

A sampling-based approach to solve Sobol' Indices using variance deconvolution for arbitrary uncertainty distributions

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INTRODUCTION

Global sensitivity analysis (GSA) seeks to assess the relative contributions of various uncertainty sources to the uncertainty in one or more computation outputs. Such rank-ordering of contributions enables informed decisions such as down-selection of which uncertainty sources to further study and identification of where to invest additional effort in reducing the overall uncertainty. Perhaps the most common tool for GSA are Sobol' Indices (SI) [1]. Common approaches to computing SI include through the Saltelli sampling methods [2] and direct computation following the construction of a polynomial chaos surrogate model [3].

We seek to compute SI using a stochastic solver, here a Monte Carlo radiation transport (MC RT) solver, that describe the relative variance contributions from two different aleatoric uncertainty sources, which are sources for which the uncertainty is due to real random effects as opposed to epistemic uncertainty where the uncertainty is due to lack of knowledge. We examine a parametric aleatoric uncertainty source (e.g., an uncertain cross section value) and a non-parametric uncertainty source (e.g., stochastic media). Stochastic media (SM) are comprised of constituent materials that are modeled as being randomly mixed within the medium—except in special cases, they cannot be described by a distribution on an interval.

While the Saltelli sampling methods have been carefully optimized for application with deterministic solvers, their optimization does not consider selection of parameters that drive the statistical noise produced by stochastic solvers. Likewise, while surrogate-based approaches, such as use of a polynomial chaos expansion, can be efficient for uncertainty sources for which the probability basis function is known and well-behaved, they cannot be straightforwardly applied when one or more of the uncertainty sources cannot be easily characterized with a well-behaved probability basis. Therefore, we seek to develop efficient methods for computing SI in the presence of stochastic solver noise (e.g., MC RT) and non-parametric aleatoric uncertainty (e.g., SM) that are amenable to embedding within a stochastic solver.

In [4] and previous, related work, we proposed a variance deconvolution approach by which to remove stochastic solver noise from a numerically computed output variance driven by an aleatoric uncertainty source and thereby enable unbiased computation of aleatoric uncertainty when using a stochastic solver. We successfully applied an early version of this method to stochastic media transport problems [5] to enable characterization of the variance caused by the stochastic material mixing. In Ref. [6], we applied variance deconvolution to solve for SI in a transport problem with uniformly distributed uncertainty sources and demonstrated that the method was more efficient

than the Saltelli approach when using a stochastic solver for at least some cases. In recent work, we proposed a symbolic notation for describing the difference between parametric and non-parametric uncertainty sources and derived expressions to solve for conditional variance terms [7].

In this contribution, we propose a new, unbiased, sampling-based method for solving SI when using a stochastic solver via application of variance deconvolution that is applicable even when involving non-parametric aleatoric uncertainty sources. This approach is simpler than our previous iteration [6] for using variance deconvolution to solve for SI with stochastic solvers; incorporates our improved variance deconvolution estimator [4]; builds on our recently proposed notation and derivations for describing different types of aleatoric uncertainty sources [7]; and demonstrates not only computation of variance caused by a non-parametric uncertainty source [5], but also the ability to solve relative variance contributions of parametric and non-parametric uncertainty sources through SI. We numerically corroborate the method by proposing a new, attenuation-only transport problem involving stochastic material mixing and an uncertain cross section and deriving closed-form transport solutions. We use the same example problem to demonstrate the usefulness of the method for ranking the importance of uncertainty contributions. We leave as topics for future work the optimization of model parameter selection and efficiency comparison with other methods such as the Saltelli and surrogate-based approaches.

Whereas we present cross section uncertainty and stochastic media as, respectively, a parametric and a non-parametric uncertainty source, it is worth noting that the numerical model we present for each is actually parametric, that our method does not rely on the parametric property of either (but our closed-form solutions rely on both), and that these designations have been chosen primarily to be illustrative since stochastic media is often a non-parametric uncertainty source.

SI GENERATION

As we recently proposed [4, 7], let η denote statistical sampling of a stochastic solver, ω denote dependence on an aleatoric uncertainty source that we cannot—or choose to assume that we cannot—characterize with a known distribution on an interval, and let ξ represent an aleatoric uncertainty source that we can characterize with a known distribution on an interval. Without loss of generality, in this summary, η denotes sampling of a Monte Carlo radiation transport (MC RT) solver, ω denotes dependence on stochastic media (SM) configuration, and ξ denotes cross section uncertainty.

We seek to characterize a quantity of interest (QoI), in our problem transmittance through a slab, that is dependent on

the aleatoric uncertainty sources: $Q(\xi, \omega)$. The transmittance is the expectation of transmittance tallies, though, in practice, only a finite number (N_η) of particle histories can be simulated to approximate $Q(\xi, \omega)$:

$$Q(\xi, \omega) \stackrel{\text{def}}{=} \mathbb{E}_\eta[f(\xi, \omega, \eta)] \approx \tilde{Q}_{N_\eta}(\xi, \omega) \stackrel{\text{def}}{=} \frac{1}{N_\eta} \sum_{j=1}^{N_\eta} f(\xi, \omega, \eta^{(j)}), \quad (1)$$

where the tilde represents an approximation polluted with MC RT sampling noise and $f(\xi, \omega, \eta)$ is a function of a sample of the aleatoric uncertainty sources and the MC RT solver.

Similarly, the expectation of the QoI as a function of the cross section uncertainty is

$$\mathbb{P}_\xi(\xi) \stackrel{\text{def}}{=} \mathbb{E}_\omega[Q(\xi, \omega)] \approx \tilde{\mathbb{P}}_{N_\omega}^\xi(\xi) \stackrel{\text{def}}{=} \frac{1}{N_\omega} \sum_{k=1}^{N_\omega} \tilde{Q}_{N_\eta}(\xi, \omega^{(k)}), \quad (2)$$

where $\mathbb{P}_\xi(\xi)$ is the expectation of the QoI averaged over N_ω SM realizations for a value of the uncertain cross section and $\tilde{\mathbb{P}}_{N_\omega}^\xi(\xi)$ is an approximation of that quantity polluted by MC RT and SM sampling noise.

We recently solved for an expression for the variance due to the parametric uncertainty as a function of the expectation of the non-parametric uncertainty [7]:

$$\text{Var}_\xi[\mathbb{P}_\xi(\xi)] = \text{Var}_\xi[\tilde{\mathbb{P}}_{N_\omega}^\xi(\xi)] - \frac{\mathbb{E}_\xi[\text{Var}_\omega[\tilde{Q}_{N_\eta}(\xi, \omega)]]}{N_\omega}, \quad (3)$$

in which $\text{Var}_\xi[\tilde{\mathbb{P}}_{N_\omega}^\xi(\xi)]$ is a polluted estimate of $\text{Var}_\xi[\mathbb{P}_\xi(\xi)]$ computed using N_η particle histories on each of N_ω SM realizations and $\frac{1}{N_\omega} \mathbb{E}_\xi[\text{Var}_\omega[\tilde{Q}_{N_\eta}(\xi, \omega)]]$ is the average statistical pollution caused by MC RT histories and SM variability. While $\text{Var}_\xi[\mathbb{P}_\xi(\xi)]$ cannot be correctly computed by sampling with a finite number of N_η and N_ω , it is straightforward to compute a de-polluted (unbiased) estimator for the desired conditional variance by tallying the other two terms and finding the difference. We have called this process of deconvolving an easily computed, but polluted, variance into a noise term and the desired de-polluted variance “variance deconvolution.”

A minor conceptual step of recognizing that aleatoric variance can be comprised of both parametric and non-parametric contributions enables us to generalize another of our previously established applications of variance deconvolution [4] to solve for the total aleatoric variance while de-polluting from MC RT noise. This is expressed as

$$\text{Var}_{\xi, \omega}[Q(\xi, \omega)] = \text{Var}_{\xi, \omega}[\tilde{Q}_{N_\eta}(\xi, \omega)] - \mathbb{E}_{\xi, \omega}[\sigma_{RT, N_\eta}^2(\xi, \omega)], \quad (4)$$

where $\text{Var}_{\xi, \omega}[Q(\xi, \omega)]$ is the total aleatoric variance, $\text{Var}_{\xi, \omega}[\tilde{Q}_{N_\eta}(\xi, \omega)]$ is a polluted estimate of it when using N_η MC RT histories, and $\sigma_{RT, N_\eta}^2(\xi, \omega)$ is the 1-sigma statistical uncertainty (aka, standard error of the mean) on an estimate of $Q(\xi, \omega)$ when using N_η histories: $\sigma_{RT, N_\eta}^2(\xi, \omega) \stackrel{\text{def}}{=} \frac{1}{N_\eta} \text{Var}_\eta[f(\xi, \omega, \eta)]$.

We make the new observation that Eqs. (3) and (4) enable unbiased (de-polluted) computation of the Sobol main effect for the parametric contribution to the aleatoric uncertainty:

$$S_\xi = \frac{\text{Var}_\xi[\mathbb{P}_\xi(\xi)]}{\text{Var}_{\xi, \omega}[Q(\xi, \omega)]}. \quad (5)$$

Furthermore, we contribute the new observation that it is mathematically valid to switch all occurrences of ξ with ω and all occurrences of ω with ξ in Eqs. (1)-(5). The result of this observation is that we not only have the means to compute unbiased estimates of the Sobol main effect for the parametric contribution to the total aleatoric variance in the presence of MC RT noise, but, through the law of total variance, we can compute the Sobol main and total effects for both the parametric and non-parametric contributions:

$$S_\xi = \frac{\text{Var}_\xi[\mathbb{P}_\xi(\xi)]}{\text{Var}_{\xi, \omega}[Q(\xi, \omega)]} = 1 - \frac{\mathbb{E}_\xi[\text{Var}_\omega[Q(\xi, \omega)]]}{\text{Var}_{\xi, \omega}[Q(\xi, \omega)]} = 1 - S_{T_\omega} \quad (6a)$$

$$S_\omega = \frac{\text{Var}_\omega[\mathbb{P}_\omega(\omega)]}{\text{Var}_{\xi, \omega}[Q(\xi, \omega)]} = 1 - \frac{\mathbb{E}_\omega[\text{Var}_\xi[Q(\xi, \omega)]]}{\text{Var}_{\xi, \omega}[Q(\xi, \omega)]} = 1 - S_{T_\xi} \quad (6b)$$

A caveat is that, to make practical use of this approach to solve for $\text{Var}_\omega[\mathbb{P}_\omega(\omega)]$, it must be known how to hold ω constant while resampling ξ . For example, depending on the SM model used, it may not be known how to maintain the same SM realization while resampling a ξ parameter such as the average chord length of a constituent material.

Though we do not demonstrate here, this procedure can be used to solve for the Sobol main and total effects for any subset of parametric and non-parametric contributions to the total aleatoric variance.

CLOSED-FORM SOLUTIONS

To verify the accuracy of the method described in the previous section, we propose a simple test problem and derive closed-form solutions to various terms of interest. For brevity, we show only key steps in deriving closed-form solutions.

The test problem geometry is a one-dimensional slab with three regions of thicknesses r_1, r_2 and r_3 and a mono-energetic beam source incident on the first region. The slab contains three absorption-only materials with total cross sections $\Sigma_{t,1}, \Sigma_{t,2}$ and $\Sigma_{t,3}$. Region 1 contains N_{tot} subcells of equal width $\Delta x = r_1/N_{tot}$, each of which can contain either Material 1 with probability p_1 or Material 2 with probability $(1 - p_1)$. The number of cells in Region 1 containing Material 1 in a realization of this stochastic medium can be represented as a sample from the binomial probability density function (PDF), $N_1(\omega) \sim \mathcal{B}(N_{tot}, p_1)$, where ω represents the non-parametric aleatoric uncertainty of N_1 . Region 2 simply contains Material 2. Region 3 contains Material 3, whose cross section $\Sigma_{t,3}(\xi)$ is a function of parametric aleatoric uncertainty $\xi \sim \mathcal{U}(-1, 1)$.

The problem quantity of interest, transmittance T through the slab, is a function of the optical thickness τ of each region:

$$\begin{aligned} \tau_1 &= N_1(\omega) \Delta x \Sigma_{t,1} + (N_{tot} - N_1(\omega)) \Delta x \Sigma_{t,2} \\ &= N_1(\omega) \Delta x (\Sigma_{t,1} - \Sigma_{t,2}) + r_1 \Sigma_{t,2} \end{aligned} \quad (7)$$

$$\tau_2 = r_2 \Sigma_{t,2} \quad (8)$$

$$\begin{aligned} \tau_3 &= r_3 \Sigma_{t,3} = r_3 (\Sigma_{t,3}^0 + \Sigma_{t,3}^\Delta \xi) \\ &= r_3 \Sigma_{t,3}^0 + r_3 \Sigma_{t,3}^\Delta \xi \end{aligned} \quad (9)$$

where $\Sigma_{t,3}(\xi) = \Sigma_{t,3}^0 + \Sigma_{t,3}^\Delta \xi$, $\Sigma_{t,3}^0$ is the mean total cross section, and $\Sigma_{t,3}^\Delta$ the deviation from the mean. The transmittance is

therefore a function of both the non-parametric and parametric aleatoric uncertainties,

$$T = T(\xi, \omega) = k \exp(-k_1 N_1(\omega)) \exp(-k_3 \xi) \quad (10)$$

where

$$k = \exp[-r_1 \Sigma_{t,2} - r_2 \Sigma_{t,2} - r_3 \Sigma_{t,3}^0] \quad (11a)$$

$$k_1 = \Delta x (\Sigma_{t,1} - \Sigma_{t,2}) \quad (11b)$$

$$k_3 = -r_3 \Sigma_{t,3}^\Delta \quad (11c)$$

The p^{th} -order raw moment of $T(\xi, \omega)$ is

$$\begin{aligned} \mathbb{E}_{\xi, \omega}[T^p(\xi, \omega)] &= \mathbb{E}_\xi[\mathbb{E}_\omega[T^p(\xi, \omega)]] \\ &= \int_\omega \int_\xi d\xi d\omega k^p \exp(-k_1 p N_1(\omega)) \exp(-k_3 p \xi) \\ &= k^p \frac{\sinh[k_3 p]}{k_3 p} \sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp(-k_1 p x) \end{aligned} \quad (12)$$

where $B_\omega(x)$ represents the PDF of the binomial variable $N_1(\omega)$ being equal to x :

$$\begin{aligned} B_\omega(x) &\stackrel{\text{def}}{=} \Pr(N_1 = x | N_{\text{tot}}, p_1) \\ &= \frac{N_{\text{tot}}!}{x!(N_{\text{tot}}-x)!} p_1^x (1-p_1)^{(N_{\text{tot}}-x)} \end{aligned} \quad (13)$$

Eq. (12) enables computation of the variance of $T(\xi, \omega)$ over both aleatoric uncertainties, $\mathbb{V}ar_{\xi, \omega}[T(\xi, \omega)]$, by expanding the expression for variance,

$$\mathbb{V}ar_{\xi, \omega}[T(\xi, \omega)] = \mathbb{E}_{\xi, \omega}[T^2(\xi, \omega)] - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2. \quad (14)$$

This is the denominator of the main and total effect SIs. For comparison with numerical results, we calculate analytic solutions for the numerators in Eqs. (6a) and (6b). Taking $\mathbb{V}ar_\xi[\mathbb{P}_B(\xi)]$ to indicate the variance of the conditional mean of $T(\xi, \omega)$ given ξ , over all ξ , we find that

$$\begin{aligned} \mathbb{V}ar_\xi[\mathbb{P}_B(\xi)] &= \mathbb{E}_\xi[\mathbb{P}_B^2(\xi)] - \mathbb{E}_\xi[\mathbb{P}_B(\xi)]^2 \\ &= \mathbb{E}_\xi[\mathbb{P}_B^2(\xi)] - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2. \end{aligned} \quad (15)$$

The second term is the first-order raw moment of $T(\xi, \omega)$, calculable from Eq. (12). The first term, the second-order raw moment of $\mathbb{P}_B(\xi)$, is

$$\begin{aligned} \mathbb{E}_\xi[\mathbb{P}_B^2(\xi)] &= \int_\xi d\xi k^2 \exp(-k_3 \xi) \left(\sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp(-k_1 x) \right)^2 \\ &= \frac{k^2 \sinh[2k_3]}{2k_3} \left(\sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp(-k_1 x) \right)^2 \end{aligned} \quad (16)$$

Inserting Eqs. (14) and (15) into Eq. (6a) yields

$$S_\xi = \frac{\frac{k^2 \sinh[2k_3]}{2k_3} \left(\sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp(-k_1 x) \right)^2 - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2}{\mathbb{E}_{\xi, \omega}[T^2(\xi, \omega)] - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2}. \quad (17)$$

Following the same process to calculate $\mathbb{V}ar_\omega[\mathbb{P}_B(\omega)]$ yields

$$S_\omega = \frac{\frac{k^2 \sinh^2[k_3]}{k_3^2} \left(\sum_{x=0}^{N_{\text{tot}}} B_\omega(x) \exp(-2k_1 x) \right) - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2}{\mathbb{E}_{\xi, \omega}[T^2(\xi, \omega)] - \mathbb{E}_{\xi, \omega}[T(\xi, \omega)]^2}. \quad (18)$$

Given these closed-form solutions for the main effect SIs, Eqs. (6a) and (6b) provide closed-form solutions for the total effect SIs.

RESULTS

We solve two numerical problems each using the problem description from the previous section with $r_1 = r_2 = r_3 = 1.0$, $\Sigma_{t,1} = 3.0$, $\Sigma_{t,2} = 0.1$, $\Sigma_{t,3}^0 = 1.0$, and $p_1 = 0.3$. For Problem 1, $N_{\text{tot}} = 10$ and $\Sigma_{t,3}^\Delta = 0.25$. For Problem 2, $N_{\text{tot}} = 100$ and $\Sigma_{t,3}^\Delta = 0.75$.

For each quantity on both problems, we use $N_\eta = 20$. For each problem, we first solve for the average transmittance ($\mathbb{E}_{\xi, \omega}[T(\xi, \omega)]$) and combined aleatoric variance ($\mathbb{V}ar_{\xi, \omega}[Q(\xi, \omega)]$) using 10,000 samples of the aleatoric uncertainty space (i.e., ξ and ω). We then use $N_\omega = 10$ and $N_\xi = 1000$, for a total of 10,000 aleatoric samples, to solve for $\mathbb{V}ar_\xi[\mathbb{P}_B(\xi)]$. Next, we use $N_\xi = 10$ and $N_\omega = 1000$, for a total of 10,000 aleatoric samples, to solve for $\mathbb{V}ar_\omega[\mathbb{P}_B(\omega)]$. For each of these numerically computed quantities, we average the computed quantities over 40 repetitions and use those repetitions to compute a standard error of the mean (SEM) for the quantity. Closed-form values, numerically computed mean and SEM values, and error in numerical values reported as number of 1-sigma SEMs are reported in Table I. In addition to the above-mentioned quantities, to enable numerical interrogation and reproducibility, we report intermediate computed values for $\mathbb{V}ar_{\xi, \omega}[\tilde{Q}_{N_\eta}(\xi, \omega)]$ and $\mathbb{E}_{\xi, \omega}[\sigma_{RT, N_\eta}^2(\xi, \omega)]$.

SI are computed using Eq. (6). To compute these quantities from the total aleatoric variance and each conditional variance, statistical uncertainties are propagated using the standard error propagation formula for independent variables

$$s_f = \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 s_x^2 + \left(\frac{\partial f}{\partial y}\right)^2 s_y^2 + \left(\frac{\partial f}{\partial z}\right)^2 s_z^2 + \dots} \quad (19)$$

Error is computed compared to closed-form solutions in terms of number of standard deviations and listed in Table I.

We first observe that all numerically computed values agree with closed-form solutions within no more than 1.58 standard deviations, that the error is usually less than 1 standard deviation, and that the error is stochastically either positive or negative. This degree and form of agreement with closed-form solutions corroborates the new numerical method.

We secondly observe the SI of these two problems to gain insight to their practical value: whereas the transmittance and overall aleatoric variance for each problem are roughly the same, our numerically computed SI provide a formal mechanism by which to measure that the SM provide the majority of the variance (~90%) in Problem 1 and, by contrast, the uncertain cross section provides the majority of the variance (~90%) in Problem 2.

TABLE I. Closed-form and Numerically Computed Values

	Problem 1				Problem 2			
	Closed	Numerical	SEM	Error	Closed	Numerical	SEM	Error
Unconditional Mean and Variance				Unconditional Mean and Variance				
$E_{\xi,\omega}[T(\xi,\omega)]$	0.1387816	0.1387030	0.0001423	0.55σ	0.1395753	0.1396815	0.0001744	-0.61σ
$Var_{\xi,\omega}[\tilde{Q}_{N_\eta}(\xi,\omega)]$	N/A	0.0094396	0.0000240	N/A	N/A	0.0097554	0.0000291	N/A
$E_{\xi,\omega}[\sigma_{RT,N_\eta}^2(\xi,\omega)]$	N/A	0.0057908	0.0000048	N/A	N/A	0.0058113	0.0000058	N/A
$Var_{\xi,\omega}[Q(\xi,\omega)]$	0.0036845	0.0036488	0.0000226	1.58σ	0.0039277	0.0039441	0.0000271	-0.61σ
Conditional Variance Values				Conditional Variance Values				
$Var_\omega[\mathbb{P}_B(\omega)]$	0.0032181	0.0031919	0.0000324	0.81σ	0.0003430	0.0003469	0.0000102	-0.38σ
$Var_\xi[\mathbb{P}_B(\xi)]$	0.0003996	0.0004065	0.0000090	-0.77σ	0.0035227	0.0035377	0.0000225	-0.67σ
Sobol Indices				Sobol Indices				
S_ω	0.8734261	0.8747955	0.0103919	-0.13σ	0.0873300	0.0879516	0.0026643	-0.23σ
S_ξ	0.1084529	0.1114180	0.0025490	-1.16σ	0.8968785	0.8969538	0.0083963	-0.01σ
S_{T_ω}	0.8915471	0.8885820	0.0025490	1.16σ	0.1031215	0.1030462	0.0083963	0.01σ
S_{T_ξ}	0.1265739	0.1252045	0.0103919	0.13σ	0.9126700	0.9120484	0.0026643	0.23σ

CONCLUSIONS

We leverage the recently established variance deconvolution method to propose a new, unbiased method for computing SI when using a stochastic solver such as a MC RT solver. We demonstrate that, since this method does not rely on the parametric property of uncertainty sources, as long as samples of each uncertainty source can be kept constant while the other uncertainty sources are resampled, this approach can not only solve SI for well-behaved parametric aleatoric uncertainty sources such as uncertain cross section values, but also for challenging non-aleatoric uncertainty sources such as stochastic media. To enable numerical testing of the new method, we derive closed-form solutions for a radiation transport test problem involving stochastic media and an uncertain cross section value. Numerical results agree with closed-form solutions within statistical uncertainty corroborating the numerical approach. Via two numerical test problems, we demonstrate the ability of SI to rank the fractional contribution of each uncertain input (including SM) to the output uncertainty.

In future work, we plan to examine applications with more than two aleatoric uncertainty sources, to compare the method's efficiency to other methods, to optimize the method's efficiency by re-using samples to contribute to computing more than one term, and to apply the method to more complicated transport problems such as those with scattering.

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