

# Application of the DiffeRential Evolution Adaptive Metropolis (DREAM) Method for Uncertainty Quantification in Inverse Transport Problems

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## INTRODUCTION

In the problem of inverse radiation transport, measurements of particle leakages from radioactive source/shield systems are used to infer unknown parameters within the systems. This reconstruction can be accomplished by finding the physical parameters of the unknown system that minimize the difference between calculated detector responses and measured detector responses. In recent years, a variety of optimization algorithms has been successfully applied to this task [1–4], but studies in quantification of uncertainties in the final calculated parameters for the unknown system have been limited, despite the fact that these parameters were determined by using information from detector measurements that contain inherent uncertainties. The Levenberg-Marquardt method employed in Ref. [1] provides a covariance matrix that gives a measure of uncertainty for problems in which errors are normally distributed and the model is linear in its parameters [5]. Reference [4] also provided quantified uncertainties in reconstructed parameters, although the method for propagating them from measurement uncertainties was not identified.

In order to further address the issue of uncertainty quantification in inverse problems, we recently applied the generalized linear-least squares (GLLS) approach in tandem with the Levenberg-Marquardt optimization method [6]. This method was found to be adept at quantifying uncertainty for problems with relatively few (~2–3) unknown parameters but tended to break down for larger numbers of unknowns. In this work, we apply the DiffeRential Evolution Adaptive Metropolis (DREAM) [7] method for uncertainty quantification to inverse problems with larger numbers of unknown parameters.

## APPLICATION OF DREAM TO INVERSE TRANSPORT PROBLEMS

### Markov Chain Monte Carlo Methods

Markov Chain Monte Carlo (MCMC) methods provide a generalized methodology for obtaining the posterior distribution of the unknown parameters in an inverse transport problem. This posterior distribution  $p(\mathbf{u}|M_o)$  represents the probability of a model  $\mathbf{u}$  (where  $\mathbf{u}$  is a vector representing postulated values for the unknown

parameters) given observed measurements  $M_o$ . This distribution is proportional to a likelihood function times a prior probability distribution. For this study, it was assumed that the prior distribution contains an equal probability that the parameter lies somewhere within its constraints, and a probability of zero that the parameter lies outside its constraints. The likelihood function was defined as

$$p(M_o|\mathbf{u}) = \exp\left[-\frac{1}{2}\sum_{d=1}^D\left(\frac{M_d(\mathbf{u}) - M_{d,o}}{\sigma_d}\right)^2\right], \quad (1)$$

where  $D$  is the total number of detector measurements,  $M_d(\mathbf{u})$  is the calculated response for detector  $d$  for postulated parameter set  $\mathbf{u}$ ,  $M_{d,o}$  is the observed measurement for detector  $d$ , and  $\sigma_d$  is the uncertainty in the measurement for detector  $d$ . The goal of the inverse problem is to find the regions for which  $p(M_o|\mathbf{u})$  is at or near its maximum.

In the traditional MCMC approach, a single Markov chain is employed. The chain begins at some initial parameter set  $\mathbf{u}_t$  [for which  $p(\mathbf{u}_t|M_o)$  is calculated], and then a trial parameter set is created. The posterior  $p(\mathbf{u}_{t+1}|M_o)$  is calculated for this trial parameter set, and this trial set is either accepted or rejected according to the Metropolis acceptance probability

$$\alpha(\mathbf{u}_t, \mathbf{u}_{t+1}) = \min\left[\frac{p(\mathbf{u}_t|M_o)}{p(\mathbf{u}_{t+1}|M_o)}, 1\right]. \quad (2)$$

According to Eq. (2), if the trial point has a posterior smaller than the current chain state (i.e., parameters  $\mathbf{u}_{t+1}$  yield a closer match between calculated and observed measurements), then the acceptance probability is 1 and the chain is moved to the trial state. If parameters  $\mathbf{u}_{t+1}$  do not lead to a closer match between calculated and observed measurements, they are still accepted with a probability equal to  $p(\mathbf{u}_t|M_o)/p(\mathbf{u}_{t+1}|M_o)$ . The chain progresses in this way until it creates the full posterior distribution describing the probabilities for the values of the unknown parameters.

### The DREAM Method

Traditional MCMC approaches have generally been inefficient because trial parameters are either too close to the current point (leading to a high acceptance rate but slow convergence to the posterior distribution) or they are

too far from the current point (leading to a low acceptance rate). The issue of choosing trial parameters has been explored for many years. The DREAM algorithm has been particularly successful at finding appropriate trial parameters. DREAM has been shown to greatly increase the speed of the MCMC process and has also been shown to be highly successful for solving difficult optimization problems in the presence of noise [8]. DREAM employs simultaneous multiple Markov chains (generally 3–5) and uses the differential evolution [9] algorithm to generate trial points for each chain.

Suppose we have a set of  $N$  chains, each containing a postulated parameter set  $\mathbf{u}_i$  ( $i = 1, \dots, N$ ). For chain  $i$ , the differential evolution approach generates a trial point according to

$$\mathbf{u}_{i,trial(inter)} = \mathbf{u}_i + \gamma(\mathbf{u}_{R1} - \mathbf{u}_{R2}) + \mathbf{e}_i. \quad (3)$$

In Eq. (3),  $\mathbf{u}_{R1}$  and  $\mathbf{u}_{R2}$  are the current states of two randomly selected chains that are different from chain  $i$  and different from each other. The term  $\gamma$  is a scalar parameter generally set equal to  $2.38/\sqrt{2m}$ , where  $m$  is the number of unknown parameters in the problem. The term  $\mathbf{e}_i$  is a small scalar value, generated randomly for each  $i$  and equally likely to be positive or negative, used to increase diversity in the trial chain values. The subscript *inter* on  $\mathbf{u}_{i,trial(inter)}$  indicates that this is an intermediate trial; the final trial state occurs after the differential evolution crossover operation. The crossover operation is used to choose whether the final trial vector will take parameter  $u^j, j = 1, \dots, M$  from  $\mathbf{u}_{i,trial(inter)}$  or its parent vector  $\mathbf{u}_i$ . This selection process follows the rule (for chain  $i$  and parameter  $j$ ):

$$u_{i,trial}^j = \begin{cases} u_{i,trial(inter)}^j, & \text{if rand} < CR, \\ u_i^j, & \text{otherwise,} \end{cases} \quad (4)$$

where rand is a random number between 0 and 1 and CR is called the crossover probability, which may be 1/3, 2/3, or 1. The value of CR is chosen at random from one of these three options for each crossover operation. In the case of multiple chains, the Metropolis ratio [Eq. (2)] becomes

$$\alpha(\mathbf{u}_1, \dots, \mathbf{u}_N; \mathbf{u}_{1,trial}, \dots, \mathbf{u}_{N,trial}) = \min \left[ \frac{p(\mathbf{u}_1|M_o) + \dots + p(\mathbf{u}_N|M_o)}{p(\mathbf{u}_{1,trial}|M_o) + \dots + p(\mathbf{u}_{N,trial}|M_o)}, 1 \right]. \quad (5)$$

The original DREAM algorithm was extended to what is called the DREAM(ZS) method [10], where the terms  $\mathbf{u}_i$ ,  $\mathbf{u}_{R1}$ , and  $\mathbf{u}_{R2}$  correspond to parameter values drawn from an archive of past chain states rather than from the current chain states. This method of sampling

from past states was shown to be more effective than the original DREAM algorithm [10].

It is the DREAM(ZS) method that has been implemented in this work. This method begins by creating a (random) archive of potential solutions. The values of  $\mathbf{u}_i$ ,  $\mathbf{u}_{R1}$ , and  $\mathbf{u}_{R2}$  in Eq. (3) are then created by drawing a random solution from the archive, and the method proceeds to update the chains according to Eqs. (3)–(5). Every  $m^{\text{th}}$  generation (where  $m$  is usually  $\sim 10$ ), the current chain states are added to the archive so that as the algorithm progresses the archive grows, generally adding [due to the selection performed by the Metropolis ratio, Eq. (5)] better solutions until the chains approach the region of the actual parameter values. The time spent searching for this region is generally referred to as the “burn-in” period. Once the algorithm reaches the maximum number of generations, the burn-in results are discarded and the remainder of the archive is used to build the posterior distribution and calculate the means and standard deviations of the unknown parameters. In this work, the burn-in period is defined to be half of the total number of generations (specified in advance by the user). After the burn-in results are discarded, the archive values can be used to calculate a mean value and standard deviation for each unknown parameter.

The DREAM method has been implemented into INVERSE, Los Alamos National Laboratory’s toolset for solving inverse transport problems. When analyzing decay gamma rays, INVERSE uses only the peaks in the spectrum. Therefore, in this work, transport calculations used in the DREAM method are performed using a deterministic ray-tracing routine [11].

## NUMERICAL TEST CASES

Consider the geometry shown in Fig. 1. An 8.741-cm radius source of highly enriched uranium (HEU) of 94.73%  $^{235}\text{U}$  and 5.27%  $^{238}\text{U}$  (by weight) is surrounded by layers of lead (12.4–12.9 cm) and aluminum (12.9–13.2 cm) shielding. The simulated total leakages from the system for the 144-, 186-, 766-, and 1001-keV uranium emission lines are given in Table I. These leakages were generated using MCNP and have uncertainties representative of actual measurements using a high-purity germanium detector.

Two test cases will be considered. In the first, only a single parameter is unknown. This case is used to illustrate the equivalence of uncertainties obtained by the Levenberg-Marquardt/GLLS method of Ref. [6] and the DREAM method. In the second test case, four unknown parameters are considered. This case illustrates the application of DREAM to a problem in which the GLLS method is unable to accurately quantify uncertainties.

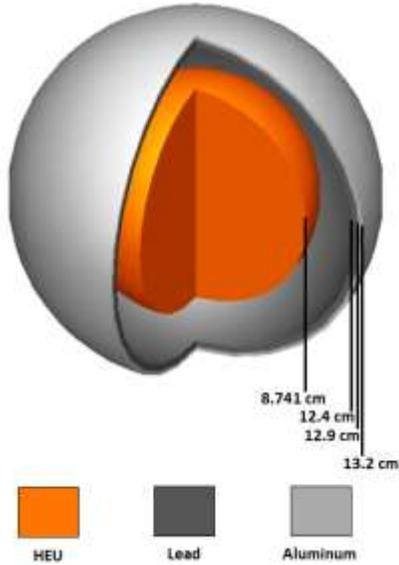


Figure 1. Test Geometry.

TABLE I. Simulated  $4\pi$  Leakage Measurements for the Test Geometry

Energy Line (keV)	Simulated Measurement ( $\gamma/s$ )
144	$9.96 \times 10^{-1} \pm 0.56\%$
186	$4.67 \times 10^3 \pm 0.12\%$
766	$2.53 \times 10^3 \pm 4.26\%$
1001	$9.86 \times 10^3 \pm 2.32\%$

### Test Case 1

In the first numerical test problem, only the 8.741-cm source radius was unknown. Ten independent trials of the Levenberg-Marquardt/GLLS method and the DREAM algorithm were considered. In each independent trial of the Levenberg-Marquardt/GLLS method, a different initial guess for the unknown parameter was used, while each independent trial of DREAM used a different random number seed. In all 10 trials, the GLLS method calculated a radius of  $8.766 \pm 0.054$  cm. In all 10 DREAM trials, the radius was calculated to be 8.766 cm, and the uncertainty ranged from 0.053 cm to 0.055 cm. The similar results obtained by the two methods suggest, but do not prove, that the uncertainties are accurately quantified. We are working on methods to verify these uncertainties.

### Test Case 2

In the second numerical test problem, the three internal radii (8.741, 12.4, and 12.9 cm) and the weight fractions of the uranium source were considered to be unknown. In 20 independent trials, the Levenberg-Marquardt/GLLS approach was unable to successfully locate the unknown parameters and accurately quantify

uncertainty in them. In 18 of the trials, an uncertainty of 100% was calculated for at least one parameter. In the two other trials, highly imprecise (though accurate) values ( $5.550 \pm 4.440$  cm and  $5.352 \pm 4.643$  cm) were calculated for the source radius. In none of the 20 cases was the parameter set leading to the global minimum between the measured and calculated detector fluxes found.

The DREAM method successfully found the parameters corresponding to the region near the global minimum of the likelihood function and quantified uncertainties in each of 20 independent trials. The average calculated values and uncertainties (95% confidence intervals) for the parameters using the DREAM method are given in Table II. The actual parameter values fall well within the calculated uncertainty bands obtained by the DREAM method, suggesting that the uncertainty bands are reasonable. However, we are working on methods to verify that the calculated uncertainty bands are accurate. We are also exploring the reason why slight discrepancies occur for the calculated values and uncertainties of the source radius across the 20 test trials.

## CONCLUSIONS

Recently, the generalized linear-least squares (GLLS) method was applied to uncertainty analysis in inverse transport problems. This method was demonstrated to be highly effective for problems with a relatively small ( $\sim 2-3$ ) number of unknown parameters but broke down when more unknown parameters were considered. Therefore we have implemented the Differential Evolution Adaptive Metropolis (DREAM) method for uncertainty quantification for more difficult inverse problems. The increased performance of the DREAM method over the GLLS method for a problem with four unknown parameters has been demonstrated.

Future work with uncertainty analysis for inverse transport problems includes determining when to use GLLS or to use DREAM, implementing a method to automatically detect when DREAM has sufficiently sampled the posterior distribution, and making improvements to DREAM so that it requires fewer transport calculations to accurately quantify uncertainty. In order for DREAM to be applicable to more than spherically symmetric geometries, it will be necessary to implement parallelization into the algorithm. This is an area of current research. Also, as mentioned above, we are investigating methods to verify the accuracy of the DREAM uncertainties.

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TABLE II. Results of 20 Independent Trials of the DREAM Method for Test Case 2

Trial	Radius 1 (cm)	Radius 2 (cm)	Radius 3 (cm)	<sup>235</sup> U Weight Fraction	Run Time (s)
1	9.396 ± 2.306	12.39 ± 0.29	12.89 ± 0.29	0.9525 ± 0.0157	114.2
2	9.374 ± 2.289	12.39 ± 0.29	12.89 ± 0.29	0.9528 ± 0.0157	114.5
3	9.322 ± 2.248	12.39 ± 0.29	12.89 ± 0.30	0.9524 ± 0.0155	114.0
4	9.256 ± 2.263	12.40 ± 0.29	12.90 ± 0.30	0.9519 ± 0.0155	114.1
5	9.476 ± 2.299	12.37 ± 0.28	12.87 ± 0.28	0.9534 ± 0.0156	114.0
6	9.186 ± 2.089	12.41 ± 0.28	12.91 ± 0.29	0.9515 ± 0.0147	114.2
7	9.466 ± 2.415	12.38 ± 0.29	12.88 ± 0.30	0.9533 ± 0.0164	114.2
8	9.330 ± 2.189	12.39 ± 0.28	12.89 ± 0.29	0.9525 ± 0.0151	115.0
9	9.254 ± 2.252	12.40 ± 0.29	12.90 ± 0.30	0.9518 ± 0.0154	113.8
10	9.297 ± 2.276	12.39 ± 0.30	12.90 ± 0.30	0.9522 ± 0.0158	114.0
11	9.269 ± 2.157	12.39 ± 0.28	12.90 ± 0.28	0.9521 ± 0.0150	114.4
12	9.390 ± 2.218	12.38 ± 0.27	12.88 ± 0.28	0.9529 ± 0.0150	113.5
13	9.525 ± 2.357	12.37 ± 0.28	12.87 ± 0.28	0.9537 ± 0.0158	119.8
14	9.315 ± 2.194	12.39 ± 0.27	12.89 ± 0.28	0.9525 ± 0.0149	114.7
15	9.479 ± 2.484	12.38 ± 0.29	12.88 ± 0.30	0.9534 ± 0.0165	114.6
16	9.351 ± 2.399	12.40 ± 0.31	12.90 ± 0.31	0.9524 ± 0.0164	114.1
17	9.320 ± 2.316	12.40 ± 0.29	12.90 ± 0.30	0.9523 ± 0.0161	113.5
18	9.329 ± 2.365	12.40 ± 0.28	12.90 ± 0.29	0.9524 ± 0.0160	116.0
19	9.359 ± 2.258	12.39 ± 0.28	12.89 ± 0.29	0.9526 ± 0.0153	116.6
20	9.356 ± 2.201	12.38 ± 0.27	12.88 ± 0.28	0.9527 ± 0.0151	114.2