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Case Study

Inversion of potential field data using the finite element method on parallel computers

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ABSTRACT

In this paper we present a formulation of the joint inversion of potential field anomaly data as an optimization problem with partial differential equation (PDE) constraints. The problem is solved using the iterative Broyden–Fletcher–Goldfarb–Shanno (BFGS) method with the Hessian operator of the regularization and cross-gradient component of the cost function as preconditioner. We will show that each iterative step requires the solution of several PDEs namely for the potential fields, for the adjoint defects and for the application of the preconditioner. In extension to the traditional discrete formulation the BFGS method is applied to continuous descriptions of the unknown physical properties in combination with an appropriate integral form of the dot product. The PDEs can easily be solved using standard conforming finite element methods (FEMs) with potentially different resolutions. For two examples we demonstrate that the number of PDE solutions required to reach a given tolerance in the BFGS iteration is controlled by weighting regularization and cross-gradient but is independent of the resolution of PDE discretization and that as a consequence the method is weakly scalable with the number of cells on parallel computers. We also show a comparison with the UBC–GIF GRAV3D code.

1. Introduction

The inversion of geophysical data is the solution of an optimization problem subject to constraints in the form of partial differential equations (PDEs). A PDE constraint provides a prediction of measured quantities for a given geological model and is sometimes referred to as the *forward model*. The cost function to be minimized defines the data misfit of the prediction to the observational data. In the case of weakly constrained geology, which we are particularly interested in for this paper, a regularization term (Tikhonov and Arsenin, 1977) for the geological model is added to the cost function in order to obtain convergence towards the simplest model realization. In fact, the additional regularization guarantees the uniqueness and existence of a solution of the optimization problem. A framework for magnetic data has been developed by Li and Oldenburg in the mid-1990s (Li and Oldenburg, 1996) and later extended to gravity anomaly data (Li and Oldenburg, 1998). It is now widely used in the exploration industry (Oldenburg and Pratt, 2007). The approach is based on a discrete representation of the geological model and a continuous representation of the forward model using Green's functions. Various improvements have been added, in particular regularization [e.g. Zhdanov, 2009; Portniaguine and Zhdanov, 1999], solving large-scale problems using conjugate gradient based solvers (Zhdanov and Tolstaya, 2004), and sparsification of the sensitivity matrix (Li and Oldenburg, 2003).

In this paper we present a formulation of the inversion problem for potential field data which is consistent with the use of the finite element method (FEM) (Zienkiewicz et al., 2013) to construct for the model representation, the cost function gradient and the potential fields. Using FEM provides a variety of advantages over the conventional Green's function approach. Firstly, it allows for more general forms of the forward model for the potential fields, for instance self-demagnetization (Lelièvre and Oldenburg, 2006). Secondly, the discretization is spatially sparse and does not require sparsification when solving large-scale problems. Finally, well-developed technology is available to handle large-scale FEM problems on parallel compute architectures, see e.g. Heroux and et al. (2005).

In contrast to conventional inversion methods working on a discrete version of the problem the method proposed in this paper is applied directly to the problem in continuous form. It is based on the iterative limited-memory Broyden–Fletcher–Goldfarb–Shanno (BFGS) method (Nocedal and Wright, 2006). An evaluation of the cost function to be minimized requires the solution of the forward problem, and an additional PDE for the so-called adjoint defect (Plessix, 2006) needs to be solved to calculate the cost

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function gradient. The inverse of the Hessian operator of the regularization part of the cost function – again defined through the solution of a PDE – is used as preconditioner for the BFGS iterations in order to accelerate its convergence and to improve its robustness. In accordance with the FEM method the involved PDEs – these are the PDE constraint, the adjoint PDE and the preconditioner – are solved in weak form. Summations over cell values of physical properties as used in the conventional BFGS version are replaced by appropriate integrals due to the different representation of the unknown introduced here. These can be evaluated exactly for a FEM representation of the physical properties. At the limit of convergence our approach returns a solution that is identical to results using the all-at-once method, e.g. Haber and Ascher (2001). However our approach avoids building a system of three coupled PDEs and still solves an optimization problem without (directly) introducing a Lagrangian multiplier for the constraint.

In the following we will discuss the solution of joint inversion of gravity and magnetic anomaly data sets. In the case of strong correlation it is assumed that a functional relationship between density and susceptibility is available, e.g. from borehole logs. Then the geological structure can be represented through a single property function which is constructed analogously to a single inversion with a single regularization term, but two independent forward models need to be considered. An alternative is to assume weak correlation between density and susceptibility based on geometrical alignment, with two property functions used as proxies for density and susceptibility. Driven by the idea that there is still a single geological structure present, the contours of the property functions should be aligned, in particular in regions of strong contrast. This can be achieved by maximizing a covariance measure of the contour orientation. We use the cross-gradient term of the property functions (Gallardo and Meju, 2004).

This paper is organized as follows. In Section 2 we formulate the joint inversion problems. Sections 3 and 4 discuss the calculation of the cost function gradient and the application of the BFGS method to the continuous inversion problem, respectively. Section 5 gives a brief introduction into FEM and its parallelization. Numerical experiments for two- and three-dimensional data are presented in Section 6 including a comparison with the UBC–GIF GRAV3D code. As a key result the experiments show that the number of BFGS steps is in fact independent of the mesh resolution demonstrating the effectiveness of the chosen preconditioning strategy. As a consequence the presented method is computationally scalable with the number of FEM cells subject to the use of a computationally scalable FEM solver.

2. Problem formulation

Given is a bounded domain $\Omega \subset \mathbb{R}^3$ covering a subsurface region for which rock properties are to be calculated, as well as a region above ground in which data for the potential field anomalies have been obtained. The task is to provide a possible distribution of rock properties in the subsurface region which fits the measured anomalies.

2.1. The potential field problem

Rock features in the subsurface are described by a real valued property function m defined on Ω. It is assumed that the density distribution is given in the form

$$\rho = a \cdot m + b \tag{1}$$

with spatially variable coefficients a and b. In practice the density ρ is an anomaly defining deviation from a homogeneous background density. For some applications a reference density distribution ρ_{ref} and depth weighting factor α is introduced (Li and Oldenburg, 1998) for which Eq. (1) takes the form $\rho = \alpha^{-1}m + \rho_{ref}$. The magnetization is similarly described in the form

$$\vec{M} = \vec{A} \cdot m + \vec{B} \tag{2}$$

where the coefficients $\vec{A}$ and $\vec{B}$ consider inducing magnetic field, depth weighting and a reference susceptibility model (Li and Oldenburg, 1996). The unknown property function m is to be calculated through the inversion. In parts of the domain – in particular in the regions above ground – density and/or magnetization may be known. For these locations the property function is set to zero and appropriate choices for the coefficients in Eqs. (1) and (2) can be taken. For reasons of numerical stability it is assumed that values of m are scaled between zero and one. The method presented in this paper can easily be extended to cases where the dependence of density and magnetization on the property function is non-linear. For the sake of simplicity we present the linearized version only.

Forces due to density or to magnetization are derived from scalar potentials Φ solving a partial differential equation (PDE). The PDE is solved in its weak form (Zienkiewicz et al., 2013) which is given as

$$\int_\Omega \vec{\nabla}^t \Psi \cdot \vec{\nabla} \Phi \, dx = \int_\Omega \left(\Psi \cdot (a \cdot m + b) + \vec{\nabla}^t \Psi \cdot (\vec{A} \cdot m + \vec{B}) \right) dx \tag{3}$$

for all admissible potentials Ψ. In this context a function Ψ on the domain is called an 'admissible potential' if it is sufficiently smooth and is zero on the top of the domain in the same way as the potential field Φ. The symbol $\vec{\nabla}$ refers to the gradient operator, and $\vec{\nabla}^t \Psi$ is a short form for the transposed vector $(\vec{\nabla}\Psi)^t$. When solving for the gravity potential we set $\vec{A}$ and $\vec{B}$ to zero, and for the magnetic potential we set a and b to zero. It is pointed out that the weak formulation implicitly imposes the boundary condition

$$\vec{n}^t \cdot \vec{\nabla} \Phi = \vec{n}^t \cdot (\vec{A} \cdot m + \vec{B}) \tag{4}$$

with surface outer normal field $\vec{n}$ on all parts of the domain boundary except on the top of the domain where the potentials are set to zero.

2.2. Data misfit function

For a given property function m the data misfit function D measures the deviation of the resulting accelerating forces from the scalar potential Φ solving the forward problem (3) from the measured data d. We use the form

$$D(\Phi) = \frac{1}{2} \int_\Omega (\vec{w}^t \cdot \vec{\nabla} \Phi - d)^2 \, dx \tag{5}$$

where d are the measured data for the acceleration force and the vector $\vec{w} = (w_i)$ sets the orientation in which the acceleration force has been measured. In practical applications one sets $w_i(\vec{x})$ to $1/\sigma$ if at location $\vec{x}$ the ith component of the acceleration force has been measured as $d(\vec{x})/\sigma$ with a known error $\sigma > 0$. At all other locations $\vec{x}$ and for all other components i one sets $w_i(\vec{x}) = 0$ and $d(\vec{x}) = 0$. Notice that $\vec{w}$ is non-zero on a very small portion of the domain. It is pointed out that summation over various surveys including overlapping regions can be added but is omitted here for the sake of a simpler presentation.

2.3. The inversion problem

If a functional relationship between susceptibility and density