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Automatic estimation of the regularization parameter in 2D focusing gravity inversion: application of the method to the Safo manganese mine in the northwest of Iran

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Abstract
We investigate the use of Tikhonov regularization with the minimum support stabilizer for underdetermined 2D inversion of gravity data. This stabilizer produces models with non-smooth properties which is useful for identifying geologic structures with sharp boundaries. A very important aspect of using Tikhonov regularization is the choice of the regularization parameter that controls the trade-off between the data fidelity and the stabilizing functional. The $L$-curve and generalized cross-validation techniques, which only require the relative sizes of the uncertainties in the observations, are considered. Both criteria are applied in an iterative process; at each iteration a value for the regularization parameter is estimated. Suitable values for the regularization parameter are successfully determined in both cases for synthetic, but practically relevant, examples. Whenever the geologic situation permits, it is easier and more efficient to model the subsurface with a 2D algorithm, rather than to apply a full 3D approach. Then, because the problem is smaller it is appropriate to use the generalized singular value decomposition to solve the problem efficiently. The method is applied to a profile of gravity data acquired over the Safo mining camp in Maku, Iran, which is well known for manganese ores. The presented results demonstrate success in reconstructing the geometry and density distribution of the subsurface source.

Keywords: focusing inversion, 2D gravity, regularization parameter, $L$-curve, generalized cross validation

(Some figures may appear in colour only in the online journal)

1. Introduction
Gravity inversion allows us to reconstruct models of subsurface density distribution using data measured on the surface. There are two important ambiguities in the inversion of gravity data. Theoretical ambiguity is caused by the nature of gravity; many equivalent sources in the subsurface can produce the same data at the surface. Algebraic ambiguity occurs when parameterization of the problem creates an underdetermined situation with more unknowns than observations. This means that there is no unique density distribution which satisfies the observed data. Further, the measurement process at the Earth’s surface is necessarily error-contaminated and such errors can introduce arbitrarily large changes in the reconstructed solutions; namely the solutions are sensitive to errors in the measurements. Thus, the inversion of gravity data with undersampling is a typical example of an ill-posed problem that requires the inclusion of a priori information in order to find a feasible reconstruction.

Tikhonov regularization is a well-known and well-studied method for stabilizing the solutions of ill-posed problems (e.g. Hansen 1998, Vogel 2002). The objective function of
the Tikhonov formulation includes a data fidelity (misfit term), and a stabilizing term that controls the growth of the solution with respect to a chosen weighted norm. The choice of the weighting for the regularization term impacts the properties of the solution. For example, a smoothing stabilizer which employs the first or second derivative of the model parameters, as in e.g. Li and Oldenburg (1996, 1998), produces smooth images of the subsurface density distribution. There are, however, situations in which the potential field sources are localized and have material properties that vary over relatively short distances. Then, a regularization that does not penalize sharp boundaries should be used. Last and Kubik (1983) presented a compactness criterion for gravity inversion that seeks to minimize the volume of the causative body. This concept was developed by introducing minimum support (MS) and minimum gradient support (MGS) stabilizers (Portniaguine and Zhdanov 1999, Zhdanov 2002); which are applied iteratively, generating repeatedly updated weighted quadratic stabilizers.

In any regularization method, the trade-off between the data fit and the regularization terms is controlled by a regularization parameter. Methods to find this regularization parameter, called parameter-choice methods, can be divided into two classes (Hansen 1998): (i) those that are based on knowledge of, or a good estimate of, the error in the observations, such as Morozov’s discrepancy principle (MDP), and (ii) those that, in contrast, seek to extract such information from the observations, such as the L-curve or generalized cross-validation (GCV) methods. The use of the MDP is dominant in papers related to potential field inversion (e.g. Li and Oldenburg 1996, 1998), and the original paper for focusing inversion (Portniaguine and Zhdanov 1999). In many practical applications, little knowledge about the noise or error in the data measurement is available. The MDP then reduces to a trial and error procedure for finding the optimal regularization parameter (Li and Oldenburg 1999). Here we discuss the use of the L-curve and GCV methods for use in focusing inversion of gravity data in situations in which there is information about the relative magnitudes of the standard deviations across the measured data (Farquharson and Oldenburg 2004). Due to the iterative nature of the algorithm, the regularization parameter is determined at each iteration.

Depending on the type of problem to be tackled, gravity inversion can be carried out in either two or three dimensions (2D or 3D). 2D methods are suitable for the recovery of geologic structures such as faults, dikes and rift zones, for which the length of the source body in one direction is much longer than its extension in other directions. Then, it may be possible to consider the gravitational sources as completely invariant in the direction parallel to the length direction. Additionally, 2D sources are both easier to conceptualize and model than their 3D counterparts (Blakely 1996).

The outline of this paper is as follows. In section 2 we review the derivation of the analytic calculation of the gravity anomaly derived from a 2D cell model and then present an overview of numerical methods for focusing inversion. The use, and rationale for the use, of the generalized singular value decomposition (Paige and Saunders 1981) for the solution is given in section 2.2.1. The L-curve and GCV parameter-choice methods are discussed in section 2.3. Results for synthetic data are illustrated in section 3. The approach is applied to a profile of gravity data acquired from the Safo mining camp in Maku, Iran, in section 4. Future directions and conclusions follow in section 5.

2. Gravity modeling

2.1. The theoretical model

A simple two-dimensional model is obtained by dividing the subsurface under the survey area into a large number of infinitely long horizontal prisms in the invariant y-direction, with variations in densities only assumed for the x- and z-directions. The cross-section of the subsurface under the gravity profile for the model is shown in figure 1, in which the cells have square cross-sections and unknown densities. The dimensions of the cells are equal to the distances between two observation points. This type of parameterization, originally used by Last and Kubik (1983), could indeed be improved. Yet, increasing the resolution of the models, and hence the number of parameters, by dividing the subsurface into smaller cells, makes the problem more ill-posed. Here the unknown density is considered to be constant for each block and the data and model parameters are linearly related.

The vertical component of the gravitational attraction $g_i$ of a two-dimensional body at the origin using Cartesian coordinates is given by (Blakely 1996)

$$g_i = 2 \Gamma \rho \int \frac{\Delta x \, \Delta z}{\sqrt{x^2 + z^2}}. \tag{1}$$

Here $\Gamma$ is the universal gravitational constant and the density $\rho$ is assumed to be constant within the body. A solution of this integral for an l-sided polygon is given by (Blakely 1996)

$$g_i = 2 \Gamma \sum_{p=1}^{l} \frac{v_p}{1 + \psi_p^2} \left( \log \frac{r_{p+1}}{r_p} - \psi_p (\theta_{p+1} - \theta_p) \right). \tag{2}$$

where $\psi_p = (x_{p+1} - x_p)/(z_{p+1} - z_p)$ and $v_p = x_p - \psi_p z_p$. The variables $r_p$, $r_{p+1}$, $\theta_p$ and $\theta_{p+1}$ are as displayed for the upper side of a square block in figure 1. The term on the right-hand side of (2), which quantifies the contribution to the $i$th
datum of a unit density in the \( j \)th cell, is denoted by the kernel weight \( G_{ij} \), and is valid only at the station \( i \) for cell \( j \). The total response for station \( i \) is obtained by summing over all cells, giving

\[
g_i = \sum_{j=1}^{n} G_{ij} \rho_j, \quad i = 1, \ldots, m, \quad m < n, \tag{3}\]

which leads to the matrix equation

\[
d = Gm + e \tag{4}\]

where we have used the standard notation that vector \( d \) is the set of measurements given by the \( g_i \), \( m \) is the vector of unknown model parameters (here the densities \( \rho_j \)), and \( e \) represents the error in the measurements. The purpose of the gravity inverse problem is to find a geophysically plausible density model that reproduces \( d \).

### 2.2. Numerical approaches for focusing inversion

The conventional method for solving ill-posed inverse problems as described by (4) is based on minimization of the parametric functional

\[
P^\alpha(m) = \phi(d) + \alpha^2 S(m). \tag{5}\]

Here \( \phi(d) \) measures the data fidelity, which is usually measured by the weighted discrepancy

\[
\phi(d) = \|W_d(d - d_{\text{obs}})\|^2 , \tag{6}\]

where \( d = Gm \) is the vector of predicted data, \( d_{\text{obs}} \) is the observation and \( W_d \) is a data weighting matrix. Under the assumption that the noise \( e \) is Gaussian and uncorrelated, \( W_d = \text{diag}(1/\sigma_1, \ldots, 1/\sigma_m) \) where \( \sigma_i \) is the standard deviation of the noise in the \( i \)th datum. Following Farquharson and Oldenburg (2004), rather than always assuming that the relative magnitudes of the error can be estimated. Then for an unknown \( \sigma_i \) each \( \sigma_i \) is re-expressed as \( \sigma_i = \sigma_0 \sigma_i^* \) and \( W_d = \text{diag}(1/\sigma_1^*, \ldots, 1/\sigma_m^*) \). In (5), \( S(m) \) is a stabilizing regularization functional and \( \alpha \) is a regularization parameter.

Different choices are possible for \( S(m) \). Here we use the MS stabilizer introduced in Last and Kubik (1983) and developed in Portniaguine and Zhdanov (1999). This stabilizer generates a compact image of a geophysical model with sharp boundaries and, following Zhdanov (2002), is of the form

\[
S_{\text{MS}}(m) = (m - m_{\text{apriori}})^T (\epsilon^2 I + m^2_{\text{apriori}})^{-1} (m - m_{\text{apriori}}) \tag{7}\]

\[
W_e = (\epsilon^2 I + m^2_{\text{apriori}})^{-1/2} \tag{8}\]

where \( m_{\text{apriori}} \) and \( m_{\text{apriori}} \) are diagonal matrices of the current model parameters \( m \) and an estimate of the model parameters \( m_{\text{apriori}} \). If good a priori knowledge of the properties of the subsurface distribution exists, a full model of the expected physical properties can be used for \( m_{\text{apriori}} \), otherwise it is often set to 0. In \( W_e, \epsilon \geq 0 \) is a focusing parameter that is introduced to provide stability as \( m \to m_{\text{apriori}} \) component wise. Small values for \( \epsilon \) lead to compact models but also increase the instability in the solution. For large \( \epsilon \) the image will not be focused. In general we are interested in the case where \( \epsilon \to 0 \). A trade-off curve method can be used to select \( \epsilon \) (Zhdanov and Tolstaya 2004, Ajo-Franklin et al 2007, Vatankhah et al 2013).

It is well known that in potential data inversion the reconstructed models tend to concentrate near the surface. The depth weighting matrix, \( W_{\text{depth}} = 1/(z_j + \xi)^2 \) introduced in Li and Oldenburg (1996, 1998) and Pilkington (1997) can then be incorporated into the stabilizer term. Here \( z_j \) is the mean depth of cell \( j \) and \( \xi > 0 \) is a small number imposed to avoid singularity at the surface. The choice for \( \beta \) is important. Small \( \beta \) values provide a shallow reconstruction for the solution and large values concentrate the solution at depth. For all inversions considered here \( \beta = 0.6 \) is selected. The hard constraint matrix \( W_{\text{hard}} \) is also important for the inversion process. If field operation, geological and geophysical information are able to provide the value of the density of cell \( j \) this information should be included in \( m_{\text{apriori}} \). Then, \( W_{\text{hard}} \) is the diagonal identity matrix but with \( (W_{\text{hard}})_{jj} = 100 \) for those diagonal entries \( j \) for which information on the density is known.

Combining the diagonal weighting matrices, \( W_{\text{hard}}, W_e \) and \( W_{\text{depth}}, (5) \) is replaced by

\[
P^\alpha(m) = \|W_e(Gm - d_{\text{obs}})\|^2 + \alpha^2 \|D(m - m_{\text{apriori}})\|^2, \tag{9}\]

\[
D = W_e W_{\text{hard}} W_{\text{depth}}. \tag{10}\]

To obtain solution \( m := \arg \min_m P^\alpha(m) \) linear transformation of the original model parameters is introduced via \( m(\alpha) = m - m_{\text{apriori}} \). Then \( m(\alpha) \) solves the normal equations

\[
\left(G^T W^2_e G + \alpha^2 D^T D\right)m(\alpha) = G^T W^2_e (d_{\text{obs}} - Gm_{\text{apriori}}), \tag{11}\]

providing

\[
m = m_{\text{apriori}} + m(\alpha). \tag{12}\]

When (9) is solved iteratively due to the dependence of \( W_e \) on \( k \), we use \( m_{\text{apriori}} = (m)^{(k-1)}, m^{(0)} = 0 \) and \( D^{(k)} = W_e^{(k)} W_{\text{hard}}^{(k)} W_{\text{depth}}^{(k)} \) with

\[
w_{(k)} = \epsilon^2 (\epsilon^2 I + m^2)^{-1} \tag{13}\]

Then \( m^{(k)} \) is obtained from the iteratively regularized equation, with updated regularization parameter \( \alpha^k \),

\[
\left(G^T W^2_e G + \epsilon^2 (D^{(k)}^T D^{(k)})\right)m(\alpha^{(k)}) \tag{14}\]

\[
= G^T W^2_e (d_{\text{obs}} - Gm^{(k-1)}), \tag{15}\]

yielding

\[
m^{(k)} = m^{(k-1)} + m(\alpha^{(k)}). \tag{16}\]

This technique in which the weighting in \( W_e \) is frozen at each iteration, creating the possibility of solving the problem using the standard Tikhonov update, was introduced in the context of focusing inversion in Zhdanov (2002). Because the MS stabilizer tends to produce the smallest possible anomalous domain we follow the approach of Portniaguine and Zhdanov (1999) and Boulanger and Chouteau (2001) to produce a reliable image of the subsurface when using focusing inversion. Based on geologic information, upper and lower bounds, \( m_{\text{min}} \leq m_j \leq m_{\text{max}}, \) can be determined for the model parameters. If during the iterative process a given density value falls outside the bounds, projection is employed to force the value back to the exceeded value, and a hard constraint is imposed at that cell via \((W_{\text{hard}})_{jj} = 100\).
2.2.1. Numerical solution by the generalized singular value decomposition. We now discuss the numerical procedure for finding the solution to (13). For large scale problems, iterative methods such as conjugate gradients, or other Krylov methods, should be employed to find \( m(\alpha^{(k)}) \) (e.g. Hansen 1998). For small scale problems it is feasible to use the singular value decomposition (SVD) for the matrix \( \hat{G} = W_2G \), when matrix \( D \) is the identity. Otherwise the generalized singular value decomposition (GSVD) (Paige and Saunders 1981), is needed. But again, it is effective to use it for this problem because it facilitates efficient determination of the regularization parameter. We assume \( \hat{G} \in R^{m \times n}, m < n, D \in R^{m \times m} \) and \( N(G) \cap N(D) = 0, \) where \( N(G) \) is the null space of the matrix \( G \). Then there exist orthogonal matrices \( U \in R^{m \times m}, V \in R^{n \times n} \) and a nonsingular matrix \( X \in R^{n \times n} \) such that \( \hat{G} = U X, D = V M X^T \) where \( \Lambda \) of size \( m \times n \) is zero except for entries \( 0 < \Lambda_{1, q+1} \lesssim \ldots \Lambda_{m, n} < 1 \) with \( q = n - m, M \) is diagonal of size \( n \times n \) with entries \( 1 = M_{1, 1} = \ldots = M_{q, q} > M_{q+1, q+1} = \ldots = M_{n, n} > 0 \). The generalized singular values of the matrix pair \( \hat{G}, D \) are \( \gamma_i = \lambda_i/\mu_i \), where \( \gamma_1 = \ldots = \gamma_q = 0 < \gamma_{q+1} \lesssim \ldots \lesssim \gamma_n \), and \( \Lambda^T \Lambda = \text{diag}(0, \ldots, 0, \lambda_1^2, \ldots, \lambda_n^2), M^T M = \text{diag}(1, \ldots, 1, \mu_1^2, \ldots, \mu_n^2) \) and \( \lambda_1^2 + \mu_1^2 = 1, \forall i = 1 : n, \) i.e. \( M^T M + \Lambda^T \Lambda = I_n \).

Using the GSVD, introducing \( u_i \) as the \( i \)th column of matrix \( U \) and \( \gamma_i \) as the \( i \)th diagonal element of \( \Lambda \), we may immediately write the solution of (13) as

\[
m(\alpha^{(k)}) = \sum_{i=q+1}^{n} \frac{\gamma_i^2}{\gamma_i^2 + (\alpha^{(k)})^2} \frac{u_i^T M^{(k)} x}{\lambda_i} (X^T)_i^{-1},
\]

\[
m^{(k)}(\alpha) = \sum_{i=q+1}^{n} \frac{\gamma_i^2}{\gamma_i^2 + (\alpha^{(k)})^2} (X^T)_i^{-1} f_i = \frac{\gamma_i^2}{\gamma_i^2 + (\alpha^{(k)})^2},
\]

\[
q < i \leq n, \quad f_i = 0, \quad 1 \leq i \leq q,
\]

where \( (X^T)_i^{-1} \) is the \( i \)th column of the inverse of the matrix \( X^T \) and \( f_i \) are the filter factors. Therefore the algorithm proceeds by first updating the matrix \( W_2 \) at step \( k \) using (12), calculating the GSVD for the matrix pair \( [\hat{G}, G^{(k)}] \) and then updating \( m^{(k)} \) using (16) which depends on \( \alpha^{(k)} \).

Three criteria are used to terminate the iterative procedure. Following Farquharson and Oldenburg (2004) the iteration is seen to have converged and is thus terminated when either (i) a sufficient decrease in the functional is observed, \( p^{(k)}(\alpha) - p^{(k-1)}(\alpha) < \tau (1 + P^{(k)}) \), or (ii) the change in the density satisfies \( \| m^{(k-1)} - m^{(k)} \| < \tau \sqrt{1 + \| m^{(k)} \|} \). If neither of these conditions is satisfied by an upper limit on the number of iterations, the procedure is terminated without convergence as measured in this manner. The parameter \( \tau \) is taken as \( \tau = 0.01 \) for the inversions considered here.

The remaining issue is the determination of the regularization parameter at each step of the iteration. As noted, when \( a \) priori information in the form of the standard deviations on the noise in the data is available, the MDP can be used to find \( \alpha \). Here, in the absence of the exact information on the error in the data we investigate the use of the L-curve and GCV methods to find \( \alpha^{(k)} \) for which the formulation using the GSVD is advantageous.

2.3. Regularization parameter estimation

2.3.1. The L-curve. The L-curve approach developed by Hansen (1992, 1998) for linear inverse problems is a robust criterion for determining the regularization parameter. It is based on the trade-off between the norm of the regularized solution and the norm of the corresponding fidelity term residual as the regularization parameter varies. According to Hansen (1992, 1998), when these two norms are plotted on a log–log scale, the curve has an L shape with an obvious corner. This corner separates the flat and vertical parts of the curve where the solution is dominated by regularization errors and perturbation errors, respectively. Picking \( \alpha_{opt} \) as the \( \alpha \) responsible for the corner point gives the optimal trade-off between the two terms, and the corresponding model is selected as the optimal solution. For \( \alpha > \alpha_{opt} \) the regularized solution does not change dramatically, while the residual does. In contrast, for \( \alpha < \alpha_{opt} \) the regularized solution increases rapidly with little decrease in the residual. Because of the relation of \( \alpha_{opt} \) with the shape of the curve, Hansen (1998) recommends estimating \( \alpha_{opt} \) by finding the maximum of the local curvature in the neighborhood of the dominant corner of the plot. Although the L-curve technique can be robust for problems generating well-defined corners, it may not work so well in other cases. For an underdetermined problem the recovered model can change more slowly with the degree of regularization (Li and Oldenburg 1999), and the L-curve is thus smoother. This makes it difficult to find the maximum point of curvature of the curve. On the other hand, given the solution of the regularized problem in terms of the GSVD, as in (15), finding the L-curve is relatively efficient and is thus one of the conventional ways to estimate \( \alpha_{opt} \).

It was shown by Farquharson and Oldenburg (2004) that the L-curve choice for \( \alpha \) at early iterations may be too small which may lead to the inclusion of excessive structure in the model that needs to be eventually removed, hence requiring more iterations for the inversion. Hence here we follow the approach suggested by Farquharson and Oldenburg (2004) and impose a so-called cooling process in which \( \alpha^{(k)} \) is given by \( \alpha^{(k)} = \max(\alpha^{(k-1)}, \alpha^*) \) where \( 0.01 \leq c \leq 0.5 \) and \( \alpha^* \) is the point of maximum curvature of the L-curve. Moreover, choosing a relatively large value for \( \alpha^* \) improves the performance of the algorithm. We use \( \alpha^* = \max(\gamma_i/\mu_i) \) which work well for the presented inversion examples.

2.3.2. Generalized cross validation. The major motivation for using the GCV to find an optimal value for \( \alpha \) is that a good value should predict missing data values. Specifically, if an arbitrary measurement is removed from the data set, then the corresponding regularized solution should be able to predict the missing observation. The choice of \( \alpha \) should be independent of an orthogonal transformation of the data (Hansen 1998). The GCV functional is given by

\[
\text{GCV}(\alpha) = \frac{\| \tilde{G}_m(\alpha) - \tilde{F} \|^2}{\text{trace}(\tilde{I}_m - \tilde{G} G(\alpha))^2} = \frac{\| \tilde{G}_m^{(k)} - \tilde{d}_{obs} \|^2}{(m - \sum_{i=q+1}^{n} f_i)^2},
\]

\[
= \frac{\| \sum_{i=q+1}^{n} (1 - f_i) u_i^T M^{(k)} x \|^2}{(m - \sum_{i=q+1}^{n} f_i)^2};
\]

\[
= \frac{\| \tilde{G}_m^{(k)} - \tilde{d}_{obs} \|^2}{(m - \sum_{i=q+1}^{n} f_i)^2}, \quad (17)
\]
where the final expressions follow immediately from the GSVD, with \( G(\alpha) = (\tilde{G}^T \tilde{G} + \alpha^2 D^T D)^{-1} \tilde{G}^T \). Here the numerator is the squared residual norm and the denominator is effectively the square of the number of degrees of freedom (Hansen 1998). It can be shown that the value of \( \alpha \) which minimizes the expected value of the GCV function is near the minimizer of the expected value of the predictive mean-square error, \( \| \hat{G} m(\alpha) - d_{\text{exact}} \|^2 / \) (Hansen 1998). Hence, finding the minimum for GCV(\( \alpha \)) should lead to a reasonable estimate for \( \alpha \). We have seen in our experiments that when the GCV does not fail, in which case it produces a very small \( \alpha \), it usually leads to a value of \( \alpha \) which is slightly larger than the optimal value. Failure occurs when GCV(\( \alpha \)) is almost flat near the optimal alpha, leading to numerical difficulties in computing its minimum. The cooling procedure, as described for the L-curve, is also applied to the GCV estimation of \( \alpha^{(k)} \) but with \( \alpha^* \) now chosen as the current minimum of the GCV function. For clarity we summarize in algorithm 1 the steps for the inversion that are applied at each iteration. Here we state this for the L-curve method. The GCV solutions are found equivalently but at all steps using the L-curve instead the GCV method is applied.

**Algorithm 1.** The steps taken for the inversion at every iteration assuming the use of the L-curve to find the regularization parameter.

Step 1. Calculate the GSVD for matrix pair \([\tilde{G}, D]\).

Step 2. Calculate the solutions, and the associated L-curve function, for a range of \( \alpha \), the optimal \( \alpha \) is found using the L-curve.

Step 3. The cooling process is implemented for deciding whether the obtained \( \alpha \) from step 2 should be used or not.

Step 4. With \( \alpha \) from step 3, the model parameters are computed using equation (16).

Step 5. Density limits are implemented on model parameters, from step 4, and then \( W_e \) and \( W_{\text{hard}} \) are updated.

Step 6. Data misfit, \( S(m) \) and related parameters are computed for model parameters obtained from step 5.

Step 7. If the termination criteria are satisfied the iteration terminates. Otherwise, the a priori density model is set as equal to the density model from step 5 and the iteration returns to step 1.

**Figure 2.** In figure (a) the synthetic model of a body set in a grid of square cells each of size 10 m, the density contrast of the body is 1 gr cm\(^{-3}\). Figure (b) shows the gravity anomaly due to the synthetic model contaminated by uncorrelated noise with \( \eta_1 = 0.03 \) and \( \eta_2 = 0.001 \). The exact anomaly is indicated by the solid line and the contaminated data by the symbols.

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L-curve criterion is more focused. This feature was present in all the examples we have analyzed; inversion using GCV always provide a smoother reconstruction than that obtained using the L-curve. Figures 4(a) and (b) demonstrate the progression of the solutions with iteration \( k \) for the data fidelity \( \phi(d^{(k)}) \), the stabilizer \( S(m^{(k)}) \), the parametric functional \( P^* (m^{(k)}) \), and regularization parameter, \( \alpha^k \), again for the L-curve and GCV, respectively, for this first example. In our experience the behavior indicated is consistent when using the GCV to find the regularization parameter \( \alpha \); it generally decreases initially, but then increases to converge to a fixed value. On the other hand, for the L-curve the progression of \( \alpha^k \) is more erratic, generally oscillating in final iterations toward a converged value as shown in figure 4(a). Manual intervention may then be needed to force the overall convergence of the algorithm (Ajo-Franklin et al 2007). The main problem in using the L-curve, as mentioned in section 2.3.1, is its smooth shape, that makes it difficult to find the corner, namely the point of maximum curvature. To illustrate we plot the L-curve for all iterations in figure 5(a), showing that overall the approach is successful, although at a given middle iteration the apparent corner is missed, see figure 5(c). Still, the starting and final iterations in figures 5(b) and (d) do find useful corners.

The same formulation was used to generate two further synthetic data sets, with quantitative results shown also in table 1. Noise generated using \( \eta_1 \) equal to 0.01 and 0.05 was considered, with \( \eta_2 = 0.001 \) in both cases. The results of the inversions are illustrated in figures 6 and 7, respectively. We note from table 1 that the fidelity values at convergence are less than the \( \chi^2 \) measure of the noise, that always \( \chi^2_{L-curve} < \chi^2_{GCV} \), but that there is no fixed conclusion about the relation between the final relative errors and fidelity estimates by the L-curve and GCV inversions. We conclude that both the GCV and the L-curve are successful in providing reasonable solutions. It should be noted that increasing the focusing parameter \( \varepsilon \) can yield solutions which are not focused, especially as shown in figure 7.

To assess both the impact of the choice of the bounds on the convergence properties for the solution and the choice of the regularization parameter \( \alpha \), we investigated two additional situations. First we implemented the same problem as given in figure 2, with noise \( \eta_1 = 0.03 \) and \( \eta_2 = 0.001 \), but inverted now with upper bounds on the density changed to 2 gr cm\(^{-3}\). The results are illustrated in figure 8 and detailed as before in table 1. We see that the solutions are more focused, as anticipated from the previous work of Portniaguine and Zhdanov (1999) but the relative error overall is increased and
Figure 5. The $L$-curve for all iterations; in each case the circle shows the point with maximum curvature. In figures (b)–(d) we show the individual curves at iteration 1, 10 and the final stage.

Figure 6. Density model obtained from inverting the data of figure 2(b) with MS stabilizer and noise level with $\eta_1 = 0.01$ and $\eta_2 = 0.001$. The regularization parameter was found using in (a) the $L$-curve; and in (b) the GCV.

Figure 7. Density model obtained from inverting the data of figure 2(b) with MS stabilizer and noise level with $\eta_1 = 0.05$ and $\eta_2 = 0.001$. The regularization parameter was found using in (a) the $L$-curve; and in (b) the GCV.
Figure 8. Density model obtained from inverting the first data set, $\eta_1 = 0.03$ and $\eta_2 = 0.001$, with MS stabilizer and density limits $0 \text{gr cm}^{-3} \leq m_j \leq 2 \text{gr cm}^{-3}$. The regularization parameter was found using in (a) the $L$-curve; and in (b) the GCV.

Figure 9. Density model obtained from inverting the first data set, $\eta_1 = 0.03$ and $\eta_2 = 0.001$, with smoothness stabilizer. In (a) and (b) density limits are $0 \text{gr cm}^{-3} \leq m_j \leq 1 \text{gr cm}^{-3}$, in (c) and (d) density limits are $0 \text{gr cm}^{-3} \leq m_j \leq 2 \text{gr cm}^{-3}$. The regularization parameter was found using in (a) and (c) the $L$-curve; and in (b) and (d) the GCV.

the fidelity of the solution is also decreased. However, it is of greater interest for the purposes of this study to observe that the performance of the parameter choice techniques is independent of the upper bound, and the parameters are found to be stably independent of the constraint bounds. To determine the necessity of using the MS instead of a smoothness stabilizer, we also considered the results obtained using a smoothness stabilizer, i.e. the $W_s$ in (9) replaced with the approximation for the second derivative of the model parameters, for the situations in figures 3 and 8. These results are also detailed in table 1 and illustrated in figures 9(a), (b) and (c), (d), respectively. They demonstrate the relative insensitivity to density limits of the smoothness-stabilizer obtained solutions. However, the solutions lack the contrast that is achieved using the MS regularization. Overall, the solutions obtained with GCV are apparently more robust than those obtained with the $L$-curve. It should be noted that using a non-$L_2$ measure of the derivative in geophysical inversion leads to a strongly piecewise constant, or blocky, reconstruction with sharp jumps, see for example Farquharson and Oldenburg (1998).

4. Numerical results: real data

4.1. Geological context

The data used for inversion was acquired over the Safo mining camp in Maku, Iran, which is well known for manganese ores. Geologically this area is located in the Khoy ophiolite zone, in the northwest of Iran. Some manganese and iron–manganese deposits are found within sedimentary pelagic rocks and radiolarian cherts which are accompanied by Khoy ophiolite (Imamalipour 2005). Most of these deposits have little reserve; the Safo deposit is the only viable area distinguished so far for mining. In the Safo deposit, depositions of manganese have been found to occur in different horizons within pelagic rocks. Mineralogically, pyrolusite, bixibite, braunite and hematite are the main minerals present in ore, of which pyrolusite is the dominant ore (Imamalipour 2005), and calcite with quartz and barite present as minor phases. The banded, massive and disseminated textures are seen in orebodies. Manganese content varies from 7.4% to 69.1% in different regions of the area (Imamalipour 2005).
4.2. Gravity anomaly

The area of the gravity survey extends between UTM coordinates [438 276 438 609] west and [4342 971 4343 187] north, Z38. The gravity survey was performed by the gravity branch of the Institute of Geophysics, University of Tehran. The measurements were corrected for effects caused by instrument and tidal drift, latitude, free air and the Bouguer correction, to yield the Bouguer gravity anomaly, figure 10(a).

The Bouguer anomaly displays extreme magnitudes in the central of the area in the north–south direction, related to mineral occurrence which has high density contrast with the host rocks. This geological structure is therefore clearly suitable for using a 2D algorithm. The residual anomaly was obtained by subtracting the regional anomaly from the Bouguer anomaly using a polynomial fitting method, figure 10(b). One of the recommended steps in potential field inversion is upward continuation of data to a height of half the thickness of the shallowest cell which removes near surface effects without noticeably degrading the data. Figure 11 shows upward continuation of the residual data up to 2.5 m.

4.3. Inversion result

A profile of the anomaly (SA) consisting of 49 data measurements, sampled every 5 m, is chosen for inversion. The subsurface is divided into $49 \times 15$ square cells of size 5 m, hence in this case $m = 49$ and $n = 735$. Based on geological information (Imamalipour 2005), the background density is set to $2.8 \text{ gr cm}^{-3}$ and the density limits for the inversion are $2.4 \text{ gr cm}^{-3} \leq \rho_j \leq 4.7 \text{ gr cm}^{-3}$. The maximum number of iterations was set to 20. Each datum is assigned a Gaussian error as in the simulated cases, here with $\eta_1 = 0.05$ and $\eta_2 = 0.001$. Figures 12(a) and (b) illustrate the reconstructed density models from the inversion of profile SA using the $L$-curve and GCV methods for estimating the regularization parameter, yielding $\alpha_{L\text{-curve}}^* = 0.69$ and $\alpha_{GCV}^* = 4.87$ respectively.

Figure 10. (a) The Bouguer anomaly. (b) The residual anomaly, over the Safo manganese mine.

Figure 11. Upward continuation of the residual anomaly to height 2.5 m.

Figure 12. The density models obtained by inverting field gravity data (profile SA). The regularization parameter was found using in (a) the $L$-curve; in (b) the GCV.
Figures 13(a) and (b) illustrate the profile of the anomaly (SA) which is used for the inversion, indicated by the stars, and the resulting values obtained from reconstructed models in figures 12(a) and (b), denoted in each case by the circles. Both solutions clearly represent the density contrast and geometry for the occurrence of manganese ore. The horizontal extension of the obtained model is about 30 m and vertical extension shows a depth interval approximately between 5 m and 35 m. These results are close to those obtained by bore-hole drilling on the site, which show extension of manganese ores from 3–4 to 25–30 m in the subsurface along the north–south direction (Noorizadeh 2010). The data fidelity, the stabilizer, the parametric functional and regularization parameter, with iteration $k$, are shown in figures 14(a) and (b). The convergence histories have properties for the practical data that are similar to those for the simulated data sets.

5. Conclusion

Tikhonov regularization with the minimum support stabilizer has been demonstrated to yield non-smooth solutions and is thus an appropriate approach for recovery of geological structures with sharp boundaries. The presented algorithm is flexible and allows variable weighting in the stabilizer, including depth weighting, a priori density ranges for the domain and the inclusion of hard constraints for the a priori information in the inversion process. The L-curve and GCV criteria for estimating the regularization parameter were discussed, and characteristics of each of them in obtaining a solution were introduced. Numerical tests using synthetic data have demonstrated the feasibility of applying both methods in the iteratively reweighted algorithm. The regularization parameter is seen to converge as the number of iterations increases. Although the GCV method leads to inverse solutions which are slightly smoother than those obtained by the L-curve method, both recovered models are close to the original model. For this small-scale problem, it is shown that the GSVD can be used in the algorithm, demonstrating the filtering of the solution. Moreover, this use of the GSVD, which might generally be assumed to be too expensive, is beneficial and worthwhile in the context of regularization parameter estimation as shown here. For large-scale problems it is
anticipated that a randomized GSVD needs to be developed, along the lines of the randomized SVD that was introduced by Liberty et al. (2007). Finally the method was used on a profile of gravity data acquired over the Safo manganese mine in the northwest of Iran. The result shows a density distribution in the subsurface from about 5 to 35 m in depth and about 30 m horizontally. Future work will consider the inclusion of statistical weighting in the solution and the use of regularization parameter estimation using statistical approaches (Mead and Renaut 2009).

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