Multifidelity Monte Carlo Estimation of Variance and Sensitivity Indices[*]

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Abstract. Variance-based sensitivity analysis provides a quantitative measure of how uncertainty in a model input contributes to uncertainty in the model output. Such sensitivity analyses arise in a wide variety of applications and are typically computed using Monte Carlo estimation, but the many samples required for Monte Carlo to be sufficiently accurate can make these analyses intractable when the model is expensive. This work presents a multifidelity approach for estimating sensitivity indices that leverages cheaper low-fidelity models to reduce the cost of sensitivity analysis while retaining accuracy guarantees via recourse to the original, expensive model. This paper develops new multifidelity estimators for variance and for the Sobol' main and total effect sensitivity indices. We discuss strategies for dividing limited computational resources among models and specify a recommended strategy. Results are presented for the Ishigami function and a convection-diffusion-reaction model that demonstrate up to $10\times$ speedups for fixed convergence levels. For the problems tested, the multifidelity approach allows inputs to be definitively ranked in importance when Monte Carlo alone fails to do so.

1. Introduction. Sensitivity analysis plays a central role in modeling and simulation to support decision making, providing a rigorous basis on which to characterize how input uncertainty contributes to output uncertainty. This allows identification of the most significant sources of input uncertainty as well as identification of uncertain inputs whose variation contributes minimally to output variability. Such sensitivity analyses arise in a wide variety of applications—for example, for models with uncertain inputs of high dimension, it is often necessary to reduce the input dimension in order to make tractable the tasks of policy optimization, robust design optimization, and reduced-order modeling. Variance-based global sensitivity analysis quantifies the relative effect of input uncertainties on the output uncertainty via the calculation of sensitivity indices, enabling the prioritization of inputs with larger

influence on the output (e.g., by fixing relatively unimportant inputs). Estimates of these sensitivity indices are typically obtained via Monte Carlo integration, which often requires many model evaluations to obtain accurate sensitivity estimates. This work presents a multifidelity formulation—leveraging approximate models to accelerate convergence—for Monte Carlo estimation of sensitivity indices. In particular, we develop and analyze new multifidelity estimators for variance and for the Sobol' main and total effect sensitivities.

Sensitivity analysis plays an important role in the development and analysis of numerical models; see [20] for a comprehensive review. In addition to the classical local approach, entailing deterministic calculation of partial derivatives, a multitude of global approaches exist, which seek to characterize how the overall input uncertainty affects the uncertainty of the model output. These include screening methods [30], correlation ratios [16, 24, 25, 46], variance-based methods [11, 18, 36, 40, 45, 50], entropy-based methods [28], and moment-independent methods [3, 4, 8, 41]. Our interest is in the Sobol' variance-based sensitivity indices [50], which attribute portions of output variance to the influence of individual inputs and their interactions and have been used in a variety of applications [1, 7, 14, 34, 47].

Sobol' sensitivity indices are typically estimated via Monte Carlo methods, using "fixing methods" which estimate sensitivity indices by holding one or more inputs constant while varying the others. Rather than using an inner and outer Monte Carlo loop to do so, Saltelli et al. propose a method that allows computation of all sensitivity indices using a single loop [44]. Saltelli's method is commonly used in application, but the number of function evaluations required per Monte Carlo sample scales linearly with the number of uncertain input parameters. This, combined with the sublinear convergence rate of the root mean-squared error (RMSE) of Monte Carlo estimators, means that computation of Sobol' sensitivities quickly becomes computationally prohibitive when the model is expensive and the dimension of the input is high. To address this, several authors have proposed estimators with improved precision, including [22, 29, 35]. These estimators have reduced variance relative to those initially proposed by Sobol', although some of them are biased. To achieve further acceleration, other previous work [1, 2, 19, 49] has achieved speedups by replacing the expensive model with cheaper low-fidelity models (sometimes referred to as metamodels or surrogates). One drawback of these approaches is that estimation based on the surrogate model introduces bias relative to the high-fidelity model, and procedures for error estimation exist only in limited settings [15, 23, 51]. We develop a multifidelity approach which combines the high-fidelity model with low-fidelity models, resulting in computational speedups and retaining accuracy.

Multifidelity formulations have in recent years been shown to provide significant computational gains in Monte Carlo estimation for uncertainty propagation and for optimization under uncertainty [39]. For uncertainty propagation, multifidelity formulations use surrogate models to reduce the cost of Monte Carlo estimators. The multilevel Monte Carlo method employs a hierarchy of coarse grids and exploits the known relationships between error and cost at each grid level [13] and has been used to accelerate the convergence of variance estimation [2]. In stochastic collocation, the outputs of a low-fidelity model are corrected with a discrepancy model that accounts for the difference between the high- and the low-fidelity model [12]. Multifidelity stochastic collocation approaches have been shown to have bounded error and fast convergence [31, 52]. The multifidelity Monte Carlo (MFMC) method [32, 38] accelerates the estimation of model statistics by using general surrogate models as control

variates. In the particular case of optimization under uncertainty, the control variate can be formed using the high-fidelity model's autocorrelation across the design space—i.e., using model evaluations from previous optimization iterates at nearby design points as a so-called information reuse control variate [33].

Here, we build on the MFMC method [38] and present new multifidelity estimators for the variance and main effect sensitivity indices. Multifidelity formulations which target estimation of Sobol' indices have been presented in [15, 26, 27, 37]. The work in [15] considers a setting where, in addition to having random inputs, the model itself is stochastic. We do not consider that setting here. In [27], the Sobol' indices are sampled from a Gaussian process which approximates a high-fidelity computer code. In this approach, lower-fidelity models can be introduced via a cokriging model, thus increasing the quality of the Gaussian process approximation without incurring additional evaluations of the expensive high-fidelity model. In [37], the Sobol' indices are obtained from a polynomial chaos expansion derived from a low-fidelity model with a correction polynomial chaos expansion derived from the difference between the low- and the high-fidelity model at some inputs. In both [27, 37], the Sobol' indices are obtained for a surrogate model, and the multifidelity formulation serves to efficiently increase the quality of the surrogate employed. This means that the result will be biased relative to the original high-fidelity model. In contrast, our approach samples directly from the high-fidelity model to ensure that our estimates are unbiased. Our approach is most closely related to the control variate formulation of [26], which uses the first-order terms of the analysis-of-variance (ANOVA) decomposition as the control variate. Our framework is also based on control variates but does not restrict the type or number of surrogate models used. Additionally, the work in this paper presents a strategy for distributing work among the available models given a limited computational budget.

Section 2 introduces the Sobol' variance-based sensitivity indices and Monte Carlo estimation procedure. Section 3 introduces our multifidelity formulations for variance and sensitivity index estimation, presents their accuracy guarantees, and discusses model management strategies. Results are presented for an analytical example in section 4 and for a numerical example in section 5. Conclusions are presented in section 6.

2. Setting. In this section, we introduce Sobol' global sensitivity analysis. Subsection 2.1 presents the underlying mathematical theory and defines the Sobol' main and total effect sensitivity indices. Subsection 2.2 introduces the corresponding Monte Carlo estimators.

2.1. Variance-based global sensitivity analysis. Consider a model $f : \mathcal{Z} \to \mathcal{Y}$ that maps a d-dimensional input $z \in \mathcal{Z} \subset \mathbb{R}^d$ to a scalar output $y \in \mathcal{Y} \subset \mathbb{R}$ of our system of interest. The input domain $\mathcal{Z} = \mathcal{Z}_1 \times \cdots \times \mathcal{Z}_d$ is the product of the domains $\mathcal{Z}_1, \ldots, \mathcal{Z}_d \subset \mathbb{R}$. Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space with sample space Ω, σ-algebra $\mathcal{F}$, and probability measure $\mathbb{P}$, and let $Z : \Omega \to \mathcal{Z}$ be a random vector $Z = (Z(1), \ldots, Z(d))^T$ with independent components $Z(i) : \Omega \to \mathcal{Z}_i$ for $i = 1, \ldots, d$. Because the components of Z are independent, the probability density function $\mu(z)$ is the product of its marginals $\mu(z) = \mu_1(z(1))\mu_2(z(2)) \cdots \mu_d(z(d))$. We now consider Z as an uncertain input to model f and $f(Z)$ as the uncertain output. If f is square-integrable with respect to μ, then the mean $\mathbb{E}[f(Z)] = \int f(z) \, \mu(\mathrm{d}z)$ and variance $\mathbb{V}\mathrm{ar}[f(Z)] = \int (f(z) - \mathbb{E}[f(Z)])^2 \, \mu(\mathrm{d}z)$ of f are finite, and $f(z)$ may be expressed as the sum

of functions of subsets of its inputs [17],

$$(1) \qquad f(z) = f_0 + \sum_{i=1}^{d} f_i(z(i)) + \sum_{1 \le i < j \le d} f_{i,j}(z(i), z(j)) + \cdots + f_{1,2,\ldots,d}(z) = \sum_{u \subseteq \mathcal{I}} f_u(z(u)),$$

with $\mathcal{I} = \{1, \ldots, d\}$, $z(u) = \{z(i) : i \in u\}$, and the component functions $f_u : \bigotimes_{i \in u} \mathcal{Z}_i \to \mathcal{Y}$ for $u \subseteq \mathcal{I}$. This expression is unique if we enforce the following orthogonality condition:

$$(2) \qquad \int f_u(z(u)) \, \mu_j(\mathrm{d}z(j)) = 0 \quad \forall j \in u, \forall u \subseteq \mathcal{I}.$$

The decomposition given by (1) satisfying (2) is known as the ANOVA high-dimensional model representation (ANOVA HDMR) because the orthogonality ensures $f_0 = \mathbb{E}[f(Z)]$ and $\mathbb{E}[f_u(Z)] = 0$ for $u \subseteq \mathcal{I}, u \ne \emptyset$, which allows the variance $V = \sigma^2 = \mathbb{V}\mathrm{ar}[f(Z)]$ to then be decomposed as [50]

$$\mathbb{V}\mathrm{ar}[f(Z)] = \int f^2(Z) \, \mu(\mathrm{d}z) - f_0^2$$

$$= \sum_{i=1}^{d} \mathbb{V}\mathrm{ar}[f_i(Z(i))] + \sum_{1 \le i < j \le d} \mathbb{V}\mathrm{ar}[f_{i,j}(Z(i), Z(j))] + \cdots + \mathbb{V}\mathrm{ar}[f_{1,2,\ldots,d}(Z)].$$

Sobol' defined the sensitivity indices $s_u = \mathbb{V}\mathrm{ar}[f_u(Z(u))]/V$ for $u \subseteq \mathcal{I}$ [50]. Of particular interest are the Sobol' indices for subsets $u \subseteq \mathcal{I}$ with cardinality $|u| = 1$, which are the portions of the output variance that can be attributed to the influence of a single input alone, denoted

$$(3) \qquad V_j = \mathbb{V}\mathrm{ar}_{\mu_j}[f_j(Z(j))].$$

We are also interested in the total variance contributed by the input $Z(j)$, denoted

$$(4) \qquad T_j = \sum_{\{u : j \in u\}} \mathbb{V}\mathrm{ar}_{\mu_u}[f_u(Z(u))].$$

This allows us to define the Sobol' main and total effect sensitivity indices for input j as the fraction of variance contributed by $Z(j)$ alone and by the sum of contributions influenced by $Z(j)$, respectively.

Definition 2.1. *The Sobol' main effect sensitivity index for input j is given by*

$$(5) \qquad s_j \equiv \frac{V_j}{V} = \frac{\mathbb{V}\mathrm{ar}_{\mu_j}[f_j(Z(j))]}{\mathbb{V}\mathrm{ar}[f(Z)]}, \qquad j = 1, \ldots, d.$$

Definition 2.2. *The Sobol' total effect sensitivity index for input j is given by*

$$(6) \qquad s_j^t \equiv \frac{T_j}{V} = \frac{\sum_{\{u : j \in u\}} \mathbb{V}\mathrm{ar}_{\mu_u}[f_u(Z(u))]}{\mathbb{V}\mathrm{ar}[f(Z)]} = \frac{\mathbb{E}_{\mu_{\bar{j}}}[\mathbb{V}\mathrm{ar}_{\mu_j}[f(Z)|Z(\bar{j})]]}{\mathbb{V}\mathrm{ar}[f(Z)]},$$

where $\bar{j}$ denotes the set of all inputs excluding the jth input, i.e., $\bar{j} = \mathcal{I} \setminus \{j\}$.

2.2. Monte Carlo estimation of variance and sensitivity indices.

Variance estimation. Let $\{z_1, \ldots, z_n\}$ denote $n \in \mathbb{N}$ independent realizations of the input Z. The sample mean and variance are given by

$$
(7) \qquad \hat{E} = \frac{1}{n} \sum_{i=1}^{n} f(z_i) \text{ and } \hat{V} = \frac{1}{n-1} \sum_{i=1}^{n} (f(z_i) - \hat{E})^2,
$$

respectively. The variance estimator has expected value $\mathbb{E}[\hat{V}] = \mathbb{V}\mathrm{ar}[f(Z)]$ and variance $\mathbb{V}\mathrm{ar}[\hat{V}] = \frac{1}{n}(\delta - \frac{n-3}{n-1}\sigma^4)$, where $\delta = \mathbb{E}[(f(Z) - \mathbb{E}[f(Z)])^4]$ is the fourth central moment of f [9].

Sensitivity index estimation. The sensitivity indices in Definitions 2.1 and 2.2 are typically estimated via Monte Carlo integration, using "fixing methods" to estimate V_j and T_j. These methods use a second set of n independent realizations of Z, denoted $\{z'_1, \ldots, z'_n\}$. Define

$$
(8) \qquad y_i^{(j)} = (z'_i(1), \ldots, z'_i(j-1), z_i(j), z'_i(j+1), \ldots, z'_i(d)).
$$

The estimator for V_j (resp., T_j) is the empirical covariance of the data set of $f(y_i^{(j)})$ and $f(z_i)$ (resp., $f(z'_i)$) pairs, and $\hat{s}_j$ and $\hat{s}_j^t$ are obtained by normalizing by $\hat{V}$ given by (7). The main effect Sobol' estimator is given by [50]

$$
(9) \qquad \hat{V}_{j,\mathrm{sobol}} = \frac{1}{n} \sum_{i=1}^{n} f(z_i) f\left(y_i^{(j)}\right) - \hat{E}^2,
$$

with $\hat{E}$ given by (7). To estimate main effect sensitivities in d inputs using (9), we require $(d+1)$ function evaluations per Monte Carlo sample, i.e., a total of $n \times (d+1)$ evaluations of f.

Variants on the Sobol' estimator exist, including the Saltelli estimator [43], which modifies the Sobol' estimator (9) by dividing the sum by $(n-1)$ rather than n, and the work by Janon et al. [22], which shows that replacing $\hat{E}$ with the alternative sample mean estimator $\tilde{E} = \frac{1}{2n} \sum_{i=1}^{n} (f(z_i) + f(y_i^{(j)}))$ lowers the variance of the s_j estimator in the asymptotic limit. The bias of these estimators is of order $\mathcal{O}(1/n)$. In [36], Owen introduces a bias-corrected version of the Janon estimator, given by

$$
(10) \qquad \hat{V}_{j,\mathrm{owen}} = \frac{2n}{2n-1} \left(\frac{1}{n} \sum_{i=1}^{n} f(z_i) f\left(y_i^{(j)}\right) - \left(\frac{\hat{E} + \hat{E}'}{2}\right)^2 + \frac{\hat{V} + \hat{V}'}{4n} \right),
$$

where $\hat{E}$, $\hat{E}'$ and $\hat{V}$, $\hat{V}'$ are the sample means and variances, respectively, estimated using $z_1, \ldots, z_n$ and $z'_1, \ldots, z'_n$, respectively.

To estimate T_j, the estimator introduced by Homma and Saltelli [18] is given by

$$
(11) \qquad \hat{T}_{j,\mathrm{homma}} = \hat{V} - \left(\frac{1}{n-1} \sum_{i=1}^{n} f(z'_i) f\left(y_i^{(j)}\right) - \hat{E}^2 \right).
$$

This estimator has an $\mathcal{O}(1/n)$ bias. Owen suggests an alternative estimator,

$$
(12) \qquad \hat{T}_{j,\mathrm{owen}} = \frac{1}{2n} \sum_{i=1}^{n} \left(f(z'_i) - f\left(y_i^{(j)}\right) \right)^2,
$$

which is an unbiased estimator of T_j [36].

Although the Saltelli estimators are the most widely cited in the literature, the unbiased alternatives are better suited to the multifidelity theory we develop in section 3. Given the popularity of the Saltelli estimators, however, we will present results for multifidelity estimators based both on the Saltelli estimators as well as on their unbiased alternatives.

3. Multifidelity global sensitivity analysis approach. We now consider the multifidelity setting where we have K models: In addition to our high-fidelity model f, which we will hence denote $f^{(1)}$, we also have $K - 1$ surrogate models $f^{(k)}$ for $k = 2, \ldots, K$. In contrast to multilevel methods, the surrogates $f^{(k)}$ are not limited to hierarchical discretizations but may include projection-based reduced models, support vector machines, data-fit interpolation and regression, and simplified-physics models. This section introduces multifidelity estimators that leverage all available models to provide efficient estimators for the variance and the Sobol' main and total effect indices.

3.1. MFMC variance estimation. Let $\mathbf{m} = [m_1, \ldots, m_K] \in \mathbb{N}^K$ be a vector with $m_1 > 0$ and $m_l \geq m_k$ for $l > k$. We draw m_K realizations of Z, denoted $z_1, \ldots, z_{m_K} \in \mathcal{Z}$. Let $\hat{V}_n^{(k)}$ denote the unbiased Monte Carlo sample variance of $\mathbb{Var}[f^{(k)}(Z)]$ evaluated using the first n realizations of z, given by (7). We can now introduce our multifidelity variance estimator.

Proposition 3.1. *The multifidelity variance estimator given by*

$$(13) \qquad \hat{V}_{\mathrm{mf}} = \hat{V}_{m_1}^{(1)} + \sum_{k=2}^{K} \alpha_k \left(\hat{V}_{m_k}^{(k)} - \hat{V}_{m_{k-1}}^{(k)} \right)$$

is an unbiased estimator of $\mathbb{Var}[f^{(1)}(Z)]$. In (13), $\alpha_2, \ldots, \alpha_K$ are control variate coefficients which will be determined by the model management strategy (see subsection 3.3).

Proof. It follows from linearity of expectation that $\mathbb{E}[\hat{V}_{\mathrm{mf}}] = \mathbb{E}[\hat{V}_{m_1}^{(1)} + \sum_{k=2}^{K} \alpha_k (\hat{V}_{m_k}^{(k)} - \hat{V}_{m_{k-1}}^{(k)})] = \mathbb{E}[\hat{V}_{m_1}^{(1)}] + \sum_{k=2}^{K} \alpha_k(\mathbb{E}[\hat{V}_{m_k}^{(k)}] - \mathbb{E}[\hat{V}_{m_{k-1}}^{(k)}])$. Since $\mathbb{E}[\hat{V}_n^{(k)}] = \mathbb{Var}[f^{(k)}(Z)]$ for $n \geq 2$, $\mathbb{E}[\hat{V}_{m_k}^{(k)}] - \mathbb{E}[\hat{V}_{m_{k-1}}^{(k)}] = \mathbb{Var}[f^{(k)}(Z)] - \mathbb{Var}[f^{(k)}(Z)] = 0$ for $k = 1, \ldots, K$. $\mathbb{E}[\hat{V}_{\mathrm{mf}}(Z)] = \mathbb{Var}[f^{(1)}(Z)]$ follows. ∎

Note that $\hat{V}_{m_k}^{(k)}$ reuses m_{k-1} function evaluations used to compute $\hat{V}_{m_{k-1}}^{(k)}$. We now prove a lemma that will help us assess the quality of the MFMC variance estimator.

Lemma 3.2. *Let $\hat{V}_n^{(k)}(Z)$, $n \leq m_K$ denote the Monte Carlo variance estimator computed with model $f^{(k)}$ at the first n input realizations in the set $\{z_i\}_{i \in \mathbb{N}, 1 \leq i \leq m_K}$. Without loss of generality, let $m \geq n$. Then the covariance of two estimators $\hat{V}_m^{(k)}(Z)$ and $\hat{V}_n^{(l)}(Z)$ is given as follows for $1 \leq k, l \leq K$:*

$$(14) \qquad \mathbb{Cov}[\hat{V}_m^{(k)}(Z), \hat{V}_n^{(l)}(Z)] = \begin{cases} \frac{1}{m}(q_{k,l}\tau_k\tau_l + \frac{2}{m-1}\rho_{k,l}^2\sigma_k^2\sigma_l^2) & \text{if } k \neq l \\ \frac{1}{m}(\delta_k - \frac{m-3}{m-1}\sigma_k^4) & \text{if } k = l, \end{cases}$$

where $\rho_{k,l} = \frac{\mathbb{Cov}[f^{(k)}(Z), f^{(l)}(Z)]}{\sigma_k\sigma_l}$, the Pearson product-moment correlation coefficient between $f^{(k)}(Z)$ and $f^{(l)}(Z)$; σ_k is the standard deviation of $f^{(k)}(Z)$; δ_k is the fourth moment of

$f^{(k)}(Z)$; τ_k is the standard deviation of $g^{(k)}(Z) = (f^{(k)}(Z) - \mathbb{E}[f^{(k)}(Z)])^2$; and $q_{k,l} = \frac{\mathbb{C}\text{ov}[g^{(k)}(Z), g^{(l)}(Z)]}{\tau_k \tau_l}$.

Proof. Using $k_\beta = f^{(k)}(z_\beta)$ and $l_\gamma = f^{(l)}(z_\gamma)$ as shorthand, note that

$$\mathbb{C}\text{ov}[\hat{V}_m^{(k)}(Z), \hat{V}_n^{(l)}(Z)] = \frac{1}{4m(m-1)n(n-1)} \sum_{a=1}^{m} \sum_{b=1}^{m} \sum_{c=1}^{n} \sum_{d=1}^{n} \mathbb{C}\text{ov}[(k_a - k_b)^2, (l_c - l_d)^2].$$

Let $\chi_{abcd} = \mathbb{C}\text{ov}[(k_a - k_b)^2, (l_c - l_d)^2]$. If $\{a,b\} \cap \{c,d\} = \emptyset$ or if $a = b$ or $c = d$, then $\chi_{abcd} = 0$. Otherwise, if $\{a,b\} = \{c,d\}$, then $\chi_{abcd} = 2q_{k,l}\tau_k\tau_l + 4\rho_{k,l}^2\sigma_k^2\sigma_l^2$. There are $2n(n-1)$ such terms. Otherwise, when $|\{a,b\} \cap \{c,d\}| = 1$, $\chi_{abcd} = q_{k,l}\tau_k\tau_l$. There are $4n(n-1)(m-2)$ such terms, so

$$\mathbb{C}\text{ov}[\hat{V}_m^{(k)}(Z), \hat{V}_n^{(l)}(Z)] = \frac{2n(n-1)(2q_{k,l}\tau_k\tau_l + 4\rho_{k,l}^2\sigma_k^2\sigma_l^2) + 4n(n-1)(m-2)q_{k,l}\tau_k\tau_l}{4m(m-1)n(n-1)}$$

(15)
$$= \frac{1}{m}\left(q_{k,l}\tau_k\tau_l + \frac{2}{m-1}\rho_{k,l}^2\sigma_k^2\sigma_l^2\right).$$

When $k = l$, note that (15) can be rewritten as $\frac{1}{m}(q_{k,l}\tau_k\tau_l + \rho_{k,l}^2\sigma_k^2\sigma_l^2 - \frac{(m-3)}{m-1}\rho_{k,l}^2\sigma_k^2\sigma_l^2)$, $\rho_{k,k} = q_{k,k} = 1$, and $\tau_k^2 + \sigma_k^4 = \delta_k$. ∎

We can now make a statement about the quality of the MFMC estimator.

Theorem 3.3. *The variance of the MFMC variance estimator* (13) *is given by*

(16)

$$\mathbb{V}\text{ar}[\hat{V}_{\text{mf}}(Z)] = \frac{1}{m_1}\left(\delta_1 - \frac{m_1-3}{m_1-1}\sigma_1^4\right) + \sum_{k=2}^{K}\alpha_k^2\left(\frac{1}{m_{k-1}}\left(\delta_k - \frac{m_{k-1}-3}{m_{k-1}-1}\sigma_k^4\right) - \frac{1}{m_k}\left(\delta_k - \frac{m_k-3}{m_k-1}\sigma_k^4\right)\right)$$

$$+ 2\sum_{k=2}^{K}\alpha_k\left(\frac{1}{m_k}\left(q_{1k}\tau_1\tau_k + \frac{2}{m_k-1}\rho_{1k}^2\sigma_1^2\sigma_k^2\right) - \frac{1}{m_{k-1}}\left(q_{1k}\tau_1\tau_k + \frac{2}{m_{k-1}-1}\rho_{1k}^2\sigma_1^2\sigma_k^2\right)\right).$$

Proof. The variance of a sum of random variables is the sum of their covariances:

$$\mathbb{V}\text{ar}[\hat{V}_{\text{mf}}(Z)] = \mathbb{V}\text{ar}[\hat{V}_{m_1}^{(1)}] + \sum_{k=2}^{K}\alpha_k^2\left(\mathbb{V}\text{ar}[\hat{V}_{m_k}^{(k)}] + \mathbb{V}\text{ar}[\hat{V}_{m_{k-1}}^{(k)}]\right)$$

$$+ 2\sum_{k=2}^{K}\alpha_k\left(\mathbb{C}\text{ov}[\hat{V}_{m_1}^{(1)}, \hat{V}_{m_k}^{(k)}] - \mathbb{C}\text{ov}[\hat{V}_{m_1}^{(1)}, \hat{V}_{m_{k-1}}^{(k)}]\right)$$

(♯)
$$+ 2\sum_{k=2}^{K}\alpha_k \sum_{j=k+1}^{K}\alpha_j\left(\mathbb{C}\text{ov}[\hat{V}_{m_k}^{(k)}, \hat{V}_{m_j}^{(j)}] - \mathbb{C}\text{ov}[\hat{V}_{m_k}^{(k)}, \hat{V}_{m_{j-1}}^{(j)}]\right)$$

(♭)
$$- 2\sum_{k=2}^{K}\alpha_k \sum_{j=k+1}^{K}\alpha_j\left(\mathbb{C}\text{ov}[\hat{V}_{m_{k-1}}^{(k)}, \hat{V}_{m_j}^{(j)}] - \mathbb{C}\text{ov}[\hat{V}_{m_{k-1}}^{(k)}, \hat{V}_{m_{j-1}}^{(j)}]\right)$$

$$- 2\sum_{k=2}^{K}\alpha_k^2\mathbb{C}\text{ov}[\hat{V}_{m_k}^{(k)}, \hat{V}_{m_{k-1}}^{(k)}].$$

Using the covariances from Lemma 3.2, since $m_1 \leq \cdots \leq m_K$, the covariance terms in ♯ and ♭ will cancel, and Theorem 3.3 follows. ∎

3.2. Multifidelity sensitivity index estimation. We draw a second set of m_K realizations of Z, denoted $z_1', \ldots, z_{m_K}' \in \mathcal{Z}$. Let $y_i^{(j)}$ be defined as in subsection 2.2; i.e., $y_i^{(j)}$ is the ith realization of this second set, z_i', whose jth component has been replaced by the jth component of z_i, the ith input realization in the original set. For each j, the set $\{y_i^{(j)} : i = 1, \ldots, m_K\}$ is used to estimate the sensitivity index corresponding to the jth input variable.

Let $\hat{V}_{j,n}^{(k)}$ and $\hat{T}_{j,n}^{(k)}$ denote the estimators of V_j and T_j given by (10) and (12), respectively, evaluated using model $f^{(k)}$ at the first n pairs $(z, y^{(j)})$. We now introduce our multifidelity sensitivity index estimators.

Theorem 3.4. *Using the Owen estimators for $\hat{V}_{j,n}^{(k)}$ and $\hat{T}_{j,n}^{(k)}$ given by (10) and (12), the multifidelity estimators for V_j and T_j given by*

$$(17) \qquad \hat{V}_{j,\mathrm{mf}} = \hat{V}_{j,m_1}^{(1)} + \sum_{k=2}^{K} \alpha_k \left(\hat{V}_{j,m_k}^{(k)} - \hat{V}_{j,m_{k-1}}^{(k)} \right)$$

and

$$(18) \qquad \hat{T}_{j,\mathrm{mf}} = \hat{T}_{j,m_1}^{(1)} + \sum_{k=2}^{K} \alpha_k \left(\hat{T}_{j,m_k}^{(k)} - \hat{T}_{j,m_{k-1}}^{(k)} \right)$$

are unbiased estimators of V_j and T_j, where $\alpha_2, \ldots, \alpha_K$ are control variate coefficients.

Since (10) and (12) are unbiased [36], the proof is analogous to that of Proposition 3.1. We can then evaluate $\hat{s}_{j,\mathrm{mf}} = \hat{V}_{j,\mathrm{mf}}/\hat{V}_{\mathrm{mf}}$ and $\hat{s}_{j,\mathrm{mf}}^t = \hat{T}_{j,\mathrm{mf}}/\hat{V}_{\mathrm{mf}}$. These ratios of estimators are biased estimators for the sensitivity indices s_j and s_j^t. However, since $\hat{V}_{j,\mathrm{mf}}$, $\hat{T}_{j,\mathrm{mf}}$, and $\hat{V}_{\mathrm{mf}}$ are all unbiased estimators, our sensitivity index estimator is consistent with the best practices in Monte Carlo Sobol' index estimation [36, 43].

We note that the Saltelli estimators could also be used within (17) and (18) to create a "Saltelli-based" multifidelity estimator. Given the popularity of the Saltelli estimators, we present results for both the Owen-based and the Saltelli-based formulations in sections 4 and 5. However, since the expectation of the multifidelity estimator is the expectation of $\hat{V}_{j,m_1}^{(1)}$ (resp., $\hat{T}_{j,m_1}^{(1)}$), the $\mathcal{O}(1/n)$ bias of the Saltelli estimators will be preserved in a Saltelli-based multifidelity formulation and may in fact be exacerbated by the fact that m_1 is ideally a small number.

3.3. Model management. Let w_k, $k = 1, \ldots, K$ denote the time it takes to evaluate $f^{(k)}$ once, and let $p \in \mathbb{R}_+$ be our computational budget. We are interested in determining the coefficients α_i and the numbers of model evaluations $\mathbf{m}$ so as to efficiently use the computational time available to us. In [38], analytical α_k and m_k assignments that minimize the MSE of the MFMC mean estimate given a fixed computational budget are presented. This result is restated in Theorem 3.5.

Theorem 3.5. *If the K models $f^{(1)}, \ldots, f^{(K)}$ satisfy $|\rho_{1,1}| > \cdots > |\rho_{1,K}|$ and have costs satisfying*

$$\frac{w_{k-1}}{w_k} > \frac{\rho_{1,k-1}^2 - \rho_{1,k}^2}{\rho_{1,k}^2 - \rho_{1,k+1}^2},$$

for $k = 2, \ldots, K$, and the components of $\mathbf{r}^* = [r_1^*, \ldots, r_K^*]^T$ are given by

$$r_k^* = \sqrt{\frac{w_1(\rho_{1,k}^2 - \rho_{1,k+1}^2)}{w_k(1 - \rho_{1,2}^2)}},$$

then, given a maximum computational budget p, the assignments $\alpha_k^* = \frac{\rho_{1,k}\sigma_1}{\sigma_k}$ and $m_1^* = \frac{p}{\mathbf{w}^T\mathbf{r}^*}$, $m_k^* = m_1^* r_k^*$ for $k = 2, \ldots, K$ minimize the MSE of the multifidelity mean estimator given by

$$\tag{19} \hat{E}^{MF} = \hat{E}_{m_1}^{(1)} + \sum_{k=2}^{K} \alpha_k \left(\hat{E}_{m_k}^{(k)} - \hat{E}_{m_{k-1}}^{(k)} \right),$$

where $\hat{E}_{m_k}^{(k)}$ is the sample mean computed using model k and the first m_k samples in the multifidelity approach.

For variance estimation, we formulate an optimization problem to minimize the MSE of the MFMC variance estimate:

$$\tag{20a} \min_{\alpha_2, \ldots, \alpha_K, m_1, \ldots, m_K} \mathbb{V}\mathrm{ar}[\hat{V}_{\mathrm{mf}}]$$

$$\tag{20b} \text{s.t. } 0 < m_1 \leq m_2 \leq \cdots \leq m_K \text{ and } \sum_{k=1}^{K} w_k m_k \leq p.$$

Solving the nonlinear optimization problem (20) yields optimal α_i and m_i assignments. In practice, the model statistics $(\rho_{1,k}, \sigma_k, \delta_k, q_{1,k}, \tau_k)$ which enter into the objective function (16) are unknown and must be estimated, making (20) an optimization under uncertainty. One way to treat this is to estimate these model statistics in a pilot run with a small number of samples. However, the resultant model allocation may be sensitive to variation in these estimates since the objective function (20a) has fourth-order dependencies on these statistics. When estimates for Sobol' indices are also desired, in principle a similar optimization problem could be formulated, but the difficulties resulting from unknown model statistics are compounded both by the fact that statistics would need to be estimated for individual terms of the ANOVA decomposition (1) and by the fact that the optimization becomes multiobjective. Finding a different optimal allocation for each sensitivity index is likely to be sensitive to statistic estimates and therefore impractical.

In contrast, the Theorem 3.5 allocation depends only on $\rho_{1,k}$ and σ_k, and the dependencies are at most second-order. Additionally, the work [38] has demonstrated that this allocation is insensitive to estimates of unknown model statistics. In application, mean estimates are often desired in addition to variance and sensitivity estimates. It is thus both more practical and more robust to use the same mean-optimal Theorem 3.5 allocation to estimate the variance and all sensitivity indices. Because each Monte Carlo sample for sensitivity index estimation requires $(d + 2)$ function evaluations (of which two evaluations are independent and may be used for mean and variance estimation), we use Theorem 3.5 with an effective budget $p_{\mathrm{eff}} = p/(d + 2)$. This effective budget is then distributed across the available models, and the same set of samples is used to estimate the mean, variance, and sensitivity indices.

We will show in section 4 that the reduction in mean-squared error (MSE) achieved by using this heuristic allocation is comparable to that obtained by solving (20). Our recommendation for practice is therefore to use the Theorem 3.5 heuristic allocation for the estimation of variance and sensitivity indices.

Remark. We have noted that our proposed framework can accommodate surrogate models of any type. For some models, such as polynomial chaos expansions and Gaussian processes, the variances V_j (5) and T_j (6) can be analytically determined. If such a model were the Kth (lowest-fidelity) model, we could take advantage of this by using the analytical values for $\hat{V}_{m_K}^{(K)}$, $\hat{V}_{j,m_K}^{(K)}$, and $\hat{T}_{j,m_K}^{(K)}$ while still sampling the model for the estimates $\hat{V}_{m_{K-1}}^{(K)}$, $\hat{V}_{j,m_{K-1}}^{(K)}$, and $\hat{T}_{j,m_{K-1}}^{(K)}$. This would free some portion of the budget to allow additional higher-fidelity evaluations.

4. Analytical example. We first demonstrate our method on an analytical example for which model statistics are known. This allows us to validate the theory developed in subsection 3.1 and to compare the two suggested model management approaches for multifidelity variance estimation and sensitivity analysis.

4.1. Ishigami function and models. The Ishigami function was first introduced in [21] and has been frequently used to test methods for sensitivity analysis and uncertainty quantification [18, 42, 48]. The function is given by

$$(21) \qquad f(Z) = \sin Z_1 + a \sin^2 Z_2 + b Z_3^4 \sin Z_1, \quad Z_i \sim \mathcal{U}(-\pi, \pi)$$

and has ANOVA HDMR decomposition $f(Z) = f_0 + f_1(Z_1) + f_2(Z_2) + f_{13}(Z_1, Z_3)$ with

$$f_0 = a/2, \qquad f_1(Z_1) = \left(1 + b\frac{\pi^4}{5}\right) \sin Z_1,$$

$$f_2(Z_2) = a \sin^2 Z_2 - a/2, \text{ and } f_{13}(Z_1, Z_3) = b \sin Z_1 \left(Z_3^4 - \frac{\pi^4}{5}\right).$$

The variance is $\mathbb{V}\text{ar}[f(Z)] = \frac{1}{2} + \frac{a^2}{8} + \frac{\pi^4 b}{5} + \frac{\pi^8 b^2}{18}$, and the component variances are $V_1 = \frac{1}{2}(1 + b\frac{\pi^4}{5})^2$, $V_2 = \frac{a^2}{8}$, $V_{13} = \pi^8 b^2(\frac{1}{18} - \frac{1}{50})$. We set the constants $a = 5$ and $b = 0.1$ as in [1, 42], yielding $\mathbb{V}\text{ar}[f(Z)] \approx 10.845$ and sensitivities given in Table 1.

To investigate the performance of our proposed multifidelity estimation approach, we treat the Ishigami function (21) as the high-fidelity model and use the correlated functions given in Table 2 as low-fidelity models. To apply our model management strategy, we assign artificial computational costs w_k to each of these functions, so that our model hierarchy satisfies the assumptions of Theorem 3.5. In this case, the exact correlation coefficients and standard deviations are known. The models, weights, and model statistics are tabulated in Table 2.

Table 1

Main and total effect sensitivity indices for Ishigami function (21) with constants $a = 5$, $b = 0.1$.

	Z_1	Z_2	Z_3
Main effect s_i^m	0.401	0.288	0
Total effect s_i^t	0.712	0.288	0.311

Table 2

Model functions, statistics, and weights used for numerical tests on the Ishigami function, $a = 5$, $b = 0.1$.

Model	μ_k	σ_k	ρ_{1k}	τ_k	q_{1k}	δ_k	w_k
$f^{(1)} = \sin Z_1 + a \sin^2 Z_2 + b Z_3^4 \sin Z_1$	2.5	3.29	1	22.2	1	492	1
$f^{(2)} = \sin Z_1 + 0.95a \sin^2 Z_2 + b Z_3^4 \sin Z_1$	2.375	3.25	0.9997	19.1	0.9997	475	0.05
$f^{(3)} = \sin Z_1 + 0.6a \sin^2 Z_2 + 9b Z_3^2 \sin Z_1$	1.5	3.53	0.9465	23.0	0.9442	528	0.001

4.2. Results for Ishigami function. We use the models in Table 2 in our multifidelity approach to estimate the mean, variance, and sensitivity indices of the Ishigami function ($f^{(1)}$) using computational budgets ranging from 200 to 20000. Multifidelity estimates are computed using two approaches to model management: a heuristic multifidelity approach which uses the Theorem 3.5 allocation and effective budget $p_{\text{eff}} = p/(d+2)$ and the variance-optimal approach obtained by numerically solving the optimization problem (20) using p_{eff}.

We compare the two multifidelity approaches to each other as well as to vanilla Monte Carlo estimation for a fixed computational cost. The m_k and α_k assignments yielded by these two approaches are tabulated in Table 3 with the analytically predicted estimator MSE. The number of function evaluations allocated to each model is very similar in both multifidelity approaches, and the resultant reduction in variance is of similar magnitude, so our recommendation to use the mean-optimal allocation given by Theorem 3.5 is justified. We thus present only results for the mean-optimal model management approach in Figure 1. For computational budgets of 200, 2000, and 20000, 100 replicates of the estimators are computed, and the replicate sample variance is evaluated. The dashed lines in Figures 1 show the MSE predicted by our analysis (see (16)). We note good agreement between the predicted MSE and the replicate sample variance.

Our multifidelity approach has the same convergence rate as Monte Carlo, and the MSE of the multifidelity variance estimator is approximately 50 times lower than that of the Monte Carlo estimator with the same cost. For a fixed convergence level, this translates to a $50\times$ speedup relative to Monte Carlo for variance estimation. Thus, by assigning the lower-fidelity models most of the work, we are able to achieve a variance estimator MSE of approximately 0.1 with a computational budget of 200 compared to the budget of 10000 that would be required to achieve the same level of convergence using Monte Carlo.

Table 3

Number of samples per model and weights for a computational budget of $p = 200$, $p_{\text{eff}} = 40$. For variance and mean estimation, the number of function evaluations per model is $2m_k$ because two of the $d+2$ evaluations per sample needed for sensitivity estimation are independent. Note the similarity of the multifidelity allocations optimized for mean and variance estimation and the small difference in the resultant variance estimator MSE.

|	Monte Carlo	MF mean-optimal		MF variance-optimal	
	m_k	m_k	α_k	m_k	α_k
$f^{(1)}$	20	7	1	8	1
$f^{(2)}$	–	461	1.013	447	1.015
$f^{(3)}$	–	9589	0.8825	9070	0.9455
MSE	4.71	0.080		0.078	

Variance estimation convergence
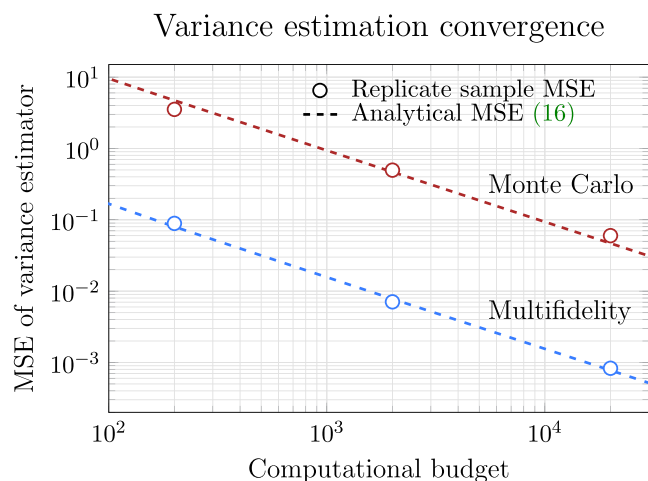
Figure 1. *Convergence of multifidelity variance estimates. One hundred estimator replicates are computed at $p = 200, 2000, 20000$. The multifidelity approaches optimized for mean and variance estimation perform essentially identically, so only the mean-optimal approach is shown (see Table 3).*
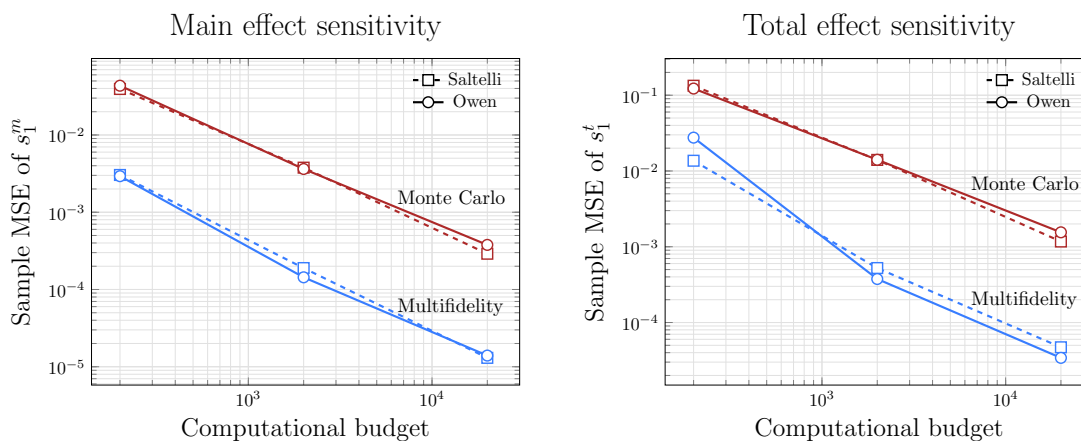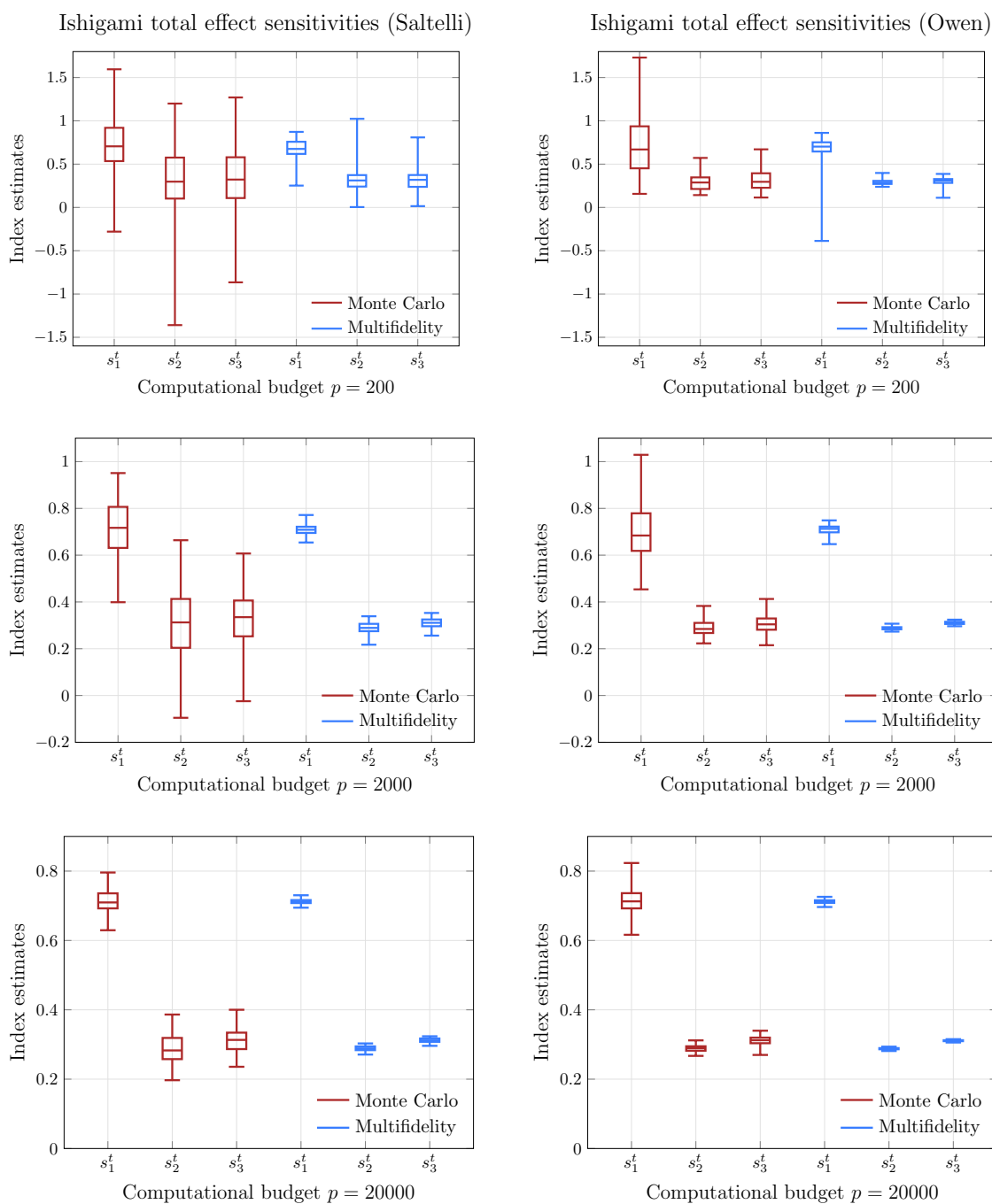

Figure 2. *Convergence comparison of multifidelity vs. Monte Carlo sensitivity index estimators for the first parameter of the Ishigami function. One hundred replicates are computed with computational budgets $p = 200, 2000, 20000$, and the replicate sample MSE is shown. Main and total effect sensitivities are shown on the left and right, respectively.*

Convergence of the sensitivity estimators in just the first parameter is shown in Figure 2. In this plot, we can see that the multifidelity approach is able to reduce the estimator MSE by an order of magnitude, corresponding to speedups of just under a factor of 10. For this example, the performance of the Saltelli and Owen estimators is similar. Figures 3 and 4 show the results of Monte Carlo and multifidelity global sensitivity analysis. Box plots for 100 replicates are shown, and estimators using both the Saltelli and the Owen estimators for the index numerators are shown. We note that the Owen total index estimator converges on small sensitivity indices faster than the the Saltelli estimator. In all cases, the multifidelity estimator has a reduced variance relative to its Monte Carlo counterpart.
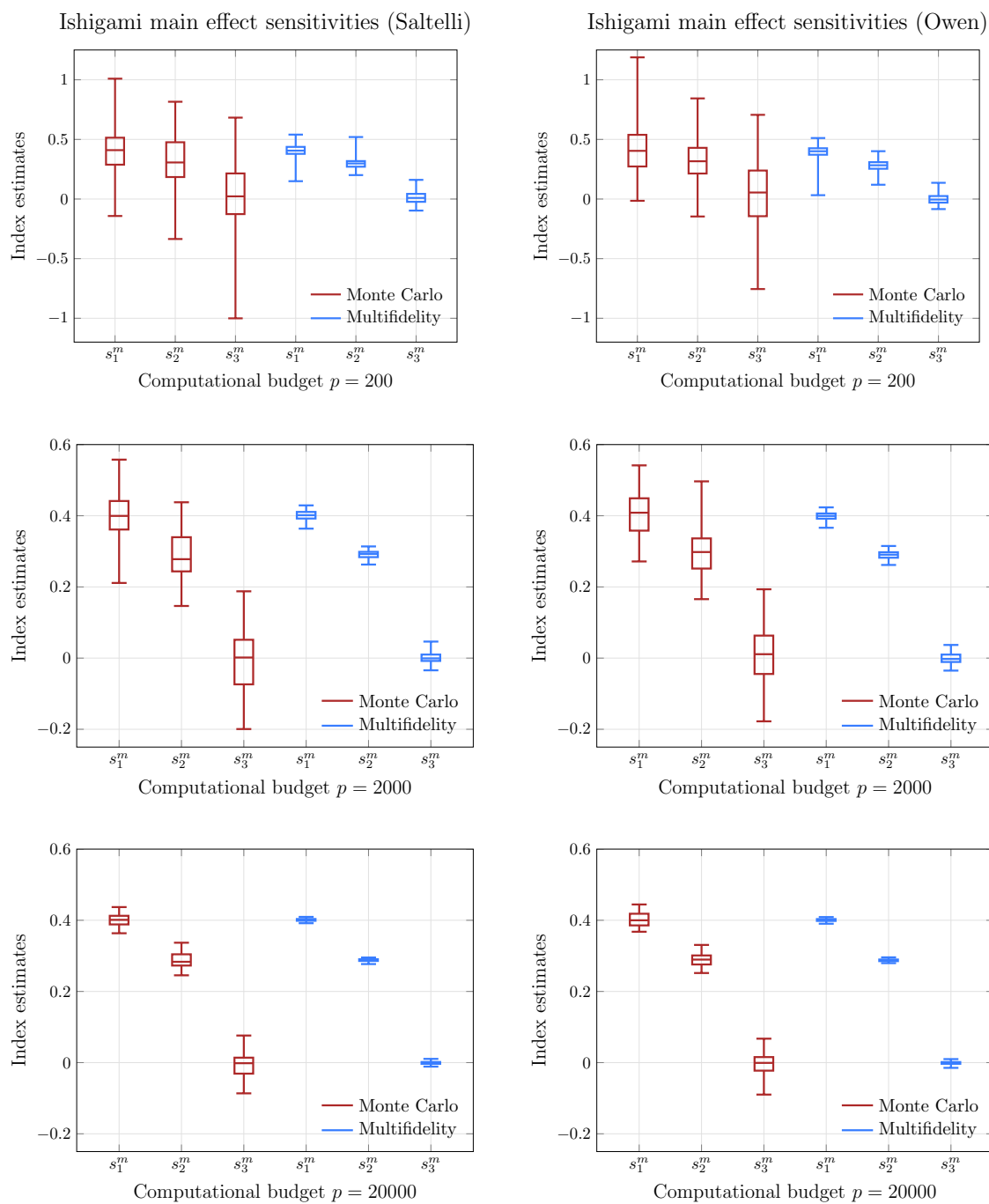
Figure 3. *Comparison of multifidelity vs. Monte Carlo estimates of main effect sensitivities for the Ishigami function* (21) *with computational budgets $p = 200, 2000, 20000$. Box plots are of 100 estimator replicates. Left and right plots use the Saltelli and Owen estimators, respectively. The multifidelity estimators achieve desired accuracy faster than the MC estimators, allowing definitive ranking of inputs with $p = 2000$, while Monte Carlo barely achieves this at $p = 20000$.*

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Figure 4. *Comparison of multifidelity vs. Monte Carlo estimates of total effect sensitivities for the Ishigami function* (21) *with computational budgets* $p = 200, 2000, 20000$. *Box plots are of 100 estimator replicates. Left and right plots use the Saltelli and Owen estimators, respectively. Note that the Owen estimators outperform the Saltelli estimators on small sensitivity indices.*

5. Numerical results. We now demonstrate our method on a 2D hydrogen combustion model with five parameters, detailed in [5] and summarized in subsection 5.1. The models used for the multifidelity approach are described in subsection 5.2, and results from numerical experiments are presented and discussed in subsection 5.3.

5.1. Convection-diffusion-reaction (CDR) problem. We consider a domain $\Omega \subset \mathbb{R}^2$ with boundary Γ which assumes a premixed flame at constant, uniform pressure with constant, divergence-free velocity field and equal, uniform molecular diffusivities for all species and temperatures. The dynamics of the system are described by a CDR equation,

$$(22) \qquad \frac{\partial \mathbf{x}}{\partial t} = \Delta \mathbf{x} - U \nabla \mathbf{x} + \mathbf{s}(\mathbf{x}, \mathbf{p}) \text{ in } \Omega,$$

subject to Dirichlet boundary conditions $\mathbf{x}|_{\Gamma_D} = \mathbf{x}_D$ on the left boundary of the domain and Neumann boundary conditions $\mathbf{x}_{\Gamma_N} = \mathbf{x}_N$ on all other boundaries (see Figure 5). We consider the steady problem, where our output of interest is the maximum temperature in the chamber. The thermochemical composition is given by $\mathbf{x}(\mathbf{p}, t) = [Y_F, Y_O, Y_P, T]^T \in \mathbb{R}^n$, where Y_F, Y_O, and Y_P are the mass fractions of the fuel, oxidizer, and product, respectively, and T is the temperature. The molecular diffusivity is κ, U is the velocity field, and $\mathbf{s}$ is the nonlinear reaction source term. The input parameter vector is given by $\mathbf{p} = [A, E, T_i, T_0, \phi]$, where A and E are parameters of the Arrhenius equation; T_i and T_0 are the Dirichlet temperatures on $\Gamma_{D,i}$ and $\Gamma_{D,0}$, respectively; and ϕ is the fuel:oxidizer ratio of the premixed inflow.

The reaction modeled is a one-step hydrogen combustion given by

$$2\mathrm{H}_2 + \mathrm{O}_2 \rightarrow 2\mathrm{H}_2\mathrm{O},$$
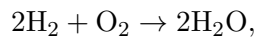
where hydrogen is the fuel, oxygen acts as the oxidizer, and water is the product. The source term is modeled as in [10]:

$$(23) \qquad s_i(\mathbf{x}, \mathbf{p}) = \nu_i \left(\frac{W_i}{\rho}\right) \left(\frac{\rho Y_F}{W_F}\right)^{\nu_F} \left(\frac{\rho Y_O}{W_O}\right)^{\nu_O} A \exp\left(-\frac{E}{RT}\right), \, i = F, O, P$$

$$(24) \qquad s_T(\mathbf{x}, \mathbf{p}) = s_P(\mathbf{x}, \mathbf{p})Q$$

where A is the pre-exponential factor of the Arrhenius equation, E is the activation energy, W_i is the molecular weight of species i, ρ is the density of the mixture, R is the universal gas
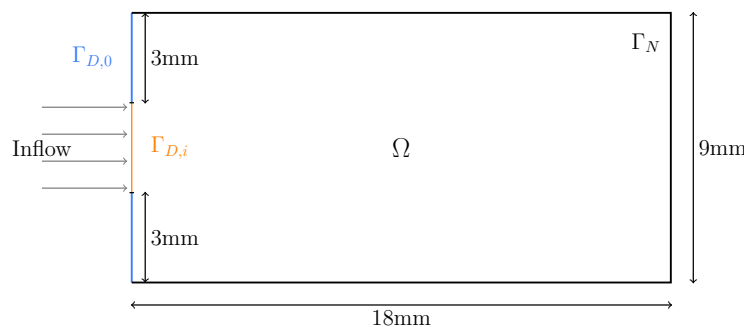

Figure 5. *Schematic of reacting flow domain*

constant, and Q is the heat of the reaction. We allow the parameters $\mathbf{p} = [A, E, T_i, T_0, \phi]$ to vary in the domain $\mathcal{D} = [5.5 \times 10^{11}, 1.5 \times 10^{12}] \times [1.5 \times 10^3, 9.5 \times 10^3] \times [200, 400] \times [850, 1000] \times [0.5, 1.5]$ and assume that A and E are log-uniformly distributed in their domains, while T_i, T_0, and ϕ are assumed to be uniformly distributed in their domains. The velocity field is assumed to be $U = (50, 0)\frac{\text{cm}}{\text{s}}$, and the diffusivities are $\kappa = 2.0\frac{\text{cm}^2}{\text{s}}$. The density is $\rho = 1.39 \times 10^{-3}\frac{\text{gr}}{\text{cm}^3}$. The molecular weights W_i are $2.016\frac{\text{gr}}{\text{mol}}$, $31.9\frac{\text{gr}}{\text{mol}}$, and $18\frac{\text{gr}}{\text{mol}}$ for H_2, O_2, and H_2O, respectively, and the heat of reaction is $Q = 9800\text{K}$, with universal gas constant $R = 8.314472\frac{\text{J}}{\text{mol}\cdot\text{K}}$.

5.2. CDR models. The high-fidelity model for the problem described in subsection 5.1 is a finite-difference solver which discretizes the spatial domain Ω into a 73×37 grid, resulting in 10804 degrees of freedom (the mass fractions of each of the three chemical species as well as the temperature at each grid point). A POD-DEIM reduced model [6] with 19 POD basis functions and 1 DEIM basis function is used as the low-fidelity model (see [5] for details of the model reduction approach applied to this reacting flow problem). This yields a correlation coefficient with the full model of approximately 0.95. Statistics for these models computed using 2.4 million samples are tabulated in Table 4.

5.3. CDR results. The models tabulated in Table 4 are used in our multifidelity approach to estimate the mean, variance, and sensitivity indices of the reacting flow problem using computational budgets ranging from 100 to 10000 minutes. Multifidelity estimates are computed using the mean-optimal allocation resulting from estimated model statistics and an effective computational budget $p_{\text{eff}} = p/(d+2)$, as above. For each multifidelity replicate, the statistics $\rho_{1,i}$ and σ_i are estimated using just 10 samples, and these rough estimates are used to compute the model allocation and weights for the multifidelity approach. We present and discuss results for the Owen estimators, which we recommend, and compare to results for the Saltelli estimators, which are widely used.

Figures 6 and 7 contain box plots of the estimator replicates at different computational budgets. We note that the multifidelity estimator has a reduced variance relative to the Monte

Table 4

*Model statistics for the high- and low-fidelity models for the reacting flow problem.*

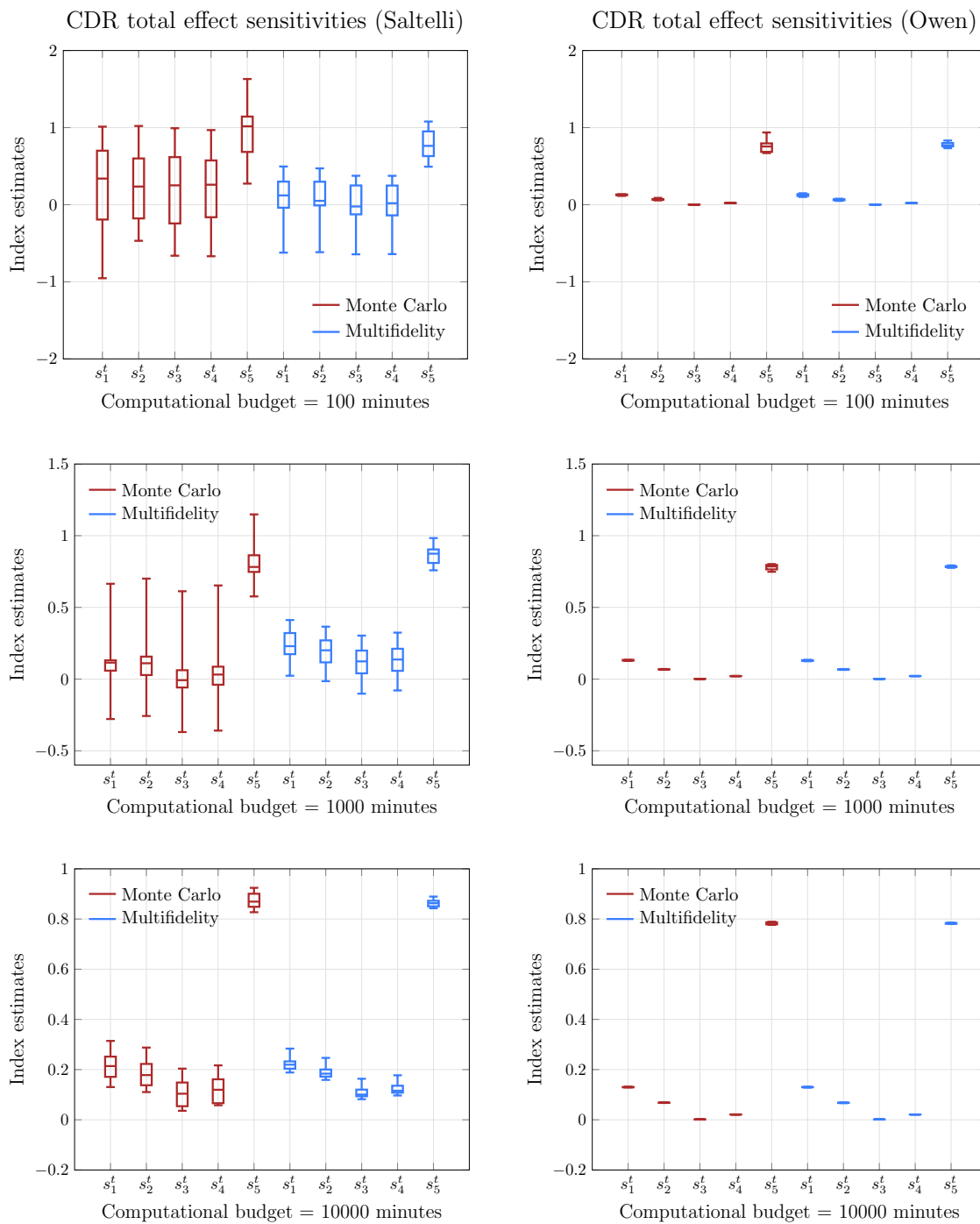| model		μ_i	σ_i	ρ_{1i}	w_i
High-fidelity (FD)	$f^{(1)}$	1406	276.1	1	1.94
Low-fidelity (POD-DEIM)	$f^{(2)}$	1349	356	0.95	6.2e-3

Table 5

Mean number of samples per model and weights for index estimator replicates computed with a budget of $p = 100$ minutes, $p_{\text{eff}} = 14.3$ minutes. For each replicate, the values of m_k and α_k are determined from estimates of ρ_k and σ_k arising from just 10 samples.

	Monte Carlo	MF mean-optimal	
	m_k	m_k	α_k
$f^{(1)}$	441	401	1
$f^{(2)}$	–	12811	0.667
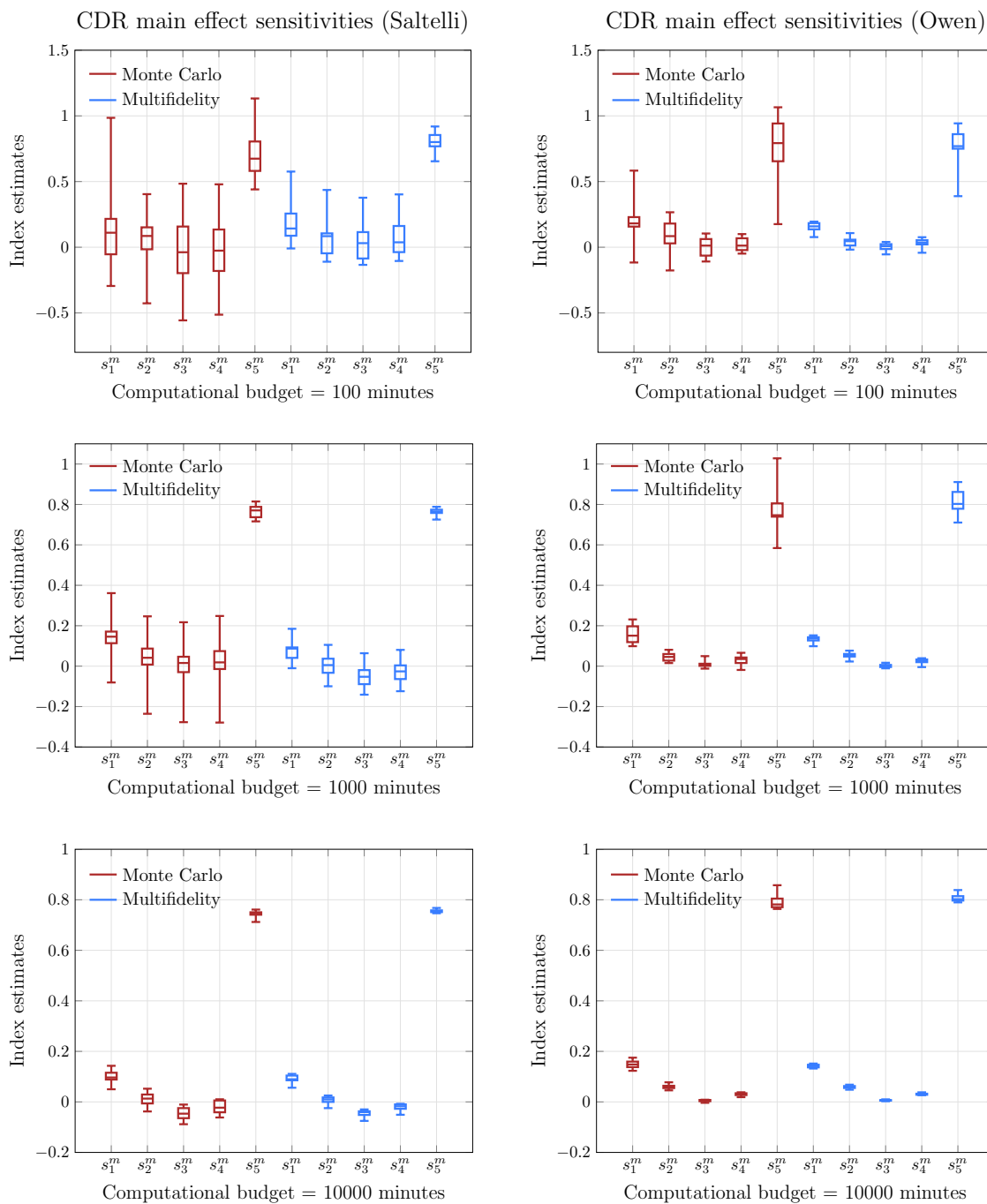
Figure 6. *Box plots of 100 main sensitivity index estimate replicates with vanilla Monte Carlo estimates in red and multifidelity estimates in blue. The multifidelity estimator outperforms the Monte Carlo estimator, and the Owen estimator outperforms the Saltelli estimator.*

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Figure 7. *Box plots of 100 total sensitivity index estimate replicates with vanilla Monte Carlo estimates in red and multifidelity estimates in blue. The Owen estimator significantly outperforms the Saltelli estimator. The multifidelity method outperforms a vanilla Monte Carlo approach for all Saltelli indices but only achieves efficiency gains relative to the Owen estimator in the s_5^t estimate.*

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Carlo estimator, even under the uncertainty of using very rough estimates for $\rho_{1,i}$ and σ_i. The exception to this are the Owen estimators for the small total sensitivity indices—in these cases, the Owen Monte Carlo estimator has a slightly smaller variance than that of the Owen multifidelity estimator. In this case, however, the true value of the sensitivity index is closer to zero, and the estimator variances are similar in magnitude. In all cases, the Owen estimators have smaller variances than the Saltelli estimators.

We now take a closer look at the results for main effect sensitivity indices Figure 6. We note that with a computational budget of 100 minutes, the Owen multifidelity approach can determine with certainty (i.e., no minimal overlap in box plot ranges) that the fifth input (ϕ) has the highest main effect sensitivity index and is able to effectively differentiate between all five sensitivity indices with a computational budget of 10000 minutes. Using standard Monte Carlo with the Owen estimators yields a higher variance which leads to a significantly impaired ability to rank inputs with a low computational budget. At higher computational budgets, however, the ability to rank inputs using the Owen estimators and standard Monte Carlo is comparable the multifidelity Owen approach. The multifidelity Saltelli estimators also have smaller variance than their Monte Carlo counterparts, but even at each computational budget tested, the Saltelli approaches have larger variance than their Owen counterparts, and the Saltelli estimators are not able to effectively rank the smaller sensitivity indices even at the highest computational budget. Convergence results for the main effect sensitivities for E and ϕ are shown in Figure 8. Convergence results for the total effect sensitivity estimates are shown in Figure 9. For the sensitivity indices close to zero, our multifidelity implementation performs worse than the vanilla Monte Carlo method, but we achieve gains similar to those achieved in the main effect indices for the estimate of the larger total index. This is also evident in Figure 7, where it is also clear that the Owen estimators significantly outperform their Saltelli counterparts. We note that larger gains can be achieved with a more accurate low-fidelity model, even for small sensitivity indices.

We plot the running mean of the estimator replicates with the replicate standard deviations for E and ϕ in Figures 10 and 11. These plots clearly show the biasedness of the Saltelli estimators—note that the running mean approaches the asymptote from above. Finally, in
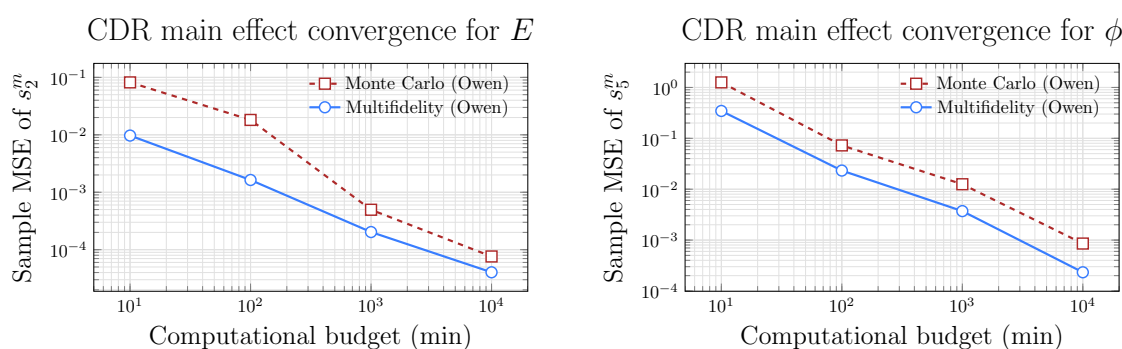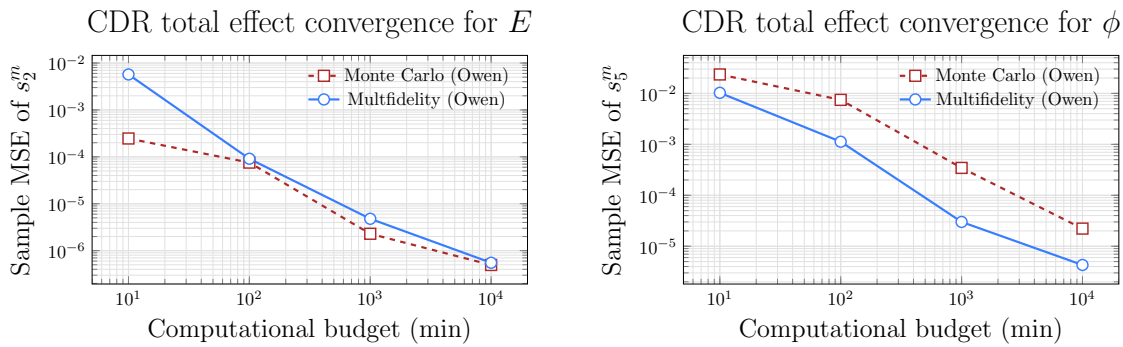

Figure 8. *Sample MSE of main sensitivity estimates using high-fidelity Monte Carlo and MFMC. Results for one small (for E) and one large sensitivity (for ϕ) are shown.*

Figure 9. *Sample MSE of total sensitivity estimates using high-fidelity Monte Carlo and MFMC. Results for one small (for E) and one large (for ϕ) sensitivity are shown; the Owen estimators are so efficient that the multifidelity approach does not achieve efficiency gains for small sensitivity indices.*
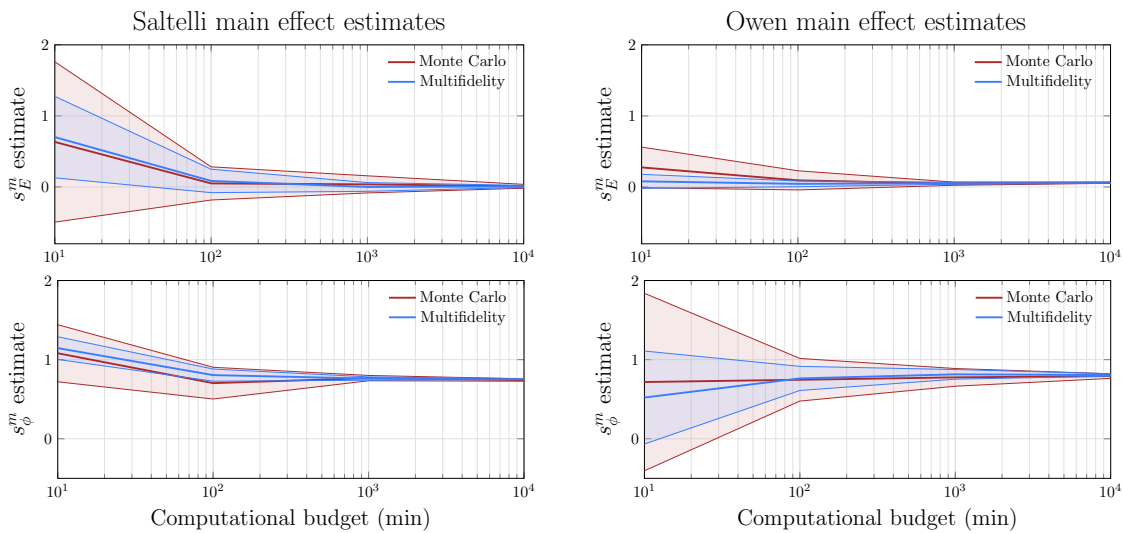

Figure 10. *Running mean of main effect sensitivity index estimator replicates with replicate standard deviation. The Saltelli estimator is biased, and its running mean approaches the asymptote from above, while the Owen estimators are unbiased.*

Figure 12, we show the root mean square error (RMSE) relative to the "true" sensitivity (estimated using 2.4 million samples) for the Owen estimators. The RMSE is shown for the high-fidelity Monte Carlo estimator, our multifidelity approach, and the low-fidelity Monte Carlo estimator. While using the low-fidelity model leads to estimators with small variance, the bias relative to the high-fidelity model can be the same order as the sensitivity index. Thus, even a low-fidelity model that exhibits fairly good correlation with the high-fidelity model may lead to incorrect estimates of sensitivity indices. This emphasizes the importance of our rigorous multifidelity formulation.
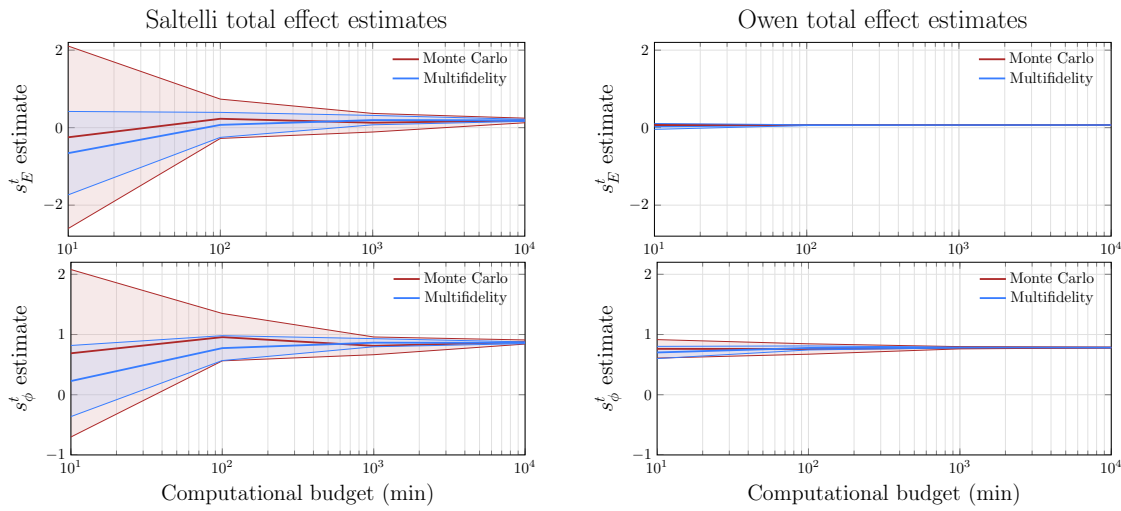
Figure 11. *Running mean of total effect sensitivity index estimator replicates with replicate standard deviation. The Owen total effect estimators significantly outperform the Saltelli estimators for both large and small sensitivity indices.*
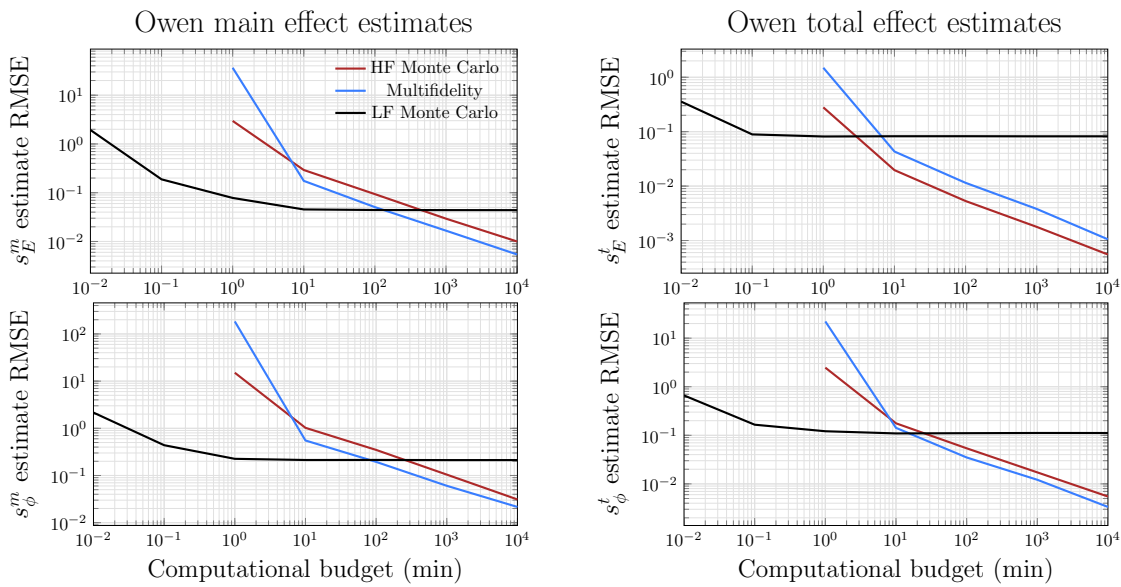
Figure 12. *RMSE of Owen-based Sobol' index estimates computed with (red) high-fidelity model only, (blue) multifidelity approach, and (black) low-fidelity model only. RMSE is calculated relative to "truth" value estimated using 2.4 million high-fidelity samples (corresponds to a computational budget of approximately 50 days). The multifidelity approach converges to the true value, while using the low-fidelity model alone leads to a bias that is of the same order as the sensitivity index despite having a 0.95 correlation with the high-fidelity model.*

6. Conclusions. We have introduced new multifidelity estimators for output variance as well as the Sobol' main and total effect indices. These multifidelity formulations use evaluations of low-fidelity models to reduce estimator variance while using the high-fidelity to retain accuracy guarantees consistent with current best practices in Sobol' index estimation. Notably, the accuracy guarantees of our formulation require the use of the unbiased Sobol' numerator estimators proposed by Owen rather than the more commonly used Saltelli estimators. We derived an expression for the variance of our multifidelity variance estimator and formulated an optimization problem to obtain an optimal model management strategy given limited computational resources. This optimization problem can be efficiently solved, but it is parametrized by model statistics which in general are unknown and must be estimated. In practice, because we often desire a mean estimate in addition to variance and sensitivity index estimates, we recommend using the mean-optimal model management strategy (Theorem 3.5) developed in [38] as a heuristic for variance and sensitivity estimation as well: This approach is simple and fairly insensitive to variation in the estimates of model statistics and also performs nearly as well as the variance-optimal allocation in the analytical example examined in section 4 and is thus a reasonable general strategy.

The results for the analytical and numerical examples in sections 4 and 5 demonstrate the efficacy of the proposed multifidelity framework for reducing the variance of variance and Sobol' index estimators. We use low-fidelity models with ≈ 0.95 correlation with the high-fidelity model to demonstrate $2\times$ to $10\times$ variance reductions corresponding to $3\times$ to $10\times$ speedups. We note that larger gains may be achieved with more highly correlated low-fidelity models.

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