SAND2022-3023C

Numerical Investigation on the Performance of a Variance Deconvolution Estimator

Kayla Clements,*,† Gianluca Geraci,† and Aaron Olson,†

*Oregon State University, clemekay@oregonstate.edu
†Sandia National Laboratories, ggeraci@sandia.gov, aolson@sandia.gov

INTRODUCTION

In radiation transport problems, uncertainty quantification (UQ) can be used to characterize and propagate the effects of uncertain input parameters; we refer to this variance caused by uncertain parameters as parametric variance. Monte Carlo (MC) sampling is one method to obtain statistics of the system's quantities of interest (QoIs) that we wish to evaluate with UQ. In the case of a QoI obtained from Monte Carlo radiation transport (MC RT) computations, UQ MC sampling can function as a wrapper around the MC RT solver. MC RT solvers produce results whose variance is inversely proportional to the square root of the number of particle histories used; we refer to this variance as statistical variability. Though increasing the number of particle histories will decrease this statistical variability, it is often necessary to control the growth of the overall computational burden by limiting the number of particle histories used in each MC RT computation. In this contribution, we show how the statistical variability from this limited number of particle histories propagates to the variance of the QoI, compounding with the parametric variance, and that this increase must be accounted for to obtain reliable UQ results. We named this process –estimating and removing the MC RT statistical variability from the measured total variance –variance deconvolution.

Recently, we developed a novel variance deconvolution estimator which uses tallies already generated during MC RT computations to accurately and efficiently estimate the parametric variance, without carrying the contribution of the statistical variability [1]. Preliminary results suggested that the most efficient variance estimator can be obtained for given computational cost by using specific numbers of UQ samples and particle histories. In this work, we present thorough numerical studies for RT problems with and without scattering to further develop our understanding of how this trade-off affects estimator performance.

VARIANCE DECONVOLUTION

We first develop some background on the variance deconvolution estimator following the presentation in [1]. In the case of a general RT problem, the quantity of interest Q can be understood as a function of a vector of d input parameters, $\xi \in \Xi \subseteq \mathcal{R}^d$. Several code evaluations can be performed for values of ξ sampled from the joint probability density function $p(\xi)$. These samples are then used to evaluate the desired statistics, *e.g.* mean and variance. The interested reader can refer to [2] for an in depth presentation of MC sampling estimators or [3] for an in depth review of MC RT. The non-deterministic behavior of MC RT codes provides a challenge to this process. Each UQ realization $Q(\xi^{(i)})$ from an MC RT code is the result of an averaging over a finite number of particle histories. If we use $f(\xi^{(i)}, \eta^{(j)})$ to indicate the jth particle history corresponding to the ith sample, the QoI can be approximated as

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

where N_η indicates the number of particle histories per parameter sample and $\mathbb{E}_\eta[\cdot]$ is a shorthand to indicate the expected value over realizations drawn with respect to the variable η. We note here that η is used here only to notionally represent the MC RT stochastic behavior and that its value may not be, in general, controllable or known.

Straightforward computation of the parametric variance from the samples of $\tilde{Q}$ unfortunately does not yield accurate results. Instead, the limited number of particle histories N_η embeds a statistical variability that propagates to the measurable variance of $\tilde{Q}$. Although $\mathbb{V}ar_\xi[\tilde{Q}] \to \mathbb{V}ar_\xi[Q]$ as $N_\eta \to \infty$, we want to understand how to accurately compute the parametric variance of $\tilde{Q}$ using a limited, and possibly small, number of histories N_η. This result can be obtained rigorously by applying the Law of Total Variance to $\mathbb{V}ar[\tilde{Q}]$,

$$\begin{aligned}\mathbb{V}ar\left[\tilde{Q}\right] &= \mathbb{V}ar_\xi\left[\mathbb{E}_\eta\left[\tilde{Q}\right]\right] + \mathbb{E}_\xi\left[\mathbb{V}ar_\eta\left[\tilde{Q}\right]\right] \\ &= \mathbb{V}ar_\xi\left[Q\right] + \mathbb{E}_\xi\left[\frac{\sigma_\eta^2}{N_\eta}\right] \\ &= \mathbb{V}ar_\xi\left[Q\right] + \mathbb{E}_\xi\left[\sigma^2_{RT,N_\eta}\right],\end{aligned} \quad (2)$$

where σ_η^2 is defined as the variance of the histories over N_η for each fixed UQ parameter, *i.e.* $\sigma_\eta^2(\xi) \stackrel{\text{def}}{=} \mathbb{V}ar_\eta[f(\xi, \eta)]$, and $\sigma^2_{RT,N_\eta}(\xi) \stackrel{\text{def}}{=} \sigma_\eta^2(\xi)/N_\eta$ is the corresponding MC RT solver variance [1]. The expression above relates the true parametric variance of the QoI, $\mathbb{V}ar_\xi[Q]$, and the expected value (over the parameter space) of the statistical variability introduced by the MC RT computations, σ^2_{RT,N_η}. Both terms contribute to the total variance $\mathbb{V}ar[\tilde{Q}]$, the only variance directly observable from numerical experiments.

Practical implementation

As previously discussed, the QoI Q can only be approximated with $\tilde{Q}$, the variance of which can be considered to be polluted by the MC RT statistical variability. On the other hand, $\tilde{Q}$ can be re-evaluated for several samples of ξ, making $\mathbb{V}ar_\xi[\tilde{Q}]$ an accessible quantity; unlike $\mathbb{V}ar_\xi[Q]$, it can be directly estimated by taking the variance over the number of UQ samples N_ξ. Similarly, given multiple particle histories per UQ sample, it is possible to estimate the term $\sigma_\eta^2 = \mathbb{V}ar_\eta[f]$ at each ith UQ parameter location, and therefore estimate σ^2_{RT,N_η}. The true parametric variance can then be obtained.

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As $\mathbb{V}ar[\tilde{Q}]$ and $\mathbb{E}_\xi[\sigma^2_{RT,N_\eta}]$ are exact only at the limit of infinite N_ξ, a sample estimator counterpart of the variance deconvolution in Equation 2 is necessary,

$$\mathbb{V}ar_\xi[Q] \approx S^2 = \tilde{S}^2 - \hat{\mu}_{\sigma^2_{RT,N_\eta}}, \tag{3}$$

where S^2 and $\tilde{S}^2$ represent the sample estimators for the true parametric (*i.e.* inaccessible) and polluted variances, respectively, and $\hat{\mu}_{\sigma^2_{RT,N_\eta}}$ indicates the sample mean of the MC RT variance over N_ξ. Assuming the tallies of each particle history are accessible, we can define the two estimators as

$$\begin{aligned}\tilde{S}^2 &= \frac{1}{N_\xi - 1}\sum_{i=1}^{N_\xi}\left(\tilde{Q}(\xi^{(i)}) - \frac{1}{N_\xi}\sum_{k=1}^{N_\xi}\tilde{Q}(\xi^{(k)})\right)^2 \\ \hat{\mu}_{\sigma^2_{RT,N_\eta}} &= \frac{1}{N_\xi}\sum_{i=1}^{N_\xi}\frac{\sigma^2_\eta(\xi^{(i)})}{N_\eta},\end{aligned} \tag{4}$$

where the term σ^2_η is approximated, for each ith UQ sample, with an additional sample variance estimator

$$\begin{aligned}\sigma^2_\eta(\xi^{(i)}) &\approx \hat{\sigma}^2_\eta(\xi^{(i)}) \\ &= \frac{1}{N_\eta - 1}\sum_{j=1}^{N_\eta}\left(f(\xi^{(i)},\eta^{(j)}) - \frac{1}{N_\eta}\sum_{k=1}^{N_\eta} f(\xi^{(i)},\eta^{(k)})\right)^2.\end{aligned} \tag{5}$$

By solving for $\tilde{S}^2$, σ^2_η, and $\hat{\mu}_{\sigma^2_{RT,N_\eta}}$, we can calculate S^2, and estimate of $\mathbb{V}ar_\xi[Q]$. Ref. [1] shows that S^2 is an unbiased estimator for $\mathbb{V}ar_\xi[Q]$.

The idea of the variance deconvolution, in RT applications, was previously introduced in [4] and presented in the context of an embedded UQ strategy dubbed Embedded VAriance DEconvolution (EVADE). Moreover, EVADE has been successfully adopted in RT computations in the presence of stochastic media, as in [5]. The original EVADE estimator presented in [4] was derived for an approximation of $\tilde{Q}$ obtained with a single particle history. The interested reader can refer to [1] for an in depth discussion of the relationship between the two estimators and numerical comparisons. Both estimators are unbiased, although the variance of the newer estimator summarized thus far is smaller in all analysis scenarios we have considered.

In the present work, we significantly extend our understanding of the deconvolution strategy by investigating the trade-off between the number of UQ samples N_ξ and the number of particle histories N_η. Because only one history was used to calculate the total polluted variance in the original EVADE estimator, the variance of an estimate of S^2 using a prescribed estimator cost $C = N_\xi \times N_\eta$ was minimized when the lowest possible number of particle histories was used. Preliminary results from [1] found that the minimum variance of the newer estimator did not necessarily correspond to the minimum number of histories in the tested problem. To investigate this, we performed numerical studies varying the ratio of N_η to N_ξ for a prescribed estimator cost for a given problem, results of which are discussed in the numerical section.

PROBLEM DESCRIPTION

A short description of the problem used in the numerical investigation follows. We consider the stochastic, one-dimensional, neutral-particle, mono-energetic, steady-state radiation transport equation with a normally incident beam source of magnitude one. The slab has fixed boundaries, i.e. $x \in [0, L]$, and contains a total of M material sections separated by fixed boundaries. The problem is solved both as an attenuation-only problem and with isotropic scattering included. For both scenarios, the stochastic total cross section of each material is assumed to be uniformly distributed. In the scenario which includes scattering, the ratio $c = \Sigma_s/\Sigma_t$ of scattering to total cross section is distributed uniformly and independently of Σ_t. For each region m, Σ_t and c are defined using

$$\Sigma_{t,m}(\xi_m) = \Sigma^0_{t,m} + \Sigma^\Delta_{t,m}\xi_m \tag{6a}$$

$$c_m(\xi_m) = c^0_m + c^\Delta_m\xi_m \tag{6b}$$

where $\cdot^0$ represents the average value and $\cdot^\Delta$ the deviation from the mean. Furthermore, a random parameter $\xi_m \sim \mathcal{U}[-1, 1]$ is used to represent the variability of $\Sigma_{t,m}(\xi) \sim \mathcal{U}[\Sigma^0_{t,m} - \Sigma^\Delta_{t,m}, \Sigma^0_{t,m} + \Sigma^\Delta_{t,m}]$. For cases with scattering, the scattering ratio c_m is defined analogously. In the attenuation-only case, the number of uncertain parameters is equal to the number of materials, *i.e.* $\xi \in \mathbb{R}^d$ with $d = M$, whereas in the case of both attenuation and scattering $d = 2M$.

For the attenuation-only case, the estimate S^2 can be compared to its analytic counterpart. By using the pth raw moment for the transmittance, as shown in [4],

$$\mathbb{E}[T^p] = \prod_{m=1}^{d} exp\left[-p\Sigma^0_{t,m}\Delta x_m\right]\frac{sinh\left[p\Sigma^\Delta_{t,m}\Delta x_m\right]}{p\Sigma^0_{t,m}\Delta x_m}, \tag{7}$$

the parametric variance can be obtained as $\mathbb{V}ar[T] = \mathbb{E}[T^2] - \mathbb{E}[T]^2$. It is also possible to compute the variance $\mathbb{E}_\xi[\sigma^2_{RT,N_\eta}]$ in closed form for this problem, using $\sigma^2_{RT,N_\eta} = \frac{T(\xi)}{N_\eta}(1 - T(\xi))$.

NUMERICAL RESULTS

In this section, we present the performance of the described variance estimator for two UQ analysis scenarios, attenuation-only and attenuation with scattering. We consider a 1D slab with 3 material sections[1], and report in Table I the right boundary location, average total cross section, and deviation from the cross section mean for each of the material sections for both problems, as well as the analogous information for the scattering ratio for the isotropic scattering problem. In Table II, we report the mean QoI and parametric variance computed with closed-form solutions where available; numerical benchmark solutions with $N_\eta = 10^5$, $N_\xi = 10^3$ ($C = 10^8$); and using one typical repetition of our variance deconvolution method with $N_\eta = 10^1$, $N_\xi = 10^3$ ($C = 10^4$), for reference[2].

[1]The approach can be extended to higher number of sections without any modifications to the algorithm.

[2]Note that for the deconvolved results, this is only one realization of a stochastic problem, which converges to the benchmark over many repetitions.

TABLE I. Problem parameters.

	Problem Parameters			Scattering Parameters	
	x_R	$\Sigma^0_{t,m}$	$\Sigma^\Delta_{t,m}$	$c^0_{s,m}$	$c^\Delta_{s,m}$
m = 1	2.0	0.90	0.70	0.50	0.40
m = 2	5.0	0.15	0.12	0.50	0.40
m = 3	6.0	0.60	0.50	0.50	0.40

TABLE II. Mean QoI and parametric variance. Numerical benchmark computed with $N_\eta = 10^5$, $N_\xi = 10^3$ ($C = 10^8$); variance deconvolution computed with $N_\eta = 10^1$, $N_\xi = 10^3$ ($C = 10^4$); and closed-form solutions where available.

Attenuation Only			
	Benchmark	Deconvolved	Analytic
$\mathbb{E}[T]$	8.915E-2	8.870E-2	8.378E-2
S^2_T	5.789E-3	5.768E-3	5.505E-3
Scattering			
	Benchmark	Deconvolved	-
$\mathbb{E}[T]$	1.299E-1	1.209E-1	-
S^2_T	9.710E-3	9.825E-3	-
$\mathbb{E}[R]$	1.386E-1	1.336E-1	-
S^2_R	8.251E-3	7.703E-3	-

To better understand where the variance of the novel estimator is minimized, we solve the described RT problem using Woodcock-delta tracking with analog Monte Carlo methods for an estimator cost $C = N_\xi \times N_\eta$ of 200, 500, 1000, 1500, 2000, and 5000 for a variety of N_η values. We repeat the estimator evaluation over 25,000 repetitions to evaluate its statistics. We report $\mathbb{V}ar[S^2]$ for both the attenuation-only and isotropic scattering case, where $S^2 = \mathbb{V}ar[T]$ or $\mathbb{V}ar[R]$, in Table III. The exact parametric variance is calculable for the attenuation-only case, so we also compare the estimate of S^2 for the attenuation-only case to the analytic solution using Mean Square Error (MSE), which we also report in Table III.

For the attenuation-only case, we see that $\mathbb{V}ar[S^2]$ first decreases as a function of N_η, reaches its minimum at $N_\eta = 10$, then gradually increases again. We only report up values up to $N_\eta = 100$, because after this $\mathbb{V}ar[S^2]$ just continues to increase. The varied N_η value is the number of histories per sample, meaning that even in the case where $N_\eta = 2$, the actual QoI (transmittance, reflectance) is still being calculated over the full estimator cost. To better see the trend, Figure 1 shows $\mathbb{V}ar[S^2]$ as a function of N_η on a log-log scale for the attenuation-only case. We can see clearly here that $\mathbb{V}ar[S^2]$ is not minimized by running with the lowest possible number of histories, and a tradeoff does indeed exist between the number of UQ samples N_ξ and the number of particle histories N_η; this is not the case for the previous estimator in [1] with most problems. We can see the same trend in the isotropic scattering case, and when $S^2 = \mathbb{V}ar[T]$, $\mathbb{V}ar[S^2]$ is also minimized at $N_\eta = 10$.

We see a similar trend for the isotropic scattering problem where S^2 is $\mathbb{V}ar[R]$, the parametric variance of the reflectance tally. However, in this case $\mathbb{V}ar[S^2]$ is minimized at $N_\eta = 20$, rather than $N_\eta = 10$. While both transmittance and reflectance are influenced by the addition of scattering and

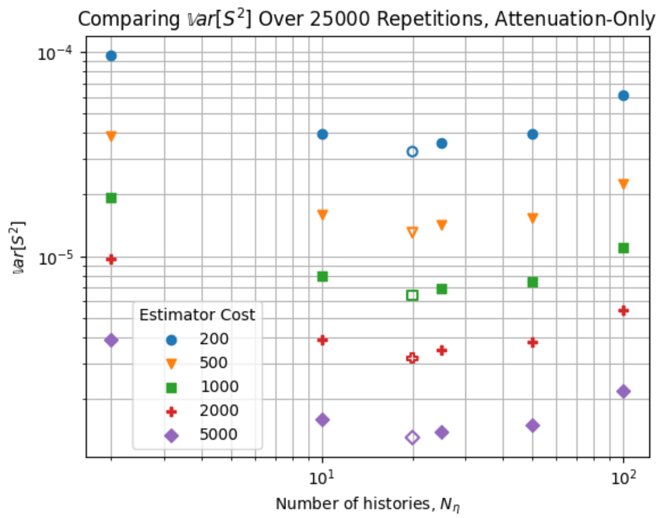

Fig. 1. $\mathbb{V}ar[S^2]$ as a function of N_η for a variety of total estimator costs, log-log plot. Unfilled point is minimum $\mathbb{V}ar[S^2]$.

the stochastic scattering ratio, the reflectance tally is likely more sensitive to this scattering ratio, and requires more radiation transport tallies to resolve than the transmittance tally. This demonstrates that the optimal number of N_ξ and N_η can differ between different QoIs even within the same problem, motivating further investigation to allow the analyst to choose these parameters in an informed way. Figure 2 compares the trends for the attenuation-only estimate of $\mathbb{V}ar[T]$ to the isotropic scattering estimate of $\mathbb{V}ar[T]$ and $\mathbb{V}ar[R]$.

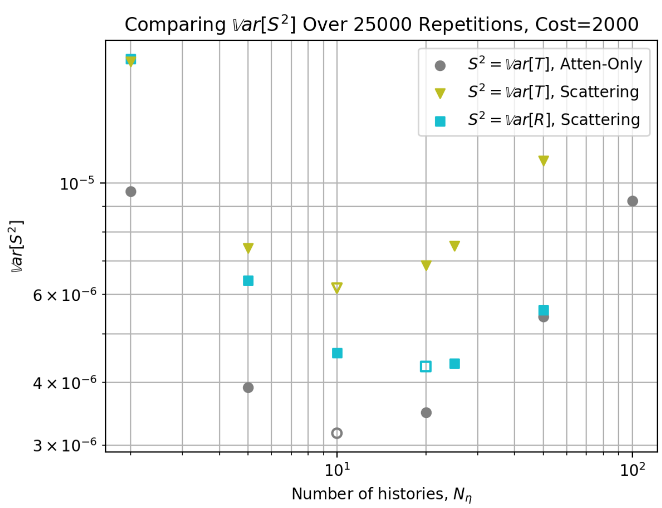

Fig. 2. $\mathbb{V}ar[S^2]$ as a function of N_η for the attenuation-only and scattering cases. Log-log plot, estimator cost $N_\xi \times N_\eta = 2000$. Unfilled point is minimum $\mathbb{V}ar[S^2]$.

CONCLUSIONS AND FUTURE WORK

For a stochastic radiation transport problem solved using MC RT methods, simply performing uncertainty quantification

TABLE III. The variance (and MSE, where applicable) of the estimate of S^2 over 25,000 repetitions for both the attenuation-only and scattering problems.

Attenuation-Only Problem									
	$\mathbb{V}ar[S^2]$					$MSE[S^2]$ (Exact $\mathbb{V}ar[T] = 5.505E-3$)			
N_η	Estimator Cost 200	500	2000	5000	N_η	Estimator Cost 200	500	2000	5000
2	9.584E-05	3.887E-05	9.626E-06	3.879E-06	2	1.332E-10	9.106E-13	3.176E-11	5.565E-11
5	3.970E-05	1.597E-05	3.907E-06	1.586E-06	5	1.119E-09	3.600E-14	3.734E-11	4.169E-11
10	**3.241E-05**	**1.303E-05**	**3.168E-06**	**1.297E-06**	10	7.155E-10	2.692E-10	5.997E-12	1.308E-11
20	3.568E-05	1.414E-05	3.482E-06	1.384E-06	20	2.576E-10	1.026E-10	8.893E-12	4.168E-11
100	1.327E-04	3.866E-05	9.218E-06	3.656E-06	100	3.678E-10	6.301E-09	1.424E-10	3.323E-11

Scattering Problem									
	$\mathbb{V}ar[S^2]$, Transmittance					$\mathbb{V}ar[S^2]$, Reflectance			
N_η	Estimator Cost 200	500	2000	5000	N_η	Estimator Cost 200	500	2000	5000
2	1.730E-04	6.921E-05	1.749E-05	6.996E-06	2	1.786E-04	7.085E-05	1.770E-05	7.140E-06
5	7.664E-05	2.963E-05	7.424E-06	2.882E-06	5	6.574E-05	2.592E-05	6.392E-06	2.591E-06
10	**6.329E-05**	**2.461E-05**	**6.175E-06**	**2.488E-06**	10	4.792E-05	1.852E-05	4.586E-06	1.861E-06
20	7.360E-05	2.775E-05	6.852E-06	2.753E-06	20	**4.656E-05**	**1.758E-05**	**4.303E-06**	**1.694E-06**
25	8.090E-05	3.102E-05	7.499E-06	3.012E-06	25	4.963E-05	1.836E-05	4.371E-06	1.771E-06
100	2.987E-04	8.572E-05	1.897E-05	7.456E-06	100	1.661E-04	4.169E-05	8.476E-06	3.241E-06

with MC sampling would over-estimate the parametric variance; it fails to consider that the total variance has been polluted by the statistical variability of the MC RT solver. In [1], we developed a novel variance deconvolution method which estimates the parametric variance of a QoI by removing this statistical variability from the polluted total variance. Preliminary numerical investigations showed that the variance of this estimate of parametric variance could be minimized by optimizing the ratio of UQ samples N_ξ to particle histories N_η, providing the most accurate estimate for a given computational cost.

In this work, we performed numerical studies for an attenuation-only and isotropic scattering problem over a range of total computational costs, using Woodcock-delta tracking with analog Monte Carlo. We found that the variance of the estimate of $\mathbb{V}ar[T]$ followed a consistent trend of decreasing as N_η increased, reaching a minimum, then increasing again, for the problem defined with and without scattering. In both the attenuation-only and scattering cases, this minimum was at $N_\eta = 10$ across all tested costs. A similar trend was observed in the isotropic scattering case for a QoI of reflectance, though the minimum was at $N_\eta = 20$. Though further investigation is needed, these studies allow us to better understand how to apply this variance deconvolution method for the most accurate estimate of parametric variance. As we continue developing this estimator, we hope to corroborate these numerical findings with an analytic, closed-form solution for the variance of the estimate of $\mathbb{V}ar[S^2]$.

ACKNOWLEDGMENTS

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government. This work was supported by the Center for Exascale Monte-Carlo Neutron Transport (CEMeNT) a PSAAP-III project funded by the Department of Energy, grant number DE-NA003967.

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