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Comparison of Differential Operator and Malliavin Sensitivity Methods for Particle Transport

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ABSTRACT

The differential operator technique has been widely used in the particle transport community for estimating the sensitivity of Monte Carlo estimates to problem parameters. Techniques like stochastic calculus-based Malliavin estimators have been developed and applied to the calculation of financial derivatives. The interest in the differential operator and Malliavin sensitivity methods is the ability to reuse the existing Monte Carlo samples. We present comparisons between these methods for the estimation of sensitivities on a non-scattering transport problem. Both methods differ depending upon the tallies used for the underlying Monte Carlo approximation of the response functional. Both methods provide accurate sensitivities approximations but differ in their statistical uncertainties.

KEYWORDS: differential operator, Malliavin, sensitivities, Monte Carlo

1. INTRODUCTION

Local sensitivities are the impact of a problem parameter's variation on a model response. These are useful in performing sensitivity analysis as part of uncertainty quantification. The transport community has utilized the differential operator method, described by Rief [1], for the calculation of sensitivities [2]. Another class of sensitivity estimators has been developed in the financial derivatives community based upon the work of Paul Malliavin [3]; see the books [4,5] for an introduction. These Malliavin sensitivity methods are of minimal variance for Brownian motion [7] but to our knowledge have not been applied to linear particle transport. See the technical report [6] for recent developments specific to particle simulations, including a review of various sensitivity methods and their use in gradient-based optimization methods. The interest in the differential operator and Malliavin sensitivity methods is the ability to reuse the existing Monte Carlo samples. Both methods determine weightings that are applied to Monte Carlo samples and so can be efficiently applied. This is in stark contrast to finite-difference approaches that require further Monte Carlo samples to be computed.

This investigation of sensitivity methods is motivated in part by limitations with existing methods. One specific limitation with the differential-operator method is in the calculation of sensitivities to boundary locations in the presence of scattering. One approach to this limitation has been proposed [8]. Here we investigate a non-scattering problem to facilitate comparison of the differential operator and Malliavin methods in a problem with a boundary-location sensitivity, though there are alternative methods for non-scattering transport problems [9].

We also remark that by the result in [11], we can calculate an approximation to the adjoint problem using the same set of Monte Carlo samples used to approximate the Boltzmann transport solution. Since these transport problems can be identified as expectations over formally defined stochastic processes, the methods presented in this paper allow for the reuse of those same samples to calculate sensitivities for the adjoint problem.

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The remainder of this paper is organized as follows. In Section 2, we define a non-scattering transport problem with an internal boundary. For a particle transmission current, we derive the differential operator sensitivity estimator due to variation in the position of an internal boundary in Section 3. We derive a Malliavin sensitivity estimator for the same quantity in Section 4. In Section 5, we provide numerical results comparing these two sensitivity estimators.

2. TRANSPORT PROBLEM

For comparison of the sensitivity methods, we define a simplified one-dimensional slab problem with two regions, as illustrated in Fig. 1. Each region contains a material that is a pure absorber, meaning that any particle interaction is an absorption event. We are interested in calculating the expected number or rate of escape of particles from the right side of the problem and the sensitivity of that quantity to the position of the boundary between the two regions, while the external escape boundaries of the problem remain at fixed locations.

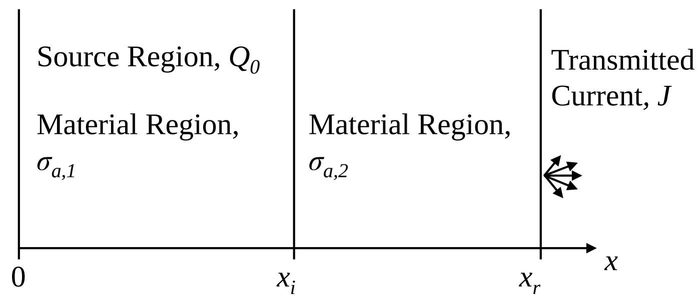

Figure 1: Transmitted current J and the parameters associated with the boundary value problem (1)

More precisely, we solve

$$\mu \frac{\partial \psi(x,\mu)}{\partial x} + \sigma_a(x)\psi(x,\mu) = Q(x,\mu)\,, \tag{1a}$$

with vacuum boundary conditions and where the cross section and source are given by

$$\sigma_a(x) = \sigma_{a,1}\, \mathbb{1}_{(0,\,x_i)}(x) + \sigma_{a,2}\, \mathbb{1}_{(x_i,\,x_r)}(x)\,, \tag{1b}$$

$$Q(x,\mu) = \frac{Q_0}{x_i} \mathbb{1}_{(0,\,x_i)}(x) \mathbb{1}_{(0,\,1)}(\mu)\,. \tag{1c}$$

$\mathbb{1}_{(a,b)}(x)$ is an indicator function defined as equal to 1 when x is in the interval (a, b) and 0 otherwise, $\sigma_{a,k}$ is the absorption cross section in region k, μ is the cosine of the angle of the particle direction with respect to the positive x direction, x_i is the location of the interface between the two regions, and x_r is the location of the right boundary of the problem.

The solution ψ of the boundary-value problem (1) at x_r and positive μ is

$$\psi(x_r,\mu) = \frac{Q_0}{\mu\, x_i}\, \mathbb{1}_{(0,\,1)}(\mu) \int_0^{x_i} r(x_s, x_i)\, dx_s\,,$$

where

$$r(x_s; x_i) = \exp\left(-\sigma_{a,1}\frac{x_i - x_s}{\mu}\right) \exp\left(-\sigma_{a,2}\frac{x_r - x_i}{\mu}\right) \tag{2}$$

is the probability that the particle reaches at least x_r before absorption with the particle source position x_s.

We can now estimate the transmitted current at x_r, an expected value, as

$$J = \int_0^1 \mu \psi(x_r, \mu) d\mu = Q_0 \int_0^1 \int_0^{x_i} \frac{r(x_s; x_i)}{x_i} \, dx_s \, d\mu \,. \tag{3}$$

If ξ is a uniformly distributed random number over the interval $(0,1)$ then the source position can be described via the relationship $x_s = \xi x_i$ and

$$R(\xi; x_i) = r(\xi x_i; x_i) = \exp\left(-\sigma_{a,1} \frac{(1-\xi)x_i}{\mu}\right) \exp\left(-\sigma_{a,2} \frac{x_r - x_i}{\mu}\right) \tag{4}$$

is the probability that a particle sampled at a location in the left interval $(0, x_i)$ reaches x_r before absorption. In this problem, it is possible to directly compute R_n for each sampled source particle n because we know the solution ψ of the boundary value problem (1). However, in general the solution is cast as a Neumann series [10].

Another expression for the probability that the particle reaches at least x_r before absorption is

$$t(x_s; x_i) = \int_0^\infty \mathbb{1}_{\{t > \ln r(\xi x_i; x_i)\}}(t) \, e^{-t} \, dt \,, \tag{5a}$$

which follows from the equality

$$r(x_s; x_i) = \int_{\ln r(\xi x_i; x_i)}^\infty e^{-t} \, dt \,.$$

In analogy to the discussion preceding (4), we define the random variable

$$T(\xi x_i; x_i) = \mathbb{1}_{\{-\frac{\mu}{\sigma_{a,1}} \ln(1-\xi_1) > (1-\xi)x_i\}} \mathbb{1}_{\{-\frac{\mu}{\sigma_{a,1}} \ln(1-\xi_2) > x_r - x_i\}}, \tag{5b}$$

where ξ_1 and ξ_2 are independent uniform random numbers on (0,1). Terms of the form $-\frac{\ln(1-\xi)}{\sigma}$ represent rate σ exponentially distributed numbers denoting the distance to an interaction in the x-dimension. Each indicator function is determining whether or not the particle escapes the material region and because the probability $t(x_s; x_i)$ is the expected value of the random variable $\mathbb{1}_{\{t > \ln r(\xi x_i; x_i)\}}$ under the unit-rate exponential distribution, we have

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} T(\xi_n x_i; x_i) = t(\xi x_i; x_i) \,. \tag{6}$$

Putting all of this together, we can approximate the transmission current response

$$J = Q_0 \int_0^1 \int_0^1 r(\xi x_i; x_i) \, d\xi \, d\mu \tag{7a}$$

$$= \lim_{N \to \infty} \frac{Q_0}{N} \sum_{n=1}^{N} R(\xi_n x_i; x_i) \tag{7b}$$

or

$$J = Q_0 \int_0^1 \int_0^1 t(\xi x_i; x_i) \, d\xi \, d\mu \tag{8a}$$

$$= \lim_{N \to \infty} \frac{Q_0}{N} \sum_{n=1}^{N} T(\xi_n x_i; x_i) \,. \tag{8b}$$

The distinction between the two estimators is that the former tallies random numbers in the unit interval determined by an analytical form of the solution ψ and the latter tallies exponentially distributed binary random variables representing an analog Monte Carlo method. The nature of the resulting Monte Carlo approximations is also distinct. In the former tally, the integrand is deterministic and the Monte Carlo approximation is for the double integral. In contrast, the latter tally has the Monte Carlo approximation given by (6) for the integrand $t(\xi x_i; x_i)$ representing an expected value.

Recall that the interest in the differential operator and Malliavin sensitivity methods is the ability to reuse the existing Monte Carlo samples. The goal is to determine weightings $\rho(\xi_n, \mu_n)$ or $\tau(\xi_n, \mu_n)$ so that

$$\frac{\mathrm{d}J}{\mathrm{d}x_i} = \lim_{N\to\infty} \frac{Q_0}{N} \sum_{n=1}^{N} R(\xi_n x_i; x_i)\, \rho(\xi_n, \mu_n) \tag{9a}$$

$$= \lim_{N\to\infty} \frac{Q_0}{N} \sum_{n=1}^{N} T(\xi_n x_i; x_i)\, \tau(\xi_n, \mu_n)\,. \tag{9b}$$

We remark that the weightings $\rho(\xi_n, \mu_n)$ or $\tau(\xi_n, \mu_n)$ are likely to be distinct because the nature of the Monte Carlo approximations are distinct as discussed following (8).

3. DIFFERENTIAL OPERATOR SENSITIVITY

The two different tallies (7) and (8) lead to distinct differential operator sensitivities. The differential operator sensitivity using (7) is

$$\begin{aligned}\frac{\mathrm{d}J}{\mathrm{d}x_i} &= Q_0 \int_0^1 \int_0^1 \frac{\partial}{\partial x_i} r(\xi x_i; x_i)\, d\xi\, d\mu \\ &= Q_0 \int_0^1 \int_0^1 r(\xi x_i; x_i) \Big(\frac{\sigma_{a,2} - \sigma_{a,1}}{\mu} + \xi \frac{\sigma_{a,1}}{\mu}\Big) d\xi\, d\mu \end{aligned}\tag{10}$$

which can be approximated as

$$S_{\mathrm{DO}}^{N} = \frac{Q_0}{N} \sum_{n=1}^{N} R(\xi_n x_i; x_i) \Big(\frac{\sigma_{a,2} - \sigma_{a,1}}{\mu_n} + \xi_n \frac{\sigma_{a,1}}{\mu_n}\Big)\,. \tag{11}$$

In contrast, the differential operator sensitivity using (8) is

$$\begin{aligned}\frac{\mathrm{d}J}{\mathrm{d}x_i} &= Q_0 \int_0^1 \int_0^1 \frac{\partial}{\partial x_i} t(\xi x_i; x_i)\, d\xi\, d\mu \\ &= Q_0 \int_0^1 \int_0^1 \frac{\partial}{\partial x_i} \Big(\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} T(\xi_n x_i; x_i) \Big)\, d\xi\, d\mu \\ &= Q_0 \int_0^1 \int_0^1 \Big(\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \frac{\partial}{\partial x_i} T(\xi_n x_i; x_i) \Big)\, d\xi\, d\mu \end{aligned}\tag{12}$$

where we formally replaced the differentiation of a limit of a sum with the limit of the sum differentiation terms. In practice, the approximation

$$\frac{\partial}{\partial x_i} T(\xi_n x_i; x_i) \approx T(\xi_n x_i; x_i) \Big(\frac{\sigma_{a,2} - \sigma_{a,1}}{\mu_n} + \xi_n \frac{\sigma_{a,1}}{\mu_n}\Big) \tag{13}$$

is assumed to hold to obtain

$$\tilde{S}_{\mathrm{DO}}^{N} = \frac{Q_0}{N} \sum_{n=1}^{N} T(\xi_n; x_i) \Big(\frac{\sigma_{a,2} - \sigma_{a,1}}{\mu_n} + \xi_n \frac{\sigma_{a,1}}{\mu_n}\Big)\,. \tag{14}$$

In other words, we assume that the sensitivity weightings $\rho(\xi_n, \mu_n)$ or $\tau(\xi_n, \mu_n)$ discussed in (9) needed to reuse the existing Monte-Carlo samples are the same.

4. MALLIAVIN WEIGHTINGS

The two different tallies (7) and (8) lead to the distinct Malliavin sensitivities. To arrive at a weighting consistent with the Malliavin approach using (7), the derivative on the transmission current (3) can also be evaluated using the Leibniz rule, i.e.,

$$\begin{aligned}\frac{\mathrm{d}J}{\mathrm{d}x_i} &= Q_0 \frac{\mathrm{d}}{\mathrm{d}x_i} \int_0^1 \int_0^{x_i} \frac{r(x_s;x_i)}{x_i}\, dx_s\, d\mu \\ &= Q_0 \int_0^1 \frac{r(x_i;x_i)}{x_i}\, d\mu + Q_0 \int_0^1 \int_0^{x_i} r(x_s;x_i) \frac{\partial}{\partial x_i}\frac{1}{x_i}\, dx_s\, d\mu + Q_0 \int_0^1 \int_0^{x_i} \frac{1}{x_i}\frac{\partial}{\partial x_i} r(x_s;x_i)\, dx_s\, d\mu \\ &= \frac{1}{x_i} Q_0 \int_0^1 \int_0^{x_i} r(x_i;x_i)\frac{1}{x_i}\, dx_s\, d\mu \; - \frac{1}{x_i} J + Q_0 \int_0^1 \int_0^{x_i} \frac{r(x_s;x_i)}{x_i}\Big(\frac{\sigma_{a,2}-\sigma_{a,1}}{\mu}\Big)\, dx_s\, d\mu \end{aligned} \quad (15)$$

where we used the equality

$$\int_0^1 r(x_i;x_i)\frac{1}{x_i}\, d\mu = \frac{1}{x_i} \int_0^1 \int_0^{x_i} r(x_i;x_i)\frac{1}{x_i}\, dx_s\, d\mu\,.$$

A Monte Carlo approximation for (15) results in

$$S^N_{\text{Mall}} = \frac{Q_0}{N}\sum_{n=1}^{N} \exp\Big(-\sigma_{a,2}\frac{x_r - x_i}{\mu_n}\Big)\frac{1}{x_i} + \frac{Q_0}{N}\sum_{n=1}^{N} R(\xi_n x_i; x_i)\Big(\frac{\sigma_{a,2}-\sigma_{a,1}}{\mu_n} - \frac{1}{x_i}\Big) \quad (16)$$

where the third term of (15) exploits the approximation of (10) by (11). Note that both terms in the latter parentheses have units of reciprocal length and the exponential in the first term is the probability that the particle survives to x_r given that it starts at x_i. We also remark that the approximation is a naïve Monte Carlo approach for the Malliavin sensitivity.

In contrast, a weighting consistent with the Malliavin approach using (8), i.e.,

$$\frac{\mathrm{d}J}{\mathrm{d}x_i} = Q_0 \frac{\mathrm{d}}{\mathrm{d}x_i} \int_0^1 \int_0^{x_i} \frac{t(x_s;x_i)}{x_i}\, dx_s\, d\mu$$

stumbles into difficulties similar to those encountered by the differential operator approach; see (12). The Malliavin counterpart to (14) is

$$\tilde{S}^N_{\text{Mall}} = \frac{Q_0}{N}\sum_{n=1}^{N} \exp\Big(-\sigma_{a,2}\frac{x_r - x_i}{\mu_n}\Big)\frac{1}{x_i} + \frac{Q_0}{N}\sum_{n=1}^{N} T(\xi_n x_i; x_i)\Big(\frac{\sigma_{a,2}-\sigma_{a,1}}{\mu_n} - \frac{1}{x_i}\Big) \quad (17)$$

where we assume the approximation (13) holds so that the sensitivity weightings $\rho(\xi_n, \mu_n)$ or $\tau(\xi_n, \mu_n)$ discussed in (9) are the same.

5. NUMERICAL RESULTS

To assess the accuracy and performance of these sensitivity methods, we consider a set of test problems. Source particles are isotropic and uniformly distributed in the left region, which has a cross section of $\sigma_{a,1}$. The boundary between the two regions is at x_i. The right region has cross section $\sigma_{a,2}$ and extends from the boundary at x_i to x_r. The transmitted particle current is tallied at the x_r boundary of the problem. Results are normalized to a source strength of $Q_0 = 1$.

All test problems have a total slab width of $x_r = 2$. The values examined for the material interface location, x_i, and the cross sections, $\sigma_{a,1}$ and $\sigma_{a,2}$, are given in Table 1. The first three test problems, with the same cross section in both regions, are only testing sensitivity to the extent of the source region. The other six test problems also test sensitivity due to the change in the cross section at the material interface.

Table 1: Parameter values for test problems.

	1	2	3	4	5	6	7	8	9
x_i	0.5	1.0	1.5	0.5	1.0	1.5	0.5	1.0	1.5
$\sigma_{a,1}$	1.0	1.0	1.0	0.5	0.5	0.5	2.0	2.0	2.0
$\sigma_{a,2}$	1.0	1.0	1.0	2.0	2.0	2.0	0.5	0.5	0.5

In Table 2 we provide semi-analytical solutions for the current, J, and sensitivity to the interface position, S, for the test problems. The results shown in Table 3 are the senstivities calculated using the differential operator method, S_{DO}, and the Malliavin method, S_{Mall}. The standard deviations of the mean for the estimated sensitivities are provided as $\sigma_{S_{\text{DO}}}$ and $\sigma_{S_{\text{Mall}}}$. These estimated statistical errors indicate that both methods provide estimates of the sensitivity that are in statistical agreement with the solutions in Table 2. Further, we observe that the two methods provide different levels of statistical uncertainty, indicating that for different problems one of the methods will have an advantage over the other in terms of computational efficiency. That is, one method will reach a specific level of statistical uncertainty with fewer particles simulated and less computational expense than the other.

The results shown in Table 4 are the senstivities calculated using the T_n simulation method instead of the R_n method. Again, results are given for both the differential operator method, $\tilde{S}_{\text{DO}}$, and the Malliavin method, $\tilde{S}_{\text{Mall}}$. As expected, the additional random sampling increases the statistical variance in both the estimation of the current (not shown) and of the sensitivities. Despite the inconsistency between the derivation method and the tally method, we still observe that the results are in statistical agreement with the benchmark results and that the two sensitivity methods provide different levels of statistical uncertainty.

Table 2: Benchmark results for test problems.

	1	2	3	4	5	6	7	8	9
J	0.05321	0.07956	0.12765	0.00917	0.02768	0.09127	0.11353	0.10265	0.10602
S	0.03977	0.06894	0.13266	0.01972	0.06307	0.23080	-0.04025	-0.00615	0.01953

Table 3: Results for test problems using R_n tally estimators.

	1	2	3	4	5	6	7	8	9
S_{DO}	0.03977	0.06875	0.13242	0.01972	0.06306	0.23056	-0.04017	-0.00599	0.01946
S_{Mall}	0.03982	0.06900	0.13279	0.01969	0.06324	0.23093	-0.04004	-0.00608	0.01981
$\sigma_{S_{\text{DO}}}$	0.00005	0.00009	0.00017	0.00002	0.00007	0.00020	0.00010	0.00009	0.00011
$\sigma_{S_{\text{Mall}}}$	0.00004	0.00006	0.00009	0.00002	0.00006	0.00018	0.00024	0.00032	0.00045

Table 4: Results for test problems using T_n tally estimators.

	1	2	3	4	5	6	7	8	9
$\tilde{S}_{\text{DO}}$	0.03925	0.06867	0.13248	0.01965	0.06310	0.23039	-0.04181	-0.00686	0.01871
$\tilde{S}_{\text{Mall}}$	0.03954	0.06882	0.13199	0.01956	0.06348	0.23214	-0.04029	-0.00597	0.01934
$\sigma_{\tilde{S}_{\text{DO}}}$	0.00044	0.00026	0.00022	0.00004	0.00018	0.00049	0.00131	0.00100	0.00101
$\sigma_{\tilde{S}_{\text{Mall}}}$	0.00020	0.00028	0.00042	0.00021	0.00039	0.00078	0.00030	0.00023	0.00023

6. CONCLUSIONS

We have compared the differential operator method, which has been widely used within the transport community, with the Malliavin sensitivity method on a non-scattering transport problem, Numerical results demonstrated that the two methods provided estimates of the sensitivity that were in statistical agreement with analytical results. In some cases the Malliavin sensitivity calculations provided improved computational efficiency. These efficiency gains indicate that the method warrants further investigation. Future work that extends these sensitivity evaluations to more general transport problems that include scattering is desirable as is investigation of the consequence of applying Monte Carlo approximation to fundamentally distinct tallies; see the discussion following (8). In general, conditions for the convergence of the sensitivity estimators to the derivative of the expectations, and whether the same weightings can be used given the distinct tallies would benefit from further analyses.

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REFERENCES

[1] H. Rief, "A synopsis of Monte Carlo perturbation algorithms", *Journal of Computational Physics*, Vol. 111(1), pp. 33-48 (1994). doi:10.1006/jcph.1994.1041.

[2] A. K. Hess, J. S. Hendricks, G. W. McKinney, L. L. Carter, "Verification of the MCNP$^{\text{TM}}$ Perturbation Correction Feature for Cross-Section Dependent Tallies", Technical Report LA-13520, Los Alamos National Laboratory (1998).

[3] P. Malliavin, "Stochastic calculus of variations and hypoelliptic operators", *Proc. Int. Symp. on Stochastic Differential Equations* Kyoto, 1976, pp. 195-263, New York (1976).

[4] P. Glasserman, *Monte Carlo Methods in Financial Engineering*, Applications of mathematics: stochastic modelling and applied probability, Springer (2004). doi:10.1007/978-0-387-21617-1.

[5] S. Asmussen, P. W. Glynn, *Stochastic Simulation: Algorithms and Analysis*, Stochastic Modelling and Applied Probability, Springer New York (2007). doi:978-0-387-69033-9.

[6] S. D. Bond, B. C. Franke, R. B. Lehoucq, J. D. Smith, S. A. McKinley, “Sensitivity Analyses for Monte Carlo Sampling-Based Particle Simulations”, Techical Report SAND2022-12721, Sandia National Laboratories (2022).

[7] E. Fournié, J.-M. Lasry, J. Lebuchoux, P.-L. Lions, N. Touzi, “Applications of Malliavin calculus to Monte-Carlo methods in finance II”, *Finance and Stochastics*, Vol. 5, pp. 201-236 (2001).

[8] T. P. Burke, B. C. Kiedrowski, “Monte Carlo Perturbation Theory Estimates of Sensitivities to System Dimensions”, *Nuclear Science and Engineering*, Vol. 189, pp. 199-223 (2018).

[9] J. A. Favorite, K. C. Bledsoe, D. I. Ketcheson, “Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products”, *Nuclear Science and Engineering*, Vol. 163, pp. 73-84 (2009).

[10] J. Spanier, E. M. Gelbard, *Monte Carlo Principles and Neutron Transport Problems*, Addison-Wesley Publishing Company (1969).

[11] J.D. Smith, R.B. Lehoucq, B.C. Franke, “A Stochastic Calculus Approach to Boltzmann Transport,” In *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering* (2023).