Application of Generalized Linear Least-Squares for Uncertainty Quantification in Inverse Transport Problems

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INTRODUCTION

Recently, inverse transport problems in spherical and cylindrical source/shield systems have been successfully solved using various optimization algorithms, including Levenberg-Marquardt [1,2], Differential Evolution [3], and Mesh Adaptive Direct Search [4]. In all of these approaches, the inverse problem was solved by finding the physical parameters of the unknown system that minimize the difference between calculated detector responses and measured detector responses. However, the uncertainties in the final calculated parameters of the unknown system were not accounted for, despite the fact that they are determined by using information from detector measurements that contain inherent uncertainties. In this work, we apply the generalized linear least-squares (GLLS) approach to quantify the uncertainties of the calculated parameters. This approach is an adaptation of that used by the TSURFER [5] module of Oak Ridge National Laboratory's SCALE code system, in which the GLLS method is used to quantify uncertainties in k_{eff} in critical systems.

APPLICATION OF GLLS TO INVERSE TRANSPORT PROBLEMS

Los Alamos National Laboratory's code INVERSE is used to apply various optimization methods to solve inverse transport problems. The goal of all of these methods is to minimize a χ^2 difference between a set of measured detector responses and detector responses calculated using postulated values for the unknown parameters of the system,

$$\chi^2 \equiv \sum_{d=1}^{D} \left(\frac{M_{d,0} - M_d(\mathbf{u})}{\sigma_{d,0}} \right)^2 . \tag{1}$$

In Eq. (1), $M_{d,0}$ is the measured value for detector response, d, $M_d(\mathbf{u})$ is the value of the detector response calculated using a set of postulated parameters $\mathbf{u}$, and $\sigma_{d,0}$ is the uncertainty in the measurement for response d. INVERSE has been shown to successfully find the parameters $\mathbf{u}$ that minimize χ^2 but has previously not quantified the uncertainties in these calculated parameter values.

Application of the GLLS method for uncertainty analysis in inverse problems is a two-step process. In the first step, INVERSE uses an optimization algorithm to determine the system parameters that lead to the closest match between calculated detector responses and the mean values of the measured detector responses. In this step, uncertainties are used to formulate χ^2 but not to compute uncertainties in unknown parameters. In the second step, the GLLS approach is used to further reduce discrepancies between the calculated and measured responses. By adjusting all of the data which contribute uncertainty to the system (the calculated values for the unknown parameters and the detector measurement values) within their uncertainty bands (utilizing sensitivity coefficients calculated by INVERSE), the overall consistency between calculated and measured values is maximized. If the original set of calculated parameters and the measured detector responses are consolidated in a consistent manner (i.e., correctly accounting for uncertainties), then the adjusted responses and adjusted physical parameters will be better estimates of the true values, because the revised responses and parameters are based upon more information than was available in either the original calculations or measurements alone. Using the additional information in the adjustment process will reduce all sources of uncertainty, including the uncertainties in the calculated model parameters (prior to GLLS adjustment, uncertainties in the model parameters are assumed to be 100%).

NUMERICAL TEST PROBLEMS

Except where otherwise stated, the optimization algorithm used by INVERSE was a hybridization of Differential Evolution and Levenberg-Marquardt, where the former is used to establish an accurate initial guess and the latter is used for fine-tuning. This process is described in [6].

Cylindrical Geometry

Consider the sample cylindrical geometry shown in Fig. 1. A source of highly enriched uranium (HEU) containing 94.73% ^{235}U and 5.27% ^{238}U is surrounded by layers of nickel and aluminum shielding. The source region has a radius of 4.00 cm, and the axial locations of the source bottom and top are at $z = 2.00$ cm and $z = 6.00$ cm, respectively. All three of these dimensions are assumed to be unknown. Uncollided photon fluxes for the four strongest emission lines of uranium (144, 186, 766, and 1001 keV) are measured at two locations outside the geometry, (r,z) = (9.00 cm, 4.00 cm), and (r,z) = (0.00 cm, 8.00 cm). Measured detector responses were simulated using MCNP with a small number of particle histories in order to simulate the uncertainty associated with actual measurements. The simulated measurements and their uncertainties are given in Table I.

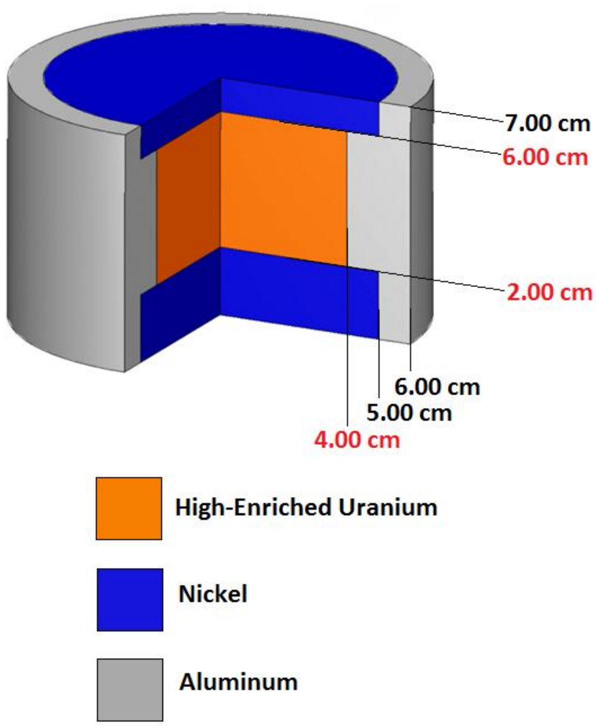

Fig. 1. Cylindrical Test Geometry. Dimensions shown in red are unknown.

In the inverse analysis step, INVERSE determined the source radius to be 4.021 cm and the bottom and top of the source to be at 2.012 cm and 5.997 cm. Without uncertainty quantification, there is no information on the confidence in these values after this first step. After the GLLS step, however, we have a high confidence in the calculated solution. After GLLS adjustment and uncertainty quantification, the uranium radius is calculated to be 3.980 ± 0.110 cm, the uranium bottom is calculated to be 2.091 ± 0.158 cm, and the uranium top is calculated to be 5.993 ± 0.015 cm. The results for this test problem are presented in Table II.

Table I. Simulated Detector Measurements for the Cylindrical Inverse Problem

Detector Location 1 (r, z) = (9.00 cm, 4.00 cm)	
Energy Line (keV)	**Simulated Measurement**
144	$6.72 \times 10^{1} \pm 10.46\%$
186	$6.36 \times 10^{2} \pm 8.02\%$
766	$5.84 \times 10^{-1} \pm 4.70\%$
1001	$2.19 \times 10^{0} \pm 2.46\%$
Detector Location 2 (r, z) = (0.00 cm, 8.00 cm)	
Energy Line (keV)	**Simulated Measurement**
144	$6.63 \times 10^{1} \pm 12.32\%$
186	$1.21 \times 10^{3} \pm 8.71\%$
766	$2.12 \times 10^{0} \pm 3.19\%$
1001	$8.23 \times 10^{0} \pm 1.84\%$

Table II. Results of the Cylindrical Inverse Problem

Parameter	**Actual Value (cm)**	**Results of Step 1 Inverse Analysis (cm)**	**Results of Step 2 GLLS Adjustment and Uncertainty Quantification (cm)**
Radius of Uranium Cylinder	4.000	4.021	3.980 ± 0.110
Bottom of Uranium Cylinder	2.000	2.012	2.091 ± 0.158
Top of Uranium Cylinder	6.000	5.997	5.993 ± 0.015

Spherical Geometry

Now consider the geometry shown in Fig. 2. A sphere of HEU of radius 5.032 cm is surrounded by a shell of stainless steel with inner radius 6.000 cm and outer radius 7.000 cm. All three of these radii are unknown. The total (4π) leakage from the system was simulated using MCNP, resulting in the detector responses shown in Table III.

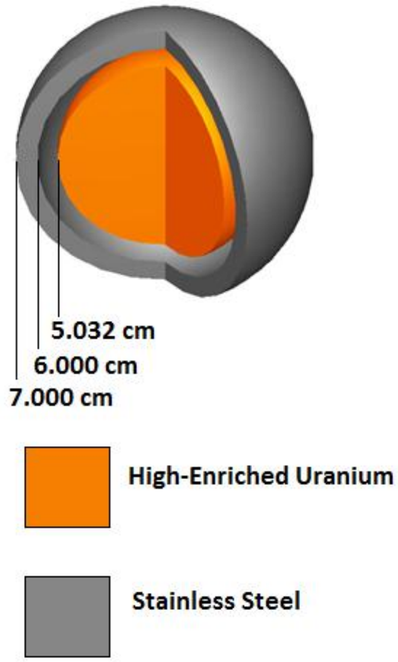

Fig. 2. Spherical Test Geometry. All three dimensions are unknown.

Table III. Simulated Measurements for the Spherical Test Geometry

Energy Line (keV)	Simulated Measurement
144	$3.895 \times 10^4 \pm 0.352\%$
186	$5.770 \times 10^5 \pm 0.110\%$
766	$8.481 \times 10^2 \pm 4.09\%$
1001	$3.158 \times 10^3 \pm 2.19\%$

Again using the Levenberg-Marquardt method, the INVERSE optimization step calculated the source radius and inner and outer shield radii to be 5.050 cm, 15.648 cm, and 16.838 cm, respectively. The source radius is calculated with high accuracy, but the shield radii are very inaccurate. The GLLS step quantifies this. Following GLLS adjustment and uncertainty quantification, the radius of the uranium sphere is calculated to be 5.050 ± 0.030 cm, and the inner and outer shield walls are calculated to be 15.671 ± 11.455 cm and 16.852 ± 11.490 cm, respectively. Thus, the GLLS method correctly identifies that we should have a high confidence in the calculation of the source radius but very low confidences in the calculated shield radii. This matches physical expectations, because for uncollided photons the 4π leakage is highly dependent on the thickness of the shield but largely independent of its position. The results for the spherical test problem are given in Table IV.

Table IV. Results of the Spherical Inverse Problem

Parameter	Actual Value (cm)	Results of Step 1 Inverse Analysis (cm)	Results of Step 2 GLLS Adjustment and Uncertainty Quantification (cm)
Radius of Uranium Source	5.032	5.050	5.050 ± 0.030
Inner Shield Radius	6.000	15.648	15.671 ± 11.455
Outer Shield Radius	7.000	16.838	16.852 ± 11.490

One interesting question to consider is whether the calculated uncertainties are dependent on the initial guess used by the Levenberg-Marquardt method. Since the GLLS procedure employs the derivatives of the measured responses with respect to the values calculated for the unknown parameters in the inverse analysis step, any initial guess that finds the global optimum will result in the same calculated values and uncertainties for the unknown quantities. What if, however, the initial guess is poor and the Levenberg-Marquardt method falls into a local minimum? To analyze this question, the spherical test problem was run without using Differential Evolution to generate an initial guess. Instead, poor initial guesses of 1.000 cm, 2.300 cm, and 3.100 cm were used for the source and inner and outer shell radii, respectively. In this case, the inverse analysis step fell into a local minimum corresponding to radii of 1.287 cm, 2.69871 cm, and 2.69872 cm. In the GLLS step, uncertainties of 100% were calculated for all three of these dimensions. Thus, GLLS was able to identify that we should have no confidence in the calculated values. Further testing is being conducted to study the general performance of GLLS at identifying local optima.

SUMMARY AND CONCLUSIONS

The generalized linear least-squares method has been applied for uncertainty quantification in spherical and cylindrical inverse transport problems. The GLLS methodology is the second step in a two-step process now employed by Los Alamos National Laboratory's inverse transport analysis code INVERSE. In the first step, INVERSE identifies the unknown parameters of the radioactive source/shield system without quantifying the parameter uncertainties. In the second step, the GLLS method is used to further adjust the calculated parameters and quantify the uncertainties of these parameters. In two numerical test problems, the GLLS method correctly identified the calculated parameters for which we should have a high degree of confidence and those for which we should have a low degree of confidence.

The GLLS method assumes that variations in the measured responses depend linearly on the physical parameters in the system. This assumption leads to a computationally inexpensive approach for uncertainty quantification. While the linearity assumption was valid for the numerical test problems considered here, it is likely not valid for all inverse problems. A method of nonlinear uncertainty analysis, the Data Assimilation technique, was also recently shown to be successful in uncertainty quantification of inverse problems [7]. Therefore, our future work will include determining the classes of inverse transport problems where the linearity assumption breaks down and examining the application of nonlinear uncertainty quantification methods to those problems.

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