Higher order Sobol’ indices

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June 2013

Abstract
Sobol’ indices measure the dependence of a high dimensional function on groups of variables defined on the unit cube $[0,1]^d$. They are based on the ANOVA decomposition of functions, which is an $L^2$ decomposition. In this paper we discuss generalizations of Sobol’ indices which yield $L^p$ measures of the dependence of $f$ on subsets of variables. Our interest is in values $p > 2$ because then variable importance becomes more about reaching the extremes of $f$. We introduce two methods. One based on higher order moments of the ANOVA terms and another based on higher order norms of a spectral decomposition of $f$, including Fourier and Haar variants. Both of our generalizations have representations as integrals over $[0,1]^{kd}$ for $k \geq 1$, allowing direct Monte Carlo or quasi-Monte Carlo estimation. We find that they are sensitive to different aspects of $f$, and thus quantify different notions of variable importance.

1 Introduction

Sobol’ indices (Sobol’, 1990) are the standard way to measure the importance of variables and subsets of variables for a black box function defined on the unit cube $[0,1]^d$. These measures are used in applications in aerospace engineering and climate models among many others.

Sobol’s indices are based on the ANOVA decomposition of $[0,1]^d$, which is an $L^2$ method. An aeronautics-astronautics engineering student, Gary Tang, asked us about how to construct an alternative to Sobol’ indices that would identify which variables are most important when one is especially interested in the extreme values taken on by the function. In this paper we address that problem by considering alternative measures based on other criteria that place greater emphasis on extremes than $L^2$ does.

Perhaps the simplest way to get an index more sensitive to extremes in $f$ is to replace the target function $f(x)$ by a transformed version such as $|f(x)|$ or $\exp(f(x))$ or $1_{f(x) \geq M}$ for a threshold $M$ and so on, followed by an application of
the usual Sobol’ indices. This approach will often be reasonable. In some cases though, it may complicate the problem. For example, if \( f \) is a sum of functions of one variable at a time, then \( f^2 \) involves pairwise interactions that were not present in \( f \), and \( 1_{f(x) \geq M} \) may involve interactions of all orders. Furthermore, if \( f \) only takes two values, such as 0 or 1 (e.g., safe versus dangerous outcomes), then transforming it to take two different values does not help. As a result, we consider new generalizations.

The ANOVA can be developed as an analysis of \( L^2[0,1]^d \), or as a synthesis of Fourier, Walsh or other basis expansions. Both of these methods can be used to make \( L^p \) generalizations. Additionally, the Sobol’ indices satisfy some identities that can be directly generalized. These approaches coincide for \( p = 2 \), but they differ for \( p \neq 2 \).

An outline of this paper is as follows. Section 2 introduces our notation and reviews the ANOVA and Sobol’ indices. Section 3 presents some related non-\( L_2 \) concepts, median polish and analysis of skewness, from the literature. One of our methods includes a crossed-effects extension of the analysis of skewness as a special case. Section 4 presents a generalization based on extending one of Sobol’s identities to \( p \)th order moments. The identity yields a representation of the index as an integral of dimension \( dp \) or lower. For even integers \( p \geq 2 \) we show that the resulting estimates are nonnegative and increase when any set of variables is replaced by a superset. Section 5 presents a generalization based on the synthesis from a Fourier expansion. When \( p \geq 2 \) is an even integer, then the resulting importance measures are sums of \( p \)th powers of the moduli of the function’s Fourier coefficients. Yet they can still be estimated directly by a high dimensional quadrature, based on an identity like one of Sobol’s. That integral can be converted into one of dimension \( d(p - 1) \) or lower. We also provide a version based on Walsh functions, which again has nonnegativity and additivity when \( p \geq 2 \) is an even integer and also has an integral representation for quadrature. For odd \( p \), we include a ‘Dirichlet kernel trick’ that produces non-negative importance measures based on \( L_p \) norms of Fourier or Walsh coefficients. That method also allows one to favor certain parts of the spectrum.

Section 6 illustrates our importance measures on test functions that are sums or products. We use such examples to confirm that our measures focus on variables that bring \( f \) towards extreme values. For product functions, and even \( p \), our spectral measures find that the most important variables are those whose spectrum is sparsest. Our moment measure, for \( p = 4 \), favors variables with high kurtosis and with mean and skewness of the same sign. We look also at the important special case a rectangular spike: \( f(x) = \prod_{j=1}^{d} 1_{x_j \leq \epsilon_j} \). When \( f \) measures hitting a small region like this the variable with the smallest \( \epsilon_j \) is the most important one, at least when all \( \epsilon_j \) are small. Both moment and Fourier measures favor small \( \epsilon_j \). For additive functions, having no interactions, we find that the spectral measures place all their importance on singleton sets. The moment measure does this for third but not fourth moments. Section 7 has a discussion.
2 Notation

We are given a real-valued function $f$ defined on $[0,1]^d$ for $d \geq 1$ and we are interested in quantifying the importance of $f$ of various subsets of the variables in the set $\mathcal{D} = \{1,2,\ldots,d\}$.

We make frequent use of subsets of $\mathcal{D}$ as indices. The complement of $u \subseteq \mathcal{D}$ is $u^c = \mathcal{D} - u$, or simply $-u$ when that is typographically more convenient. The cardinality of $u$ is $|u|$. For $x \in [0,1]^d$, the point $x_u \in [0,1]^{|u|}$ is made up of $x_j$ for $j \in u$ and $dx_u = \prod_{j \in u} dx_j$. We use $u \subset v$ to mean that $u$ is a proper subset of $v$ (i.e., $u \subsetneq v$).

We often make a new point from components of two old points. If $x, z \in [0,1]^d$ and $u \subseteq \mathcal{D}$, then $y \equiv x_u \cdot z_{-u}$ is the point in $[0,1]^d$ with $y_j = x_j$ for $j \in u$ and $y_j = z_j$ for $j \notin u$.

2.1 ANOVA of $[0,1]^d$

The ANOVA decomposition represents $f(x)$ via

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

(1)

where the functions $f_u$ are defined recursively by

$$f_u(x) = \int_{[0,1]^{d-|u|}} \left( f(x) - \sum_{v \subsetneq u} f_v(x) \right) dx_{-u}.$$  

(2)

From usual conventions, $f_\emptyset(x) = \mu \equiv \int_{[0,1]^d} f(x) \, dx$ for all $x \in [0,1]^d$. The function $f_u$ only depends on $x_j$ for $j \in u$. For $f \in L^2[0,1]^d$, these functions satisfy $\int_0^1 f_u(x) \, dx_j = 0$ when $j \in u$, from which it follows that $\int f_u(x) f_v(x) \, dx = 0$ for $u \neq v$ and that

$$\sigma^2 = \sum_{u \subseteq \mathcal{D}} \sigma_u^2$$

(3)

where $\sigma^2 = \int (f(x) - \mu)^2 \, dx$, $\sigma_\emptyset^2 = 0$ and $\sigma_u^2 = \int f_u(x)^2 \, dx$ for $u \neq \emptyset$. The name ANOVA stands for analysis of variance, as given by (3). This decomposition goes back to Hoeffding [1948].

Sobol’ [1969] obtained the decomposition (1) by a different route, described next. Let $\phi_k$ for $k \in \mathbb{I}$ be a complete orthonormal basis for $L^2[0,1]$, where $\mathbb{I}$ is a countable index set containing a 0 element, with $\phi_0(x) = 1$, $\forall x \in [0,1]$. We can form the tensor product basis $\phi_k(x) = \prod_{i=1}^d \phi_{k_i}(x_i)$, for $k \in \mathbb{I}^d$ and then $f(x) = \sum_{k \in \mathbb{I}^d} \beta_k \phi_k(x)$ where $\beta_k = \int f(x) \phi_k(x) \, dx$. Then, with $0$ a vector of $d$ zeros, and $\mathbb{I}_0$ the nonzero members of $\mathbb{I}$,

$$f_u(x) = \sum_{k_u \in \mathbb{I}_0^{|u|}} \beta_{k_u \cdot 0_{-u}} \phi_{k_u \cdot 0_{-u}}(x)$$

(4)
recovers the functions defined at (2), and \( \sigma_u^2 = \sum_{j \in 1^{|u|}} \beta_j^2 \cdot \mathbf{o}_{-u} \). Sobol' (1969) used Haar functions for his ‘decomposition into summands of different dimensions’ given by (1). Where Hoeffding has an analysis, Sobol’ has a synthesis of variance.

2.2 Sobol’ indices and identities

The importance of variable \( j \in D \) is due in part to \( \sigma_{\{j\}}^2 \), but also due to \( \sigma_u^2 \) for other sets \( u \) with \( j \in u \). More generally, we may be interested in the importance of a subset \( u \) of the variables.

Sobol’ introduced two measures of variable subset importance, which we denote

\[
\tau_u^2 = \sum_{v \subseteq u} \sigma_v^2, \quad \text{and} \quad \tau_u^2 = \sum_{v \cap u \neq \emptyset} \sigma_v^2.
\]

These satisfy \( \tau_u^2 \leq \tau_v^2 \) and \( \tau_u^2 + \tau_{-u}^2 = \sigma^2 \). Sobol’ usually normalized these quantities by \( \sigma^2 \), yielding global sensitivity indices \( \tau_u^2 / \sigma^2 \) and \( \tau_{-u}^2 / \sigma^2 \). We will use the unnormalized versions.

It is an elementary consequence of the ANOVA definitions that

\[
\iint f(x) f(x_u: z_{-u}) \, dx \, dz = \mu^2 + \tau_u^2
\]

and

\[
\frac{1}{2} \iint (f(x) - f(x_{-u}: z_u))^2 \, dx \, dz = \tau_u^2.
\]

We write these integrals over \((x, u) \in [0,1]^{2d}\), although the first really only uses \(2d - |u|\) components and the second uses \(d + |u|\).

The great convenience of Sobol’ measures is that they can be directly estimated by integration without bias. We do not need to explicitly estimate, square, integrate and sum the individual ANOVA terms. As a consequence, we can avoid numerical optimization and bias corrections.

It is computationally convenient to replace equation (5) by

\[
\iint f(x)(f(x_u: z_{-u}) - f(z)) \, dx \, dz = \tau_u^2,
\]

because it eliminates the need to subtract an estimate of \( \mu \). Equation (7) was developed independently in Saltelli (2002) and by Mauntz (2002), and it performs better when \( \tau_u^2 \) is small. For discussion and another estimator, see Owen (2012a).

2.3 Generalizations

We have three different ways to generalize the ANOVA to higher moments. First, we can generalize the original ANOVA decomposition by noticing that the
integrals in it minimize a quadratic quantity, and then replacing that quadratic by a higher order moment. Second, we can generalize the Sobol’ indices directly, replacing the integrals of products of pairs of function values by integrals of products of three or more function values. Third, we can generalize Sobol’s synthesis.

3 Related literature

In this section we consider two non-$L_2$ methods from the literature. A natural approach to generalizing the ANOVA to $p \neq 2$ begins with the probabilistic interpretation of $f_u(x)$ as a conditional expectation

$$f_u(x) = \mathbb{E}\left( f(x) - \sum_{v \subset u} f_v(x) \mid x_u \right).$$

For any $x_u \in [0, 1]^d$

$$f_u(x) = \arg\min_m \mathbb{E}\left( \left( f(x) - \sum_{v \subset u} f_v(x) - m \right)^2 \mid x_u \right).$$

Just as the conditional expectation minimizes conditional variance, we may generalize the ANOVA to moments $p \geq 1$, via

$$f_u^{(p)}(x) = \arg\min_m \mathbb{E}\left( |f(x) - \sum_{v \subset u} f_v^{(p)}(x) - m|^p \mid x_u \right).$$

This generalization satisfies $f(x) = \sum_u f_u^{(p)}(x)$ through the definition of $f_u^{(p)}$, but the terms in it are not generally orthogonal. Nor do they decompose $\int |f(x)|^p \, dx$, nor do they generally integrate to 0 over $x_j$ for $j \in u$. If $|f|$ is bounded, then there is a $p = \infty$ version corresponding to a statistic called the.midrange.

It is cumbersome to minimize norms other than $L_2$ to define alternatives to $f_u$. The one example we found for this approach is the median polish method, in the next section. It uses $p = 1$, which might be expected to place less emphasis on extremes of $f$ than the ANOVA, and is based on conditional medians.

3.1 Median polish

Tukey [1977] describes the median polish algorithm for a two dimensional table of numbers $X_{ij}$, $i = 1, \ldots, I$ and $j = 1, \ldots, J$. The median polish algorithm generates a decomposition

$$X_{ij} = a_i + b_j + R_{ij}.$$

Starting with $a_i = b_j = 0$ and $R_{ij} = X_{ij}$, it alternates between row steps

$$m_i \leftarrow \text{median}(R_{i1}, \ldots, R_{iJ}), \quad 1 \leq i \leq I$$

and column steps

$$m_j \leftarrow \text{median}(R_{1j}, \ldots, R_{IJ}), \quad 1 \leq j \leq J$$



5
\[ a_i \leftarrow a_i + m_i, \quad 1 \leq i \leq I \]
\[ R_{ij} \leftarrow R_{ij} - m_i, \quad 1 \leq i \leq I, 1 \leq j \leq J \]
and analogous column steps. Siegel (1983) shows that the algorithm converges when all of the \( X_{ij} \) are rational numbers. While median polish will converge to a result where every row and column of \( R_{ij} \) has median 0, the result does necessarily have the \( L_1 \) minimizing values of \( a_i \) and \( b_j \). For a table of data with an even number \( I = 2k \) of rows, Siegel (1983) gets better results via the ‘low median’, which is the \( k \)'th smallest value, instead of the median which averages the \( k \)'th and \( k + 1 \)'st values. In principal one could evaluate \( f \) on a grid embedded in \([0, 1]^2\) and apply the median polish algorithm. While there may be reasonable ways to generalize median polish to \( d > 2 \), the necessity of estimating the additive components in order to measure them is computationally unattractive.

### 3.2 Analysis of skewness

Wang (2001) defines an analysis of skewness for problems in biology. Let \( X_{ij} \) be a measure on animal \( j = 1, \ldots, n_i \) from population \( i = 1, \ldots, I \). Here animals are nested within populations and the appropriate analysis of variance is:

\[
\sum_{i=1}^{I} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{..})^2 = \sum_{i=1}^{I} n_i (\bar{X}_{i.} - \bar{X}_{..})^2 + \sum_{i=1}^{I} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{i.})^2.
\]

An analogous analysis of skewness is

\[
\sum_{i=1}^{I} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{..})^3 = \sum_{i=1}^{I} n_i (\bar{X}_{i.} - \bar{X}_{..})^3 + \sum_{i=1}^{I} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{i.})^3
\]

\[+ 3 \sum_{i=1}^{I} (\bar{X}_{i.} - \bar{X}_{..}) \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_{i.})^2.
\]

The terms above correspond to skewness of group means, skewness of observations within groups and a third term measuring the correlation of within group variance and the group mean. The relative sizes of these terms have been interpreted in terms of driven versus passive trends in evolutionary biology. The total skewness can be negative as can any of its terms.

The analysis is centered on \( \bar{X}_{..} \) which is not generally the minimizer of \( \sum_{i} \sum_{j} |X_{ij} - m|^3 \) over \( m \in \mathbb{R} \). Similarly, \( \bar{X}_{i.} \) minimizes \( \sum_{j} |X_{ij} - m|^2 \) not \( \sum_{j} |X_{ij} - m|^3 \). In other words, this method is not based on generalizing the successive minimization property of ANOVA terms.

For functions on the unit cube, we can develop an analysis of skewness. A crossed decomposition is more appropriate than a nested one. Let \( f(x) = \mu + \sum_{u \neq \emptyset} f_u(x) \) be the ANOVA decomposition of \( f \). Then

\[
\int (f(x) - \mu)^3 \, dx = \sum_{u \neq \emptyset} \sum_{v \neq \emptyset} \sum_{w \neq \emptyset} \int f_u(x) f_v(x) f_w(x) \, dx
\]
The product \( f_u f_v f_w \) has mean zero if there is some index \( j \) that belongs to precisely one of the sets \( u, v, w \). There can be more nonzero terms than nonempty subsets of \( D \). For example \( f_{(1,2)}(x)f_{(2,3)}(x)f_{(1,3)}(x) \) need not integrate to zero. After eliminating the terms that must be zero, we find that \( \int (f(x) - \mu)^3 \, dx \) equals

\[
\sum_{u \neq \emptyset} \int f_u(x)^3 \, dx + \sum_{u \neq \emptyset} \sum_{v \neq \emptyset} \sum_{z \subseteq u \cap v} \int f_u(x)f_v(x)f_{(u \Delta v) \cup z} \, dx.
\]

For example, with \( d = 2 \), there are 3 nonempty subsets of \( \{1, 2\} \) providing 27 combinations for \( u, v \) and \( w \) of which only 12 vanish, yielding

\[
\int (f(x) - \mu)^3 \, dx = \int f_{\{1\}}(x)^3 \, dx + \int f_{\{2\}}(x)^3 \, dx + \int f_{\{1,2\}}(x)^3 \, dx \\
+ 3 \int f_{\{1\}}(x)f_{\{2,1\}}^2(x) \, dx + 3 \int f_{\{2\}}(x)f_{\{1,2\}}^2(x) \, dx \\
+ 6 \int f_{\{1\}}(x)f_{\{2\}}(x)f_{\{1,2\}}(x) \, dx.
\]

Our moment based method in Section 4 provide crossed decompositions for \( d \) dimensions and \( p' \)th powers. The terms are sums together into \( 2^d - 1 \) effects.

4 Generalizing the Sobol’ identity

Instead of generalizing the ANOVA to higher moments, we find it more convenient to directly generalize the identity (5) which yields \( \mu^2 + \tau^2 \). We are generalizing \( \mu^2 + \tau^2 \) instead of \( \tau^2 \), because the minimizer of \( \int |f(x) - m|^p \, dx \) over \( m \), is the mean when \( p = 2 \), but is otherwise not easy to identify.

Where (5) uses 2 points in \([0,1]^d\) with common \( x_u \), our generalization works via \( p \geq 2 \) such points. Define \( \tau^{(p)} \) via

\[
\tau^{(p)}_u + \mu^p = \int \cdots \int \prod_{k=1}^p f(x_u : z^{(k)}_u) \, dx \prod_{k=1}^p dz^{(k)} \tag{8}
\]

where \( z^{(1)}, \ldots, z^{(p)} \in [0,1]^d \). This integral is over \([0,1]^{(p+1)d}\) but only uses \(|u| + p(d - |u|)\) components. For \( p = 2 \), we get the usual Sobol’ sensitivity indices (plus \( \mu^2 \)). The desirable property of (8) is that it is a multivariable integral and may be estimated by Monte Carlo or quasi-Monte Carlo sampling without requiring any numerical optimization.

When we seek to estimate \( \tau^{(p)}_u \) it is necessary to subtract an estimate of \( \mu^p \). One approach, generalizing an estimate studied in Janon et al. (2012) is to use

\[
\tau^{(p)}_u = \frac{1}{n} \sum_{i=1}^n \prod_{k=1}^p f(x_{i,u} : z^{(k)}_{i,u}) - \hat{\mu}^p, \tag{9}
\]
\[
\hat{\mu} = \frac{1}{np} \sum_{i=1}^{n} \sum_{k=1}^{p} f(x_{i,u} : z_{i,u}^{(k)}).
\] (10)

A second approach, generalizing an estimate in Mauntz (2002) and Saltelli (2002) takes

\[
\hat{\tau}^{(p)} = \frac{1}{n} \sum_{i=1}^{n} \left( \prod_{k=1}^{p} f(x_{i,u} : z_{i,u}^{(k)}) - \prod_{k=1}^{p} f(z_{i}^{(k)}) \right),
\] (11)
a sample version of the identity

\[
\tau^{(p)}(u) = \int \left( \prod_{k=1}^{p} f(x_{u} : z_{-u}^{(k)}) - \prod_{k=1}^{p} f(z_{i}^{(k)}) \right) dx \prod_{k=1}^{p} dz^{(k)}.
\]

Equation (11) provides unbiased estimates of \(\tau^{(p)}(u)\). Even for \(p = 2\) it is known that neither estimate (9) or (11) is always better than the other. For instance Owen (2012b) finds that (11) is more accurate in some examples with small \(\tau^{2}_u\), while (9) is better on some examples with large \(\tau^{2}_u\).

The most interesting cases are \(p = 3\), which gives us a skewness measure for each subset of variables, and \(p = 4\), the smallest even power above 2. For even integers \(p \geq 4\) we get nonnegative measures that are increasing in \(u\) as shown below. We will use

\[
f_u(x) = \sum_{v \subseteq u} f_v(x) = \mathbb{E}(f(x) \mid x_u),
\] (12)

when \(x \sim U[0,1]^d\).

**Proposition 1.** For integer \(p \geq 1\), \(\hat{\tau}^{(p)} + \mu^p = \mathbb{E}(f^p_u(x_u))\).

**Proof.** Define \(h(x) = f(x) - f_u(x_u)\) and \(y_k = x_u : z_{-u}^{(k)}\), for \(k = 1, \ldots, p\). Then \(\mathbb{E}(h(y_j) \mid x_u) = 0\) and

\[
\mu^p + \hat{\tau}^{(p)} = E\left( E\left( \prod_{k=1}^{p} (f_u(x_u) + h(y_k)) \mid x_u \right) \right)
= E\left( E(f^p_u(x_u) \mid x_u) \right)
= E(f^p_u(x_u)). \quad \Box
\]

**Theorem 1.** Let \(f \in L^p[0,1]^d\) for an even integer \(p \geq 2\). Then \(\hat{\tau}^{(p)}(u) \leq \hat{\tau}^{(p)}(v)\) holds when \(u \subseteq v \subseteq D\).

**Proof.** It suffices to consider the case where \(v = u \cup \{j\}\) for \(j \not\subseteq u\). Let \(h(x) = f_v(x) - f_u(x_u) = \sum_{w \subseteq u} f_{w \cup \{j\}}(x)\). Then by Proposition 1

\[
\mu^p + \hat{\tau}^{(p)} = E(f^p_u(x_u)) = E((f_u(x_u) + h(x))^p)
\]
\[ = \mathbb{E}(\mathbb{E}(f(x_u) + h(x))^p | x_u) \]
\[ \geq \mathbb{E}(\mathbb{E}(f(x_u))^p | x_u) = \mu^p + \tau^{(p)} \]
by convexity of the function \( \varphi(y) = y^p \).

From Theorem 1 we see that \( \tau^{(p)} \) has some important properties for a subset importance quantity when \( p \) is an even integer. First \( \tau^{(p)} \geq \tau^{(p)}_{\emptyset} = 0 \), and so the importance of every subset is nonnegative. Second, increasing the number of components in a subset does not make the measure smaller. Both of these properties also hold for the measure \( \tau^{(p)} = \mathbb{E}(\varphi(f(x_u))) - \varphi(\mu) \) for convex non-negative functions \( \varphi \), but when \( \varphi(y) \) is even power of \( y \), we have a convenient estimation formula based on (8) that lets us avoid having to compute an estimate of \( f \).

Odd power variable measures like \( \tau^{(3)} \) do not have the nesting property of Theorem 1 and they can take negative values. Such negative values may be informative and interpretable. For example if \( \tau^{(3)} \{1\} < 0 \) while \( \tau^{(3)} \{2\} > 0 \) this may indicate that controlling \( x_1 \) is more important for attaining (or avoiding) very small values of \( f \) while \( x_2 \) is more important for large values of \( f \).

5 Generalizing the synthesis

In this section we introduce a multilinear operator that allows a generalization of the synthesis approach to ANOVA. We use two different bases, Fourier and Walsh.

5.1 Fourier synthesis

For \( 0 \leq j < p \) let \( f_j : [0,1]^d \to \mathbb{R} \) have a Fourier expansion

\[ f_j(x) = \sum_{k \in \mathbb{Z}^d} \hat{f}_j(k)e^{2\pi ik \cdot x}. \]

For any \( j \in \{0,1,\ldots,p-1\} \) let its successor be \( j+ \equiv j + 1 \mod p \) and its predecessor be \( j- \equiv j - 1 \mod p \). Our multilinear operator is

\[ \langle f_0, \ldots, f_{p-1} \rangle_p = \int_{[0,1]^d} \prod_{j=0}^{p-1} f_j(\{(-1)^j(x_j - x_{j+})\}) \, dx_0 \cdots dx_{p-1}, \quad (13) \]

where \( \{z\} = z - \lfloor z \rfloor \) is the fractional part of \( z \) (componentwise).

The following result is the fundamental lemma, giving a multilinear orthogonality property of the operator on Fourier functions.

**Lemma 1.** Let \( p \geq 2 \) be an integer and \( k_0, \ldots, k_{p-1} \in \mathbb{Z}^d \) and let \( \phi_k(x) = e^{2\pi ik \cdot x} \). Then

\[ \langle \phi_{k_0}, \ldots, \phi_{k_{p-1}} \rangle_p = \begin{cases} 1, & k_j = (-1)^j k_0, \quad j = 1, \ldots, p-1 \\ 0, & \text{otherwise.} \end{cases} \]
Proof. For $p$ even we have
\[
\langle \phi_{k_0}, \ldots, \phi_{k_{p-1}} \rangle_p = \prod_{j=0}^{p-1} \int_{[0,1]^d} e^{2\pi i \sum_{j=0}^{p-1} k_j \langle x_j, x_j \rangle} \, dx_j 
\]
and for $p$ odd we have
\[
\langle \phi_{k_0}, \ldots, \phi_{k_{p-1}} \rangle_p = \prod_{j=1}^{p-1} \int_{[0,1]^d} e^{2\pi i (-1)^j (k_j + k_j -) \cdot x_j} \, dx_j \int_{[0,1]^d} e^{2\pi i (k_0 - k_{p-1}) \cdot x_0} \, dx_0.
\]
The integrals are 1 if $k_j = (-1)^j k_0$ for $0 \leq j < p$ and 0 otherwise, which implies the result.

The function $\langle \cdot, \ldots, \cdot \rangle_p$ is symmetric and multi-linear. For integers $p \geq 2$ we will use
\[
\sigma_p(f) = \langle f, \ldots, f \rangle_p
\]
\[
= \sum_{k_0, \ldots, k_{p-1} \in \mathbb{Z}^d} \prod_{j=0}^{p-1} \hat{f}(k_j) \int_{[0,1]^d} e^{2\pi i \sum_{j=0}^{p-1} (-1)^j k_j \langle x_j, x_j \rangle} \, dx_0 \ldots dx_{p-1}
\]
\[
= \sum_{k \in \mathbb{Z}^d} \hat{f}(k)^{\lfloor p/2 \rfloor} \hat{f}(-k)^{\lfloor p/2 \rfloor}.
\]
If $f$ is a real-valued function we have $\hat{f}(-k) = \overline{\hat{f}(k)}$. If $p$ is an even integer we therefore get
\[
\langle f, \ldots, f \rangle_p = \sum_{k \in \mathbb{Z}^d} |\hat{f}(k)|^p.
\]
The ANOVA decomposition $f(x) = \sum_{u \subseteq \mathcal{D}} f_u(x)$, has terms
\[
f_u(x) = \sum_{k_u \in \mathbb{Z}^{|u|}} \hat{f}(k_u : 0_{-u}) e^{2\pi i k_u \cdot x_u}.
\]
The diagonality of the multilinear operator \[\langle \cdot, \ldots, \cdot \rangle_p\] yields a $p$-fold orthogonality for the ANOVA terms:

Lemma 2. Let $f$ be as above and let $f = \sum_u f_u$ be the ANOVA decomposition of $f$. Then for all $u_0, \ldots, u_{p-1} \subseteq \mathcal{D}$, such that there are $i, j \in \{0, \ldots, p-1\}$ with $u_i \neq u_j$, we have
\[
\langle f_{u_0}, \ldots, f_{u_{p-1}} \rangle_p = 0.
\]

Proof. If $u_i \neq u_j$, then $k_{u_j : 0_{-u_j}} \neq -k_{u_i : 0_{-u_i}}$ for all $k_{u_j} \in \mathbb{Z}^{|u_j|}$ and $k_{u_i} \in \mathbb{Z}^{|u_i|}$. Then
\[
\int_{[0,1]^d} e^{2\pi i (k_{u_j : 0_{-u_j}} - k_{u_i : 0_{-u_i}}) \cdot x} \, dx = 0.
\]
The result follows now from Lemma 1.
**Lemma 3.** Let \( f \) be as above and let \( f = \sum_u f_u \) be the ANOVA decomposition of \( f \). Then we have
\[
\sigma_p(f) = \sum_u \sigma_p(f_u).
\]

**Proof.** Recall that \( \langle f_{u_0}, \ldots, f_{u_{p-1}} \rangle_p = 0 \) unless \( u_0 = \cdots = u_{p-1} \). Therefore expanding \( \sigma_p(f) = \langle f, \cdots, f \rangle_p \) yields
\[
\sum_{u_0, \ldots, u_{p-1} \subseteq \mathcal{D}} \langle f_{u_0}, \ldots, f_{u_{p-1}} \rangle_p = \sum_{u \subseteq \mathcal{D}} \langle f_u, \ldots, f_u \rangle_p = \sum_{u \subseteq \mathcal{D}} \sigma_p(f_u). \tag{14}
\]

The aim is to estimate \( \sigma_p(f_u) \) or sums of those. We investigate this in the following. For \( u \subseteq \mathcal{D} \), define \( \tau_p[u] \) via
\[
\tau_p[u] + \mu_p = \sum_{u \subseteq \mathcal{D}} |\hat{f}(k_u \cdot \mathbf{0} - u)|^p = \sum_{v \subseteq u} \sigma_p(f_v). \tag{15}
\]

**Theorem 2.** Let \( f \in L^p[0,1]^d \), for integer \( p \geq 2 \), with ANOVA decomposition \( f = \sum_u f_u \). Then for any \( u \subseteq \mathcal{D} \) we have
\[
\tau_p[u] + \mu_p = \sum_{v \subseteq u} \sigma_p(f_v). \tag{16}
\]

**Proof.** Using the Fourier series representation of \( f \) and Lemma 1 we obtain
\[
\tau_p[u] + \mu_p = \sum_{k_u \in \mathbb{Z}^{|u|}} |\hat{f}(k_u \cdot \mathbf{0} - u)|^p = \sum_{v \subseteq u} \sigma_p(f_v). \tag{17}
\]

Theorem 2 shows that the importance measures \( \tau_p[u] \) are sums of contributions \( \sigma_p(f_v) \) from \( v \subseteq u \). This generalizes a property of the ANOVA to \( p \geq 2 \).

Theorem 2 can be generalized in the following way. Let \( f_0, \ldots, f_p-1 \) be functions in \( L^p[0,1]^d \) for integer \( p \geq 2 \) with Fourier coefficients \( \hat{f}_j(k) \), and \( \mu_j = \int f_j(x) \, dx \). Next we set
\[
\tau_p^0[f_0, \ldots, f_p-1] + \prod_{j=0}^{p-1} \mu_j
\]
\[
= \int_{[0,1]^d} \prod_{j=0}^{p-1} f_j((-1)^j \{x_{u,j} - x_{u,j+} \} \cdot y_{-u,j}) \prod_{j=0}^{p-1} dx_{u,j} \prod_{j=0}^{p-1} dy_{-u,j}.
\]

Then
\[
\tau_p^0[f_0, \ldots, f_p-1] + \prod_{j=0}^{p-1} \mu_j = \sum_{k_u \in \mathbb{Z}^{|u|}} \prod_{j=0}^{p-1} \hat{f}_j((-1)^j k_u \cdot \mathbf{0} - u). \tag{18}
\]

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5.2 Walsh synthesis

Here we replace the Fourier functions by the Walsh functions in an integer base $b \geq 2$. For $b = 2$, the coefficients of Walsh functions are real values. The index set is $I = \mathbb{N}_0$ and then $I_* = \mathbb{N}$.

For a non-negative integer $k$ with base $b$ representation

$$k = \kappa_n b^n + \cdots + \kappa_2 b^2 + \kappa_0,$$

with $\kappa_i \in \{0, 1, \ldots, b-1\}$, we define the Walsh function $\text{wal}_k : [0, 1) \to \{z \in \mathbb{C} : |z| = 1\}$ by

$$\text{wal}_k(x) := e^{2\pi i (\kappa_0 + \cdots + \kappa_n)/b},$$

for $x \in [0, 1)$ with base $b$ representation $x = x_1 b^{-1} + x_2 b^{-2} + \cdots$ (unique in the sense that infinitely many of the $x_i$ must be different from $b - 1$).

For dimension $s \geq 2$, $x = (x_1, \ldots, x_s) \in [0, 1)^s$ and $k = (k_1, \ldots, k_s) \in \mathbb{N}_0^s$ we define $\text{wal}_k : [0, 1)^s \to \{z \in \mathbb{C} : |z| = 1\}$ by

$$\text{wal}_k(x) := \prod_{j=1}^s \text{wal}_{k_j}(x_j).$$

For more information on Walsh functions see Chrestenson (1955); Fine (1949); Walsh (1923).

Let $f_j : [0, 1]^d \to \mathbb{R}$ have a Walsh series expansion of the form

$$f_j(x) = \sum_{k \in \mathbb{N}_0^d} \hat{f}_\text{wal}(k) \text{wal}_k(x).$$

For $x, y \in \{z \in \mathbb{R} : z \geq 0\}$ with base $b$ expansion $x = \sum_{i=-\infty}^{-w} x_i b^i$ and $y = \sum_{i=-\infty}^{-w} y_i b^i$ (unique in the sense that infinitely many of the $x_i$ and $y_i$ must be different from $b-1$) we set $x \oplus y = \sum_{i=-\infty}^{-w} z_i b^i$ where $z_i = x_i - y_i \pmod{b}$ and $z_i \in \{0, \ldots, b-1\}$. For vectors $x$ and $y$ we define the operation $\oplus$ componentwise. Similarly we set $x \oplus y$ where we change the definition of $z_i$ to $z_i = x_i + y_i \pmod{b}$. We define $\ominus x = 0 \ominus x$ and $(\ominus 1)^j x = x$ if $j$ is even and $\ominus x$ otherwise.

We now define

$$\langle f_0, \ldots, f_{p-1} \rangle_{p, \text{wal}} = \int_{[0,1]^d} \prod_{j=0}^{p-1} f_j((\ominus 1)^j(x_j \ominus x_{j+})) \, dx_0 \cdots dx_{p-1}.$$
All the remaining results and definitions can therefore be obtained in an analogous manner. In particular for functions $f$ with ANOVA decomposition $f = \sum_u f_u$ we have

$$
\sigma_{p,\text{wal}}(f) = \sum_{u \subseteq D} \sigma_{p,\text{wal}}(f_u),
$$

where

$$
\sigma_{p,\text{wal}}(f) \equiv \langle f, \ldots, f \rangle_{p,\text{wal}} = \sum_{k \in \mathbb{N}_0^d} \left| \hat{f}_{\text{wal}}(k) \right|^{p/2} \left| \hat{f}_{\text{wal}}(\ominus k) \right|^{p/2}.
$$

If $p$ is even and $f$ a real-valued function, then we get

$$
\sigma_{p,\text{wal}}(f) \equiv \langle f, \ldots, f \rangle_{p,\text{wal}} = \sum_{k \in \mathbb{N}_0^d} \left| \hat{f}_{\text{wal}}(k) \right|^p.
$$

**Lemma 5.** Let $f$ be as above and let $f = \sum_u f_u$ be the ANOVA decomposition of $f$. Then we have

$$
\sigma_{p,\text{wal}}(f) = \sum_u \sigma_{p,\text{wal}}(f_u).
$$

The proof of Lemma 5 follows by the same arguments as the proof of Lemma 3.

We may estimate $\sigma_{p,\text{wal}}(f_u)$ or their sums in the same way we did for their Fourier analogues $\sigma_p(f_u)$. For $u \subseteq D$, define $\tau_{u,\text{wal}}^{[p]}$ via

$$
\tau_{u,\text{wal}}^{[p]} + \mu_{\text{wal}}^p = \int_{[0,1]^d} \prod_{j=0}^{p-1} f \left( \{ (\ominus 1)^j (x_{u,j} \ominus x_{u,j+}) \} : y_{-u,j} \right) \prod_{j=0}^{p-1} dx_{u,j} \prod_{j=0}^{p-1} dy_{u,j}.
$$

Here $\tau_{\emptyset,\text{wal}}^{[p]} = 0$.

**Theorem 3.** Let $f \in L^p[0,1]^d$, for integer $p \geq 2$, with ANOVA decomposition $f = \sum_u f_u$. Then for any $u \subseteq D$ we have

$$
\tau_{u,\text{wal}}^{[p]} + \mu_{\text{wal}}^p = \sum_{u \subseteq u} \sigma_{p,\text{wal}}(f_u).
$$

The proof of this result follows along the same lines as the proof of Theorem 2.

In general, for $p > 2$, $\sigma_p(f)$ and $\sigma_{p,\text{wal}}(f)$ are different and the Walsh measure will depend on the base $b$ that was used. Parseval’s identity implies that $\sigma_2(f) = \sigma_{2,\text{wal}}(f)$.

### 5.3 Change of variable and dimension reduction

Our $p$-fold inner products are defined through a $pd$ dimensional integral. But they are equivalent to a $(p-1)d$ dimensional integral.
Lemma 6. For integers $p \geq 2$ and $d \geq 1$, let $f_0, f_1, \ldots, f_{p-1} \in L^p([0,1]^d)$. Then

$$\int_{[0,1]^d} \prod_{j=0}^{p-1} f_j(\{(-1)^j(x_j - x_{j+})\}) \prod_{j=0}^{p-1} dx_j$$

$$= \int_{[0,1]^d} f_0(y_0) f_1(y_1) \cdots f_{p-2}(y_{p-2}) f_{p-1}(\{y_0 - y_1 + \cdots + (-1)^{p-2}y_{p-2}\}) \prod_{j=0}^{p-2} dy_j.$$

Proof. We prove it for $p = 4$; the general case uses the same argument. For $x_0, \ldots, x_3 \in [0,1]^d$ let $y_0, \ldots, y_3$ be defined by

$$\begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \end{pmatrix} \mod 1$$

where both the matrix multiplication and the modulus are taken component-wise. This transformation has Jacobian 1 almost everywhere. To simplify the integrals, we extend each $f_j$ to a periodic function on $\mathbb{R}^d$, allowing us to remove the $\{\cdots\}$ operation. Making the change of variable,

$$\begin{align*}
\prod_{j=0}^{p-1} f_0(x_0 - x_1) f_1(x_2 - x_1) f_2(x_2 - x_3) f_3(x_0 - x_3) dx_0 dx_1 dx_2 dx_3 \\
= \prod_{j=0}^{p-1} f_0(y_0) f_1(y_1) f_2(y_2) f_3(y_0 - y_1 + y_2) dy_0 dy_1 dy_2 dy_3 \\
= \prod_{j=0}^{p-1} f_0(y_0) f_1(y_1) f_2(y_2) f_3(y_0 - y_1 + y_2) dy_0 dy_1 dy_2.
\end{align*}$$

Lemma 6 also applies for the Walsh case. We have

$$\int_{[0,1]^d} \prod_{j=0}^{p-1} f_j(\{(\oplus 1)^j(x_j \oplus x_{j+})\}) \prod_{j=0}^{p-1} dx_j$$

$$= \int_{[0,1]^d} f_0(y_0) f_1(y_1) \cdots f_{p-2}(y_{p-2}) f_{p-1}(\{y_0 \oplus y_1 \cdots \oplus (\oplus 1)^{p-2}y_{p-2}\}) \prod_{j=0}^{p-2} dy_j.$$

5.4 Weighted coefficients

The quantity $(f, f, \ldots, f, g)_{p+1}$ is also of interest for special choices of the function $g$. The result is to give weighted sums of powers of the Fourier (or Walsh) coefficients. We take $p$ to be an odd integer and $g$ to be a weighting function.

Of particular interest is the Dirichlet kernel

$$D_N(x) = \sum_{k \in \{-N, \ldots, N\}^d} e^{2\pi ik \cdot x} = \prod_{j=1}^d \frac{\sin(2\pi(N+1/2)x_j)}{\sin(\pi x_j)}.$$
If \( x_j = 0 \) or \( 1 \) we set \( \sin(2\pi(N + 1/2)x_j)/\sin(\pi x_j) := 2N + 1 \). For an odd integer \( p > 1 \) we have
\[
(f, \ldots, f, D_N)_p = \sum_{k \in \{-N, \ldots, N\}^d} |\hat{f}(k)|^{p-1}.
\]
The result is a non-negative importance measure for \( f \) apart from its very highest spatial frequencies. Further, for \( m \in \mathbb{Z}^d \) we have
\[
(f, \ldots, f, D_N e^{2\pi i m \cdot x})_p = \sum_{k \in \{-N, \ldots, N\}^d} |\hat{f}(k + m)|^{p-1}.
\]

The Dirichlet kernel for the Walsh system in base \( b \) is
\[
D_{m, \text{wal}}(x) = \sum_{k \in \{0, \ldots, b^m - 1\}^d} \text{wal}_k(x) = \prod_{j=1}^{d} 1_{[0, b^{-m}]}(x_j).
\]

Thus for odd integer \( p > 1 \) we have
\[
(f, \ldots, f, D_{m, \text{wal}})_{p, \text{wal}} = \sum_{k \in \{0, \ldots, b^m - 1\}^d} |\hat{f}_{\text{wal}}(k)|^{p-1}.
\]

Further, for \( a \in \mathbb{N}_0^d \) we have
\[
(f, \ldots, f, D_{m, \text{wal} a})_{p, \text{wal}} = \sum_{k \in \{0, \ldots, b^m - 1\}^d} |\hat{f}_{\text{wal}}(k \oplus a)|^{p-1}.
\]

### 6 Special case functions

Here we consider some simple functional forms for which our analysis can be carried out in closed form. The first ones are functions of product form, including rectangular spikes. We will see the effects of third and fourth moments on the \( \tau^{(p)}_u \) and the effects of spectral sparsity on \( \tau_u^{[p]} \). The second are additive functions where we will see the spectral method does not introduce any apparent interactions.

The original Sobol’ indices relate to variance components via a Moebius relation
\[
\sigma^2_u = \sum_{v \subseteq u} (-1)^{|u - v|} \tau_v^2,
\]
for \( u \neq \emptyset \). Recalling that \( \tau^{(p)}_u, \tau_u^{[p]} \) and \( \tau_u^{[p]} \) are generalizations of \( \mu^2 + \tau_v^2 \), we can define analogues of variance components via
\[
\sigma^{(p)}_u = \sum_{v \subseteq u} (-1)^{|u - v|} \tau_v^{(p)},
\]
\[
\sigma_u^{[p]} = \sum_{v \subseteq u} (-1)^{|u - v|} \tau_v^{[p]}, \quad \text{and}
\]
\[
\sigma_u^{[p], \text{wal}} = \sum_{v \subseteq u} (-1)^{|u - v|} \tau_v^{[p], \text{wal}},
\]
for \( u \neq \emptyset \). We also have \( \sigma^{(p)}_\emptyset = \sigma^{[p]}_\emptyset = \sigma^{[p], \text{wal}}_\emptyset = 0 \).
6.1 Product functions

Product functions are frequently used as examples for sensitivity measures. A notable example is [Sobol’ (1993)]. Throughout this subsection we suppose that

\[ f(x) = \prod_{j=1}^{d} h_j(x_j) = \prod_{j=1}^{d} (\mu_j + \tau_j g_j(x_j)) \quad (18) \]

for real-valued functions \( g_j \) and \( h_j \) defined on \([0,1]\). The functions \( g_j \) satisfy \( \int_0^1 g_j(x) \, dx = 0 \) and \( \int_0^1 g_j(x)^2 \, dx = 1 \).

The ANOVA components of a product function are

\[ \sigma_u^2 = \prod_{j \in u} \tau_j^2 \prod_{j \notin u} \mu_j^2, \]

for \( u \neq \varnothing \). For a product function \( \mu^2 + \zeta_u^2 = \prod_{j \in u} (\mu_j^2 + \tau_j^2) \prod_{j \notin u} \mu_j^2. \) An important subset of variables must include any \( j \) with \( \mu_j = 0 \). When \( \mu \neq 0 \) we may write

\[ \mu^2 + \zeta_u^2 = \mu^2 \prod_{j \in u} (1 + \tau_j^2 / \mu_j^2) \]

and then see that coefficients of variation \( \nu_j = \tau_j / \mu_j \) govern importance.

We need \( \int_0^1 |f(x)|^p \, dx < \infty \) to make the importance measures finite. We will use \( \gamma_j = \int_0^1 g_j^3(x) \, dx \) and \( \kappa_j = \int_0^1 g_j^4(x) \, dx \) which we assume are finite. If \( x \sim U(0,1) \), then \( \gamma_j \) is the skewness of \( g_j(x) \) and \( \kappa_j - 3 \) is the kurtosis.

Generalizing the Fourier and Walsh syntheses

To generalize the Fourier synthesis we write \( h_j(x) = \sum_{k \in \mathbb{Z}} \hat{h}_j(k)e^{2\pi ikx} \) (in mean square) for \( \hat{h}_j(k) = \int_0^1 h_j(x)e^{-2\pi ikx} \, dx \). We note that \( \mu = \prod_j \mu_j \) where \( \mu_j = \hat{h}_j(0) \). Now \( \hat{f}(k) = \prod_{j=1}^d \hat{h}_j(k_j) \) and for even \( p \geq 2 \)

\[ \begin{align*}
\zeta_u^{[p]} + \mu^p &= \prod_{j \notin u} |\mu_j|^p \sum_{k_u \in \mathbb{Z}^{\lvert u \rvert}} \prod_{j \notin u} |\hat{h}_j(k_j)|^p = \prod_{j \notin u} |\mu_j|^p \prod_{j \notin u} \left( \sum_{k_j \in \mathbb{Z}} |\hat{h}_j(k_j)|^p \right) .
\end{align*} \]

Using the alternating sum \((16)\) and simplifying, we obtain

\[ \sigma_u^{[p]} = \prod_{j \notin u} |\mu_j|^p \prod_{j \notin u} \left( \sum_{k_j \in \mathbb{Z}} |\hat{h}_j(k_j)|^p \right) \]

for \( u \neq \varnothing \). The effect is to change \( \mathbb{Z} \) to \( \mathbb{Z}_a \) in the sums.

Given two functions \( h_j \) with the same variance, the measure \( \sum_{k \in \mathbb{Z}} |\hat{h}_j(k_j)|^p \), for \( p > 2 \), is a measure of sparsity for the spectrum. It does not favor either high or low frequencies. To put more emphasis on high or low frequencies one could use weighted coefficients as outlined in subsection 5.4.

Analogous formulae hold for the Walsh synthesis. Now we write the factors of \( f \) as \( h_j(x) = \sum_{k \in \mathbb{N}_0} \hat{h}_{j,\text{wal}}(k)\text{wal}_k(x) \) for \( \hat{h}_{j,\text{wal}}(k) = \int_0^1 h_j(x)\text{wal}_k(x) \, dx \). Here
\( \mu_{wal} = \prod_j \mu_{j,wal} \) where \( \mu_{j,wal} = \hat{h}_{j,wal}(0) \) and \( \hat{f}_{wal}(k) = \prod_{j=1}^d \hat{h}_{j,wal}(k_j) \). For even \( p \geq 2 \) the same argument that we used in the Fourier case leads to

\[
\sigma_{u,wal}^{[p]} = \prod_{j \notin u} |\mu_{j,wal}|^p \prod_{j \in u} \left( \sum_{k_j \in \mathbb{N}} |\hat{h}_{j,wal}(k_j)|^p \right).
\]

for \( u \neq \emptyset \).

**Generalizing the Sobol’ identity**

When we generalize the Sobol’ identity we get

\[
\sum_{k \in \mathbb{Z}} |\hat{f}(k)|_p = \int \prod_{k=1}^p f(x_k : z_{-k}) \, dx \prod_{k=1}^p dz(k) = \prod_{j \in u} \int_0^1 h_j(x_j)^p \, dx_j \prod_{j \notin u} \mu_j^p.
\]

Where the Fourier synthesis had a \( p \)'th moment \( \sum_{k_j \in \mathbb{Z}} |\hat{h}_j(k_j)|^p \) of Fourier coefficients, this approach has an ordinary \( p \)'th moment of Fourier co-

\[
\sigma_u^{(p)} = \prod_{j \notin u} \mu_j^p \prod_{j \in u} \left( \int_0^1 h_j(x)^p \, dx - \mu_j^p \right)
\]

for \( u \neq \emptyset \).

For the generalized Sobol’ identity we can make use of the moments \( \gamma_j \) and \( \kappa_j \) of \( h_j \). The special cases of most interest have \( p = 3 \) or 4. For \( p = 3 \)

\[
\int_0^1 h_j(x)^3 \, dx = \mu_j^3 + 3 \mu_j \tau_j^2 + \gamma_j \tau_j^3
\]

and so for \( u \neq \emptyset \),

\[
\sum_{u}^{(3)} = \prod_{j \notin u} \mu_j^3 \prod_{j \in u} (\mu_j^3 + 3 \mu_j \tau_j^2 + \gamma_j \tau_j^3) - \mu^3,
\]

and

\[
\sigma_u^{(3)} = \prod_{j \notin u} \mu_j^3 \prod_{j \in u} \tau_j^2 (3 \mu_j + \gamma_j \tau_j).
\]

The \( \sigma_u^{(3)} \) are ‘components of skewness’ analogues of the components of variance \( \sigma_u^2 \). Some of these components may be negative. If every \( \mu_j > 0 \) and every \( \tau_j > 0 \), then a negative component of skewness arises if \( 3 \mu_j + \gamma_j \tau_j < 0 \) holds for an odd number of indices \( j \in u \).

Product functions illustrate one challenge with importance measures taking negative values. The same variable \( x_j \) can drive the function towards negative values through one component \( \sigma_u^{(3)} \) while driving it towards positive values through another component \( \sigma_u^{(3)} \). Similarly, whether the total effect \( \sum_u^{(3)} \) is positive or negative depends on the signs of \( \mu_j \) for \( j \notin u \). These features make \( p = 3 \) hard to interpret.
For $p = 4$, we find
\[ \int_0^1 h_j(x)^4 \, dx = \mu_j^4 + 6\mu_j^2\gamma_j^2 + 4\mu_j\gamma_j\tau_j^3 + \kappa_j\tau_j^4 \]
and so for $u \neq \emptyset$,
\[ \tau_u^{(4)} = \prod_{j \not\in u} \mu_j^4 \prod_{j \in u} \left( \mu_j^4 + 6\mu_j^2\gamma_j^2 + 4\mu_j\gamma_j\tau_j^3 + \kappa_j\tau_j^4 \right) - \mu^4, \quad \text{and} \]
\[ \sigma_u^{(4)} = \prod_{j \not\in u} \mu_j^4 \prod_{j \in u} \tau_j^2 \left( 6\mu_j^2 + 4\mu_j\gamma_j\tau_j + \kappa_j\tau_j^2 \right). \]

If $j \not\in u \neq \emptyset$ and $\mu_j \neq 0$, then
\[ \frac{\sigma_u^{(4)}}{\sigma_u^{(2)}} = v_j^2 \left( 6 + 4\gamma_j v_j + v_j^2 \kappa_j \right). \]

where $v_j = \tau_j/\mu_j$ is the $j$’th coefficient of variation.

A variable with a large absolute coefficient of variation $|v_j|$ tends to raise all of the $\sigma_u^{(4)}$ in which it participates just as it does for the $p = 2$ ANOVA case. Additionally a variable with large fourth moment $\kappa_j$ becomes more important. Variables with large skewness $\gamma_j$ become more important if $\gamma_j$ has the same sign as $\mu_j$ but less important if the opposite holds. Both of these findings are intuitively reasonable when we are interested in driving $|f|$ to its largest values.

6.2 Indicators of rectangles

A special case of the product functions are indicator (characteristic) functions of hyperrectangles. These have $h_j(x) = 1$ for $x_j \in [x_j, x_j + \epsilon_j]$ and $h_j(x) = 0$ for $x \in [0, 1) \setminus [x_j, x_j + \epsilon_j)$, so that $f(x)$ is the indicator of a hyperrectangle with volume $\prod_j \epsilon_j$. For a binary function, all of the $x_j$ have to be in their respective intervals for the function to take the high value. This means that we should expect important interactions. To model a spiky function we would have all of the $\epsilon_j$ be small. Then the most important one should be the smallest one. Here we let $\epsilon = \mu = \prod_{j=1}^d \epsilon_j$.

The generalization of Sobol’s identity works entirely with moments of $h_j$ and so without loss of generality $h_j(x) = 1$ for $x < \epsilon_j$ and is 0 otherwise. The generalization of the Walsh-based synthesis is not invariant to the interval one chooses. In this setting we prefer the Fourier-based synthesis. Shifting the interval from $[0, \epsilon_j)$ to $[x_{j+}, x_{j+} + \epsilon_j)$ for $0 \leq x_{j+} \leq 1 - \epsilon_j$ changes the phase but not the modulus of $\hat{h}_j(k)$ leaving the importance measures unchanged when $p \geq 2$ is even.

For the generalized Sobol’ index construction we find for $u \neq \emptyset$
\[ \tau_u^{(p)} = \prod_{j \in u} \epsilon_j^p \prod_{j \not\in u} \epsilon_j - \epsilon^p = \epsilon^p \left( \prod_{j \in u} \epsilon_j^{-(p-1)} - 1 \right), \quad \text{and} \]

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\[ \sigma_u^{(p)} = \prod_{j \notin u} \varepsilon_j \prod_{j \in u} (\varepsilon_j - \varepsilon_j^p) = \varepsilon_p \prod_{j \in u} (\varepsilon_j^{-(p-1)} - 1). \]

Variables with smaller \( \varepsilon_j \) are more important than those with larger \( \varepsilon_j \) and the effect is magnified at larger \( p \). Both \( \tau_u(p) \) and \( \sigma_u^{(p)} \) are always nonnegative for integers \( p \geq 2 \) without requiring \( p \) to be even.

We now consider the Fourier synthesis for even \( p \geq 2 \). After applying some trigonometric identities, we find that the key quantity there, replacing \( \varepsilon_j - \varepsilon_j^p \) satisfies

\[ \sum_{k \in \mathbb{Z}} |\hat{h}_j(k)|^p = 2 \sum_{k=1}^{\infty} \left( \frac{\sin(\pi k \varepsilon_j)}{\pi k} \right)^p \equiv T_p(\varepsilon_j). \]

Thus \( \sigma_u^{[p]} = \varepsilon_p \prod_{j \in u} T_p(\varepsilon_j)/\varepsilon_j^p \). Lemma \[\text{[\ref{lemma}]}\] gives some insight into \( T_p \) for \( \varepsilon_j < 1/2 \) as follows. For \( p = 4 \), \( \tau_u^{[4]} + \mu^4 = \prod_{j \in u} Q_4(\varepsilon_j) \) where for \( f(x) = 1 \) \( x \leq \epsilon \) and \( 0 < \epsilon < 1/2 \),

\[ Q_4(\epsilon) = \int_0^1 \int_0^1 \int_0^1 f(y_0) f(y_1) f(y_2) f(\{y_0 - y_1 + y_2\}) \, dy_0 \, dy_1 \, dy_2 \]
\[ = \int_0^\epsilon \int_0^\epsilon \int_0^\epsilon 1_{y_0 - y_1 + y_2} < \epsilon \, dy_0 \, dy_1 \, dy_2 \]
\[ = \frac{2}{3} \epsilon^3. \]

As a result we have the identity \( T_4(\epsilon) = \frac{2}{3} \epsilon^3 - \epsilon^4 \), and so for \( u \neq \emptyset \),

\[ \tau_u^{[4]} = \prod_{j \notin u} \epsilon_j \prod_{j \in u} \frac{2}{3} \epsilon_j^3 \]
\[ - \epsilon^4 = \epsilon^4 \left( \prod_{j \in u} \left( \frac{2}{3} \epsilon_j^{-(1)} - 1 \right) \right), \]
\[ \text{and}, \]
\[ \sigma_u^{[4]} = \epsilon^4 \prod_{j \in u} \left( \frac{2}{3} \epsilon_j^{-1} - 1 \right). \]

For even \( p \geq 2 \) we will find a quantity \( Q_p(\epsilon) \) like \( Q_4 \) is a \( p-1 \) dimensional volume proportional to \( \epsilon^{p-1} \). As a result, the Fourier synthesis will use importance factors which grow as \( \epsilon_j^{-1} \) compared to \( \epsilon_j^{-(p-1)} \) for the moment method.

### 6.3 Additive functions

It frequently happens that high dimensional functions encountered in practice are very nearly additive. For example Caflisch et al. \( \{1997\} \) find that a 360 dimensional function motivated by a financial valuation problem is very nearly an additive function of its inputs. It is desirable that a measure of variable importance for additive functions should only give nonzero importance to singletons \( u = \{j\} \).

Here we consider additive functions

\[ f(\mathbf{x}) = \mu + \sum_{j=1}^d h_j(x_j) \] (19)
where $f_0^1 h_j(x) \, dx = 0$, $f_0^1 h_j(x)^2 \, dx = \tau_j^2$, $f_0^1 h_j(x)^3 \, dx = \gamma_j$, and $f_0^1 h_j(x)^4 \, dx = \kappa_j$.

For even integers $p \geq 2$ we find that $\sigma_{(j)}^{[p]} = \sum_{k \neq 0} |\hat{h}_j(k)|^p$ and $\sigma_{(j),\text{wal}}^{[p]} = \sum_{k \neq 0} |\hat{h}_j(k)|^p$ are the only nonzero components.

For integer $p \geq 2$,

$$\tau_u^{(p)} + \mu^p = \int \prod_{k=1}^{p} \left[ \mu + \sum_{j \in u} h_j(x_j) + \sum_{j \notin u} h_j(y_j^{(k)}) \right] \, dx \prod_{k=1}^{p} dy^{(k)}$$

$$= \int \left[ \mu + \sum_{j \in u} h_j(x_j) \right]^p \, dx.$$

For $p = 3$, $\tau_u^{(3)} + \mu^3 = \mu^3 + 3 \mu \sum_{j \in u} \tau_j^2 + \sum_{j \in u} \gamma_j$, so that $\tau_u^{(3)} = \sum_{j \in u} (\mu \tau_j^2 + \gamma_j)$.

Next

$$\sigma_u^{(3)} = \sum_{v \subseteq u} (-1)^{|u-v|} \sum_{j \in v} (3 \mu \tau_j^2 + \gamma_j).$$

Reversing the order of summation, we find that $\sigma_u^{(3)} = 0$ for $|u| > 2$ and otherwise

$$\sigma_u^{(3)} = 3 \mu \tau_j^2 + \gamma_j,$$

compared to $\sigma_u^{(2)} = \tau_j^2$. We see that the only nonzero components of skewness for an additive function are for singletons.

The same simplification does not hold in general. For $p = 4$,

$$\tau_u^{(4)} + \mu^4 = \mu^4 + 6 \mu^2 \sum_{j \in u} \tau_j^2 + 4 \mu \sum_{j \in u} \gamma_j + \sum_{j \in u} \kappa_j + \sum_{j \in u} \sum_{k \in u \backslash \{j\}} \tau_j^2 \tau_k^2,$$

so,

$$\tau_u^{(4)} = \sum_{j \in u} (6 \mu^2 \tau_j^2 + 4 \mu \gamma_j + \kappa_j - \tau_j^4) + \left( \sum_{j \in u} \tau_j^2 \right)^2.$$

As a result

$$\sigma_u^{(4)} = \begin{cases} 6 \mu^2 \tau_j^2 + 4 \mu \gamma_j + \kappa_j - \tau_j^4, & u = \{j\} \\ 2 \tau_j^2 \tau_k^2, & u = \{j, k\}, j \neq k \\ 0, & |u| > 2. \end{cases}$$

7 Discussion

We have shown that it is possible to generalize the ANOVA decomposition to higher order methods. Working directly with either Sobol’s identities or with a synthesis of Fourier or Walsh terms both lead to measures that can be estimated by quadrature. For even values $p$ the generalizations give non-negative importance measures. For odd values of $p$ the Dirichlet kernel trick recovers non-negative importance measures for the Fourier and Walsh approaches. On test functions that we can study analytically, we see that these measures can identify variables which drive the function towards its extreme values.
Acknowledgments

We thank Gary Tang for bringing the problem to our attention. This work was supported in part by grant DMS-0906056 from the U.S. National Science Foundation. J. D. is supported in part by a Queen Elizabeth 2 Fellowship from the Australian Research Council.

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