LA-UR-12-22365

Approved for public release; distribution is unlimited.

Title: Identification of Unknown Interface Locations in a Source/Shield System Using the Mesh Adaptive Direct Search Method

Author(s): Armstrong, Jerawan C.
Favorite, Jeffrey A.

Intended for: 2012 American Nuclear Society Annual Meeting, 2012-06-24/2012-06-28 (Chicago, Illinois, United States)

Identification of Unknown Interface Locations in a Source/Shield System Using the Mesh Adaptive Direct Search Method

Jerawan C. Armstrong and Jeffrey A. Favorite
Transport Applications Group (XCP-7)
Los Alamos National Laboratory
Los Alamos, NM, USA

American Nuclear Society Annual Meeting
Chicago, Illinois
June 24-28, 2012

Abstract (not a viewgraph)

The Levenberg-Marquardt (or simply Marquardt) and differential evolution (DE) optimization methods were recently applied to solve inverse transport problems. The Marquardt method is fast but convergence of the method is dependent on the initial guess. While it has been shown to work extremely well at finding an optimum independent of the initial guess, the DE method does not provide a global optimal solution in some problems. In this paper, we apply the Mesh Adaptive Direct Search (MADS) algorithm to solve the inverse problem of material interface location identification in one-dimensional spherical radiation source/shield systems, and we compare the results obtained by MADS to those obtained by Levenberg-Marquardt and DE.

These viewgraphs accompany a summary, LA–UR–12–0119.

Introduction

- The inverse transport problem is that of determining the unknown components of a radioactive source/shield system by analyzing the system's radiation signatures.

- Solving inverse transport problem is one of great importance in global security, material safeguards, and waste management.

- We consider a source/shield system of some gamma source surrounded by some shield, where both source and shield may be multilayered but assume that a material in each layer is homogeneous.

- The inverse transport problem includes the determination of (1) material interface locations, (2) source compositions, (3) shield materials, (4) material densities, and (5) combined unknown components.

- The Levenberg-Marquardt (or simply Marquardt) and differential evolution (DE) optimization methods were recently applied to solve inverse transport problems.

- In this paper, we apply the Mesh Adaptive Direct Search (MADS) algorithm to solve the inverse problem of material interface location identification in one-dimensional spherical radiation source/shield systems, and we compare the results obtained by MADS to those obtained by Levenberg-Marquardt and DE.

Minimization Problem

- The aim of the minimization problem is to find $x_* \in X$ such that $f(x_*) \leq f(x)$ for all $x \in X$, where $f: X \to (-\infty, \infty]$ is the objective function and $X \subseteq \mathbb{R}^n$ is the feasible domain.
  - $X = \mathbb{R}^n$: unconstrained problem
  - $X \subset \mathbb{R}^n$: constrained problem
  - An unconstrained minimization problem is simpler than a constrained one.

- Iterative methods of solving optimization problems:
  - Derivative-based algorithms
    - Require information about the gradient or higher derivatives in order to search for an optimal point.
  - Derivative-free algorithms
    - Do not use any derivative information in order to search for an optimal point.
    - Methodology - generate trial points and search for an optimal point by making direct comparison of each trial solution with the "best" point obtained thus far.

- The Levenberg-Marquardt algorithm is derivative-based. The DE and MADS algorithms are derivative-free.

- The DE algorithm is population-based and the MADS algorithm is frame-based – at each iteration finitely many trial points are considered.

Problem Formulation

- The forward transport equation:

$$\hat{\mathbf{\Omega}} \cdot \vec{\nabla} \psi(r, E, \hat{\mathbf{\Omega}}) + \Sigma_t(r, E)\psi(r, E, \hat{\mathbf{\Omega}}) - \int_{4\pi} d\hat{\mathbf{\Omega}}' \int_0^\infty dE' \Sigma_s(r, E' \to E, \hat{\mathbf{\Omega}}' \to \hat{\mathbf{\Omega}})\psi(r, E', \hat{\mathbf{\Omega}}')$$

$$= q(r, E, \hat{\mathbf{\Omega}}),$$

with vacuum boundaries,

$$\psi(r_b, E, \hat{\mathbf{\Omega}}) = 0, \ \hat{\mathbf{\Omega}} \cdot \hat{\mathbf{n}} < 0.$$

- Quantities of interest are $R_g = \langle \Sigma_g \psi \rangle, g = 1, \ldots, G$ where $\Sigma_g(r, E, \hat{\mathbf{\Omega}})$ is the detector response function.

- We consider the following minimization problem:

$$\min_{x \in X} f(x) \equiv \min_{x \in X} \sum_{g=1}^{G} \left(\frac{R_{g,0} - R_g(x)}{\sigma_{g,0}} \right)^2,$$

where $R_{g,0}$ is the measured value of the flux for detector g, $R_g(x)$ is the value of the flux at detector g calculated using the postulated interface locations x, $X \subset \mathbb{R}^n$ is the set of feasible interface locations, $\sigma_{g,0}$ is the uncertainty associated with the measurement at detector g, and G is the number of detectors.

Mesh Adaptive Direct Search (MADS)

- MADS is an algorithmic framework for minimizing an objective functional $f : X \rightarrow \mathbb{R} \bigcup \{+\infty\}$ under general constraints $x \in X \neq 0 \subseteq \mathbb{R}^n$.

- MADS is a derivative-free optimization technique introduced and analyzed by Audet and Dennis [*SIAM J. Optim. 17(2006), pp. 188-217*].

- MADS has strong convergence properties, where the convergence analysis is based on Clarke's calculus for nonsmooth functions.

- MADS is an iterative method that locates an optimal solution over the feasible domain by making direct comparison of the objective function values at some trial points lying on a spatial discretization called the mesh.

- At each iteration, MADS method generates a finite number of trial points on the mesh, evaluates an objective function at some trial points with an attempt to find a point with a lower objective function value than the current best iterate point found so far, and then adapts the fineness of the mesh to approach an optimum.

Mesh Structure of MADS Method

- At each iteration k, all trial points are constructed to lie on the mesh

$$M_k = \bigcup_{x \in V_k} \{x + \Delta_k^m D z : z \in \mathbb{N}^{n_D}\},$$

where
$\Delta_k^m > 0$ is the mesh size parameter,
D is an $n \times n_D$ matrix representing a fixed finite set of n_D directions in $\mathbb{R}^n$,
$V_k \subset \mathbb{R}^n$ is the set of all previously evaluated trial points by the start of iteration k (V_0 is the set of initial trial points).

- D is called the set of mesh directions and must have the following properties: D must be positive spanning (i.e., nonnegative linear combinations of its columns must span $\mathbb{R}^n$), and $D = GZ$ where G is a nonsingular $n \times n$ matrix and Z is an $n \times n_D$ integer matrix.

- The fixed set of directions is often chosen as $D = [I_n, -I_n]$, where I_n is the $n \times n$ identity matrix. For example, $n = 2$, then $D = \left[\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \right]$ and $n_D = 4$.

- Since the mesh M_k is the union of sets over V_k, all previously evaluated trial points before iteration k lie on M_k and all new trial points can be selected around these previously evaluated points using the directions in D.

MADS Iteration

- The iteration goal is to locate an improved mesh point (i.e., a trial point on the mesh with a lower objective function value than that at the current iterate point). There are no sufficient decrease requirements on the objective function value.

- Each MADS iteration is divided into two phases.

Phase I: Generate a finite number of trial points lying on the mesh and evaluate the test for feasibility and the objective function at these trial points. Phase I consists of 2 steps: Search and Poll.

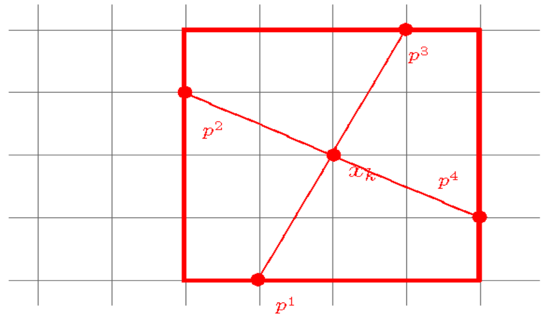
Search Step - trial points can be generated anywhere on the mesh and any strategy can be used.

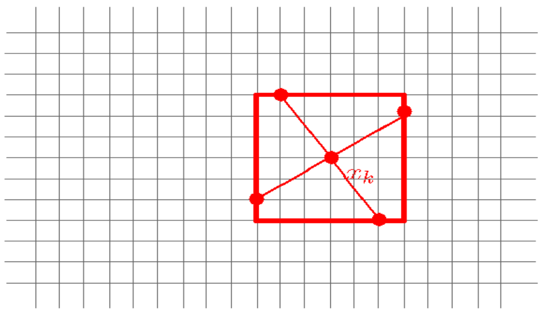
Poll Step - trial points are near the current iterate point and must be generated from a set of poll directions constructed by the MADS algorithms.

Phase II: Adapt the mesh size based on the outcome of Phase I. If an improved mesh point is found, the new mesh size must be greater than or equal to the current mesh size. Otherwise, the new mesh size must be reduced.

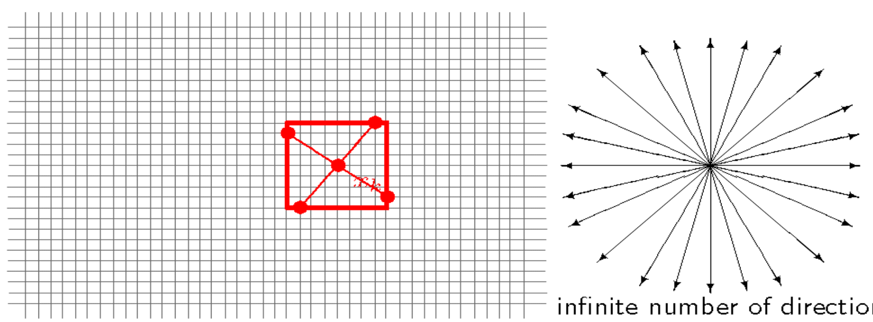
ORTHOMADS Directions for Generating Poll Trial Points

ORTHOMADS – 2008





Union of all normalized directions
grows dense in the unit sphere



infinite number of directions

- ORTHOMADS is deterministic.
  Results are reproducible on any machine.
- At any given iteration, the directions are orthogonal.

Numerical Test Implementation

- Uncollided gamma-ray leakages are computed by ray-tracing. We applied the ORTHOMADS algorithm [*Abramson, Audet, Dennis, and Le Digabel, SIAM J. Optim. 20(2009) pp. 297-319*] to identify of unknown interface locations. (The ORTHOMADS algorithm implemented in the NOMAD library is used.)

- The following MADS parameters are used:

  - A strategy for generating trial points in the Search step is: If an improved mesh point during poll iteration is found in the direction *d* then the new Search step will evaluate the objective function at a point further along in the direction *d*.

  - A set of poll directions is generated by ORTHOMADS with 2*n* directions and iteration is terminated immediately after an improved mesh point is found.

  - The updating rules of the mesh and poll sizes described in the Abramson *et al.* ORTHOMADS paper are used.

  - The extreme barrier approach (i.e., objective function values at infeasible points are set to infinity) is used to handle the closed constraints representing physical reality.

  - The stopping criteria are the objective function value is less than 1.0E-6 or the number of function evaluations is equal to 100000.

Numerical Test Results

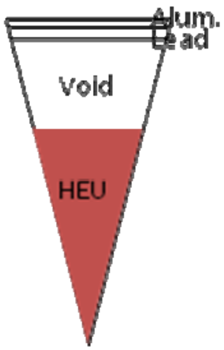


Table I. Outer Radii (cm) for the First Test Problem

Descriptor	HEU	Void	Aluminum
Actual outer radii	7.0	10.0	12.0
Initial guess	**1.0**	**2.0**	12.0
Marquardt	2.0280	11.9980	12.0
DE	7.0000	9.9998	12.0
MADS	7.0000	10.0000	12.0
Initial guess	**5.0**	**9.0**	12.0
Marquardt	6.9998	9.9999	12.0
DE	7.0000	9.9998	12.0
MADS	7.0000	10.0000	12.0

Numerical Test Results

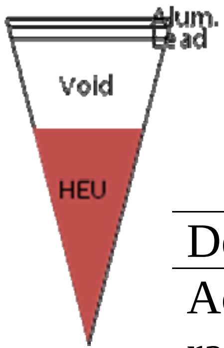


Table II. Outer Radii (cm) for the Second Test Problem

Descriptor	HEU	Void	Lead	Aluminum
Actual outer radii	8.741	12.4	12.9	13.2
Initial	**1.0**	**2.0**	**3.0**	13.2
Marquardt	2.3050	2.3162	2.6236	13.2
DE	9.4915	12.2163	12.7064	13.2
MADS	8.7410	12.4000	12.9000	13.2
Initial	**2.0**	**5.0**	**10.0**	13.2
Marquardt	6.9969	7.0125	7.3928	13.2
DE	9.4915	12.2163	12.7064	13.2
MADS	8.7410	12.4000	12.9000	13.2
Initial	**3.0**	**6.0**	**9.0**	13.2
Marquardt	7.1365	7.1414	7.5312	13.2
DE	9.4915	12.2163	12.7064	13.2
MADS	8.7410	12.4000	12.9000	13.2

Conclusions

- We applied the MADS method to solve the inverse problem of material interface location identification in one-dimensional spherical uncollided radiation source/shield systems.

- Our test problems show that the Marquardt and DE methods are not able to locate an optimal solution for some problems, but the MADS method can find a global optimal solution where convergence of the method does not depend on the initial guess and the computational time is reasonably fast.

- The MADS method produces more robust results than Marquardt and DE because both global and/or local search strategies are used in each iteration.

- We are currently working on:

    - Applying advanced features of the MADS methods to solve other radiation transport inverse problems.

    - Developing algorithms by combing the MADS methods with other search strategies to locate all global and local optimal solutions.