Generalized cross-validation and Regińska's methods for choosing the regularization parameter in 3D gravity inversion of basement relief - a hybrid MPI/OpenMP parallel algorithm

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Abstract

This paper addresses the problem of gravity inversion to determine the 3D basement relief of sedimentary basins. It is a nonlinear optimization problem where the gravity anomalies attributable to basement interfaces above which the density contrast varies continuosly with the depth are analyzed. We use the Levenberg-Marquardt (LM) algorithm which needs a key input parameter called the regularization parameter λ to deal with the singularity of the normal equation matrix in the linearized problem at each iteration. The generalized cross-validation (GCV) and Regińska's methods for estimating the optimal regularization parameter are tested through numerical experiments on a synthetic data set. Also, we implemented the LM algorithm with a hybrid message passing interface (MPI) and Open Multi-Processing (OpenMP) approach to avoid the high proccesing time. This lead to a fast and reliable algorithm, which produced satisfactory results in mapping the basement topography.

Introduction

One of the important applications of the gravimetric method is the estimation of the depth of the sediment-basement contact in a given sedimentary basin. The basement relief of a sedimentary basin generally controls the deposition of the sediments and overlying structures. Hence, the structural analysis of the basement plays a significant role in understanding the petroleum system. Generally, the gravity inversion methods for estimating the basement relief of a sedimentary basin may be grouped into two categories. The first group considers that the density contrast between the sediment and the basement is constant. The second group assumes a densisty contrast variation with the depth due to the compaction of the sediment. In the second category methods, Chakravarthi and Sundararajan (2007), for example, have assumed that the density contrast decays with the depth according to a parabolic law and have developed an inversion scheme based on the Levenberg-Marquardt algorithm to estimate the regional gravity anomaly and the depth of the 3D basement relief of the sedimentary basins. In this work, we followed the same approach proposed by Chakravarthi and Sundararajan (2007) and we introduced the generalized cross-validation and Regińska's criteria for automatic selection of optimal regularization parameter. The performance of these criteria were compared by using a synthetic data set. The validation of the GCV method by synthetic data rather than real cases, has been completely demonstrated in a previous work (Mojica and Bassrei, 2014). It's worthwhile to mention that the efficiency of the gravity inversion methods applied to the interpretation of sedimentary basins depends on the number of observations and parameters to be estimated (usuallly the number of observations and parameters are made equal), making it very poor when these are very large. Therefore, the development of efficient gravity inversion methods is of utmost importance. To adress this difficulty, recently Silva et al. (2014) proposed an improved Bott's method, which overcomes the known limitations of the Bott's method and allows a fast recovery of the basement relief. Alternatively, here we used a hybrid programming model combining MPI and OpenMP that tackles the most computationally expensive parts of the inversion procedure: The forward modeling, the Jacobian matrix computation and the search for the optimal regularization parameter through a regularization parameter choice method such as GCV or Regińska's method.

Methodology

Forward Problem

A given basin is represented by a series of rectangular prisms of known horizontal dimensions dx and dy with tops that coincide with the Earth's surface and bottoms that coincide with the interface of the basement. We assume that the gravity data are interpolated on a regular grid with coordinates x and y corresponding to the horizontal coordinates of the centers of the prisms (Figure 1).

Because $\mathbf{g} = (g_1, \ldots, g_M)^T$ is an M-dimensional vector containing the gravity observations, presumably produced by the relief of the basement of the sedimentary basin, the parameters $z_j,\ j = 1, ..., M$ to be estimated, regarding the depths of the basement in M discrete grid points are related to the ith vertical component of the gravity anomaly g_i by the nonlinear relationship:

$$g_i(x_i, y_i, z_i) = \sum_{j=1}^{M} f_i(z_j), \quad i = 1, \ \ldots \ , M. \tag{1}$$

The nonlinear function $f_i(z_j)$ at the ith point produced by the jth prism is expressed analytically in the following

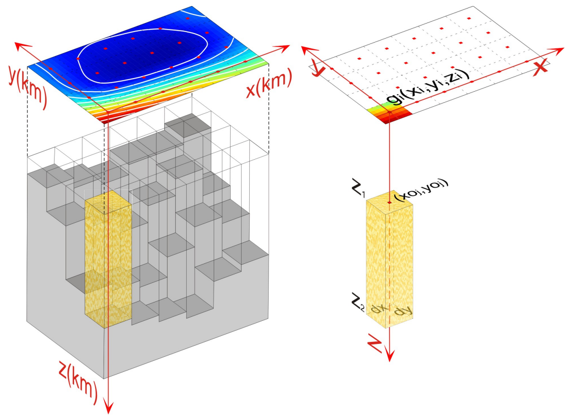


Figure 1: Schematic representation of a gravity anomaly produced by the basement interface. The sedimentary pack is discretized into a grid of 3D vertical prisms with thicknesses $(z_2 - z_1)$ that are the parameters to be estimated. The diagram on the right shows the contribution to the anomalous gravitational field $g_i(x_i, y_i, z_i)$ at the ith observation point produced by the jth prism.

equation:

$$f_i = \gamma \int_{z_1}^{z_2} \int_{yo_j - dy/2}^{yo_j + dy/2} \int_{xo_j - dx/2}^{xo_j + dx/2} \Delta\rho(z) \times \frac{z_i - z'_j}{[(x_i - x'_j)^2 + (y_i - y'_j)^2 + (z_i - z'_j)^2]^{3/2}} dx' dy' dz', \qquad (2)$$

where γ is the gravitational constant, and xo_j and yo_j are the x and y coordinates of the jth prism center, respectively. We assume that the density contrast between the basement and the sedimentary basin varies parabolically with the depth z, according to a parabolic law (Chakravarthi et al., 2002).

Inverse Problem

The nonlinear inverse problem of estimating $\mathbf{z}$ from $\mathbf{g}^{obs}$ may be formulated as the optimization problem of minimizing the cost function

$$\Phi = \sum_{k=1}^{M} (g_k^{obs} - g_k^{calc})^2, \qquad (3)$$

where, g_k^{obs} is the observed anomaly, g_k^{calc} is the calculated anomaly and M is the number of observations, which for simplicity is set equal to the number of prisms. This is minimized using the technique of Marquardt (1963). Thus, M normal equations are formulated, as follows

$$\sum_{j=1}^{M} \sum_{k=1}^{M} \frac{\partial \mathbf{g}^{calc}}{\partial z_i} \frac{\partial \mathbf{g}^{calc}}{\partial z_j} (1 + \delta_{ij}\lambda) \delta z_j = \sum_{k=1}^{M} [g_k^{obs} - g_k^{calc}] \frac{\partial \mathbf{g}^{calc}}{\partial z_i} \quad (i = 1, \ldots, M), \qquad (4)$$

where

$$\delta_{ij} = \begin{cases} 1 & \text{for} \quad i = j, \\ 0 & \text{for} \quad i \neq j. \end{cases}$$

λ is the regularization parameter and z_i represents parameters. Defining $\mathbf{J}$ as the Jacobian (the matrix of the partial derivatives) and writing (4) in matrix form, we obtain the following equation:

$$(\mathbf{J}^T \mathbf{J} + \lambda \mathbf{I}) \delta \mathbf{z} = \mathbf{J}^T \delta \mathbf{g}, \qquad (5)$$

which is solved for the correction vector $\delta \mathbf{z}$. The partial derivatives of equation (4) can be evaluated numerically or analytically. In this inversion scheme, the derivatives are calculated numerically. The variation in the parameters over the initial guess is determined using the relationship in equation (5). The updated parameters are obtained, and a new cost function is calculated using equation (3) at each iteration. The performance of the inversion scheme is evaluated using the relative Root Mean Square (RMS) error criterion related to the data and the model, which are calculated respectively, by the following equations:

$$\varepsilon_{RMS}^{g} = \frac{\sqrt{\sum_{k=1}^{M} (g_k^{obs} - g_k^{calc})^2}}{\sqrt{\sum_{k=1}^{M} (g_k^{obs})^2}} \times 100\%, \qquad (6)$$

and

$$\varepsilon_{RMS}^{z} = \frac{\sqrt{\sum_{k=1}^{M} (z_k^{true} - z_k^{est})^2}}{\sqrt{\sum_{k=1}^{M} (z_k^{true})^2}} \times 100\%. \qquad (7)$$

Automatic selection of regularization parameter

A great variety of techniques for the regularization parameter choice have been developep and well described in literature; see for instance Hansen (1998). These techniques can be broadly divided into two classes: techniques that involve the knowledge of the error norm and techniques that, in contrast, seek to extract such information from the observations. Here we discuss the use of two techniques from the latter group for the particular inverse problem previously defined.

Generalized cross-validation

The major motivation of using the GCV to find an optimal value for λ is that a good value should predict missing data values. Specifically, if an arbitrary measurement is removed from the used data, then the corresponding regularized solution should be able to predict the missing observation. The GCV functional data is given by (Wahba, 1990):

$$GCV(\lambda) = \frac{\|\mathbf{g}^{obs} - \mathbf{g}(\mathbf{z}_\lambda)\|^2}{\{Tr[\mathbf{I} - \mathbf{A}(\lambda)]\}^2}, \qquad (8)$$

where, $Tr[\cdot]$ stands for the trace of a square matrix, and

$$A(\lambda) = \mathbf{J}(\mathbf{J}^T \mathbf{J} + \lambda \mathbf{I})^{+} \mathbf{J}^T. \qquad (9)$$

The GCV method has been applied by various authors in the inversion of geophysical data (Farquharson and Oldenburg,2004; Vatankhah et al., 2014).

Regińska's method

Regińska (1996) proposed a parameter choice method related to the L-curve criterion for Tikhonov regularization. This method can be adapted without difficulty to any situation in which the regularization parameter is discrete. The method is to find the minimizer of the functional

$$\Psi_\nu(\lambda) = \|\mathbf{g}^{obs} - \mathbf{g}(\mathbf{z}_\lambda)\|^2 \|\mathbf{z}_\lambda\|^{2\nu}, \qquad \nu > 0, \tag{10}$$

where ν is a user-defined parameter. We used $\nu = 1$ in our numerical experiments.

The Regińska's method have been recently applied in the estimation of the discrete Hilbert transform (Roy, 2013), and in an improved adaptive iterative method for performing a downward continuation of the potential-field data from a horizontal plane (Zeng et al, 2013). These methods were designed for linear inverse problems, but they can also be applied to nonlinear problems, as they only require the knowledge of the residual $\mathbf{r}(\lambda) = \mathbf{g}^{obs} - \mathbf{g}(\mathbf{z}_\lambda)$ corresponding to each regularized solution.

Parallelization

The recent increase in availability of powerful multiple-core central processing units (CPUs), as well as the use of graphics processing units (GPUs) for parallelizing the calculations required for intensive computation tasks, offers a new opportunity to improve the efficiency of potential-field data inversion. Some works that consider the use of multi-CPU platforms in the field of forward/inverse gravity problems are Wilson et al. (2011), Čuma et al. (2012) and Couder-Castañeda et al. (2015). Here, we developed a parallel approach that uses a hybrid MPI/OpenMP programming model on a multi-core cluster for delaying of the high processing time of the data inversion procedure. We adopted parallelization in three key parts of the inversion algorithm.

Forward modeling subroutine: it is natural to arrange the design forward computation as loop over the observations and prisms, because the gravitational anomaly can be approximated at any point by summing the effects of all the prisms over that point. This makes using OpenMP to distribute the prisms over the threads a natural choice for parallelization.

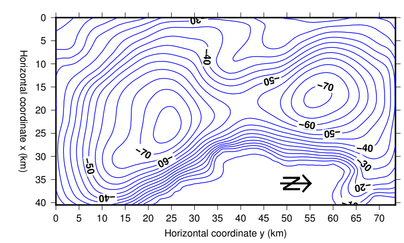
Jacobian computation: different rows of the Jacobian matrix can be computed independently from each other. Subsequently, the parallelization is performed in MPI by distributing the Jacobian matrix in row blocks among the cluster nodes, where each node is responsible for the calculation of a block matrix. Then, the matrix components (blocks) are sent to the master node in charge of the construction of the matrix.

Search for the optimal regularization parameter: the calculation of the optimal regularization parameter by GCV and Regińska's methods is a time-consuming process, because these methods need the regularized solution for each λ. The parallelization is performed using MPI to distribute a vector with various values of λ between the cluster nodes; once this distribution is made, we use OpenMP in the nodes, so that each thread within the node performs a matrix inversion using a particular value of λ.

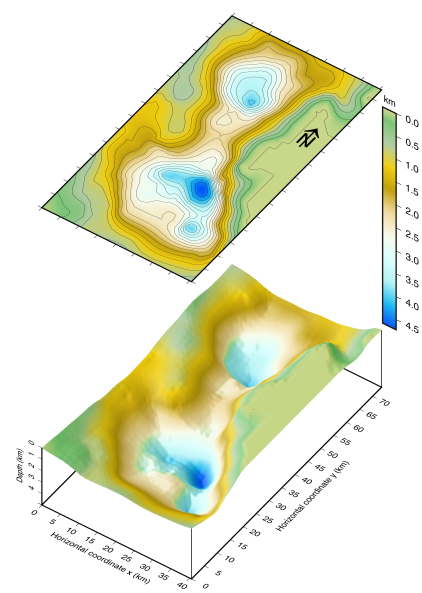
Simulations were performed on Aguia cluster from the Research Center in Geophysics and Geology at the Federal University of Bahia, which has 28 nodes divided into two groups. The first group contains 13 nodes with two quad-core Intel Xeon E5420 processors with a clock speed of 2.5GHz and 15.7GB of RAM. The second group contains 15 nodes, each of which has two quad-core Intel Xeon 5620 processors with Hyper-Threading Technology running at 2.4GHz and 23.6GB of RAM. We ran one MPI process per cluster node (using nodes of the second group), with each process launching a specific number of OpenMP threads - one thread per processor core.

Results

We evaluated the use of the GCV and Regińska's methods for a synthetic data example. The simulated basin (Figure 2b) is composed of two sub-basins interconnected in the north-south and northwest-southeast directions. The northern sub-basin has an elongated rhombohedral geometry northward and is limited by steep grades corresponding to normal faulting, whereas the southern sub-basin is a typical rift basin known as a half-graben, with its eastern edge defined by a fault in the northwest-southeast direction. It is discretized through 50×28 grid of horizontally juxtaposed rectangular prisms with horizontal dimensions of 1.5 km, tops at surface, and whose thicknesses model the basement depths.



(a)



(b)

Figure 2: (a) Noise-corrupted Bouguer anomaly (b) Contour map and perspective view of the true basement relief.

We adopted an a priori model for which the initial depth is defined by a theoretical formula Chakravarthi and Sundararajan (2007), assuming that the value of the measured gravity at each grid node is given by a horizontal infinite slab with parabolically varying density contrast (first a priori). We also considered an a priori model with a constant initial depth equal to 2.5 km (second a priori). All simulations were performed using noisy data. Basically pseudorandom Gaussian noise with zero mean and a standard deviation of 0.1 $mGal$ was added to the theoretical anomaly (Figure 2a). Due to space limitations we show only the results for the second a priori model, although all simulations are summarized in Table 1.

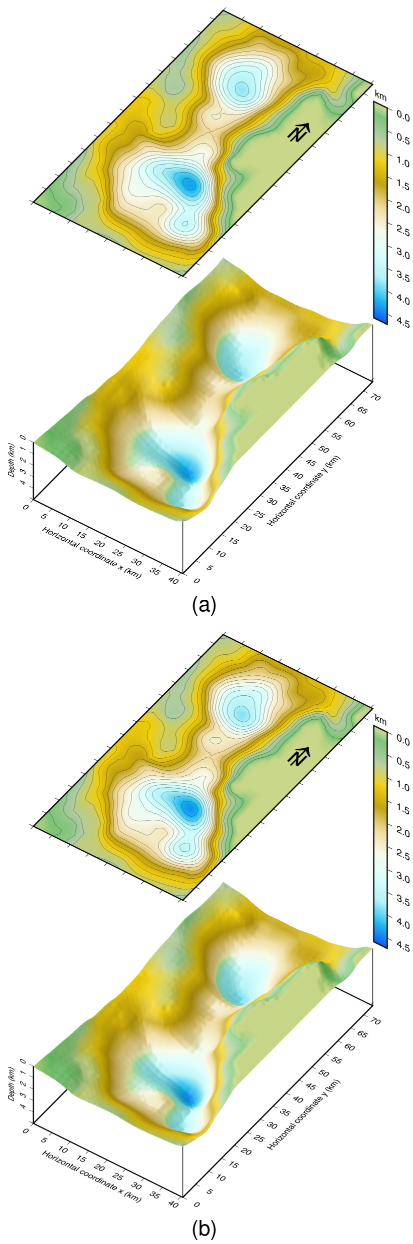


Figure 3: Contour maps and perspective views of the estimated basement reliefs using the (a) GCV and (b) Regińska's parameter-choice methods.

Figures 3a and 3b show the estimated depths of the basement relief using the GCV and Regińska's parameter-choice methods, respectively. The estimated basement reliefs (Figures 3a and 3b) show an excellent agreement with the true basement relief (Figure 2b), reflecting the good performance of both parameter-choice methods. However, from the results summarized in Table 1 it can be noticed that there is a slight difference between the errors related to the data and model for both methods. Figure 4 contains a plot of the $GCV(\lambda)$ and $\Psi_\nu(\lambda)$ curves at each iteration, which are depicted by a blue solid line with empty circles. The optimum regularization parameter is associated with the minimum of the curves.

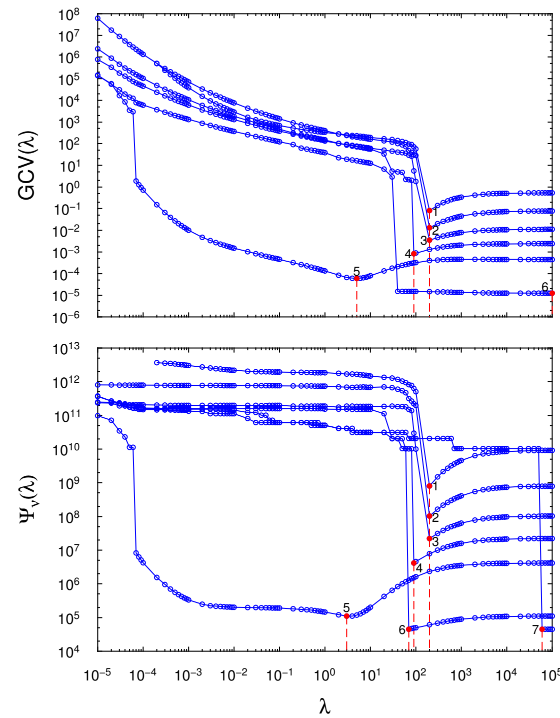


Figure 4: Plot of the $GCV(\lambda)$ and $\Psi_\nu(\lambda)$ curves (eqs. 10 and 9). The λ chosen at each iteration (number) is marked by a filled red circle and by a red vertical dashed line.

An interesting result is that the iterative process converged to the true solution in just six iterations when the GCV criterion was used with the MPI/OpenMP hybrid parallelization. In Mojica and Bassrei (2014), the GCV implementation used a pure MPI approach, and the iterative process converged in 17 iterations. This difference can be easily explained by the fact that the MPI/OpenMP implementation allows the use of a greater number of λ values (until 91).

From our experiments, we found that a combination of 12 MPI processes and 12 OpenMP threads gives an overall best performance and makes the inversion algorithm more than two orders of magnitude faster than the sequential inversion algorithm.

Conclusions

In this paper, two different methods for estimating the optimal regularization parameter λ_{best} have been tested in the problem of gravity inversion for determining the 3D relief of sedimentary basins using a synthetic

Table 1: Results of all simulations

A priori model	Method	$\varepsilon_{RMS}^{g,initial}$(%)	ε_{RMS}^{g}(%)	$\varepsilon_{RMS}^{z,initial}$(%)	ε_{RMS}^{z}(%)	Iterations	λ_{best}	Time(s)[†]
1	GCV	10.84065	0.14241	18.37159	2.30920	4	$80, 1, 60, 1\times10^5$	935
	Regińska	10.84065	0.12993	18.37159	2.10228	4	$80, 0.1, 200, 800$	864
2	GCV	64.72751	0.30886	77.77742	3.33211	6	$200, 200, 200, 90, 5, 1\times10^5$	1402
	Regińska	64.72751	0.19095	77.77742	2.85640	7	$200, 200, 200, 90, 3, 70, 6\times10^4$	1546

[†]Time obtained using 12 MPI processes, each of which using 12 OpenMP threads

data set. We conclude that both parameter-choice methods performed well in the problem addressed here. Furthermore, a parallel algorithm that tackles the most computationally expensive parts of the inversion procedure was implemented and validated using a hybrid methodology with OpenMP and MPI. This leads to a fast and reliable algorithm. In the near future, we plan to adapt our parallel inversion algorithm in order to deal with another kind of regularizations (First-order Tikhonov and Total variation regularizations) and besides, apply it in the inversion of real data.

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Acknowledgements

O. F. Mojica acknowledges the Brazilian agency CAPES for a D.Sc. scholarship. A. Bassrei would like to thank CNPq for the projects INCT-GP and 308690/2013-3 (research fellowship) and FINEP for sponsoring the CT-PETRO Network in Exploration Geophysics (Rede 01).