A simple algorithm for global sensitivity analysis with Shapley effects

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September 7, 2020

Abstract
Global sensitivity analysis aims at measuring the relative importance of different variables or groups of variables for the variability of a quantity of interest. Among several sensitivity indices, so-called Shapley effects have recently gained popularity mainly because the Shapley effects for all the individual variables are summed up to the total variance, which gives a better interpretability than the classical sensitivity indices called main effects and total effects. In this paper, assuming that all the input variables are independent, we introduce a quite simple Monte Carlo algorithm to estimate the Shapley effects for all the individual variables simultaneously, which drastically simplifies the existing algorithms proposed in the literature. We present a short Matlab implementation of our algorithm and show some numerical results.

1 Introduction
Global sensitivity analysis provides an indispensable framework in measuring the relative importance of different variables or groups of variables for the variability of a quantity of interest [10]. In particular, since his pioneering work by Sobol’ [12, 13], variance-based sensitivity analysis has been applied to a variety of subjects in science and engineering. Two classical but still major sensitivity indices are called main effect and total effect. The main effect, also called the first-order effect, measures the variance explained only by an input variable or a group of input variables, whereas the total effect is given by the total variance minus the variance explained only by the complement variables. When looking at these effects for the individual variables, the sum of the main effects is always less than or equal to the total variance, while the sum of the total effects is always larger than or equal to the total variance. In this way the classical sensitivity indices have a difficulty in normalization, and may cause some trouble when judging whether one input variable is more important than another.

∗The work of T.G. was supported by JSPS KAKENHI Grant Number 20K03744.
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Recently the connection between variance-based global sensitivity analysis and Shapley value from game theory has been studied by Owen [5]. The resulting sensitivity index defined for individual variables is called \textit{Shapley effect}. The Shapley effect takes its value between the main effect and the total effect, and importantly, the sum of the Shapley effects over all the individual variables is exactly equal to the total variance. This normalization property gives us a better interpretability in determining whether one input variable is more important than another. Moreover, the Shapley effect has been proven to remove the conceptual problem inherit to both the main and total effects when the input variables are correlated [14, 7].

In this paper we focus on the case where the input variables are independent and study Monte Carlo algorithms to estimate the Shapley effects efficiently. Building upon the previous works by Song et al. [14] and Broto et al. [1], in conjunction with the famous pick-freeze scheme [13, 8, 9, 4, 3, 2], we introduce a quite simple Monte Carlo algorithm to estimate the Shapley effects for all the individual variables simultaneously at the cost of $(d+1)N$, where $d$ denotes the number of variables and $N$ denotes the sample size. Our algorithm offers the following advantages:

1. Each Shapley effect is estimated unbiasedly.
2. The variance of the estimator is also estimated unbiasedly and decays at the canonical $1/N$ rate under some assumption.
3. The above advantages lead to an approximate confidence interval for the Shapley effect without requiring independent Monte Carlo trials.
4. The sum of the estimates for all the Shapley effects is an unbiased estimator of the total variance.

The rest of this paper is organized as follows. In Section 2 we give an overview of variance-based global sensitivity analysis and introduce several sensitivity indices. In Section 3 we present our simple Monte Carlo algorithm to estimate the Shapley effects for all the input variables simultaneously. We also show some good properties of our algorithm as explained above. Numerical experiments in Section 4 confirm the effectiveness of our algorithm for a simple test case and for a more practical example. In Appendix A we provide a short Matlab implementation of our algorithm, which we use for the test case.

2 Variance-based sensitivity analysis

2.1 ANOVA decomposition

Let $x = (x_1, \ldots, x_d) \in \Omega_1 \times \cdots \times \Omega_d =: \Omega \subseteq \mathbb{R}^d$ be a vector of input random variables. Each variable $x_j$ follows a probability distribution with density $\rho_j$ defined over the interval $\Omega_j \subseteq \mathbb{R}$. Throughout this paper we assume that all the random variables are independent with each other. Moreover, for simplicity
of notation, we write \([1 : d] := \{1, \ldots, d\}\). For a subset \(u \subseteq [1 : d]\), we denote the complement of \(u\) by \(-u = [1 : d] \setminus u\) and denote the cardinality of \(u\) by \(|u|\).

For vectors \(\mathbf{x}, \mathbf{y} \in \Omega\), we write \(\mathbf{x}_u = (x_j)_{j \in u}\) and \((\mathbf{x}_u, \mathbf{y}_{-u}) = \mathbf{z}\) with \(z_j = x_j\) if \(j \in u\) and \(z_j = y_j\) otherwise. The Cartesian product \(\prod_{j \in u} \Omega_j\) is denoted by \(\Omega_u\), and the product of density functions \(\prod_{j \in u} \rho_j(x_j)\) is denoted by \(\rho_u(\mathbf{x}_u)\) with an exception for \(u = [1 : d]\) in which case we simply write \(\rho(\mathbf{x})\).

Now let \(f : \Omega \to \mathbb{R}\) be a function which outputs a quantity of our interest. If the variance of \(f\) with respect to \(\mathbf{x}\) is finite, \(f\) can be decomposed as

\[
\sigma^2 = \int_{\Omega} (f(\mathbf{x}) - \mu)^2 \rho(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega} \left( \sum_{\emptyset \neq u \subseteq [1 : d]} \int_{\Omega_u} f_u(\mathbf{x}_u) \, d\mathbf{x}_u \right)^2 \rho(\mathbf{x}) \, d\mathbf{x}
\]

where each summand is recursively defined by

\[
f_\emptyset = \int_{\Omega} f(\mathbf{x}) \, d\mathbf{x} = \mu
\]

and

\[
f_u(\mathbf{x}_u) = \int_{\Omega_{-u}} f(\mathbf{x}) \rho_{-u}(\mathbf{x}_{-u}) \, d\mathbf{x}_{-u} - \sum_{v \subseteq u} f_v(\mathbf{x}_v)
\]

for any non-empty subset \(u\). The following lemma shows importance properties of this decomposition.

**Lemma 1.** With the notation above, the following holds true.

1. For any non-empty subset \(u\) and coordinate \(j \in u\), we have

\[
\int_{\Omega_j} f_u(\mathbf{x}_u) \rho_j(x_j) \, dx_j = 0.
\]

2. For any \(u, v \subseteq [1 : d]\), we have

\[
\int_{\Omega} f_u(\mathbf{x}_u) f_v(\mathbf{x}_v) \rho(\mathbf{x}) \, d\mathbf{x} = \begin{cases} 
\sigma_u^2 := \int_{\Omega_u} (f_u(\mathbf{x}_u))^2 \rho_u(\mathbf{x}_u) \, d\mathbf{x}_u & \text{if } u = v, \\
0 & \text{otherwise}.
\end{cases}
\]

**Proof.** We refer the reader to [6, Appendix A.3] for the proof of the special case where \(\rho_j\) is the uniform distribution over the unit interval \([0, 1]\), which can be easily generalized to a proof of this lemma.

It follows from the second assertion of Lemma 1 that the variance of \(f\) can be decomposed as

\[
\sigma^2 := \int_{\Omega} (f(\mathbf{x}) - \mu)^2 \rho(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega} \left( \sum_{\emptyset \neq u \subseteq [1 : d]} \int_{\Omega_u} f_u(\mathbf{x}_u) \, d\mathbf{x}_u \right)^2 \rho(\mathbf{x}) \, d\mathbf{x}
\]

\[
= \sum_{\emptyset \neq u, v \subseteq [1 : d]} \int_{\Omega} f_u(\mathbf{x}_u) f_v(\mathbf{x}_v) \rho(\mathbf{x}) \, d\mathbf{x} = \sum_{\emptyset \neq u \subseteq [1 : d]} \sigma_u^2.
\]
This way, the total variance $\sigma^2$ is decomposed into $2^d - 1$ terms with each term $\sigma^2_v$ being the variance of a lower-dimensional function $f_u$. This is why we call the decomposition (1) the analysis of variance (ANOVA) decomposition of $f$.

2.2 Sensitivity indices

For a non-empty subset $u \subseteq [1:d]$, the main effect and the total effect for a group of input variables $x_u$ are defined by

$$
\tau^2_u := \sum_{\emptyset \neq v \subseteq u} \sigma^2_v \quad \text{and} \quad \tau^2_{\bar{u}} := \sum_{\emptyset \neq v \subseteq [1:d], v \cap u \neq \emptyset} \sigma^2_v = \sigma^2 - \tau^2_u,
$$

respectively. We see from the definition that the main effect measures the variance explained by the variables $x_u$. On the other hand, the total effect takes into account all possible interactions with the variables $x_u$, so that we always have $\tau^2_u \leq \tau^2_{\bar{u}}$. We see from the second equality that the total effect measures the difference between the total variance and the variance explained by the complement variables $x_{\bar{u}}$.

The following identities on these effects are well-known:

$$
\tau^2_u = \int_{\Omega} \int_{\Omega} f(x) f(x_u, y_{\bar{u}}) \rho(x) \rho(y) \, dx \, dy - \mu^2,
$$

and

$$
\tau^2_{\bar{u}} = \frac{1}{2} \int_{\Omega} \int_{\Omega} (f(x) - f(y_u, x_{\bar{u}}))^2 \rho(x) \rho(y) \, dx \, dy, \quad \text{(2)}
$$

see, e.g., [6, Appendix A.6]. These identities have been used for constructing so-called pick-freeze Monte Carlo estimators of the main and total effects, respectively. We refer the reader to [13, 9, 14, 3] among many others.

Looking at these effects for an individual variable, we have

$$
\sum_{j=1}^d \tau^2_{\{j\}} = \sum_{j=1}^d \sigma^2_{\{j\}} \leq \sigma^2,
$$

and

$$
\sum_{j=1}^d \tau^2_{\{j\}} = \sum_{\emptyset \neq u \subseteq [1:d]} |u| \sigma^2_u \geq \sigma^2.
$$

Therefore, the rescaled versions of these effects, $\tau^2_{\{j\}}/\sigma^2$ and $\tau^2_{\{j\}}/\sigma^2$, are not summed up to 1. This normalization issue can be circumvented by employing a new class of sensitivity indices called Shapley effects [5]. For an individual variable $x_j$, the Shapley effect is defined as follows:

$$
\phi_j := \frac{1}{d} \sum_{u \subseteq \{j\}, |u|} (d - 1)^{d - |u|} (\tau^2_{u+j} - \tau^2_{u}) = \frac{1}{d} \sum_{u \subseteq \{j\}} \left( \frac{d - 1}{|u|} \right)^{-1} \left( \tau^2_{u+j} - \tau^2_{u} \right).
$$

(3)
Here the second equality is proven in [14, Theorem 1]. As pointed out in [5],
\[ \sum_{j=1}^{d} \phi_j = \sigma^2 \]
holds, so that the Shapley effect enables an easy interpretation when measuring
the relative importance of individual variables. Moreover, it is known from [5, Theorem 1] that
\[ \phi_j = \sum_{\emptyset \neq u \subseteq \{1:d\}} \frac{\sigma^2_u}{|u|}, \]
which leads to an inequality \( \tau^2_{(j)} \leq \phi_j \leq \tau^2_{(j)} \).

3 Monte Carlo estimator for Shapley effect

3.1 Algorithm

In this section, we introduce a simple unbiased Monte Carlo algorithm to estimate
the Shapley effects \( \phi_j \) for all \( 1 \leq j \leq d \). Although we shall use the second
expression of \( \phi_j \) in (3), it is also possible to construct a similar Monte Carlo
algorithm based on the first expression. For a start, let us consider a single value \( \phi_j \). Let \( \ell \in \{0, 1, \ldots, d-1\} \) be a uniformly distributed discrete random variable,
and given \( \ell \), let \( U_j(\ell) \subseteq \{j\} \) be a uniformly distributed random subset with
fixed cardinality \( \ell \). Then it follows from (3) and (2) that the Shapley effect for
a variable \( x_j \) is given by
\[
\phi_j = \frac{1}{d} \sum_{\ell=0}^{d-1} \binom{d-1}{\ell}^{-1} \sum_{u \subseteq \{j\}} \left( \tau_{u+j}^2 - \tau_u^2 \right)
= \mathbb{E}_\ell \mathbb{E}_{U_j(\ell)} \left[ \tau_{\ell U_j(\ell) + j}^2 - \tau_{\ell U_j(\ell)}^2 \right]
= \mathbb{E}_\ell \mathbb{E}_{U_j(\ell)} \left[ \int_\Omega \int_\Omega g_{U_j(\ell)}(x, y) \rho(x) \rho(y) \, dx \, dy \right]
= \int_\Omega \int_\Omega \mathbb{E}_\ell \mathbb{E}_{U_j(\ell)} \left[ g_{U_j(\ell)}(x, y) \right] \rho(x) \rho(y) \, dx \, dy,
\]
wherein we have defined
\[
g_{U_j(\ell)}(x, y) = \frac{1}{2} \left( f(x) - f(y_{U_j(\ell)+j}, x-U_j(\ell)) \right)^2 - \frac{1}{2} \left( f(x) - f(y_{U_j(\ell)}, x-U_j(\ell)) \right)^2
= \left( f(x) - f(y_{U_j(\ell)}, x-U_j(\ell)) + f(y_{U_j(\ell)+j}, x-U_j(\ell)+j) \right)
\times \left( f(y_{U_j(\ell)}, x-U_j(\ell)) - f(y_{U_j(\ell)+j}, x-U_j(\ell)+j) \right).
\]
This representation naturally leads to the following unbiased Monte Carlo estimator of $\phi_j$:

$$\hat{\phi}_{j,N} = \frac{1}{N} \sum_{n=1}^{N} g_{\pi^{(n)}}(x^{(n)}, y^{(n)}),$$

where $x^{(1)}, \ldots, x^{(N)}$ and $y^{(1)}, \ldots, y^{(N)}$ are i.i.d. samples generated from the density $\rho$, $\ell^{(1)}, \ldots, \ell^{(N)}$ are i.i.d. samples of $\ell \in \{0, 1, \ldots, d - 1\}$, and for each $n$, $U_j^{(n)} (\ell^{(n)})$ denotes a random sample of $U_j (\ell^{(n)})$ conditional on $\ell^{(n)}$.

The key difference from the algorithms proposed in [14] and [1] is that we directly apply the pick-freeze scheme to estimate the difference $\phi_j$ for i.i.d. permutations $\pi$. The recycling technique from [14] shares the same $\pi^{(1)}, \ldots, \pi^{(N)}$ of $[1 : d]$ for estimating all $\hat{\phi}_1, \ldots, \hat{\phi}_d$ simultaneously. In fact, if each of $\phi_1, \ldots, \phi_d$ is estimated independently, we need $3dN$ function evaluations, whereas we can reduce this cost to $(d + 1)N$ through the recycling technique by estimating all $\phi_1, \ldots, \phi_d$ simultaneously.

Let $\pi = (\pi(1), \ldots, \pi(d))$ denote a random permutation of $[1 : d]$. For a fixed $1 \leq j \leq d$, generating $\ell \in \{0, 1, \ldots, d - 1\}$ and $U_j (\ell)$ randomly is equivalent to finding $\ell$ such that $\pi(\ell + 1) = j$ and set $U_j (\ell) = \{\pi(1), \ldots, \pi(\ell)\}$. Note that we set $U_j (0)$ to the empty set. Because of this equivalence, by writing $\pi_j = \{\pi(1), \ldots, \pi(\ell)\}$ with $\ell$ satisfying $\pi(\ell + 1) = j$, we can rewrite our estimator as

$$\hat{\phi}_{j,N} = \frac{1}{N} \sum_{n=1}^{N} g_{\pi^{(n)}}(x^{(n)}, y^{(n)}),$$

for i.i.d. permutations $\pi^{(1)}, \ldots, \pi^{(N)}$ of $[1 : d]$. The recycling technique from [14] shares the same $\pi^{(1)}, \ldots, \pi^{(N)}$ for computing all of $\hat{\phi}_1, \ldots, \hat{\phi}_d, \hat{\phi}_{d,N}$, which still ensures the unbiasedness of estimators. After some rearrangements, our algorithm can be summarized as follows.

**Algorithm 1** (Monte Carlo estimation of Shapley effects for all input variables).

Let $d$ be the number of input variables and $N$ be the sample size. Initialize $\hat{\phi}_{1, N} = \ldots = \hat{\phi}_{d, N} = 0$. For $1 \leq n \leq N$, do the following:

1. Generate $x^{(n)}, y^{(n)} \in \Omega$ and $\pi^{(n)}$ randomly.
2. Let $\ell = 1$ and compute $F_n = F_{n}^{-} = f(x^{(n)})$.
3. (a) Compute $F_n^{+} = f(y^{(n)}_{\pi(1), \ldots, \pi(\ell)}, x^{(n)}_{-\pi(1), \ldots, \pi(\ell)})$.
   (b) Update
   $$\hat{\phi}_{n, \ell, N} = \hat{\phi}_{n, \ell, N} + \frac{1}{N} \left( F_n - \frac{F_n^{-} + F_n^{+}}{2} \right) \left( F_n^{-} - F_n^{+} \right).$$
   (c) Let $\ell = \ell + 1$. If $\ell \leq d$, let $F_n^{-} = F_n^{+}$ and go to Step (a).

It is obvious that we evaluate function values only $d + 1$ times for each $n$, leading to the total computational cost of $(d + 1)N$. 


3.2 Some properties

Since our Monte Carlo estimator is trivially unbiased, here we show the second and fourth properties of the estimator mentioned in Section 1. The third property immediately follows from the central limit theorem. First, let us make the second property more explicit.

**Theorem 1.** Assume that

\[ M_4(f) := \int_{\Omega} (f(x))^4 \rho(x) \, dx < \infty. \]

Then the following holds true.

1. The variance of \( \hat{\phi}_{j,N} \) is finite and decays at the rate of \( 1/N \) for all \( j \).

2. The variance of \( \hat{\phi}_{j,N} \) is estimated unbiasedly by

\[ \frac{1}{N(N-1)} \sum_{n=1}^{N} \left( g_{U_j(\ell)(n)}(x^{(n)}, y^{(n)}) - \hat{\phi}_{j,N} \right)^2. \]

**Proof.** Since the second assertion is well-known [6, Chapter 2], we only give a proof for the first assertion. Because of the independence between different samples, we have

\[ \mathbb{V} \left[ \hat{\phi}_{j,N} \right] = \mathbb{V} \left[ \frac{g_{U_j(\ell)(x,y)}}{N} \right], \]

where the variance on the right-hand side is taken with respect to \( x, y \sim \rho, \ell \in [1 : d] \) and \( U_j(\ell) \subseteq \{-j\} \). Thus it suffices to prove that \( \mathbb{V} \left[ g_{U_j(\ell)(x,y)} \right] \) is finite under the assumption \( M_4(f) < \infty \). In fact, applying Jensen’s inequality twice, we have

\[ \mathbb{V} \left[ g_{U_j(\ell)(x,y)} \right] \leq \mathbb{E} \left[ (g_{U_j(\ell)(x,y)})^2 \right] \]

\[ = \mathbb{E} \mathbb{E}_{U_j(\ell)} \left[ \int_{\Omega} \int_{\Omega} (g_{U_j(\ell)(x,y)})^2 \rho(x) \rho(y) \, dx \, dy \right] \]

\[ = \frac{1}{d} \sum_{\ell=0}^{d-1} (d-1)^{-1} \sum_{u \subseteq \{-j\}, |u| = \ell} \int_{\Omega} \int_{\Omega} \rho(x) \rho(y) \]

\[ \times \left( \frac{1}{2} (f(x) - f(y_{u+j}, x-(u+j)))^2 - \frac{1}{2} (f(x) - f(y_u, x-u))^2 \right)^2 \, dx \, dy \]

\[ \leq \frac{1}{d} \sum_{\ell=0}^{d-1} (d-1)^{-1} \sum_{u \subseteq \{-j\}, |u| = \ell} \int_{\Omega} \int_{\Omega} \rho(x) \rho(y) \]

\[ \times \left( \frac{1}{2} (f(x) - f(y_{u+j}, x-(u+j)))^4 + \frac{1}{2} (f(x) - f(y_u, x-u))^4 \right) \, dx \, dy \]
Thus we are done. □

Furthermore, the fourth property of our estimator is described as follows.

Theorem 2. With the notation above, we have

\[
\sum_{j=1}^{d} \hat{\phi}_{j,N} = \frac{1}{2N} \sum_{n=1}^{N} \left( f(x^{(n)}) - f(y^{(n)}) \right)^2,
\]

which is an unbiased estimator of the total variance \( \sigma^2 \).

Proof. For points \( x, y \in \Omega \) and permutation \( \pi \), we write

\[
[x:y](\pi, \ell) = (y_{\{\pi(1), \ldots, \pi(\ell)\}}, x_{-\{\pi(1), \ldots, \pi(\ell)\}}),
\]

for any \( 1 \leq \ell \leq d \), and let \( [x:y](\pi, 0) = x \). Then we have

\[
\sum_{j=1}^{d} \hat{g}_j(x, y) = \frac{1}{2} \sum_{\ell=1}^{d} \left[ (f(x) - f([x:y](\pi, \ell)))^2 - (f(x) - f([x:y](\pi, \ell - 1)))^2 \right]
= \frac{1}{2} \left[ (f(x) - f([x:y](\pi, d)))^2 - (f(x) - f([x:y](\pi, 0)))^2 \right]
= \frac{1}{2} \left[ (f(x) - f(y))^2 - (f(x) - f(x))^2 \right] = \frac{1}{2} (f(x) - f(y))^2.
\]

Thus we see that the equality

\[
\sum_{j=1}^{d} \hat{\phi}_{j,N} = \frac{1}{N} \sum_{n=1}^{N} \sum_{j=1}^{d} \hat{g}_{j,n}(x^{(n)}, y^{(n)}) = \frac{1}{2N} \sum_{n=1}^{N} \left( f(x^{(n)}) - f(y^{(n)}) \right)^2
\]

holds true. Moreover, we have

\[
\mathbb{E} \left[ \frac{1}{2N} \sum_{n=1}^{N} \left( f(x^{(n)}) - f(y^{(n)}) \right)^2 \right]
= \frac{1}{2N} \sum_{n=1}^{N} \mathbb{E} \left[ (f(x^{(n)}))^2 \right] + \frac{1}{2N} \sum_{n=1}^{N} \mathbb{E} \left[ (f(y^{(n)}))^2 \right] - \frac{1}{N} \sum_{n=1}^{N} \mathbb{E} \left[ f(x^{(n)})f(y^{(n)}) \right]
= \mathbb{E} \left[ (f(x))^2 \right] - (\mathbb{E}[f(x)])^2 = \sigma^2,
\]

which shows that the sum of our Shapley effect estimators is an unbiased estimator of the total variance. □
4 Numerical experiments

Finally we conduct some numerical experiments to confirm the effectiveness of our Shapley effect estimator. For the first test case, we consider Sobol’ g function which has been often used as a standard test problem in the context of global sensitivity analysis [10]. The second example is taken from [11, Section 7] which involves the assessment of structural component strength. A short implementation of our algorithm in Matlab for the first test case is available in Appendix A.

4.1 Sobol’ g function

Let us consider the case where \( \rho \) is the uniform distribution over the domain \( \Omega = [0, 1]^d \). With its simplest form, Sobol’ g function is defined by

\[
f(x) = \prod_{j=1}^{d} \frac{|4x_j - 2| + a_j}{1 + a_j},
\]

with non-negative weight parameters \( a_1, \ldots, a_d \). For this function, we can easily obtain

\[
\sigma^2 = \prod_{j=1}^{d} \left[ 1 + \frac{1}{3(1 + a_j)^2} \right] - 1 \quad \text{and} \quad \sigma^2_u = \prod_{j \in u} \frac{1}{3(1 + a_j)^2},
\]

for any non-empty \( u \subseteq [1 : d] \). Thus, for an individual variable \( x_j \), the main and total effects are given by

\[
\tau^2_j = \frac{1}{3(1 + a_j)^2} \quad \text{and} \quad \tau^2_{\{j\}} = \frac{1}{3(1 + a_j)^2} \times \prod_{\ell=1}^{d} \left[ 1 + \frac{1}{3(1 + a_\ell)^2} \right]
\]

respectively. The Shapley effect is

\[
\phi_j = \sum_{\emptyset \neq u \subseteq [1 : d]} \frac{1}{|u|} \prod_{\ell \in u} \frac{1}{3(1 + a_\ell)^2},
\]

which seems hard to simplify further.

In what follows, we set \( d = 10 \) and \( a_j = j - 1 \). With this choice of \( a_j \), the relative importance of individual variables is given by the ascending order, i.e., \( x_1 \) is the most important, \( x_2 \) is the second most important, and so on. The main and total effects of individual variables, both computed analytically, are compared in Figure 1. In fact, we can see that both of the effects decrease as the index increases.

The Shapley effects for all the input variables are estimated according to Algorithm 1. The results for two different values of \( N \) are shown in Figure 2.
Figure 1: The main and total effects of individual variables for Sobol’ g function (left and right, respectively). The effects for the label 0 denote the total variance.

Figure 2: The estimated Shapley effects of individual variables for Sobol’ g function: the result for $N = 2^{10}$ (left) and the result for $N = 2^{20}$ (right). The effects for the label 0 denote the estimated total variance. The approximate 95% confidence intervals are also shown.

With a smaller value of $N$, the result for the variable $x_{10}$, the least important variable, becomes negative. Although the Shapley effect always takes a non-negative value by definition, our Monte Carlo estimator does not ensure non-negativity. Although we do not discuss further, a similar problem happens for Monte Carlo estimation of main effects in general. As $N$ gets larger, however, all the approximate confidence intervals become smaller and even their lower endpoints take positive values for all the variables. Here, the confidence interval is constructed with the variance estimator shown in Theorem 1. It can be confirmed that the estimated Shapley effects take the values between the corresponding main and total effects, which agree with the theory. The sum of the Shapley effects is shown in the label “0”. As proven in Theorem 2, the resulting value is an unbiased estimate of the total variance. In fact, it agrees quite well with the analytical value shown in Figure 1.

The sum of the variance estimates over all the variables is computed for
Figure 3: The sum of variance estimates over all the individual variables for Sobol’ $g$ function.

Table 1: List of input variables for plate buckling example. CV denotes the coefficient of variation.

| variable | description       | mean   | CV    | distribution type |
|----------|-------------------|--------|-------|-------------------|
| $x_1$    | width             | 23.808 | 0.028 | normal            |
| $x_2$    | thickness         | 0.525  | 0.044 | log-normal        |
| $x_3$    | yield stress      | 44.2   | 0.1235| log-normal        |
| $x_4$    | elastic modulus   | 28623  | 0.076 | normal            |
| $x_5$    | initial deflection| 0.35   | 0.05  | normal            |
| $x_6$    | residual stress   | 5.25   | 0.07  | normal            |

Various values of $N$. As plotted in Figure 3, the sum decays at the rate of $1/N$ almost exactly, which can be indicated from the statement of Theorem 1. In this way one can easily check whether a sufficient convergence of estimation is achieved or not.

4.2 Plate buckling

Here we consider a more realistic example from structural engineering. As explained in [11], let us consider the buckling strength of a rectangular plate that is supported on all four edges subjected to uniaxial compression. As described in Table 1, we have $d = 6$ input random variables $x_1, \ldots, x_6$ which are related to the material, geometry and imperfection of the plate. The buckling strength is defined as a function of these variables, and is explicitly given by

$$f(x) = \left(\frac{2.1}{\lambda} - 0.9\frac{x_5}{\lambda^2}\right) \left(1 - \frac{0.75x_5}{\lambda}\right) \left(1 - \frac{2x_2x_6}{x_1}\right) \quad \text{with} \quad \lambda = \frac{x_1}{x_2} \sqrt{\frac{x_3}{x_4}}.$$

Since closed formulas for main and total effects are no longer available for this example, we estimate them for all the input variables by using the estimators proposed in the literature. We use the one from [11] for the main effects,
whereas the standard one based on the identity (2) is used for the total effects, see, e.g., [9]. The sample size is set large enough ($N = 2^{24}$) to make sure that the estimates are converged sufficiently. The results are shown in Figure 4. Interestingly, there is no clear difference between the main and total effects. This means that each variable does not have significant interactions with other variables for the buckling strength, so that the buckling strength can be effectively written as a sum of $d$ one-dimensional functions $f_{\{1\}}, \ldots, f_{\{d\}}$.

As already pointed out, the Shapley effect takes its value between the corresponding main and the total effects for each input variable. Since the difference between the latter two values is quite small in this example, it might be challenging to estimate the Shapley effect in a way that the resulting value is bracketed by them. However, our Algorithm 1 with $N = 2^{16}$ already provides good estimates for all the variables, as shown in the left panel of Figure 5. Similarly to the first test case, the variance of our estimators decays at the $1/N$ rate as indicated from the right panel of Figure 5. In this way one can reliably use our algorithm to estimate the Shapley effects simultaneously for all the input variables. In this example, we can conclude that the yield stress $x_3$ is the most important factor in controlling the buckling strength, whereas the width $x_1$ is the least one.

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Figure 5: The estimated Shapley effects of individual variables for the plate buckling example with $N = 2^{16}$ (left) and the sum of variance estimates over all the individual variables (right).

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A Matlab implementation

```matlab
n = 2^20; % sample size
d = 10; % dimension
x = rand(n,d); % Monte Carlo samples for x
y = rand(n,d); % Monte Carlo samples for y
refm = repmat(1:d,n,1); % reference matrix
 [~, pm] = sort(rand(n,d),2); % random permutation matrix

func = @(x,a)prod((abs(4.*x-2)+a)./(1+a),2); % Sobol g function
a = (0:d-1);

z = x;
fz1 = func(z,a);
fx = fz1;

phi1 = zeros(1,d); % initialization
phi2 = zeros(1,d); % initialization
for j=1:d
    qm = repmat(pm(:,j),1,d);
    ind = refm==qm;
    z(ind) = y(ind);
    fz2 = func(z,a);
    for l=1:d % update
        row = pm(:,j) == l;
        phi1(l) = phi1(l)+row.'*((fx-fz1/2-fz2/2).*(fz1-fz2))/n;
        phi2(l) = phi2(l)+row.'*((fx-fz1/2-fz2/2).*(fz1-fz2)).^2/n;
    end
    fz1 = fz2;
end

s_all = sum(phi1); % variance of function
phi2 = (phi2-phi1.^2)./(n-1); % variance of Shapley estimates

bar(0:d,[s_all,phi1]); % plot of estimates w/ confidence intervals
hold on
er = errorbar(0:d,[s_all,phi1],[0,1.96*sqrt(phi2)],[0,1.96*sqrt(phi2)]);
er.Color = [0 0 0];
er.LineStyle = 'none';
hold off
```