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Automatic estimation of regularization parameter by active constraint balancing method for 3D inversion of gravity data

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Abstract

Gravity data inversion is one of the important steps in the interpretation of practical gravity data. The inversion result can be obtained by minimization of the Tikhonov objective function. The determination of an optimal regularization parameter is highly important in the gravity data inversion. In this work, an attempt was made to use the active constrain balancing (ACB) method to select the best regularization parameter for a 3D inversion of the gravity data using the Lanczos bidiagonalization (LSQR) algorithm. In order to achieve this goal, an algorithm was developed to estimate this parameter. The validity of the proposed algorithm was evaluated by the gravity data acquired from a synthetic model. The results of the synthetic data confirmed the correct performance of the proposed algorithm. The results of the 3D gravity data inversion from this chromite deposit from Cuba showed that the LSQR algorithm could provide an adequate estimate of the density and geometry of sub-surface structures of mineral deposits. A comparison of the inversion results with the geologic information clearly indicated that the proposed algorithm could be used for the 3D gravity data inversion to estimate precisely the density and geometry of ore bodies. All the programs used in this work were provided in the MATLAB software environment.

1. Introduction

The gravity data inversion problem is the estimation of the unknown sub-surface density and its geometry from a set of gravity observations measured on the surface. Since the problem is underdetermined and non-unique, finding a stable and geologically plausible solution is feasible only with the imposition of additional information about the model [1]. Inversion is defined as a mathematical technique that automatically constructs a sub-surface physical property model using the measured data by incorporating a priori information. The recovered models must be capable of predicting the measured data adequately [2]. Determination of an optimal regularization parameter is highly important in gravity data inversion. There are different methods available for an automatic estimation of the regularization parameter in a 3D inversion [3]. There are two major ambiguities in the inversion of gravity data. Theoretical ambiguity is caused by the nature of gravity; many different sources in the sub-surface 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 [4].

In an inverse problem, the regularization parameter balances the effects of data misfit function and measure of some properties of the earth model. For linear inverse problems, several approaches have been developed for automatically estimating an appropriate regularization parameter when the observations are contaminated with Gaussian noise of uniform but an unknown standard deviation [3]. The Tikhonov regularization is a well-known and well-studied

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method for stabilizing the solution of ill-posed problems [5]. Many researchers such as Wahba (1990) [6] and Hansen (1997) [5] have used the value for the regularization parameter that minimizes the generalized cross-validation (GCV) function. Hansen (1997) has chosen the value corresponding to the point of maximum curvature on the 'L'-shaped curve obtained when ϕ_m is plotted as a function of ϕ_m for all the possible values for the regularization parameter [5].

In any regularization method, the trade-off between the data fit and the regularization term is controlled by a regularization parameter. The methods used to find this regularization parameter, called the parameter-choice methods, can be divided into two classes (Hansen (1997) [5]): (i) those that are based on knowledge of, or a good estimate of, the error in the observations such as the discrepancy principle, and (ii) those that, in contrast, seek to extract such information from the observations such as the L-curve or the GCV methods. In many practical applications, little knowledge is available about the noise or error in the data measurements. In contrast, regarding the regularization parameter as a spatially varying function λ(x,y,z), the method used is called active constraint balancing (ACB), and λ(x,y,z) is determined through the parameter resolution analysis [7]. In the ACB method, spatially varying Lagrangian multipliers (regularization parameters) are obtained by a parameter resolution matrix and the Backus-Gilbert spread function analysis [8]. Due to the iterative nature of the algorithm, the regularization parameter is determined in each iteration.

In this work, it was attempted to use the ACB method to choose the best value for the regularization parameter for the 3D linear inversion of gravity data using the Lanczos bidiagonalization algorithm. For getting the target, an algorithm was developed, which estimated this parameter. The validity of the proposed algorithm was evaluated by the gravity data acquired from a synthetic model. Then the algorithm was used for inversion of the real gravity data from the Cuba chromite deposit. The results obtained from the 3D inversion of the gravity data from this mine show that this algorithm can provide good estimates of density anomalous structures within the sub-surface.

2. Methodology

To perform inverse modeling, the sub-surface under the survey area is discretized into rectangular prisms of known sizes and positions. The density contrasts within each prism is an unknown parameter to be estimated by solving the inverse problem. A linear relationship between the density and gravity anomaly is a valid approximation; therefore, the inverse solution was obtained by solving a linear system of equations [9, 10].

$$d = Gm \tag{1}$$

In Eq. (1), G is the forward operator matrix (also called the sensitivity matrix or Kernel matrix) that maps the physical parameter space into the data space. The m vector denotes the unknown model parameters, and d is the data vector [11]. The inverse problem goal in geophysics is determining by a plausible spatial variation of one or more physical properties within the Earth, which is consistent with a finite set of geophysical observations that can be solved by formulating it as an optimization problem for an objective function such as [3-12]:

$$\phi(m) = \phi_d(m) + \lambda\phi_m(m) \tag{2}$$

The vector **m** contains the M parameters in the Earth model, ϕ_d is a measure of the data misfit, ϕ_m is a measure of some properties of the Earth model such as density, and **D** depicts the regularization matrix. Here, λ is the regularization parameter that balances the effects of ϕ_d andϕ_m [3]. The typical sum-of-squares misfit is called the misfit function:

$$\phi_d(m) = \left\| W_d \left[d^{obs} - d(m) \right] \right\|_2^2 \tag{3}$$

$$\phi(m) = \left\| Dm \right\|_2^2 \tag{4}$$

W_d is the data weighting matrix, given by $W_d = diag(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, ..., \frac{1}{\sigma_N})$. Also σ_i is a standard deviation for noise that is defined for each datum. We can replace the regularization matrix (**D**) with the depth weighting matrix (W_{depth}), which is given by $W_{depth} = diag(\frac{1}{(Z_1)^\beta}, \frac{1}{(Z_2)^\beta}, ..., \frac{1}{(Z_m)^\beta})$. The use of a ($W_{depth}$) matrix in constructing a model prevents the kernel decay [11]. The inverse problem in this work was solved as an optimization of a global objective function Eq. (1) using the iterative LSQR algorithm based on the

Lanczos bidiagonalization [13, 14]. Determination of the regularization parameter, which balances the minimization of the data misfit and model roughness may be a critical procedure to achieve both the resolution and stability.

2.1. Regularization parameter

Estimation of the regularization parameter (Lagrangian multiplier), which balances the minimization of the data misfit and model roughness, may be a critical procedure to achieve both resolution and stability.
Uchida (1993) [15] used the statistical criterion Akaike's Bayesian Information Criterion (ABIC) to determine the optimum regularization parameter. In contrast, Yi et al. (2003) [7] regarded the regularization parameter as a spatially varying function λ(x,y,z), which is named as ACB, and determines λ(x,y,z) through the parameter resolution analysis [16].
In our implementation, we adopted the spatially variable regularization parameter algorithm, in which 1 was regarded as a spatial function, determined by the parameter resolution analysis [7]. According to the ACB algorithm, the regularization parameter can be set optimally by the spread function **SP**$_i$ of the **ith** model parameter, which is defined by the parameter resolution matrix **R**. The parameter resolution matrix **R** can be obtained in the inversion process with pseudo-inverse G^{-g} multiplied by the kernel G [16].

$$R = G^{-g}G \tag{5}$$

In this work, we used the LSQR method for computation of the resolution matrix **R** in Eq. (5), This method can be be improved for a large-scale problem. where:

$$G^{-g} = (G^T G + \lambda C^T C)^{-1} G^T \tag{6}$$

The spread function, which accounts for the inherent degree of how much the i^{th} model parameter is not resolvable, is defined as:

$$SP_i = \sum_i^N \left\{ w_{ij} \left(1 - S_{ij}\right) R_{ij} \right\}^2 \tag{7}$$

In Eq. (7), N is the number of parameters and w_{ij} is a weighting factor, computed from the spatial distance between the two parameters i and j. Here, S_{ij} is a matrix used to take into account the constraint or regularization in the inversion. The value for S_{ij} is unity if C_{ij} is not zero, while it is zero when C_{ij} equals zero. In this approach, the regularization parameter $\lambda(x, y, z)$ is set by a value from the log-linear interpolation [7]:

$$\log(\lambda_i) = \log(\lambda_{\min}) + \frac{\log(\lambda_{\max}) - \log(\lambda_{\min})}{\log(SP_{\max}) - \log(SP_{\min})} \times \left\{ \log(SP_i) - \log(SP_{\min}) \right\} \tag{8}$$

where SP_{min} and SP_{max} are the minimum and maximum values for the spread function SP_i, respectively, and λ_{min} and λ_{max} are the minimum and maximum values for the regularization parameter λ(x,y,z) that must be provided by the user. With this method, we can automatically set a smaller value for λ(x,y,z) of the regularization parameter to the highly resolvable model parameter, which corresponds to a smaller value of the spread function SP_i in the inversion process, and *vice versa*. The users can choose these minimum and maximum regularization parameters by setting the variables $LambdaMin$ and $LambdaMax$.

3. Inversion tests for synthetic models

We applied our algorithm to a synthetic test to evaluate the reliability of the introduced method. The true model consisted of two different bodies embedded beneath the surface so that the density of the uniform background was zero. The density of the rectangle block was 1.0 and the square block was 2.0 g/cm^3. These bodies were buried at different depths. Figure 1a shows a perspective view of the synthetic model. The data was gathered over a grid of 1000 × 1000 m with a sample spacing of 50 m. There was 441 data, and 5% Gaussian noise of the accurate datum magnitude was added. The gravity anomaly produced by the synthetic model is shown in Figure 1b. There were 4 horizontal cross-sections in different depths for the recovered model (Figure 1c). The sub-surface was discretized into 20 × 20 × 10 = 4,000 rectangular prisms with the same size of 50 m in the x, y, and z directions. In this case, we chose the minimum and maximum values for λ to be 1 and 4, respectively. The values for λ_{min} and λ_{max} were based upon the best results. Also the choice of values was the responsibility of the user. The results obtained were compared with the results of the GCV method. The maps of depth slices through the recovered model of the GCV method are shown in Figure 2a. Figure 2b shows the maps of depth slices through the recovered model from the ACB method. The scatter plot of the predicted data versus the observed Bouguer anomaly is shown in Figures 3a and 3b, indicating a good fitness of data in both methods. The results obtained indicate an acceptable reconstruction of the synthetic multisource bodies at different depth levels below the surface. The solution was blocky and defined the depth to the top and bottom of deep bodies adequately. The results obtained indicate an acceptable reconstruction of the synthetic multisource bodies at different depth levels below the surface. According to Figure 2b, the ACB method can be an efficient model from the proposed LSQR algorithm.

Table 1. Parameters of the synthetic model.

Model number	x×y×z dimension (m)	Depth to top (m)	True density (g/cm^3)
(1)	400×200×200	-50	1
(2)	200×200×200	-100	2

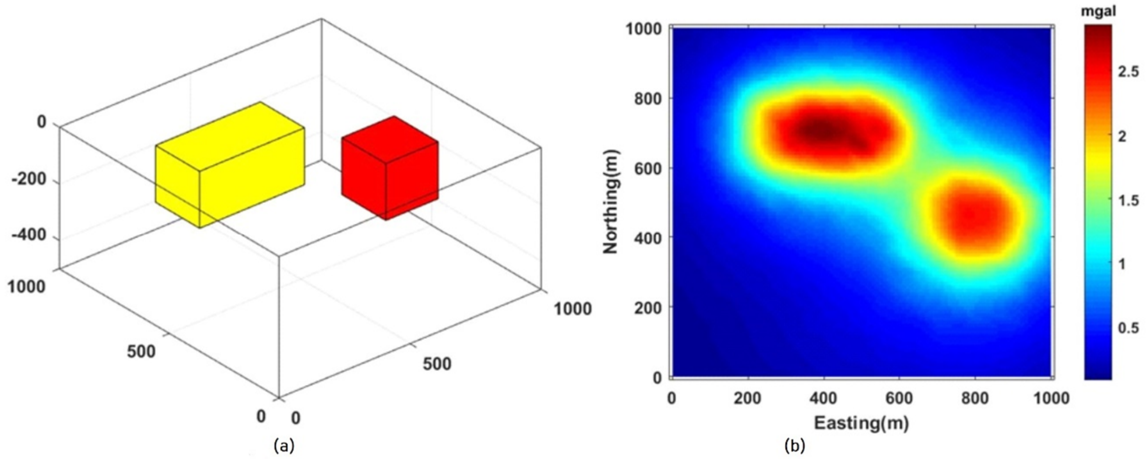

Figure 1. (a) Perspective view of the synthetic model. (b) Gravity anomaly produced by the synthetic model with 3% Gaussian noise.

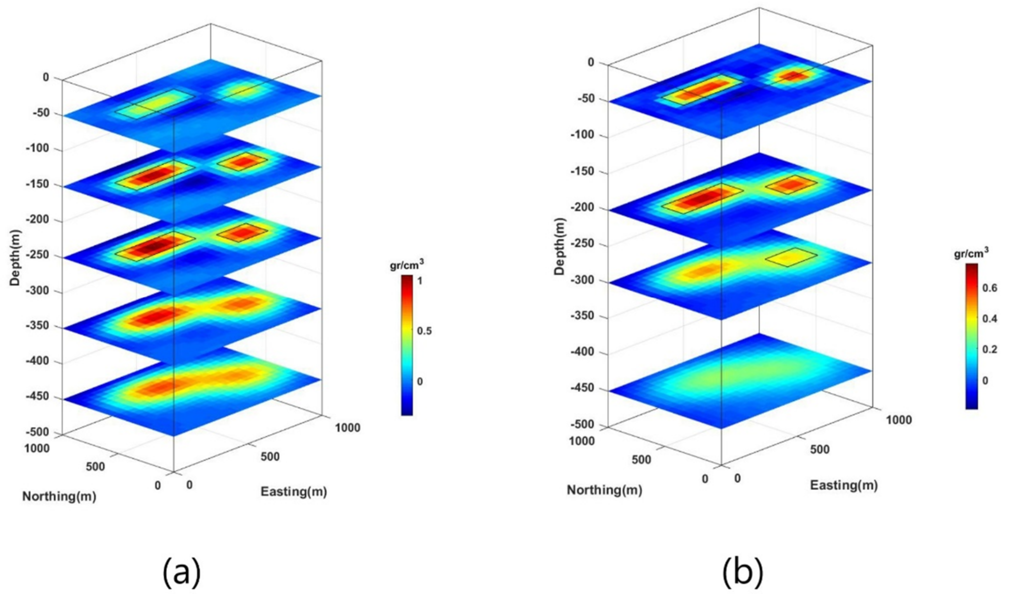

Figure 2. (a) Plan sections through the recovered density model obtained from inversion of gravity anomaly by the GCV method. (b) ACB method.

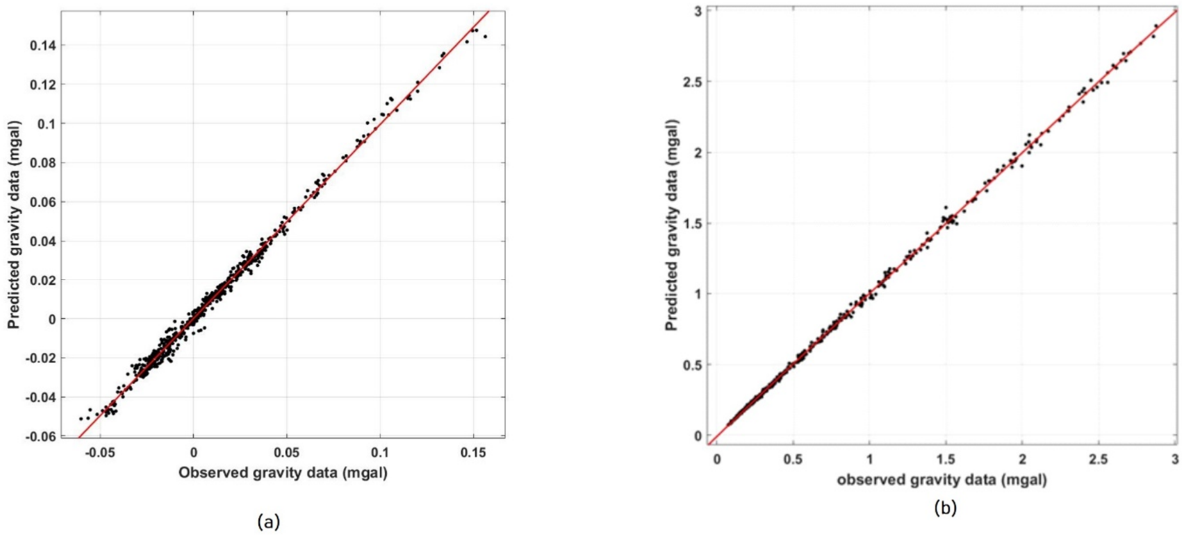

Figure 3. (a) Plot of the predicted gravity synthetic data versus the observed real data by the GCV method. (b) ACB method.

Table 2. Comparison of parameter regularization results in inversion of synthetic for the ACB and the GCV methods.

Regularization method	Time (s)	Number of iterations	Misfit
ACB	12.36	11	1.41
GCV	14.73	13	7.24

4. Inversion of field gravity data

The chromite deposits are in serpentinized Peridotite and Dunite near their contact with feldspathic rocks. The serpentinized rocks underlie the Savannah and contain feldspathic rocks, mainly Gabbro, Troctolite, and Anorthosite as well as chromite. Many feldspathic masses are not well-exposed but can be delineated by small outcrops, float, and a characteristic flora. Most of the chromite deposits are oriented so that the long axis parallels the strike of the nearest contact between the feldspathic or volcanic rocks and the serpentinized peridotite. In this work, we used a residual gravity anomaly over chromite deposits in the Holguin district, Cuba, measured by the US Geological Survey. The areas investigated were in the chromite district of the Holguin Province. The residual gravity anomaly map digitized at a grid interval of 0.2 mgal is shown in Figure 5. For a 3D inversion of the data, the sub-surface of the studied area was discretized with 28 × 23 × 10 cells in the x, y, and z directions, respectively. We The sampling data of 7 × 7 m in the digitized grid and the applied gravity method in prospecting for chromite deposits in the Holguin chromite district depends fundamentally upon the density contrast between the chromite and the surrounding country rocks. The difference in density between the chromite contained in the commercial deposits of the district and the country rock, which were serpentinized peridotite and dunite, was about 1.5 g/cm^3. The feldspathic rocks in the serpentinized peridotite and dunite had an average density of about 2.7 g/cm^3, which provided a sufficient density contrast with respect to the serpentinized rocks to cause anomalies of much the same size and magnitude as the chromite. In Figure 4, we can see the distribution of ophiolits in Cuba, and also an anomalous body with a high density contrast around the center of the studied area, which represents the Holguin deposit (Figure 5). Figure 6 shows the maps of depth slices through the recovered model from the proposed inversion methods. We can clearly see the lateral shape and extent of the main body of the deposit well-defined but for comparison, the inverse problem with the ACB method is more accurate than the GCV method for the recovered model. We obtained a good solution in agreement with the true geologic shape of chromite body and other geological studies in the area.

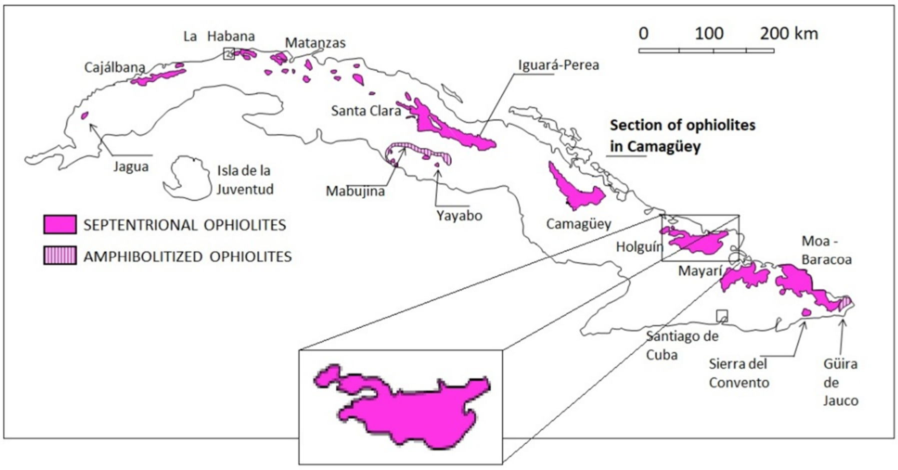

Figure 4. Distribution of ophiolits in the Holguin of Cuba.

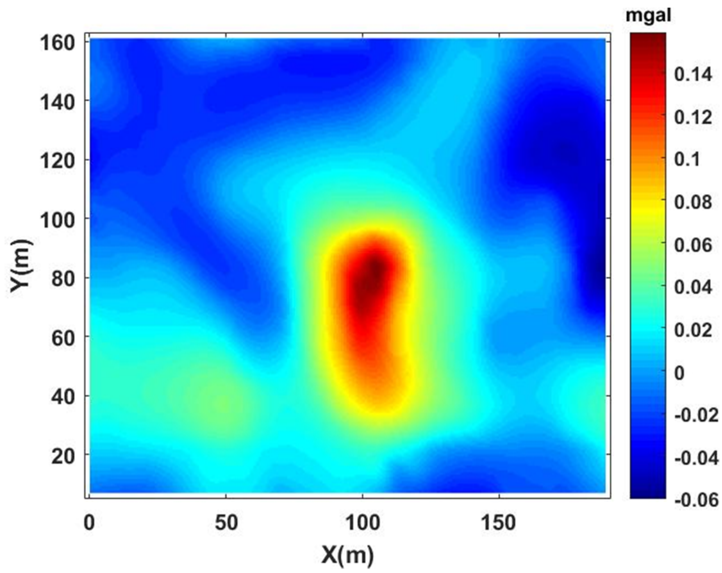

Figure 5. Holguin residual gravity map.

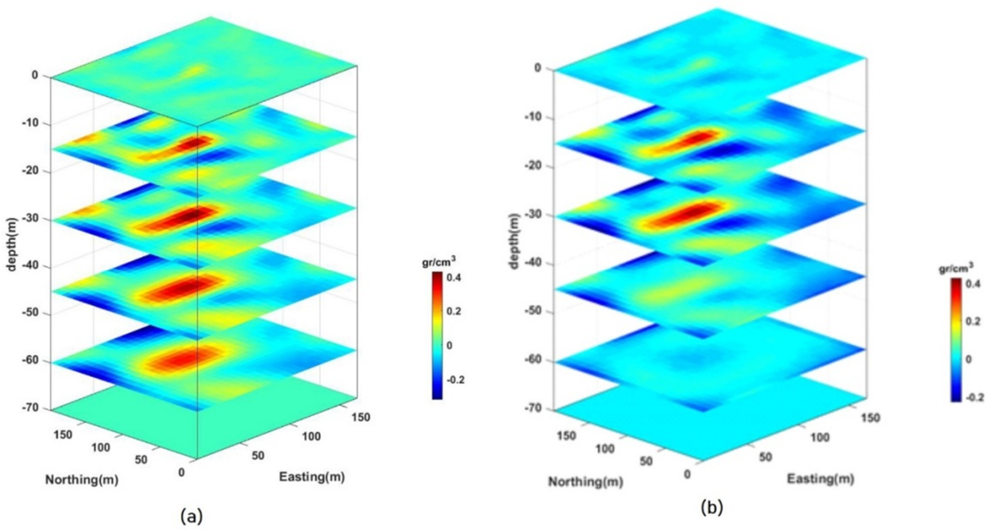

Figure 6. (a) Plan sections through the recovered density models obtained from the 3D smooth inversion of gravity anomaly using the GCV method at different depths. (b) The ACB method.

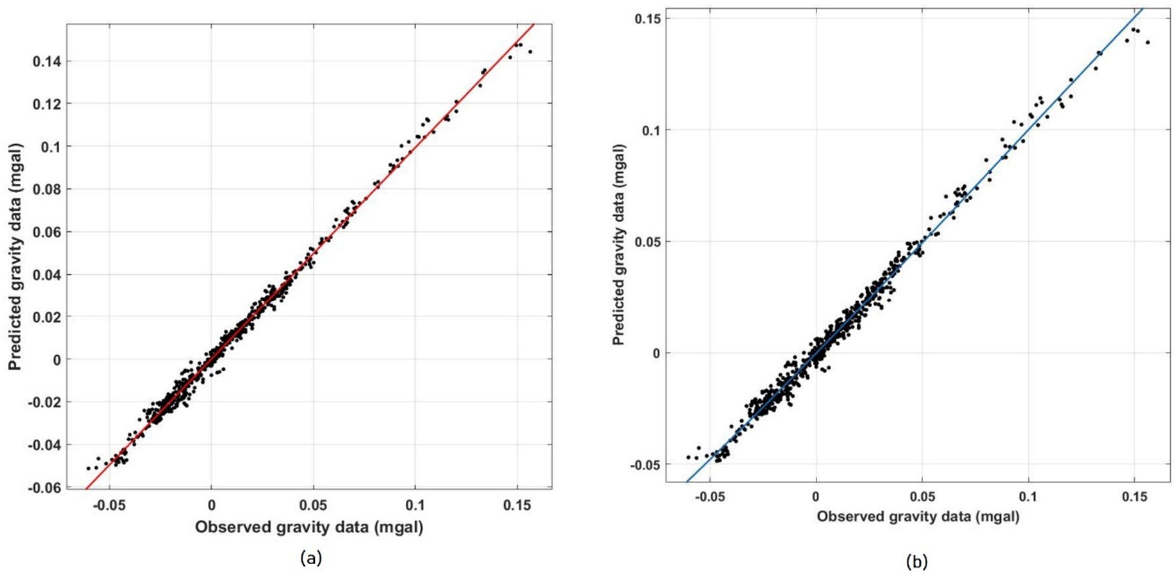

Figure 7. Data misfit between the predicted field gravity data with observed gravity data (a) GCV method. (b) ACB method.

Table 3. Comparison of parameter regularization results in inversion of real data for the ACB and the GCV methods.

Regularization method	Time (s)	Number of iterations	Misfit
ACB	9.36	9	3.42
GCV	15.61	13	8.26

The results obtained show that all the inverse algorithms with the ACB method detect the position of the orebody well, especially depth to top of the orebody.

5. Conclusions

We have developed a new algorithm for inversion of gravity data using the LSQR method. We used the active constraint balancing regularization method to choose the regularization parameter in each iteration, which is a fast and effective method for choosing the regularization parameter. In the ACB algorithm, we used the LSQR program for resolution matrix. Therefore, the proposed algorithm is efficient for large-scale problems. One of the advantages of the ACB method is the proper estimation of the lower depth of the model.

The results obtained show that the new developed 3D inversion method can produce a smooth solution, which defines the shape and extent of synthetic bodies adequately. Furthermore, this inversion algorithm was applied for inversion of a field gravity data from the Holguin deposit. It produced a model that was consistent with the available geological information of the deposit. Compression of the ACB method with other methods such as Generalized Cross-Validation (GCV) showed that the ACB method was more efficient than the GCV method for smooth inversion of gravity data.

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تخمین خودکار پارامتر منظم‌سازی با روش متعادل‌سازی قید فعال در وارون‌سازی سه‌بعدی داده‌های گرانی‌سنجی

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چکیده:

وارون‌سازی داده‌های گرانی‌سنجی یکی از مهم‌ترین مراحل در تفسیر عملی داده‌های گرانی است. نتایج وارون‌سازی می‌تواند با کمینه کردن تابع هدف تیخونوف حاصل شود. تعیین مقدار بهینه پارامتر منظم‌سازی در وارون‌سازی داده‌های گرانی از اهمیت بالایی برخوردار است. در این پژوهش، با استفاده از روش متعادل‌سازی قید فعال و الگوریتم وارون‌سازی سه‌بعدی داده‌های گرانی با استفاده از روش دوقطری‌سازی لنکزوس به محاسبه مقدار بهینه پارامتر منظم‌سازی پرداخته شده است. به منظور اعتبارسنجی الگوریتم پیشنهادی به ارزیابی این روش با استفاده از داده‌های حاصل از یک مدل مصنوعی پرداخته شده است. نتایج حاصل از داده‌های مصنوعی صحت عملکرد الگوریتم پیشنهادی را تائید می‌کند. نتایج وارون‌سازی سه‌بعدی داده‌های گرانی‌سنجی ذخایر کرومیت در کشور کوبا به خوبی نشان می‌دهد که روش دوقطری‌سازی لنکزوس می‌تواند برآورد مناسبی از توزیع چگالی و هندسه ساختارهای زیرسطحی و مواد معدنی داشته باشد. مقایسه نتایج وارون‌سازی با اطلاعات زمین‌شناسی به خوبی نشان می‌دهد که الگوریتم پیشنهادی می‌تواند تخمین مناسبی از توزیع چگالی و هندسه توده‌های معدنی ارائه دهد. تمام برنامه‌های مورد استفاده در این پژوهش در محیط نرم‌افزار متلب نوشته شده است.

کلمات کلیدی: مسئله وارون، پارامتر منظم‌سازی، متعادل‌سازی قید فعال، داده گرانی‌سنجی، ذخیره معدن هالوگین.