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A Hybrid Differential Evolution/Levenberg-Marquardt Method for Solving Inverse Transport Problems

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INTRODUCTION

Recently, the Differential Evolution (DE) optimization method was applied to solve inverse transport problems in finite cylindrical geometries and was shown to be far superior to the Levenberg-Marquardt optimization method at finding a global optimum for problems with several unknowns [1]. However, while extremely adept at finding a global optimum solution, the DE method often requires a large number (hundreds or thousands) of transport calculations, making it much slower than the Levenberg-Marquardt method. In this paper, a hybridization of the Differential Evolution and Levenberg-Marquardt approaches is presented. This hybrid method takes advantage of the robust search capability of the Differential Evolution method and the speed of the Levenberg-Marquardt technique.

OPTIMIZATION METHODS

The measurements considered in this paper are unscattered fluxes of discrete gamma-ray lines at points external to the source/shield system. Since scattering is neglected, a ray-trace technique can be used for transport calculations. This ray-trace technique, in which the angular domain of the problems is partitioned into several (hundreds or thousands) of discrete angles and the unscattered flux is calculated along each, is described in [2].

Differential Evolution

The Differential Evolution method was implemented for inverse transport problems of this type in [1]. The method uses a set of vectors $\mathbf{u}_i$, $i = 1,...,P$, that each contain a set of postulated values for the unknown parameters. P represents the total number of vectors, referred to as the population size. The fitness of each population member is determined using a χ^2 difference between a set of measured photon fluxes and fluxes calculated using the parameters of the population member. For population member i,

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

In this equation, $M_{d,0}$ is the measured value of the flux for detector d, $M_d(\mathbf{u}_i)$ is the value of the flux at detector d calculated using the set of postulated parameters $\mathbf{u}_i$ and $\sigma_{d,0}$ is the uncertainty in the measurement at detector d. In the inverse problem, we seek to find the population member with the globally minimum χ^2.

DE uses a generational process for optimization. Potential population members for generation $g+1$ are created by using weighted differences between population members of generation g. After P such children are created they are sorted in ascending order of χ_i^2. After this, a direct competition between the ith member of generation g and ith child $(i = 1,...,P)$ is implemented, with the better fit between the two becoming a member of generation $g+1$. This competition between parent and child ensures that the population members of generation $g+1$ have χ_i^2 values equal to or less than the χ_i^2 values of the corresponding population members in generation g. This generational process continues until a minimum of χ_i^2 is achieved.

Levenberg-Marquardt

The Levenberg-Marquardt (or simply Marquardt) method is a standard gradient-based optimization approach that was used to solve inverse problems in cylindrical geometries in [3]. The Marquardt method begins with an initial postulation of the unknown system parameters, then varies smoothly between the steepest-descent and inverse-Hessian methods to find a χ^2 minimum (here subscript i is dropped because Marquardt uses only a single potential solution). The Marquardt method has the advantage of requiring far fewer transport calculations to find a χ^2minimum than the Differential Evolution method. However, in problems with several unknown parameters the Marquardt method is heavily dependent on the accuracy of the initial guess for the unknown parameters. As illustrated in [1], when there are several unknown parameters this method often falls into local minima when random initial guesses are used (as would be the case for no prior information of the unknown parameter values).

Hybrid

A hybrid Differential Evolution/Marquardt method has been implemented to take advantage of the robust search capability of DE and the speed of Marquardt. In this technique, the DE method is first used to find an accurate initial guess for the Marquardt method. In order to quickly find an initial guess for Marquardt, the DE method is employed with a coarse angular partition in the ray-tracing calculations. This is accomplished by using 100 discrete values in the polar and azimuthal angles used by ray-tracing, as opposed to the 1000 discrete values we generally use. Using the parameters found with the coarse DE algorithm as initial guesses, the Marquardt method is then employed with the usual (1000 angles) angular partition to find the global minimum of χ^2.

NUMERICAL TEST PROBLEM

Consider the cylindrical geometry shown in Figure 1. The source is a cylinder of radius 2.0 cm and height 4.5 cm. Above and below the source are lead shield layers, each of radius 3.0 cm and height 0.5 cm. Outside the radial face of the source is a 1-cm thick region of void. This is all surrounded by a layer of aluminum shielding. The source has density 18.74 g/cm^3 and contains 94.73% ^{235}U and 5.27% ^{238}U (by weight). This is the same test geometry that was used in [1]. In that paper, it was shown that the Marquardt method using random initial guesses for the unknown parameters was able to determine the unknowns in just one of sixty test trials, while the DE method found the unknown parameters in all sixty test trials, but averaged over 2 hours of run time.

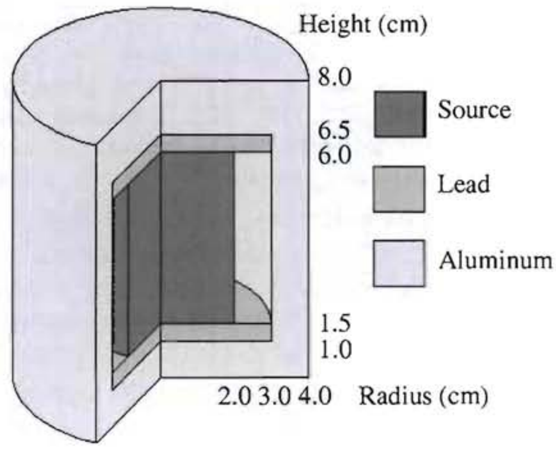

Fig. 1. Cylindrical test geometry.

Two detector locations are used here. The first lies below the geometry at a radius and height of $(r, z) = (0.0$ cm, -1.0 cm), and the second is located at $(r, z) = (10.0$ cm, 4.0 cm). At both these detector locations, the unscattered scalar photon fluxes of the 144-, 186-, 766-, and 1001-keV uranium emission lines are measured.

Measured data were simulated using two different methods. In the first, the same ray-tracing code as used in the optimization process (using 1000 discrete angles in each direction) was used. Thus, these measured data were exactly consisted with calculated data. In the second method, measurements were simulated using a Monte Carlo code, to produce less consistent, more realistic results.

In the numerical test problem, the weight fractions of ^{235}U and ^{238}U in the photon source are unknown, along with the density of the source region. Also unknown are the radial interface locations at 2.0 cm and 3.0 cm, along with the axial interface locations at 1.5 cm and 6.0 cm. The test problem thus has six unknowns (since two weight fractions must sum to 1.0, they only constitute one unknown) of three different types (dimension, density, and composition).

For the initial DE step of the hybrid algorithm a random initial population must be created. Interface locations are randomly generated within their constraints, so that the initial values for the 2.0 cm and 3.0 cm radii are randomly generated between 0.0 cm and 4.0 cm, while initial values for the 1.5 cm and 6.0 cm axial locations are randomly generated between 1.0 cm and 6.5 cm. The weight fraction of ^{235}U is generated randomly between 0.0 and 1.0, and the source density is generated randomly between 0.0 g/cm^3 and 25.0 g/cm^3. The population size used in the DE step was $P = 60$.

First consider the case of consistent measurements simulated using ray-tracing. Twenty trials of the hybrid method were run, each using different random number seeds (thus creating different initial populations for the DE step). All twenty trials found the correct parameter values, with an average run time of 23 minutes and 12 seconds. In [1], the DE method averaged over 2 hours to find these parameters. To illustrate the behavior of the hybrid method, we will consider a particular trial. Starting from the randomly generated initial population, the coarse DE method required 3 minutes and 1 second to find parameter values of

Weight Fractions: ^{235}U: 0.947487 ^{238}U: 0.052513
Source Density: 18.38 g/cm^3
Radii: 2.015 cm, 2.979 cm
Heights: 1.500 cm, 6.021 cm

Using these parameter values as the initial guess in the Marquardt method, the correct parameter values were found in 16 minutes and 24 seconds, for a total run time of 19 minutes and 25 seconds.

Using measurements simulated by Monte Carlo, all twenty trials of the hybrid method approached a minimum corresponding to parameter values of

Weight Fractions: ^{235}U: 0.9428 ^{238}U: 0.0572
Source Density: 19.43 g/cm^3
Radii: 1.858 cm, 3.400 cm
Heights: 1.498 cm, 5.694 cm

The average run time for the hybrid method was 28 minutes and 19 seconds. In [1], the DE method averaged over 2 hours of run time with Monte Carlo measurements.

CONCLUSIONS

Recently, the Levenberg-Marquardt and Differential Evolution optimization methods were applied to inverse transport problems in cylindrical radiation source/shield systems. The former technique is fast but tends to fall into a local minimum, while the latter technique is robust but is slower because it requires a much larger number of transport calculations. In this paper, a hybrid Differential Evolution/Levenberg-Marquardt approach is employed. This method first implements the DE method with a coarse angular partition in the transport calculations to find an initial guess for the Levenberg-Marquardt method that is near the global minimum. The Marquardt method then uses this guess with a fine angular partition to quickly find the global minimum. On a numerical test case, this hybrid method was found to be as robust as the DE method and to find the global optimum solution in significantly less time. The method was successful using both consistent and less-consistent, more realistic measurements.

We are currently exploring the proper size of the angular partition in the Differential Evolution to consistently create initial guesses for the Marquardt method that are accurate enough to find the global optimum in a variety of test problems. We are also exploring a hybrid DE/Marquardt method on problems that include scattering.

REFERENCES

1. K.C. BLEDSOE and J.A. FAVORITE, "A Comparison of the Differential Evolution and Levenberg-Marquardt Methods for Solving Inverse Transport Problems with Several Unknowns in Cylindrical Geometries," *Trans. Am. Nucl. Soc.*, **101**, 411-413 (2009).
2. J.A. FAVORITE, K.C. BLEDSOE, and D.I. KETCHESON, "Surface and Volume Integrals of Uncollided Adjoint Fluxes and Forward-Adjoint Flux Products," *Nucl. Sci. Eng.*, **163**, 73-84 (2009).
3. K.C. BLEDSOE and J.A. FAVORITE, "Using the Marquardt Method for Solutions of Inverse Transport Problems in Two-Dimensional Cylinders," *Trans. Am. Nucl. Soc.*, **96**, 545-547 (2007).