Variable Change Technique Applied in Constrained Inverse Transport Applications

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INTRODUCTION

The inverse transport problem is often viewed as a multi-variable optimization problem and treated using iterative minimization approaches such as a nonlinear conjugate gradient (CG) method [1]. The purpose is to infer the material properties within the object under investigation from limited information that is measured about the angular flux. Physical constraints must be imposed on the unknown material properties during the iteration process; for example the cross sections must be non-negative and the average scattering cosine must be in the interval (–1, 1). If these constraints are not imposed during the iteration, the forward-transport solver may be given a problem whose solution does not exist and the method may fail.

There are many ways that the constraints could be imposed. Our purpose in this paper is to present a variable-change technique that is simple to implement and seems to work well. The key part of this technique is to find a well-behaved function for the variable change. We describe what we have chosen, show how it is implemented, and provide results from simple test problems.

We illustrate our method using a simple one-group version of the neutron transport equation for a non-multiplying material with linearly anisotropic scattering:

$$\begin{aligned}&\underline{\Omega}\bullet\underline{\nabla}\psi(\underline{r},\underline{\Omega},t)+\Sigma_t(\underline{r})\psi(\underline{r},\underline{\Omega},t)\\&=\frac{1}{4\pi}\Sigma_s(\underline{r})\left[\phi(\underline{r},t)+3g\underline{\Omega}\bullet\underline{J}(\underline{r},t)\right]\\&+S_{ext}(\underline{r},\underline{\Omega},t)\ .\end{aligned} \tag{1}$$

Here Σ_t and Σ_s are macroscopic total and scattering cross sections and g denotes the averaging scattering cosine. These three parameters are properties of the material in the object being studied. The task of a "forward" transport problem is to solve for the angular flux ψ if the material properties (Σ_t, Σ_s, g) are provided as a function of position in the spatial domain. An inverse transport problem, on the contrary, attempts to determine the material distribution in some domain given limited information about the angular flux, ψ. Most inverse methods attempt to find the material properties (Σ_t, Σ_s, g) and then use this information to infer the material distribution within the object.

VARIABLE TRANSFORM TECHNIQUE

We start with an optimization problem: determine the material distribution that minimizes the objective function, which is defined below.

$$\Phi=\frac{1}{2}\sum_{i=1}^{N}(\frac{P_i-M_i}{M_i})^2\ . \tag{2}$$

Here Φ is the objective function, P and M are predicted and measured values respectively, and N is the total number of measurements (each of which depends on the angular flux) recorded in the system.

Deterministic optimization methods minimize the objective function in Eqn.(2) by treating the measurements P_i (and thus the objective function) as a function of the macroscopic cross sections of the materials in the object. Let $\underline{x}$ be the vector of unknowns, so that x_j is a cross section or g factor for some spatial region. The goal is to find the $\underline{x}$ that minimizes Φ. The procedure is outlined in the work of Klose, et al. [2, 3] as corrected by Scipolo [4]. We omit details here, but we note that updated iterates are produced as follows:

$$x_i^{(k+1)}=x_i^{(k)}+\alpha_{x,step}d_i^{(k)}\ , \tag{3}$$

Where the update-direction vector, $\underline{d}$, depends on several things including the gradient of the objective function:

$$\left\{d_i^{(k)},i=1..N\right\}\text{ depends on }\left\{\left.\frac{\partial\Phi}{\partial x_j}\right|^{(k)},\ j=1..N\right\}. \tag{4}$$

The components of the objective function's gradients are constructed after a forward calculation for a given iterate using the procedure described by Scipolo [4].

An updated value may be outside the physically meaningful range for the variable. If this is not corrected, then it may not be possible to perform the next forward calculation, which causes the entire method to fail.

In our problem we perform a variable change to address this issue. The new variables are not constrained; thus our procedure makes the optimization problem appear unconstrained to the minimization method. The important ingredient is a well behaved function for the variable change process. We have found simple functions that appear to work well. For cross sections we use

$$y_j = \log(\Sigma_j) \Rightarrow \frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial \Sigma_j}\frac{d\Sigma_j}{dy_j} = \frac{\partial \Phi}{\partial \Sigma_j}\Sigma_j .$$

For the anisotropic scattering factor we use

$$y_j = \tan\left(\frac{\pi}{2} g_j\right) \Rightarrow$$
$$\frac{\partial \Phi}{\partial y_j} = \frac{\partial \Phi}{\partial g_j}\frac{dg_j}{dy_j} = \frac{\partial \Phi}{\partial g_j}\frac{2}{\pi}\frac{1}{1+\tan^2\left(\frac{\pi}{2} g_j\right)} .$$

Figure 1 shows how the changed variables vary smoothly along the entire real line as the physical variables vary along their allowed ranges.

After variable changes, the new updating scheme is

$$y_i^{(k+1)} = y_i^{(k)} + \alpha_{y,step} d_{y,j}^{(k)} . \quad (5)$$

After this unconstrained update of the transformed variables, it is simple to calculate updated physical variables. As is clear from Figure 1, any value of a transformed variable will map to an allowed value of the associated physical variable.

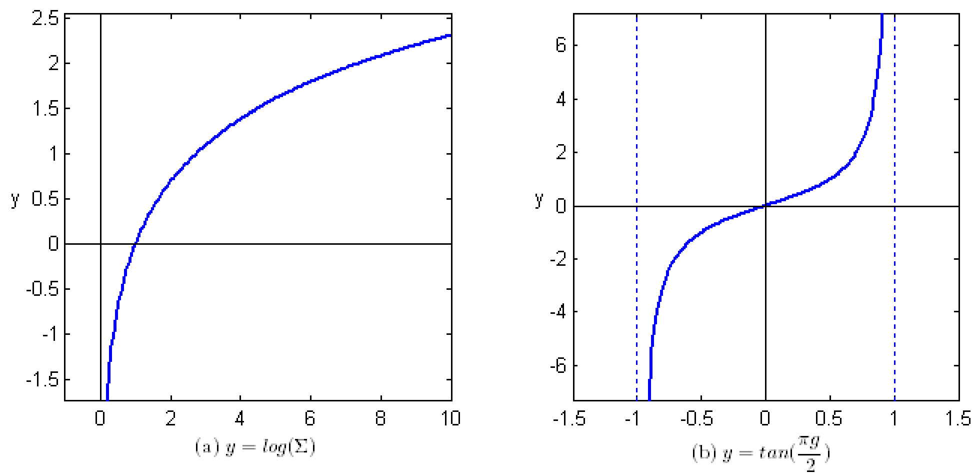

Figure 1. Variable change function for (a) cross sections and (b) average scattering cosine.

APPLICATIONS IN NEUTRON TOMOGRAPHY

We have achieved success by applying the variable change technique to some neutron tomography applications. We illustrate with a model problem with two unknown materials inside an object. Figure 2 is a schematic diagram for the problem and Table I lists the properties of the materials in the problem.

Table I. Material properties		
Material	Water	Iron
Σ_s (1/cm)	0.7362	0.96715
Σ_t (1/cm)	0.7435	1.17883
g	0.037	0.012

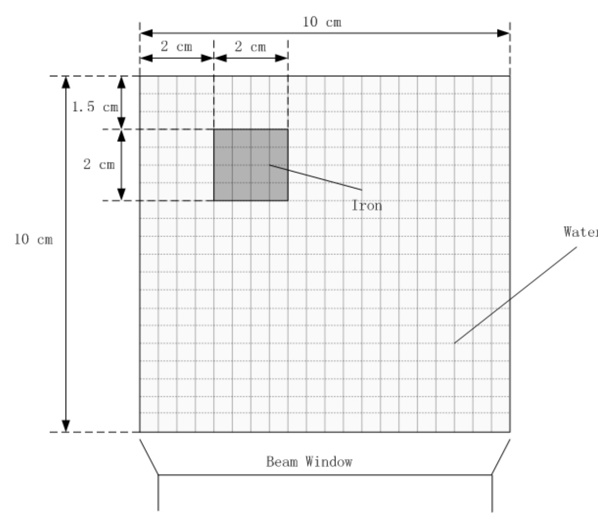

Figure 2. Schematic diagram of the test problem

In the optimization procedure, we divide the problem into 20x20 cells in X-Y Cartesian coordinate system, and build both forward and inverse updating schemes on this discretization.

When we attempt to solve this problem without our variable-change procedure, the CG algorithm attempts to drive many of the unknown parameters outside of their physical ranges. This forces the use of some sort of constraint, which we find introduces other difficulties. Our procedure avoids such complications.

The results we obtain using our variable-change procedure are illustrated in Figure 3 and 4. The problem in Figure 3 is a water-iron problem with one iron block inside a domain of water, while in Figure 4, two iron blocks are contained in the water in different places. For both problems the program started with homogeneous guess for the material distribution. The results shows that our iterative based updating scheme with variable change technique involved can identify the inclusion and roughly tell its location as well. Figure 5 is the plot of objective function in both problems changes with the number of iterations which demonstrates the efficiency of the iterative search process. The overall objective function has been reduced by a factor of 10^7 after 1000 iterations.

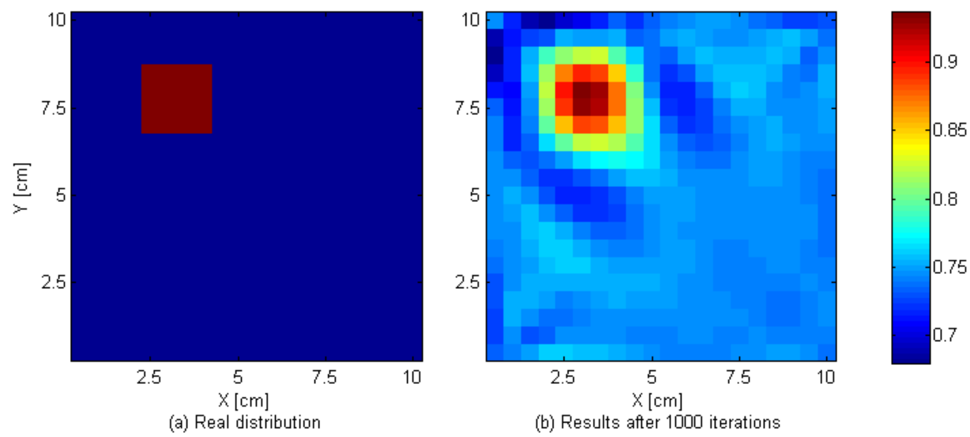

Figure 3. Total cross section distribution obtained from deterministic CG based iterative updating scheme in one iron inclusion problem. (a) Real total cross-section distribution (background material is water while the square inclusion is iron). (b) Results after 1000 CG iterations.

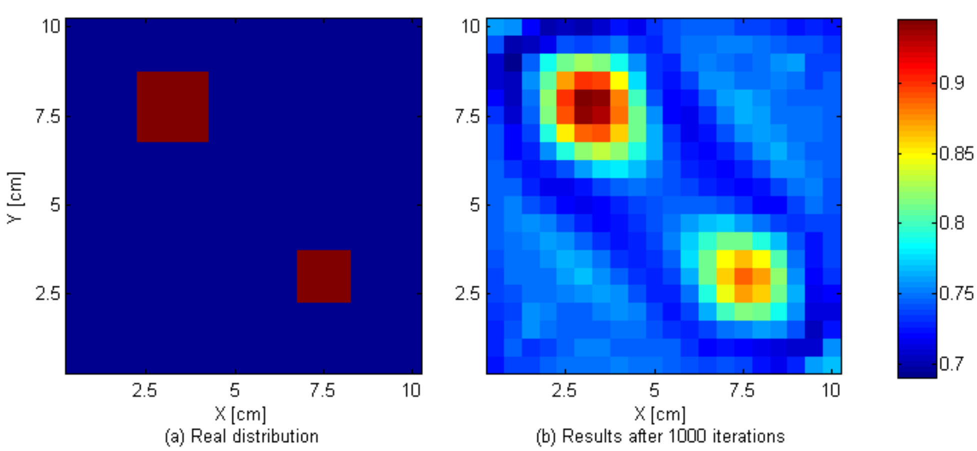

Figure 4. Total cross section distribution obtained from deterministic CG based iterative updating scheme in two-iron inclusion problem. (a) Real total cross-section distribution (background material is water while the two square inclusions are iron). (b) Results after 1000 CG iterations.

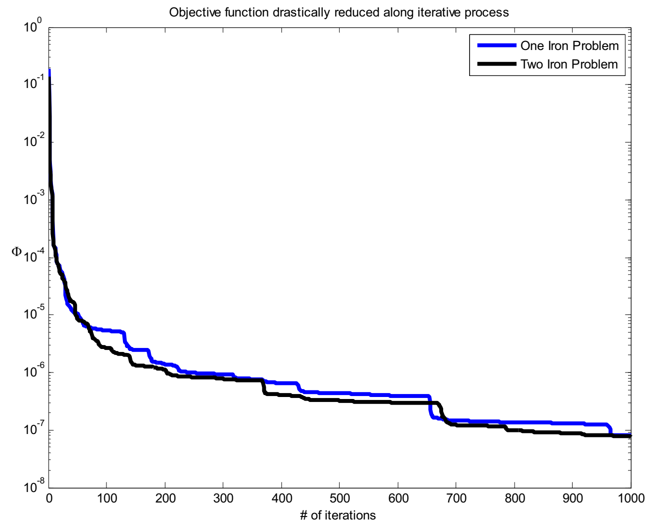

Figure 5. The objective function after each iteration.

CONCLUSIONS

We have introduced a variable change technique to convert constrained optimization into unconstrained one in inverse transport applications. Results from our neutron tomography test problems demonstrate that the method works well and is robust. The method is very easy to apply. We believe this technique may be beneficial to many gradient-based iterative optimization problems as long as the proper variable change function can be found.

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