpha$ in (2) verifies statement (A).

For statement (B), again we induct on $|\alpha|$. If $\alpha = \mathbf{0}$, statement (B) is vacuously true. Next suppose that $\alpha_j = 1$, and let $\hat{\alpha} = \alpha - \mathbf{1}^j$. Note that if

$\mathbf{0} \le \beta < \alpha$, then either $\beta < \hat{\alpha}$, or $\beta = \hat{\alpha}$, or $\mathbf{1}^j \le \beta < \alpha$, and exactly one of these three cases holds. Using this with (2), we have

$$\begin{aligned}\int_K f_\alpha(x)d\mu_j &= \int_K \int_{K^{n-|\alpha|}} f(x)d\mu_{\alpha'}d\mu_j - \sum_{0\le\beta<\alpha} \int_K f_\beta(x)d\mu_j \\ &= \int_{K^{n-|\hat{\alpha}|}} f(x)d\mu_{\hat{\alpha}'} - \sum_{0\le\beta<\hat{\alpha}} \int_K f_\beta(x)d\mu_j \\ &\quad - \int_K f_{\hat{\alpha}}(x)d\mu_j - \sum_{\mathbf{1}^j\le\beta<\alpha} \int_K f_\beta(x)d\mu_j.\end{aligned}$$

Note that the first two terms in the final expression are exactly the definition of $f_{\hat{\alpha}}(x)$. Also, since $\hat{\alpha}_j = 0$, we see that $f_{\hat{\alpha}}(x)$ is independent of $x_j$ by statement (A). Hence the third term is also exactly $f_{\hat{\alpha}}(x)$, thus cancelling the first two terms. Moreover, each integral in the final summation is 0 by induction since $\mathbf{1}^j \le \beta < \alpha$ implies $|\beta| < |\alpha|$ and $\beta_j = 1$. Thus the terms of the final expression cancel to verify statement (B).

Statement (C) is true exactly as presented in Sobol'. That is, if $\alpha \neq \beta$, then without loss there is some $j$ so that $\alpha_j = 1$ while $\beta_j = 0$. Integrating $f_\alpha f_\beta$ with respect to $x_j$ and applying statement (B) gives 0. Hence the entire integral is 0. □

## 3. Variance and sensitivity values

Next we define the variance and sensitivity values as in Sobol'.

**Definition 3.1.** Let $\alpha$ be a multi-index. Denote the variance of $f_\alpha$ by

$$D_\alpha = \int_{K^n} f_\alpha^2 d\mu - \left(\int_{K^n} f_\alpha d\mu\right)^2,$$

and denote the variance of $f$ by $D$ (replace $f_\alpha$ by $f$ in the previous expression). Define the total variance for $x_j$ to be

$$D_{T_j} = \sum_{\mathbf{1}^j\le\alpha\le\mathbf{1}} D_\alpha.$$

Define the sensitivity for $\alpha$ ($S_\alpha$) and the total sensitivity of $x_j$ ($S_{T_j}$) by

$$S_\alpha = \frac{D_\alpha}{D}, \quad S_{T_j} = \frac{D_{T_j}}{D}.$$

By abuse of notation, let $D_j = D_{\mathbf{1}^j}$ and $S_j = S_{\mathbf{1}^j}$. Note that $S_j$ is often called the main effect due to $x_j$ and $S_{T_j}$ is called the total effect due to $x_j$.

The next proposition is the main tool for computing sensitivity values via cubature. Here and below, $\|f\|_2$ denotes the $L^2$ norm of $f$ over $K^n$ with measure $\mu$.

**Proposition 3.2.** *Let $\alpha$ be a multi-index. Then*

$$\sum_{\mathbf{0}\le\beta\le\alpha} \|f_\beta\|_2^2 = \int_{K^{|\alpha|}} \left( \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} \right)^2 d\mu_\alpha.$$

In the case $\alpha = \mathbf{1}$, this statement is a version of Parseval's Theorem for the orthogonal decomposition given by the $f_\alpha$. Hence this equality may be viewed as a generalization of Parseval's Theorem to the case of partial sums of the functions in the decomposition.

*Proof.* For $\alpha = \mathbf{0}$, the statement is true by definition. Hence we assume $\alpha \neq \mathbf{0}$. Note that by (2),

$$f_\alpha(x) = \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} - \sum_{\mathbf{0}\le\beta<\alpha} f_\beta(x).$$

Hence

$$\begin{aligned}
\|f_\alpha\|_2^2 &= \int_{K^{|\alpha|}} \left( \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} - \sum_{0\le\beta<\alpha} f_\beta(x) \right)^2 d\mu_\alpha \\
&= \int_{K^{|\alpha|}} \left[ \left( \int_{K^{n-|\alpha|}} f d\mu_{\alpha'} \right)^2 - 2 \sum_{0\le\beta<\alpha} f_\beta \int_{K^{n-|\alpha|}} f d\mu_{\alpha'} + \left( \sum_{0\le\beta<\alpha} f_\beta \right)^2 \right] d\mu_\alpha.
\end{aligned}$$

Note that if $\beta < \alpha$, then $f_\beta$ depends only on the variables in $x_\alpha$ and hence is independent of the variables in $x_{\alpha'}$. Hence we may integrate the final term over $K^n$ instead of $K^{|\alpha|}$. Using this, expanding the square, and applying the orthogonality result of statement (C) gives

$$\begin{aligned}
\int_{K^{|\alpha|}} \left( \sum_{0\le\beta<\alpha} f_\beta \right)^2 d\mu_\alpha &= \int_{K^n} \sum_{0\le\beta<\alpha} \sum_{0\le\gamma<\alpha} f_\beta f_\gamma d\mu \\
&= \sum_{0\le\beta<\alpha} \int_{K^n} f_\beta^2 d\mu \\
&= \sum_{0\le\beta<\alpha} \int_{K^{|\beta|}} f_\beta^2 d\mu_\beta \\
&= \sum_{0\le\beta<\alpha} \|f_\beta\|_2^2.
\end{aligned}$$

This same idea, plus the functional decomposition of (1) implies that if $\beta < \alpha$, then

$$\begin{aligned}\int_{K^{|\alpha|}} f_\beta \left( \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} \right) d\mu_\alpha &= \int_{K^n} f_\beta f d\mu \\ &= \int_{K^n} f_\beta \sum_{0 \le \gamma \le \mathbf{1}} f_\gamma d\mu \\ &= \int_{K^n} f_\beta^2 d\mu \\ &= \int_{K^{|\beta|}} f_\beta^2 d\mu_\beta \\ &= \|f_\beta\|_2^2.\end{aligned}$$

Applying these previous two results in the expression for $\|f_\alpha\|_2^2$, we see that

$$\|f_\alpha\|_2^2 = \int_{K^{|\alpha|}} \left( \int_{K^{n-|\alpha|}} f(x) d\mu_{\alpha'} \right)^2 d\mu_\alpha - \sum_{0 \le \beta < \alpha} \|f_\beta\|_2^2.$$

Moving the final sum to the left hand side gives the proposition. □

Using this result, we express $D$ in terms of the $D_\alpha$ and express each of $D_j$ and $D_{T_j}$ as an integral, where $D$ is the variance of $f$, $D_j$ is the variance for the main effect for $x_j$, and $D_{T_j}$ is the variance for the total effect for $x_j$.

**Corollary 3.3.**

$$D = \sum_{\mathbf{0} \le \alpha \le \mathbf{1}} D_\alpha = \sum_{\mathbf{0} < \alpha \le \mathbf{1}} \|f_\alpha\|_2^2.$$

*Proof.* Note that property (B) implies that $E[f_\alpha] = 0$ when $\alpha \neq \mathbf{0}$, in which case $D_\alpha = \|f_\alpha\|_2^2$. Also, since $f_{\mathbf{0}}(x)$ is constant, $D_{\mathbf{0}} = 0$.

Applying this with the previous proposition and the formula for $f_0$ gives

$$\begin{aligned}\sum_{\mathbf{0} \le \alpha \le \mathbf{1}} D_\alpha &= \left( \sum_{\mathbf{0} \le \alpha \le \mathbf{1}} \|f_\alpha\|_2^2 \right) - \|f_0\|_2^2 \\ &= \int_{K^n} f^2 d\mu - \left( \int_{K^n} f d\mu \right)^2.\end{aligned}$$

The final expression is exactly $D$. □

**Corollary 3.4.**

$$D_j = \int_K \left( \int_{K^{n-1}} f d\mu_{\mathbf{1}^{j'}} \right)^2 d\mu_j - f_0^2.$$

*Proof.* Let $I$ denote the integral in the expression above. Proposition 3.2 implies that

$$I = \sum_{0 \le \alpha \le \mathbf{1}^j} \|f_\alpha\|_2^2.$$

Since only 0 and $\mathbf{1}^j$ satisfy the bounds on $\alpha$ in the sum, we have $I = \|f_0\|_2^2 + \|f_{\mathbf{1}^j}\|_2^2 = f_0^2 + D_j$, hence $D_j = I - f_0^2$. □

**Corollary 3.5.**

$$D_{T_j} = D + f_0^2 - \int_{K^{n-1}} \left( \int_K f \, d\mu_j \right)^2 d\mu_{\mathbf{1}^{j'}}.$$

*Proof.* By definition and properties of $D_\alpha$,

$$D_{T_j} = \sum_{\mathbf{1}^j \le \alpha \le \mathbf{1}} D_\alpha = \sum_{0 \le \alpha \le \mathbf{1}} \|f_\alpha\|_2^2 - \sum_{0 \le \alpha \le \mathbf{1}^{j'}} \|f_\alpha\|_2^2.$$

From Corollary 3.3, the first of the final two sums is $D + f_0^2$. From the proposition, the second of the final two sums is exactly the integral in the statement of this corollary. □

The following corollary follows directly from the previous corollaries using the standard proof for showing that $E[(X - \overline{X})^2] = E[X^2] - \overline{X}^2$, where $X$ is a random variable and $\overline{X} = E[X]$.

**Corollary 3.6.** *As before, let $f_0 = \int_{K^n} f d\mu$ be the mean of $f$ and $D = \int_{K^n} f^2 d\mu - f_0^2$ be the variance. Then the main effect sensitivity for $x_j$ on $f$ is*

$$S_j = \frac{1}{D} \int_K \left( \int_{K^{n-1}} (f - f_0) d\mu_{\mathbf{1}^{j'}} \right)^2 d\mu_j,$$

*and the total effect sensitivity for $x_j$ on $f$ is*

$$S_{T_j} = 1 - \frac{1}{D} \int_{K^{n-1}} \left( \int_K (f - f_0) d\mu_j \right)^2 d\mu_{\mathbf{1}^{j'}}.$$

## 4. Chebyshev interpolation and Clenshaw-Curtis quadrature

In this section we review some results about interpolation at the extrema of the Chebyshev polynomials and Clenshaw-Curtis quadrature in one dimension, then give a novel formula for evaluating the Lagrange interpolating polynomial at Chebyshev extrema. Much of this section is based on "Chebyshev Polynomials" by J.C. Mason and D.C. Handscomb [4].

Recall that the Chebyshev polynomial of the first kind of degree $d \ge 0$ is denoted $T_d$ and satisfies $T_d(\cos\theta) = \cos d\theta$. Within the interval $[-1, 1]$, the extrema of $T_d$ occur at the points $x_{d,k} = \cos(k\pi/d)$, $k = 0, \dots d$, where $d > 0$. By convention, let $x_{0,0} = 0$. Using the functional relation just given, we see that $T_d(x_{d,k}) = (-1)^k$.

In order to use sparse grid cubature as described in the next section, we need Lagrange interpolation on these extrema of $T_d$. Let $L_{d,i}(x)$ denote the degree $d$ polynomial which satisfies $L_{d,i}(x_{d,k}) = \delta_{i,k}$ for $k = 0, \dots, d$. Here and below, $\delta_{i,j} = 1$ if $i = j$ and 0 otherwise. Given a function $f$ on $[-1, 1]$, the degree $d$ polynomial interpolating $f$ on the points $x_{d,k}$ is then

$$J_d f(x) = \sum_{j=0}^{d} f(x_{d,j}) L_{d,j}(x). \tag{3}$$

From [4, p. 189], we have an alternative formulation as

$$J_d f(x) = \sum_{j=0}^{d}{}'' b_j T_j(x), \tag{4}$$

where

$$b_j = \frac{2}{d} \sum_{k=0}^{d}{}'' f(x_{d,k}) T_j(x_{d,k}),$$

and $\sum''$ means that the first and last terms are multiplied by $1/2$.

Applying this to $f(x) = L_{d,i}(x)$, we have $f(x_{d,k}) = \delta_{k,i}$, and hence $b_j = (2/d)T_j(x_{d,i})/(1 + \delta_{0,i} + \delta_{i,d})$ for $d > 0$. Since $T_j(x_{d,i}) = T_i(x_{d,j})$, we have

$$L_{d,i}(x) = \frac{2}{d(1 + \delta_{i,0} + \delta_{i,d})} \sum_{j=0}^{d}{}'' T_i(x_{d,j}) T_j(x). \tag{5}$$

We can use the interpolation $J_d f$ to produce an approximation to the integral $I(f) = \int_{-1}^{1} f(x)dx$ as follows. First, let $U_d(f) = \int_{-1}^{1} J_d f(x)dx$. By integrating (3), we obtain [4, (8.31) and (8.23)]

$$U_d(f) = \sum_{j=0}^{d} w_{d,j} f(x_{d,j}), \tag{6}$$

where

$$w_{d,j} = \frac{2}{d} \sum_{k=0}^{d}{}'' a_k T_k(x_{d,j}),$$

and

$$a_k = \int_0^{\pi} \cos k\theta \sin\theta \, d\theta.$$

The formula (6) gives $I(f)$ exactly for polynomials of degree at most $d$. For a given $d$, the weights $w_{d,j}$ may be calculated in advance, but this calculation is essentially a discrete cosine transform, and hence is not completely trivial in general. However, in the case of an interpolating polynomial, we may write down a fairly simple and well-known formula.

**Proposition 4.1.**

$$\int_{-1}^{1} L_{2d,j}(x)dx = \frac{2}{d} \sum_{k=0}^{d}{}'' \frac{1}{1 - 4k^2} \cos\left(\frac{jk\pi}{d}\right).$$

*Proof.* The result follows immediately from (6) by noting that $U_d(f)$ reduces to $w_{2d,j}$ in the case of $f = L_{2d,j}$. □

In order to approximate the variances of the previous section, we will need to integrate a product of interpolated functions. This means that we need to integrate products of the Lagrange interpolants $L_{d,j}$. Thus, we end this section by calculating such integrals. First some preliminary lemmas on sums of products of $T_j$. The first is a standard result on a kind of discrete orthogonality [4, (4.45)].

**Lemma 4.2.** *Let $d$ be a positive integer and $0 \le i, j \le d$. Then*

$$\sum_{k=0}^{d}{}'' T_i(x_{d,k}) T_j(x_{d,k}) = d \frac{\delta_{i,j}(1 + \delta_{0,i} + \delta_{i,d})}{2}.$$

Next, we need a similar result in which the point of evaluation is different for $T_j$ and $T_k$. The formula below is original to our knowledge.

**Proposition 4.3.** *Let $d_1, d_2, j_1, j_2$ be integers with $0 \le j_1 \le d_1 < d_2$ and $0 \le j_2 \le d_2$. Let $x_1 = x_{d_1,j_1}$, $x_2 = x_{d_2,j_2}$ and suppose $x_1 \ne x_2$. Then*

$$\sum_{k=0}^{d_1}{}'' T_{j_1}(x_{d_1,k}) T_{j_2}(x_{d_2,k}) = \frac{(-1)^{j_1} \sqrt{1 - x_2^2} \sin\left(\frac{j_2 d_1 \pi}{d_2}\right)}{2(x_1 - x_2)}$$

The proof is given below. Note that Lemma 4.2 fills in the gap left by the assumption that $x_1 \ne x_2$. That is, if $x_1 = x_2$, then we may replace $j_2$ with $j_1$ and $d_2$ with $d_1$ without changing the sum, in which case we may apply Lemma 4.2.

The following immediate corollary gives a method to evaluate the Lagrange basis interpolating polynomial, $L_{d,j}$ at any point $x \in [-1, 1]$ in constant time (independent of the degree) without calculating the polynomial itself or applying (5). This formula may also be derived from Lemma 6.4 of [4] using the fact that the extrema of $T_d$ are the zeros of the polynomial $(1 - x^2)U_{d-1}(x)$, where $U_{d-1}$ is the Chebyshev polynomial of the second kind.

**Corollary 4.4.** *Let $d, j$ be integers with $d > 0$ and $0 \le j \le d$, let $x_0 = \cos(j\pi/d)$, let*

$$C_{d,j} = \frac{(-1)^{j+1}}{d(1 + \delta_{0,j} + \delta_{d,j})},$$

*and let $x \in [-1, 1]$. Then*

$$L_{d,j}(x) = C_{d,j} \frac{\sqrt{1 - x^2} \sin\left(d \cos^{-1}(x)\right)}{x - x_0}, \; x \ne x_0,$$

*and $L_{d,j}(x_0) = 1$.*

Note that by replacing $x$ with $\cos\theta$, we obtain an expression analogous to $T_d(\cos\theta) = \cos(d\theta)$:

$$L_{d,j}(\cos\theta) = C_{d,j}\frac{\sin\theta\sin d\theta}{\cos\theta - \cos\left(\frac{j\pi}{d}\right)},\ \theta \neq \frac{j\pi}{d}.$$

*Proof of Corollary.* Apply (5) to the result of Proposition 4.3 to get a formula for $L_{d,j}(x_{d_2,j_2})$. Then note that $\sin(j_2 d\pi/d_2) = \sin(d\cos^{-1}(x_{d_2,j_2})$ to obtain the formula in this corollary with $x = x_{d_2,j_2}$. Finally, note that the points $x_{d_2,j_2}$ over all $d_2 > d$ and $0 \leq j_2 \leq d_2$ are dense in $[-1,1]$ and that the left and right hand functions are both continuous in $x \in [-1,1]$ , hence must be equal on all of $[-1,1]$. The continuity of the right hand side at $x = x_0$ follows from the fact that $\sin(d\cos^{-1}(x_0)) = \sin(dj\pi/d) = 0$, which implies that the right hand side has a removable singularity at $x_0$. □

Note that (6) together with this corollary gives an efficient method for evaluating the $L^2$ inner product of two Lagrange interpolating functions. That is,

$$\int_{-1}^{1} L_{d_1,j_1}(x)L_{d_2,j_2}(x)dx = \sum_{j=0}^{2d_2} w_{2d_2,j}L_{d_1,j_1}(x_{2d_2,j})L_{d_2,j_2}(x_{2d_2,j}), \tag{7}$$

which may be evaluated using Corollary 4.4 with a number of operations which is linear in the maximum degree. For this application, we may avoid the use of $\cos^{-1}$ since $\cos^{-1}(x_{2d_2,j}) = j\pi/(2d_2)$.

To prove the proposition, we use a function $S_a$ so that $S_a(x+1) - S_a(x) = \cos ax$ in order to convert the sum to a telescoping sum.

**Definition 4.5.** For $a$ real with $\sin(a/2) \neq 0$, let

$$S_a(x) = \frac{\sin\left(ax - \frac{a}{2}\right)}{2\sin\left(\frac{a}{2}\right)}.$$

**Lemma 4.6.** *For $a$ real with* $\sin(a/2) \neq 0$,

$$\sum_{k=0}^{d}\cos(ak) = S_a(d+1) + \frac{1}{2}.$$

*Proof.* Note that

$$\sin\theta - \sin\phi = 2\sin\left(\frac{\theta-\phi}{2}\right)\cos\left(\frac{\theta+\phi}{2}\right).$$

Hence

$$\sin\left(a(x+1) - \frac{a}{2}\right) - \sin\left(ax - \frac{a}{2}\right) = 2\sin\left(\frac{a}{2}\right)\cos(ax),$$

so $S_a(k+1) - S_a(k) = \cos ak$. Using this in place of $\cos(ak)$ in the sum, canceling adjacent terms, and using $S_a(0) = -1/2$ gives the result. □

*Proof of Proposition 4.3.* Let

$$a^{\pm} = \pi \left( \frac{j_1}{d_1} \pm \frac{j_2}{d_2} \right).$$

Since $j_1/d_1$ and $j_2/d_2$ are both in $[0, 1]$, the only way that $\sin(a^{\pm}/2)$ could be 0 is if $x_1 = x_2$, which is excluded by assumption. Hence $\sin(a^{\pm}/2) \neq 0$.

Note that

$$\begin{aligned} T_{j_1}(x_{d_1,k})T_{j_2}(x_{d_2,k}) &= \cos\left(\frac{j_1 k\pi}{d_1}\right)\cos\left(\frac{j_2 k\pi}{d_2}\right) \\ &= \frac{\cos(a^+k) + \cos(a^-k)}{2}. \end{aligned}$$

Applying the previous lemma and adjusting for the factors of $1/2$ for $k = 0$ and $k = d_1$ gives

$$\begin{aligned} \sum_{k=0}^{d_1}{}'' T_{j_1}(x_{d_1,k})T_{j_2}(x_{d_2,k}) = &\left(\frac{S_{a^+}(d_1+1) + S_{a^-}(d_1+1)}{2}\right) \\ &- \frac{(-1)^{j_1}}{2}\cos\left(\frac{j_2 d_1 \pi}{d_2}\right). \end{aligned} \tag{8}$$

Let $S$ denote the numerator of the first term. We expand using the definition of $S_a$, combine fractions, and use $2\sin a \sin b = \cos(a-b) - \cos(a+b)$. Writing $a_k^{\pm} = a^{\pm}d_1 + j_k\pi/d_k$ we have

$$S = \frac{\cos(a_2^+) - \cos(a_1^+) + \cos\left(a^-d_1 - \frac{j_2\pi}{d_2}\right) - \cos(a_1^-)}{\cos\left(\frac{j_2\pi}{d_2}\right) - \cos\left(\frac{j_1\pi}{d_1}\right)}.$$

Rewriting the denominator as $x_2 - x_1$ and using $\cos a + \cos b = 2\cos((a+b)/2)\cos((a-b)/2)$ to combine the first and third terms of the numerator and likewise the second and fourth terms, we get

$$S = \frac{\cos(j_1\pi)\cos\left(\frac{j_2 d_1\pi}{d_2} + \frac{j_2\pi}{d_2}\right) - \cos\left(j_1\pi + \frac{j_1\pi}{d_1}\right)\cos\left(\frac{j_2 d_1 \pi}{d_2}\right)}{x_2 - x_1}.$$

Applying the usual angle addition formula for cos, then rewriting in terms of $x_1$ and $x_2$ gives

$$\begin{aligned} S &= (-1)^{j_1}\frac{\left(x_2 T_{d_1}(x_2) - \sqrt{1-x_2^2}\sin\left(\frac{j_2 d_1\pi}{d_2}\right) - x_1 T_{d_1}(x_2)\right)}{x_2 - x_1} \\ &= (-1)^{j_1}\left(T_{d_1}(x_2) - \frac{\left(\sqrt{1-x_2^2}\sin\left(\frac{j_2 d_1 \pi}{d_2}\right)\right)}{x_2 - x_1}\right). \end{aligned}$$

Dividing by 2 and subtracting the second term in (8) cancels $T_{d_1}(x_2)$ and leaves the expression in the statement of the proposition. □

*Remark:* Note that if $d_1 = d_2$ but $\sin(a^{\pm}/2)$ is not 0, then the expression in Proposition 4.3 is 0, which agrees with the result in Lemma 4.2.

## 5. Sparse grid interpolation and cubature

As seen in section 3, the primary step in computing the sensitivity values of Sobol' is estimating an integral of the form

$$G = \int_A \left( \int_B f(x,y) d\mu_B(y) \right)^2 d\mu_A(x), \tag{9}$$

where $A = K^m$, $B = K^{n-m}$, $f : A \times B \to \mathbb{R}$. Here we assume $f$ to be smooth.

In this section we recall the basic ideas for approximating $f$ on $[-1,1]^n$ using the sparse grid techniques of Smolyak, then apply this approximation to estimate $G$. See [1] for discussion of and references for sparse grid interpolation and cubature. As in [1], we use the extrema of the Chebyshev polynomials as nodes, with the coarsest level containing a single node and the remaining levels nested. For consistency with the literature, we largely adopt the indexing in [1] as well.

Let $M_1 = 1$, $M_i = 2^{i-1} + 1$ for $i > 1$. Let $x_1^1 = 0$, and for $i > 1$ and $1 \le j \le M_i$, let $x_j^i = \cos((j-1)\pi/(M_i - 1))$. Also, with notation as in the previous section, let $L_j^i = L_{M_i-1,j-1}$ and $w_j^i = w_{M_i-1,j-1}$. To describe the range of multi-indices corresponding to a given nonnegative multi-index $\alpha$, let $M(\alpha) = (M_{\alpha_1}, \ldots, M_{\alpha_n})$. For $\mathbf{1} \le \beta \le M(\alpha)$, define $x_\beta^{\otimes\alpha} = (x_{\beta_1}^{\alpha_1}, \ldots, x_{\beta_n}^{\alpha_n})$, $w_\beta^\alpha = w_{\beta_1}^{\alpha_1} \cdots w_{\beta_n}^{\alpha_n}$, and $L_\beta^\alpha = L_{\beta_1}^{\alpha_1} \cdots L_{\beta_n}^{\alpha_n}$. Note that $w_\beta^\alpha = \int_{K^n} L_\beta^\alpha d\mu$. For $n > 1$, define

$$\mathcal{A}^{\otimes\alpha}(f) = \sum_{0 \le \beta \le M(\alpha)} f(x_\beta^{\otimes\alpha}) L_\beta^\alpha.$$

The Smolyak interpolation formula is then

$$\mathcal{A}(q,n)(f) = \sum_{q-n+1 \le |\alpha| \le q} (-1)^{q-|\alpha|} \binom{n-1}{q-|\alpha|} \mathcal{A}^{\otimes\alpha}(f). \tag{10}$$

By integrating this formula as was done to obtain (6), we obtain the standard Smolyak cubature formula to approximate the integral of $f$ over $K^n$.

To describe the accuracy of this interpolation, let $\Theta(q,n)$ be the set of all points of evaluation in (10). That is,

$$\Theta(q,n) = \bigcup_{q-n+1 \le |\alpha| \le q} \; \bigcup_{0 \le \beta \le M(\alpha)} \{x_\beta^{\otimes\alpha}\}.$$

Let $N$ denote the number of points in $\Theta(q,n)$. From [1], if $k$ is fixed, $n$ is large, and $q = n + k$, then $N \approx 2^k n^k / k!$. Moreover, assuming that $D^\alpha f$ is continuous for all $|\alpha| \le \ell$, we may define

$$\|f\| = \max\{\|D^\alpha f\|_\infty : \alpha \in \mathbb{N}_0^n, \alpha_i \le \ell\}.$$

Then [1, Theorem 8] gives the error bound

$$\|A(q,n)(f) - f\|_0 \le C_{n,\ell} N^{-\ell} (\log N)^{(n-1)(\ell+2)+1} \|f\|. \tag{11}$$

By integrating, this bound also gives an estimate for the error in approximating the integral of $f$.

## 6. Cubature for sensitivity values

There are several possible approaches to approximating the integral in (9). Here we describe two methods, each of which requires evaluation of $f$ only on the sparse grid, $\Theta$, independent of the subsets of coordinates used to determine $A$ and $B$. The first method applies the ideas used to develop integral approximations as in the previous two sections. That is, first replace the function, $f$, by an approximation using Lagrange interpolating polynomials, then integrate. This method is used to calculate the main effect coefficients, $S_j$. The second method is to use sparse-grid cubature directly on a higher dimesional space, but use projection and the symmetry of the support nodes to require evaluation of $f$ on the original set $\Theta$ only. This method is used to calculate the total effect coefficients, $S_{T_j}$. For clarity of notation, in this section we drop $d\mu_A(x)$ in favor of $dx$, etc., with the assumption that the normalizing factors remain implicit.

**Main effect values**

For the main effect coefficients, $S_j$, we need to approximate (9) in the case when $A$ is 1-dimensional. To do this, we first approximate $f$ via $\mathcal{A}(q,n)$ on a Smolyak cubature set, $\Theta$, to get an approximating function $\hat{f}$. Suppressing the precise bounds on $\alpha$ and $\beta$, we obtain

$$\hat{f}(x,y) = \sum_{\alpha,\beta} C_\alpha f(x_\beta^{\otimes\alpha}) L_\beta^\alpha(x,y),$$

where $x \in A$, $y \in B$ as in (9) and $C_\alpha$ is the coefficient in (10). Note that a given point in $\Theta$ may appear more than once in this sum since the point $x_\beta^{\otimes\alpha}$ is unchanged if a nonunit coordinate in $\alpha$ is increased by 1 and the corresponding coordinate in $\beta$ is multiplied by 2 or if $\alpha = 1$ is increased to 2 and $\beta = 1$ is increased to 2. In practice, we collect terms associated to the same point, but for exposition we keep the form above. Replacing $f$ by $\hat{f}$ and expanding the square in $G$, we get the approximation

$$\begin{aligned}\hat{G} &= \int_A \int_B \int_B \hat{f}(x,y)\hat{f}(x,z)\,dydzdx \\ &= \sum_{\alpha,\beta} \sum_{\alpha',\beta'} C_\alpha C_{\alpha'} f(x_\beta^{\otimes\alpha}) f(x_{\beta'}^{\otimes\alpha'}) \int_{A\times B\times B} L_\beta^\alpha(x,y) L_{\beta'}^{\alpha'}(x,z)\,dydzdx.\end{aligned}$$

To compute the final integral, note that the product form of $L_\beta^\alpha$ means that this integral is actually a product of one dimensional integrals. For the integral over each coordinate in $A$, we obtain an integral of a product of two interpolating polynomials as in (7), which may be evaluated as in

Corollary 4.4. For the integral over each coordinate in $B$, we obtain an integral of a single interpolating polynomial, which may be evaluated as in Proposition 4.1. In each case, this evaluation is linear in the degree of the polynomials. Moreover, each of these one dimensional integrals may be precomputed and then multiplied as needed to compute each multidimensional integral in the expression above.

To make this more explicit, let $\alpha(A)$ be the projection of $\alpha$ to the coordinates in $A$, and likewise for $\alpha(B)$. Also, let

$$(L^{\alpha}_{\beta}, L^{\alpha'}_{\beta'})_A = \int_A L^{\alpha(A)}_{\beta(A)}(x) L^{\alpha'(A)}_{\beta'(A)}(x)dx,$$

and note that

$$w^{\alpha(B)}_{\beta(B)} = \int_B L^{\alpha(B)}_{\beta(B)}(y)dy.$$

Then

$$\hat{G} = \sum_{\alpha,\beta} \sum_{\alpha',\beta'} C_{\alpha} C_{\alpha'} f(x^{\otimes\alpha}_{\beta}) f(x^{\otimes\alpha'}_{\beta'}) w^{\alpha(B)}_{\beta(B)} w^{\alpha'(B)}_{\beta'(B)} (L^{\alpha}_{\beta}, L^{\alpha'}_{\beta'})_A.$$

As noted above, $A$ is one-dimensional when computing $S_j$; without loss, we may assume that $A$ is the first coordinate direction. In this case, the expression above, which is a quadratic form, is nearly a diagonal quadratic form, except for the appearance of the inner product. In practice, for moderately large dimension, most entries in a multi-index $\alpha$ are trivial. Hence for computational efficiency, we may represent a point in $\Theta$ as the nontrivial entries in $\alpha$ and $\beta$ together with a choice of coordinate direction for each nontrivial entry. With this representation, the coefficients in the expression above depend only on the nontrivial entries in $\alpha$, $\alpha'$, $\beta$, and $\beta'$ plus whether or not the first coordinate in $\alpha$ and $\alpha'$ is trivial or not. Keeping track of this accounting and summing up over all equivalent representations of points in $\Theta$, we obtain a block representation of this quadratic form. That is, collecting terms corresponding to identical points in $\Theta$ produces $\hat{G} = v^T W v$, where $v$ is a column vector obtained by evaluating $f$ at the points of $\Theta$. However, by using the combinatorial representation of points in $\Theta$, we identify sets of pairs of points with a common value for the corresponding coefficient in the quadratic form. Reordering the rows and columns, we identify a block structure in $W$. Replacing $W$ by the matrix $\hat{W}$ formed from the coefficients in this block and replacing $v$ by $\hat{v}$ formed by summing the elements of $v$ in each block, we obtain $\hat{G} = \hat{v}^T \hat{W} \hat{v}$.

Note that, for fixed $n = \dim(A \times B)$, the set of functional evaluations is exactly $\Theta$ regardless of $m = \dim(A)$, so the time required is $O(N) = O(2^k n^k / k!)$, for fixed $k = q - n$ and large dimension $n$. In practice, $f$ may be expensive to compute, so this represents the bulk of the computational time. For completeness, we analyze the time required to compute all the $S_j$. Note that the weights $w^{\alpha}_{\beta}$ and integrals of interpolating functions may be precomputed in time $O(d^2)$, where $d = 2^k$ is the maximum degree of the interpolating polynomials $L^i_j$.

After collecting terms corresponding to multiple occurences of a given point in $\Theta$, the double sum for $\hat{G}$ may then be computed at first glance in time $O(N^2)$. However, we may reduce this estimate using the block structure described above. For a given pair, $\alpha$ and $\beta$, define the corresponding minimal represntative to be the nontrivial entries of $\alpha$, with order preserved, and the corresponding entries in $\beta$. For a given norm $n < |\alpha|$, we need to determine the nontrivial entries in $\alpha$. This can be done by distributing $t = |\alpha| - n$ balls into some number, $s$, of nonempty slots, where $1 \leq s \leq n$, which can be done in $\binom{t-1}{s-1}$ ways. For a given such choice, the number in a given slot, $t_j$, gives $M_{t_j+1} = 2^{t_j} + 1$ corresponding points in that coordinate in the sparse grid. One of these points is 0, which may be ignored since it will have been counted for smaller values of $t_j$. This gives $2^{t_j}$ points, for each slot independently, for a total of $2^t$ points corresponding to this choice of $\alpha$. This estimate is quite crude since it double counts many points, but it will suffice here. Let $R$ be the total number of representatives. Summing over $t$ and $s$ gives

$$R \leq \sum_{t=1}^{k} 2^t \sum_{s=1}^{t} \binom{t-1}{s-1}.$$

Recognizing the inner sum as $2^{t-1}$ (the total number of subsets of $t-1$ elements) and using the partial geometric sum in the outer sum gives $R \leq 2(4^k - 1)/3$. Since the sum for $\hat{G}$ is different for multi-indices which are trivial in the first slot versus those that are nontrivial in the first slot, we see that $2R$ gives an upper bound for the number of rows in $\hat{W}$. Since we can compute $\hat{v}$ from the values of $f$ on $\Theta$ in time $O(N)$, we see that after precomputation of the weights and the function evaluations, we may compute $\hat{G}$ in time $O(R^2) = O(8^k)$, which is $O(N)$ for fixed $k$ and large $n$. Finally, the mean, $f_0$, and the variance, $D$, may be computed using the standard sparse grid cubature rule, which gives time $O(N)$. Hence the total time for a single value $S_1$ is $O(N)$. To obtain all the $S_j$, we create a cyclic permutation of the points in $\Theta$ by cyclically permuting the coordinate directions: $\sigma(x_1, \ldots, x_n) = (x_2, \ldots, x_n, x_1)$. By the symmetry of the sparse grid, we have $\sigma(\Theta) = \Theta$. Computing $\hat{G}$ for $f\sigma$ allows us to compute $S_2$, and iterating gives $S_1, \ldots, S_n$. Hence we obtain

**Theorem 6.1.** *For a fixed level of approximation $k$ and large dimension $n$, the main effect sensitivity coefficients $S_j$, $j = 1, \ldots, n$, for $f$ may be computed in time $O(nN) = O(2^k n^{k+1}/k!)$. The function $f$ need be evaluated only on the sparse grid $\Theta$.*

**Total effect values**

For $S_{T_j}$, the total effect values, the set $A$ in (9) is $(n-1)$-dimensional, and the accounting as described above for $\hat{G}$ is much more involved since now the inner product $(L^{\alpha}_{\beta}, L^{\alpha'}_{\beta'})_A$ depends on the overlap pattern of the nontrivial entries in the multi-indices. In contrast, $B$ is only 1-dimensional in this case, so the integral

$$\int_A \int_B \int_B f(x,y)f(x,z)dydzdx \tag{12}$$

is only $(n+1)$-dimensional. Moreover, the symmetry of the nested sparse grid implies that if $(x,y,z) \in K^{n-1} \times K \times K$ is a point in the sparse grid of dimension $n+1$ and maximum norm $q+1$, then $(x,y)$ and $(x,z)$ are both points in the sparse grid of dimension $n$ and maximum norm $q$; that is, they are both points in $\Theta(q,n)$. Hence we may approximate the integral (12) by first evaluating $f$ on the points in $\Theta$, then using appropriate projections from $\Theta(q+1,n+1)$ to $\Theta(q,n)$ to define $g(x,y,z) = f(x,y)f(x,z)$ evaluated on $\Theta(q+1,n+1)$. Given $g$, we may then approximate (12) using the standard sparse grid cubature weights. As before, $f_0$, $D$, and the evaluations of $f$ may be done in time $O(N)$. Also as before, for fixed $k = q-n$ and large $n$, the construction of $g$ and the subsequent cubature may be done in time $O(2^k(n+1)^k/k!) = O(N)$. Using cyclic permutations as before, we have the corresponding theorem for $S_{T_j}$.

**Theorem 6.2.** *For a fixed level of approximation $k$ and large dimension $n$, the total effect sensitivity coefficients $S_{T_j}$, $j = 1,\dots,n$, for $f$ may be computed in time $O(nN) = O(2^k n^{k+1}/k!)$. The function $f$ need be evaluated only on the sparse grid $\Theta$.*

**Convergence**

Note that (11) guarantees convergence of the computed values of (9) to the true values as $q \to \infty$ (hence $N \to \infty$) under the assumption that $f$ is $C^\ell$ smooth, $\ell \geq 1$. For the method used to compute $S_{T_j}$, this follows directly by replacing $f(x,y)$ by $g(x,y,z) = f(x,y)f(x,z)$ in (11). For the method used to compute $S_j$, we need to show the convergence of $\|A(q+1,n+1)(f_1)A(q+1,n+1)(f_2) - f_1 f_2\|$ to 0 as $q \to \infty$, where $f_1(x,y,z) = f(x,y)$, $f_2(x,y,z) = f(x,z)$. But this follows immediately by adding and subtracting $A(q+1,n+1)(f_1)f_2$, using the triangle inequality, then using (11) together with the sup norm bound on $f$.

Since the calculation of $S_j$ and $S_{T_j}$ requires dividing (9) by $D$, the error in these values may be sensitive to the details of the function, particularly for functions with small variance. However, in practice, only the magnitude of one sensitivity in comparison to the others is used to guide exploration of parameter space. Since all the values $S_j$ and $S_{T_j}$ include the same factor $1/D$, we may directly compare the integrals used to determine the sensitivity values, in which case the convergence is given by (11).

## 7. Numerical results

In order to evaluate this method, we computed $S_j$ and $S_{T_j}$ for a variety of standard test functions. As noted above and in [1], the convergence for sparse grid cubature using Clenshaw-Curtis nodes depends strongly on the differentiability of the function being integrated. For discontinuous functions or functions whose first derivatives are discontinuous, the estimates from sparse grid cubature are poor to nearly useless. At the opposite extreme, for low degree polynomials, sparse grid cubature will give answers which are correct to round-off error for correspondingly low values of $q$. Since the output of many models of interest for sensitivity analysis lies between these two extremes, we have chosen a set of test functions that lie between these extremes. The test functions are the functions 1 through 4 of [1]:

1. OSCILLATORY: $f_1(x) = \cos\left(2\pi w_1 + \sum_{i=1}^{n} c_i x_i\right),$
2. PRODUCT PEAK: $f_2(x) = \prod_{i=1}^{n} (c_i^{-2} + (x_i - w_i)^2)^{-1},$
3. CORNER PEAK: $f_3(x) = \left(1 + \sum_{i=1}^{n} c_i x_i\right)^{-(n+1)},$
4. GAUSSIAN: $f_4(x) = \exp\left(-\sum_{i=1}^{n} c_i^2 (x_i - w_i)^2\right).$

We used $n = 10$ and chose values for $c_i$ and $w_i$ at random as indicated in [1].

We compared our method to the Extended FAST method of [5] and to the quasi-Monte Carlo integration method labeled the 'Richtmyer sequence' in [10]. To apply quasi-Monte Carlo, we expanded the integral as in (12) and partitioned the points so that the total number of points used to calculate all of the main effect values was roughly the same as the number of points used to calculate all of these values using the sparse grid method, and likewise for the total effect values; some version of this method is often called 'Sobol's method' [8]. We show the computed values plotted as functions of the number of points evaluated in Figures 1 (main effect value) and 3 (total effect values). Each line corresponds to the sensitivity value for one coordinate direction. Note that the sparse grid method and to a lesser extent the Extended FAST method provide relatively consistent size relationships among the various factors even for small numbers of model evaluations. That is, a common application for sensitivity analysis is to determine which parameters are the most sensitive. These results show that sparse grid and Extended FAST generally provide reasonable answers even when the number of model evaluations is relatively low.

Where possible, we also computed main effect and total effect sensitivity values analytically (using the Integrate function of Mathematica with numerical evaluation). For these cases, we show the average differences (taken over each of the 10 coordinate directions) between the approximated and exact values for both main and total effect values, plotted as functions of the number of points evaluated. We also show the maximimum and minimum relative errors, $|S - \hat{S}|/S$, where $S$ is the exact sensitivity value and $\hat{S}$ is the computed value. These results are shown in Figures 2 and 4. For the function Corner Peak, we were not able to compute analytic values in a reasonable amount of time, so we show only the values obtained rather than error values.

The error plots show that the sparse grid has good accuracy, even for small numbers of function evalutions, and good convergence as the number of function evaluations increases. The quasi-Monte Carlo method is generally less accurate but still has reasonably good convergence. The Extended FAST method is often reasonably accurate but doesn't display much improvement with the number of function evaluations. It may be that different choices in the particulars of the Extended FAST algorithm would produce better convergence; we have not tried to address this question since it represents a completely different line of inquiry.

For each of the four functions, the sparse grid method shows the best overall accuracy and convergence rates. This accuracty is especially pronounced for the relative error with a small number of function evaluations, which is in turn reflected in the plots of the sensitivity values themselves; the sparse grid values are generally in the correct order, even for a small number of function evaluations.

## 8. Conclusion

We have used sparse grid interpolation and cubature to produce a numerically accurate and efficient method for computing the main and total effect variance-based global sensitivity coefficients. This method displays good accuracy and convergence properties on functions which are known to be globally differentiable, compares favorably with existing methods, and allows for the computation of all sensitivity values from the evaluation of function on a single set of sparse grids.

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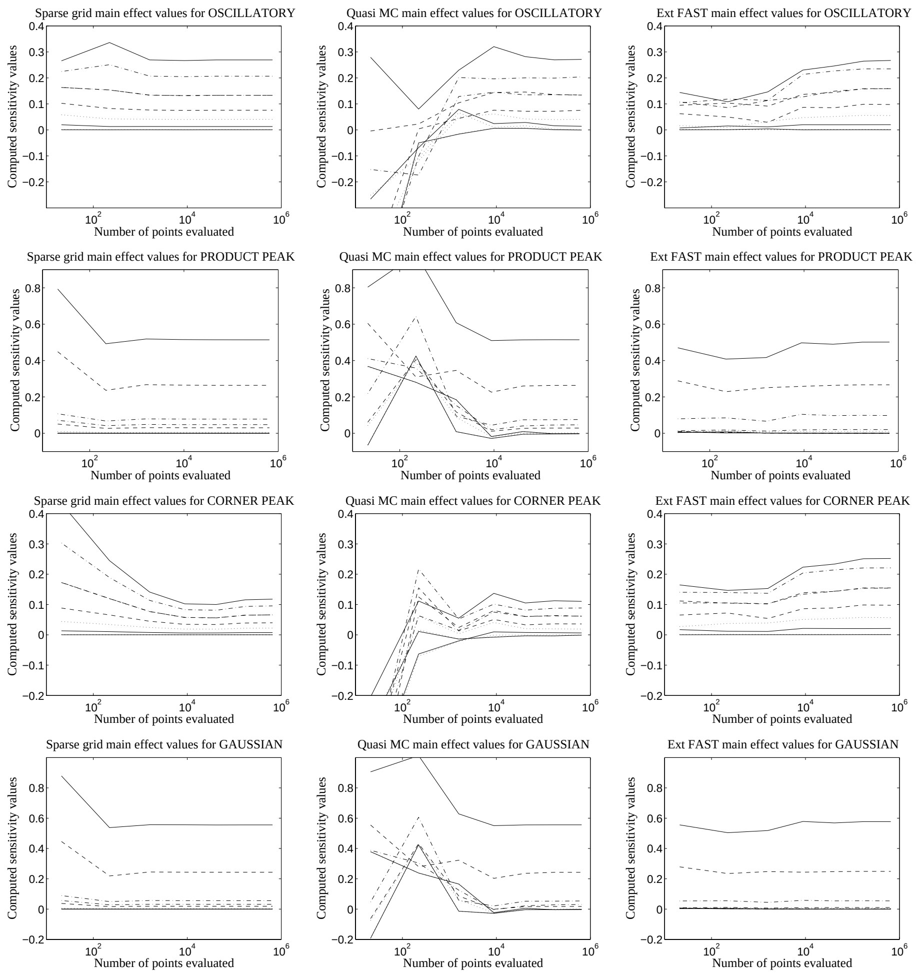


FIGURE 1. Computed main effect values plotted against number of points evaluated. Left: sparse grid method. Right: Quasi-Monte Carlo method.

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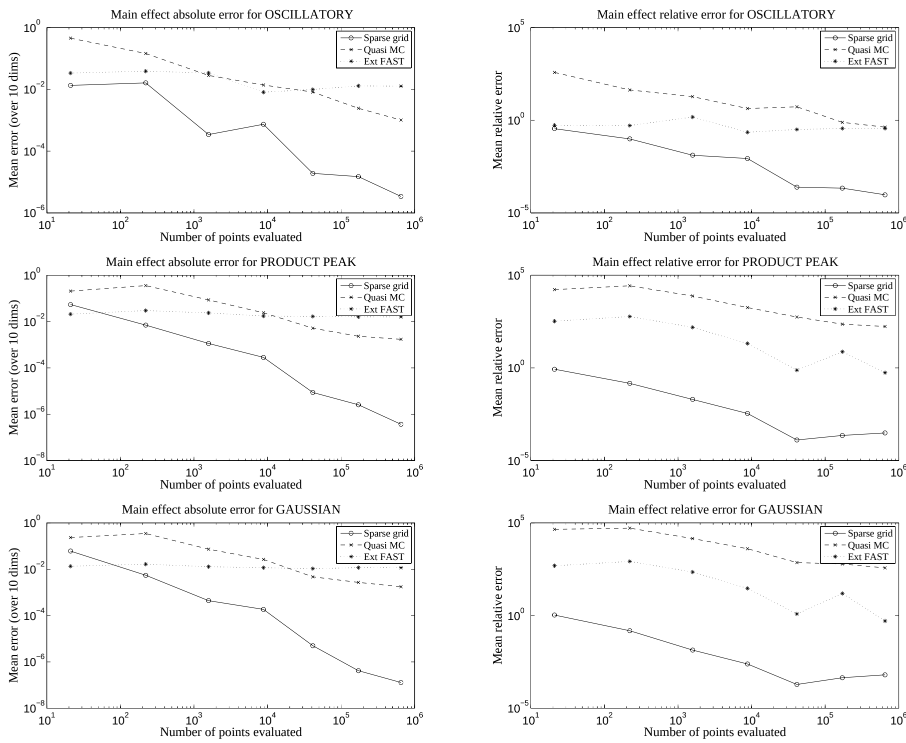


FIGURE 2. Average differences (averaged over all 10 coordinate dimensions) between approximated and true main effect values. Left: Absolute errors. Right: Relative errors.

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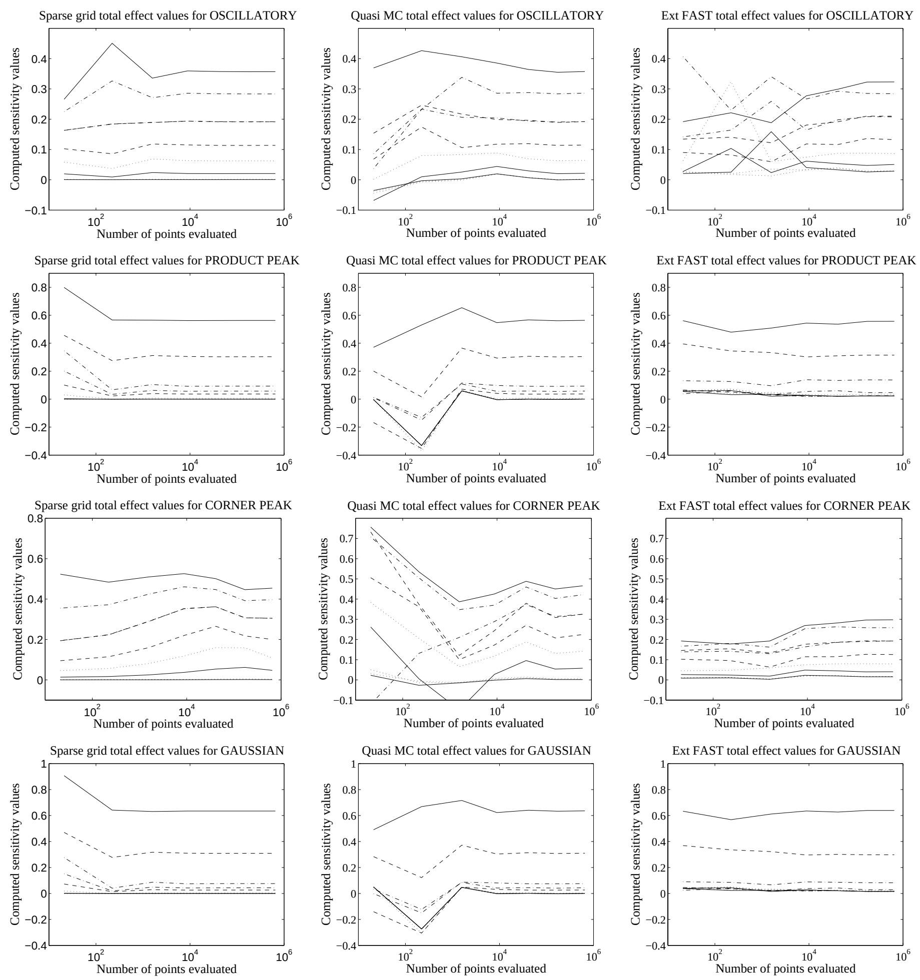


FIGURE 3. Computed total effect values plotted against number of points evaluated. Left: sparse grid method. Right: Quasi-Monte Carlo method.

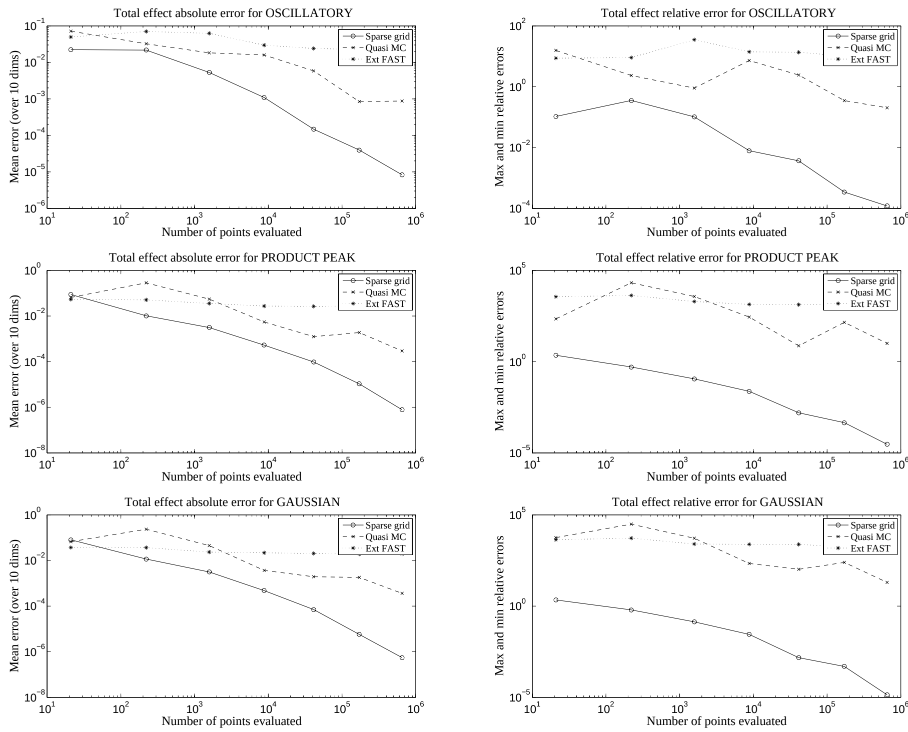


FIGURE 4. Average differences (averaged over all 10 coordinate dimensions) between approximated and true total effect values. Left: Absolute errors. Right: Relative errors.