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On estimation of stopping criteria for iterative solutions of gravity downward continuation

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2 **Abstract**

3 This article discusses methods for selecting criteria used for stopping iterative regularization
4 methods applied to solving continuation of gravity observed at or outside the Earth's
5 surface down to the geoid. This computational step is required for determination of the
6 gravimetric geoid by the Stokes approach. For surface gravity data measured with spatial
7 resolutions at the kilometer level and higher, their downward continuation becomes ill
8 posed and its solution numerically unstable. Two iterative methods often used for solving
9 this problem, namely the Landweber and conjugate gradient least-squares methods, are
10 investigated using a sample of surface gravity data synthesized from a global gravitational
11 model over a mountainous test area in Colorado, USA. Five different commonly used
12 stopping criteria are applied to both iterative methods and neither of them, except L-Curve,
13 succeed to stop the iterative process at the reasonable solution. A simple approach is
14 proposed to stop the iterative methods exploiting stochastic properties of surface gravity
15 data. Results of numerical tests suggest that a rather simple stopping criterion based on
16 stochastics parameters of surface gravity data estimated using a leave-one-out cross
17 validation procedure yields results superior to those based on the L-curve approach which is
18 best performing among the five standard methods for selecting the stopping criterion.
19 Results based on the Landweber method outperform those based on the CGLS method.
20 Iterative methods based on optimum numbers of iterations represent an alternative to
21 commonly used regularization techniques for solving ill-posed inverse problems, such as
22 Tikhonov, that require optimal estimates of regularization parameters.

23 **Key words:** Downward continuation, gravity, iterative method, inverse problem, stopping
24 criterion

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1. Introduction

Stokes's solution of the gravimetric geoid from surface gravity data requires gravity anomalies to be known on the geoid. Thus, surface gravity values observed at the topography must first be transformed into such functions of position which can be continued down to the geoid using some known mathematical technique. Helmert's gravity anomalies multiplied by their geocentric radii are harmonic functions everywhere outside the geoid; thus, they can be continued from the topography down to the geoid using an inverse solution of the Poisson integral equation in the process called the downward continuation (DWC). The spherical form of the Poisson integral equation (geoid is approximated by a mean geocentric sphere) reads for the product of the gravity anomaly Δg with the geocentric radius r (Heiskanen and Moritz, 1967; Sect. 1-6) as follows:

$$\Delta g_t(r_t, \Omega) = \frac{R}{4\pi r_t} \int_{\Omega_0} \Delta g_g(R, \Omega') K(r_t, \psi(\Omega, \Omega'), R) d\Omega', \quad (1)$$

where Ω represents the geocentric angular position (defined by the spherical latitude $-\frac{\pi}{2} \leq \varphi \leq \frac{+\pi}{2}$ and longitude $0 \leq \lambda < 2\pi$) of the gravity anomaly on the topography Δg_t (computation point) and Ω' stands for the geocentric direction of the gravity anomaly on the geoid Δg_g (integration point). R is the radius of the mean geocentric sphere approximating the geoid and r_t is the geocentric radius of the computation point at the topography. $K(r_t, \psi, R)$ is the spherical Poisson integral kernel given analytically as follows (*ibid*):

$$K(r_t, \psi, R) = R \frac{r_t^2 - R^2}{l^3(r_t, \psi, R)}, \quad (2)$$

where $l(r_t, \psi, R)$ is the Euclidian distance between the computation and integration points and ψ is their respective spherical distance. Finally, Ω_0 in Eq. (1) represents an integration domain represented by a spherical cap around the computation point defined by the

1 spherical distance $\psi_0 \ll \pi$ to which the full spatial angle is truncated due to limited
 2 geographic availability of ground gravity data.

3 The Poisson integral equation in Eq. (1) can be used for the upward continuation of the
 4 gravity anomaly from the mean geocentric sphere (representing the geoid) to the
 5 topography. Since gravity anomalies are observed on or outside the topography but
 6 required on the geoid for the purpose of the geoid determination by the Stokes integral
 7 equation, the inverse of the Poisson integral equation must actually be solved. As gravity
 8 anomalies on the topography are measured only in discrete points and the Poisson integral
 9 must be discretized for its numerical evaluation, a general system of linear equations can be
 10 formed:

$$\mathbf{A} \mathbf{x} = \mathbf{b} , \quad (3)$$

11 where the vector $\mathbf{b}$ contains gravity anomalies observed on the topography, vector $\mathbf{x}$
 12 contains sought gravity anomalies on the geoid (approximated by the mean geocentric
 13 sphere) and $\mathbf{A}$ is the design matrix with elements given for the i -th computation point and j -
 14 th integration point as follows:

$$A_{ij} = \frac{R}{4\pi r_t^i} S_j K(r_t^i, \psi_{ij}, R) , \quad (4)$$

15 where $S_j = \cos \varphi_j \Delta\varphi \Delta\lambda$ is a discrete surface element corresponding to selected
 16 discretization steps in the spherical latitude and longitude. As scattered surface gravity
 17 observations are not regularly distributed, they are usually averaged and/or interpolated to
 18 a regular coordinate grid for the numerical convenience and noise reduction. For details on
 19 various discretization schemes for continuation of gravity anomalies, see, e.g., (Vaníček et
 20 al., 1996; Huang, 2002; Huang et al., 2003; Goli et al., 2011).

21 The upward continuation, i.e., the forward problem in Eq. (3), reproduces gravity anomalies

1 given on the mean geocentric sphere to points in its outer space, i.e., to points at increasing
2 distances from gravitating masses. Thus, the upward continuation attenuates the spectrum
3 of gravity anomalies. In contrary, DWC representing its inverse amplifies exponentially their
4 spectrum. Consequently, DWC solved using the discrete Poisson integral equation easily
5 becomes an ill-posed problem with a numerically unstable solution. The system of linear
6 equations in Eq. (3) is well posed if three Hadamard's conditions are fulfilled: the solution
7 exists, is unique and stable (Hadamard, 1902). The existence and uniqueness of the solution
8 are guaranteed physically, but the solution may be unstable numerically, i.e., the solution $\mathbf{x}$
9 may represent continuously changes in the input data $\mathbf{b}$.

10 Two aspects must be considered: discretization of input gravity data and continued gravity
11 noise spectrum. The inverse of the Poisson integral may result in a well-posed problem
12 depending on the discretization of its integration domain as well as on the distance of the
13 computation point from gravitating masses. For DWC of surface gravity data, their angular
14 (spatial) resolution is a major factor influencing numerical stability of the solution. While
15 Martinec (1996) showed that DWC of surface gravity anomalies with the angular resolution
16 larger than 50 arc-sec (approximately 1.5 km at the equator) is an unstable problem, Sun
17 and Vaníček (1998) concluded that DWC of the 5 arc-min (approximately 9 km at the
18 equator) surface anomalies represents a well-posed problem even over the very rough
19 topography such as the Canadian Rocky Mountains. Tenzer and Novák (2008) investigated
20 numerical instabilities of discretized Poisson's DWC theoretically; they found that its
21 stability was depended on extreme heights of gravity points above the mean geocentric
22 sphere as well as on their angular resolution.

23 Beside discretization of the integration domain, the high-frequency noise in surface gravity
24 anomalies may also turn DWC into an unstable problem, i.e., small errors in input gravity

1 data can cause large errors in the solution. High-frequency gravity variations are mainly due
2 to observation errors and topographic gravitational effects. Reduction of observed surface
3 gravity for the topographic effects can cause large variations in the reduced gravity signal
4 particularly over mountainous areas (Heck, 2003). There exist reduction schemes which
5 smooth observed gravity but always only the high-frequency part of the signal caused by the
6 topographic effects, not the observation errors.

7 As the observation noise is an inevitable part of observed gravity, DWC of high-resolution
8 surface gravity data always needs to be regularized. Due to numerical properties of the
9 design matrix $\mathbf{A}$ in Eq. (3), its exact inverse cannot be computed and regularization is often
10 needed to find its approximate inverse. Numerous studies have been performed for
11 regularizing DWC of aerial gravitational or satellite gradiometry data, see, e.g., Novák &
12 Heck (2002), Kern (2003), Tao et al. (2004), Muller and Mayer-Guerr (2005) for aerial gravity,
13 and Xu (1992), Janák et al. (2014), Sebera et al. (2014) and Pitoňák et al. (2016) for the
14 satellite gradiometry data. The regularized solution of the Poisson DWC can be found in two
15 ways: the first solution is based on inverting the design matrix $\mathbf{A}$ called herein the direct
16 solution; for instance, Tikhonov's regularization or truncated singular value decomposition
17 (TSVD) represent two examples of often used regularization techniques. The second
18 solution, called herein the indirect solution, avoids inverting the design matrix $\mathbf{A}$; instead,
19 the solution is obtained by iterating the forward model using, e.g., Jacobi's iterative or
20 conjugate gradient (CG) techniques. Kern et al. (2003) numerically investigated various
21 regularization methods for DWC of aerial gravity data. They found that DWC errors for some
22 regularization techniques could reach up to 25 mGal. They also reported that using TSVD
23 and CG techniques these errors could be reduced down to 3 mGal. Thus, these two
24 regularization techniques were recommended for DWC of aerial data. Tao et al. (2004)

1 investigated three methods for stabilizing the downward continuation of aerial gravity data:
2 Tikhonov's regularization, point-mass modelling and an interior solution to the spherical
3 Dirichlet problem. They found out that the first two methods were more accurate and
4 stable. Moreover, choosing the regularization parameter in the direct problem influenced
5 the accuracy and stability of the inverse solution. Values of regularization parameters in the
6 direct solution and values of stopping criteria in the indirect solution affect both stability
7 and accuracy of the DWC solution.

8 DWC of surface gravity anomalies has been investigated in numerous studies. For example,
9 Huang (2002) used TSVD to regularize the indirect solution of DWC and to speed up its
10 convergence. He used surface gravity anomalies synthesized from the global gravitational
11 model EGM96 (Lemoine et al., 1998) with the angular resolution of 0.5 arc-deg. Kingdon and
12 Vaníček (2010) studied the Jacobi iterative technique to continue the surface gravity
13 anomaly down to the geoid using the discretized Poisson integral. They stopped the
14 iterative algorithm using a threshold defined as a function of the upper bound estimate of
15 the condition number of the design matrix **A**. However, this method should further be
16 investigated as it may not be applicable to other iterative techniques or to geographic areas
17 with more complex gravity anomalies.

18 The direct solution of DWC needs SVD to invert the design matrix **A**. This method is
19 applicable to small to moderate size systems of linear equations. However, in our problem,
20 i.e., for DWC of high resolution surface gravity anomalies, the number of equations equals
21 to the number of gravity observations, which means that the design matrix **A** is generally
22 very large even for block-wise DWC (surface gravity data over larger areas are divided into
23 smaller blocks which are continued per parts). For example, for a 1x1 arc-deg block with the
24 angular step of 1 arc-min and 1 arc-deg integration radius, the size of the respective system

1 of linear equations is 32400×32400 . Therefore, to regularize the direct solution of DWC
2 can computationally be very demanding. Moreover, adding any arbitrary regularization
3 parameter into the model violates physical meaning of the solution.

4 In the indirect solution, only the matrix-vector operations are needed and no matrix
5 decomposition is required. Iterative methods produce a sequence of vectors $\mathbf{x}^k, k = 1, 2, \dots$
6 until they converge to an approximate solution; see, e.g., (Hansen, 1998; Barrett et al.,
7 1994). If the design matrix $\mathbf{A}$ is ill conditioned, it contains small singular values which amplify
8 the high-frequency part of input gravity data making DWC unstable. Iterative methods
9 initially pick up those SVD components that correspond to the largest singular values of the
10 matrix $\mathbf{A}$, then converge toward the generalized solution in the presence of small singular
11 values. This phenomenon is called semi-convergence (Favati et al., 2014; Borges et al., 2015).
12 Indeed, the choice of the stopping criterion determines the number of iterations.

13 Choosing the stopping criterion is often based on differences between estimated
14 (continued) and input (observed) gravity data. Estimated statistics of the input data noise
15 are usually chosen as criteria to stop the iterative process. However, Kingdon and Vaníček
16 (2010) showed that choosing statistics of input data noise as the stopping criterion could
17 result in an incorrect solution of DWC.

18 In this article, we focus on estimating an optimal value of the stopping criterion in
19 connection with the Landweber and conjugate gradient least-squares (CGLS) methods. Our
20 task is to estimate such a stopping criterion which yields a physically meaningful indirect
21 solution for DWC of high-resolution surface gravity data. The article is organized as follows:
22 In Section 2, the ill posedness of DWC for high-resolution surface gravity anomalies is
23 investigated using discrete Picard's condition; in addition, the theory of iterative methods
24 and their semi-convergence property are briefly introduced. In Section 3, the parameter

choice rules are reviewed and their applications in the iterative DWC process are discussed. In Section 4, a new stopping criterion for the iterative DWC algorithm estimated by a cross-over validation method is proposed. Finally, Section 5 contains conclusions and recommendations.

2. Review of iterative methods

Assuming Eq. (3) represents an ill-posed but non-singular system of linear equations, to find its solution iteratively, i.e., without inverting the matrix $\mathbf{A}$, we apply the iterative algorithm of the following form:

$$\mathbf{r}_k = \mathbf{b} - \mathbf{A} \mathbf{x}_k ; \quad (5)$$

where $\mathbf{r}_k$ represents the vector of residuals after the k-th iteration. We have to consider some initial estimates $\mathbf{x}_0$ which in case of DWC of surface gravity data are usually represented by input surface gravity anomalies.

The iterative process stops when the L_2 -norm of the vector $\mathbf{r}_k$ is smaller than some predefined threshold. Other norms of the residual vector can be used depending on the selected stopping criterion. Additional parameters can be used to speed up converge of the iterative algorithm. In this study we shall consider the CGLS and Landweber iterative methods as two methods recently applied to DWC of gravity data in geodesy.

2.1 Conjugate gradient least-squares method

The conjugate gradient algorithm is used to find the numerical solution of a system of linear equations with the positive-definite design matrix $\mathbf{A}$. If the least-squares approach is used to find the unbiased solution, then we get the conjugate gradient least-squares method (CGLS). To iterate the system in Eq. (5) using the CGLS method and using the gravity at the Earth's surface as an initial solution, i.e., $\mathbf{x}_0 = \mathbf{b}$, the following algorithm is used (Hestenes and

1 Stiefel, 1952):

$$\mathbf{r}_0 = \mathbf{b} - \mathbf{A}\mathbf{x}_0$$

$$\mathbf{P}_0 = \mathbf{r}_0$$

k=0

Do while $|\mathbf{r}_k| > \delta$

$$\alpha_k = \frac{\mathbf{r}_k^T \mathbf{r}_k}{\mathbf{P}_k^T \mathbf{A} \mathbf{P}_k} \quad (6)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{P}_k$$

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{P}_k$$

$$\beta_k = \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k}$$

$$\mathbf{P}_{k+1} = \mathbf{r}_{k+1} + \beta_k \mathbf{P}_k$$

2 The iterative scheme in Eq. (6) converges to an undesirable least squares solution for small
3 threshold such as $10 \mu\text{Gal}$. Therefore, the iterative process should be terminated before the
4 solution is disturbed by the effect of the small values of SVD of the design matrix $\mathbf{A}$.

5 2.2 Landweber's method

6 The Landweber method is a rather simple and very flexible iterative method frequently used
7 in signal processing. The method proposed by Landweber (1951) has the following form:

$$\mathbf{x}_k = \mathbf{x}_{k-1} - \omega \mathbf{A}^T \mathbf{r}_{k-1}, \quad (7)$$

8 where ω is a real parameter satisfying $0 < \omega < \frac{2}{|\mathbf{A}|_2}$. $|\mathbf{A}|_2$ is the L_2 -norm of the design matrix
9 $\mathbf{A}$ which is equal to its largest singular value. The empirical parameter ω controls both
10 stability and convergence of the iterative process. If selected correctly, it increases the
11 convergence rate of the iterative method while reducing the instability of its solution. The
12 optimum value of ω for the solution of Eq. (7) reads (Strand, 1974)

$$\omega = \frac{2}{\lambda_{min} + \lambda_{max}}, \quad (8)$$

1 where λ_{min} and λ_{max} are extreme singular values of the design matrix **A**. The upper bound
 2 of λ_{max} and of the lower bound λ_{min} can be determined using Gerschgorin's theorem
 3 (Wilkinson, 1965). Unfortunately, λ_{min} cannot correctly be estimated by this theorem for
 4 high-resolution grids, e.g., for 1 arc-min and higher angular resolutions (Martinec, 1996).
 5 Assuming extreme values $\lambda_{max} < 1$ and $\lambda_{min} > 0$, we obtain $\omega = 2$.

6 **2.3 On the parameter choice in the iterative methods**

7 As mentioned above, selecting the number of iterations in the indirect solution replaces the
 8 choice of the regularization parameter in the direct solution of DWC. Many algorithms have
 9 been proposed to find optimal values of regularization parameters and of numbers of
 10 iterations. The discrepancy principle (DP), L-curve and generalized cross validation (GCV)
 11 methods belong to widely used regularization algorithms that can be applied to both direct
 12 and indirect solutions of DWC (Hansen, 1998; Kilmer and O'Leary, 2001). While DP requires
 13 an a priori knowledge of the input data noise, other methods mentioned herein are data
 14 driven methods, i.e., they do not require any initial information about the data noise.

15 Standard algorithms might not be applicable for DWC in their original forms because of the
 16 type of data used and because of the nature of the Poisson integral kernel function. Input
 17 data noise characteristics are never known precisely, so the DP rule in most cases fails. The
 18 L-curve rule often does not sufficiently turn to a definitive reasonable vertex and for GCV
 19 extensive computations are needed (Wahba, 1980). Besides these problems, which may also
 20 occur in other regularization techniques, DWC suffers from the so-called edge effects. This
 21 means that for each block additional surface gravity data outside the block are needed to
 22 account for far-zone effects omitted in the solution based on truncated integration

domains. For example, DWC of the 1x1 arc-deg block with the 1 arc-deg integration cap radius implies a system of linear equations which corresponds to 3x3 arc-deg area which contains one central block and 8 surrounding blocks; the surrounding blocks are removed from the final solution (cf. Foroughi et al. (2015)). Using additional data around the central area does not allow for the regularization parameter to be estimated optimally. Additional data in the surrounding blocks are present in the DWC process with the impact on the regularization parameter although they are not used in the solution. The edge effects also complicate finding an optimal number of iterations. In other words, the optimal iteration number for the 3x3 arc-deg computation block and for 1x1 arc-deg solution block differ.

The above-mentioned problems cause that most of known stopping criteria often fails. To demonstrate this issue, we apply five different stopping criteria suggested to iterative methods in the literature. Their list including basic characteristics can be found in Table 1. In the L-curve rule, the optimum number of iterations is defined by the corner of the plot of the logarithm of the L_2 -norm of the solution vector with respect to the logarithm of the L_2 -norm of the residual vector. In some cases, the input data noise prevents finding the vertex of the discrete L-curve. In this case, the shape of the L-curve does not have any distinct corner or there are more candidates for the corner of the L-curve. In some ill-posed problems, the plot of the logarithm of the L_2 -norm of the residual vector against the iteration number has the L-shape. Reichel and Sadok (2008) showed that the corner of the plot $(k, \log\|\mathbf{r}_k\|)$ indicates the optimum index. This rule is called the residual L-curve rule. The Reginska rule represents only a variant of the L-curve rule (Reginska, 1996). Reginska proved that the corner of the L-curve corresponding to the index k minimizes the following form:

$$\min_k(\|\mathbf{r}_k\| \|\mathbf{x}_k\|^v), \tag{9}$$

1 where $v > 0$ is a user-specified parameter. In this study $v = 2$ is adopted in all
2 computations as it was found to be optimal for DWC based on trial and error. GCV is a
3 method most commonly used for estimating values of regularization parameters in ill-posed
4 problems. GCV estimates the value of the regularization parameter by minimizing the
5 square of averaged prediction errors previously removed from the input data. This method
6 uses the so-called “leave-one-out” principle. GCV can be applied as a stopping rule in the
7 iterative methods in the form of (Kilmer and O’Leary, 2001)

$$\min_k \left(\frac{\|\mathbf{r}_k\|^2}{(n - k)^2} \right) \tag{10}$$

8 where n is the number of input data and k is the iteration number.

9

10 **Table 1:** Five stopping rules applied in the iterative methods

11 **3. Methodology**

12 To investigate the performance of the selected stopping criteria, see Table 1, for DWC of
13 surface gravity anomalies using the Landweber and CGLS iterative methods, synthetic
14 surface gravity anomalies are used. The study area bounded by $35^\circ < \varphi < 38^\circ$ in latitude
15 and by $-108^\circ < \lambda < -105^\circ$ in longitude is located in Colorado, USA. Figure 1 and Figure 2
16 show SRTM (Jarvis et al., 2008) and EGM2008 (Pavlis et al., 2012) synthetic residual
17 Helmert’s anomalies limited to the harmonic degrees 361-2190, respectively. The 0.5 mGal
18 Gaussian noise was added to synthetic surface gravity data. The synthetic data represent
19 observed gravity values with characteristics close to actual observations: used degrees
20 correspond to the spectral content of data used for recovery of the gravimetric geoid when
21 EGM and local data are combined. The value of the Gaussian noise then simulates the noise

in observed surface gravity collected by gravimeters over long periods (combining observation and positioning errors). The advantage of synthetic data is the knowledge of both input surface data as well as of their counterparts at the mean geocentric sphere. The correctness of the indirect solution can be measured in the absolute sense.

Figure 1: Topographic heights over the test area in Colorado (m).

Min = 1500.0, max = 4070.5, mean=2407.1 and STD= 498.9 m

Figure 2: Surface gravity anomalies synthesized from EGM2008 for the degrees 361-2190 over the test area in Colorado (mGal).

Min = -85.28, max = 122.92, mean = -0.79, STD = 31.23 mGal

In order to verify the need for regularizing the system of linear equations involved in DWC, the discrete Picard condition can be used (DPC, Hansen, 1990). To test the Picard condition, one 1x1 arc-deg block from the study area is considered as a test block over which surface gravity anomalies were synthesized with three different angular resolutions: 1, 2 and 5 arc-min ($37^\circ < \varphi < 38^\circ$ and $-108^\circ < \lambda < -107^\circ$). The system of linear equations (3) must be first factorized by the SVD technique (Meyer, 2000):

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T, \quad (11)$$

where $\mathbf{U}_{n \times n}$ and $\mathbf{V}_{n \times n}$ are left- and right-unitary singular matrices, respectively, and $\mathbf{\Sigma}_{n \times n}$ is a diagonal matrix containing singular values λ_i of the design matrix $\mathbf{A}$. The condition number of the matrix $\mathbf{A}$ is defined as

$$k = \frac{\lambda_{max}}{\lambda_{min}}. \quad (12)$$

1 The condition number is a tool to measure the sensitivity of the model to the input data
2 noise and to high-frequency signals in input gravity data. A large value of the condition
3 number indicates that the high-frequency signal of input gravity data will be amplified, e.g.,
4 the estimated solution may contain unwanted fluctuations. The estimated posedness of the
5 system of linear equations based on DPC depends on the coefficients of the design matrix **A**
6 as well as on spectro-stochastic properties of the input data **b**. A system of linear equations
7 is well posed if Fourier coefficients of input data **b** and of the matrix **U** (left singular matrix
8 of **A**) decay faster than singular values of the matrix **A**, i.e.,

$$\mathbf{x} = \sum_{i=1}^n \frac{\langle \mathbf{b}, \mathbf{u}_i \rangle}{\lambda_i} \mathbf{v}_i . \tag{13}$$

9 Figure 3 shows DPC and spectra of singular values of the design matrix **A** for the angular
10 resolutions of 5, 2 and 1 arc-min, respectively. Figure 3 shows increasing ratios of the
11 Fourier coefficients of the input data **b** and of the singular values of **A**, $(\frac{\langle \mathbf{b}, \mathbf{u}_i \rangle}{\lambda_i})$. Therefore, in
12 contrary to the 5 and 2 arc-min grids, DWC of the 1 arc-min surface gravity anomaly is an ill-
13 posed problem. This result confirms findings of (Martinec, 1998). Thus, DWC of the 1 arc-
14 min gravity anomaly is numerically unstable and must appropriately be regularized if gravity
15 anomalies on the geoid are solved for. In addition, the estimated condition numbers of the
16 coefficient matrix **A** are 18086.95, 84.28 and 4.26 for 1, 2 and 5 arc-min gravity anomalies,
17 respectively.

18

19 **Figure 3:** Singular values of the design matrix **A** and DPC of 5 (a), 2 (b) and 1 arc-min (c)
20 surface gravity anomalies

21

22 As high-resolution gravity anomalies are continued, surface gravity anomalies were

synthesized on the 1 arc-min grid. The test area was divided into nine 1x1 arc-deg blocks in order to solve large systems of linear equations faster. After downward continuing these blocks individually, respective solutions were merged to cover the entire test area. Foroughi et al. (2015) investigated the downward continuation of Helmert's gravity anomalies divided into 1x1 arc-deg blocks. They reported that if at least 30 arc-min data margins are considered in the DWC process, then neighboring 1x1 arc-deg blocks can safely be merged to form a seamless grid of downward continued Helmert's gravity anomalies on the geoid.

In order to evaluate the performance of the iterative methods for the tested stopping criteria, Helmert's gravity anomalies were also synthesized over the 1 arc-min grid on the geoid which we refer to here as the "*reasonable solution*". The Landweber and CGLS iterative methods were used to downward continue synthetic surface Helmert's gravity anomalies. Differences between solutions of both methods after the k -th iteration were then compared with the reasonable solution. **RMS** of the differences is considered as a measure of goodness of the solution after each iteration. As DWC is performed over nine 1x1 arc-deg blocks, the average of RMS values ($\overline{\text{RMS}}$) is considered as a validation criterion. The Landweber and CGLS iterative methods converge to an indirect solution using the five stopping rules in

Table 1. Results of the stopping rules 1 to 5 for the Landweber and CGLS methods are presented in Table 2 and

Table 3, respectively. The iteration number, for which the indirect solution with the smallest value of RMS was achieved, is indicated by k_e (the iteration for which the estimated solution best matches the reasonable solution) and k_c is the iteration number where the algorithm converges according to the stopping rules, i.e., the convergence iteration number.

Table 2: Results of the five stopping rules applied to the Landweber iterative method. RMS is in mGal, k_e is the reasonable iteration number, $\overline{\text{RMS}}$ is the mean RMS and $\text{RMS of } k_i =$

Table 3: Results of the five stopping rules applied to the CGLS iterative method. RMS is in mGal, k_e is the reasonable iteration number, $\overline{\mathbf{RMS}}$ is the mean RMS and $\mathbf{RMS of } k_i =$

11 4. Proposed new stopping criterion

As it can be seen from the results in Table 2 and Table 3, the applied stopping rules perform well enough in case of neither the Landweber method nor the CGLS method. The differences between k_e and k_c are either too large or the methods fail to converge at all. We introduce a simple approach which applies the DP criterion to stop the iterative process properly. As the input data noise must be known in DP, the leave-one-out cross-validation (LOOCV) procedure is suggested to estimate the data noise which is then used to stop the CGLS and Landweber iteration methods using DP. According to this new algorithm, the iterative process terminates when the L_2 -norm of the residual vector is smaller than the L_2 -norm of the input noise vector in the first iterative step, i.e.,

$$\|\mathbf{A} \mathbf{x}_k - \mathbf{b}\| < \tau \delta, \quad (14)$$

21 where $\mathbf{b}$ is the vector of observations, δ is the norm of the estimated data noise and τ is a

constant which can be equal to $\tau = 1$. Eq. (14) was introduced in Kingdon and Vaníček (2010), they scaled the δ based on upper estimation of the condition number of A . The degree of ill-posedness of a system of linear equation depends on both the condition number and the noise of the data; in the method suggested by Kingdon and Vaníček (2010), the condition number was only approximately estimated, and the noise of the data was set to 0.01 mGal while here we estimate the noise of the data according to the LOOCV method. In the LOOCV procedure, one observation is left out from the data as a control point and then predicted using other observations. The prediction error can be considered as a noise estimate of the input data. This method was used by (Saleh et al., 2013) for error estimation of surface gravity data over the USA. The following steps were suggested:

- 1- For each observation, neighborhood points corresponding to a small spherical radius, such as 10 arc-min, are selected as effective points.
- 2- The trend in the data is removed by fitting a bilinear 2-D polynomial.
- 3- The value of observation is predicted using Hardy's multiquadric method (Hardy, 1971) and the prediction error at each point is estimated.
- 4- RMS of the differences between predicted and observed values for all gravity points is considered as the norm of the data noise vector.

Table 4 shows results of applying proposed DP on the Landweber and CGLS iterative methods for DWC of tested nine 1×1 arc-deg blocks of surface gravity data. The comparison between values in Table 4 with those in Table 2 and Table 3 indicates that the proposed method works fine particularly in case of the Landweber method. The numerical values of RMS are comparable with those based on the residual L-curve.

Table 4: Results of the DP stopping rule (using the LOOCV estimated noise) applied to the

1 Landweber and CGLS methods. RMS is in mGal. k_e is the reasonable iteration number, $\overline{RMS}$
2 is the mean of RMS and $RMS\ of\ k_i = \sqrt{\frac{\sum(k_e - k_i)^2}{8}}$
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4 **5. Discussion of the numerical results**

5 The Landweber iterative method was applied to test amiable stopping rules in
6
7 Table 1. Statistics of results summarized in Table 2 indicate that the stopping rules of
8 Reginska and GCV fail to stop the iterative process after 30 iterations. Results based on the
9 standard L-curve rule in some blocks are way off the optimum number of iterations. The
10 residual L-curve rule gives the best results in comparison to the reasonable solution among
11 the other 4 stopping rules. The average error when using the residual L-curve rule for
12 estimation of the iteration number does not exceed 1-2 iterations.
13 According to Table 3, compared to the Landweber metod, the CGLS method performs worse
14 to stop the iterative process. Although the residual L-curve stopping rule again gives the
15 best results (smaller $RMS\ of\ k_i$) comparing to other four rules, its results are very off the
16 reasonable solution. The Reginska and GCV rules (rules 3 and 5) fail to stop the iterative
17 process in both the Landweber and CGLS iterative method.
18 In order to analyze the sensitivity of both the Landweber and CGLS methods, the block with
19 largest elevations was used to test solutions of DWC for fifty performed iterations. Figure 4
20 shows how the errors develop in course of this sensitivity analysis. The y-axis shows the
21 differences between the reasonable solution and the estimated solution for each iteration
22 number. It can be seen that the semi-convergence property in case of CGLS is more
23 pronounced than in case of the Landweber method. Therefore, finding a suitable stopping

rule is more critical for the CGLS method than for the Landweber method. Observation errors cause that the CGLS method cannot estimate the iteration number optimally. This problem is less pronounced in the Landweber method.

Figure 4: Errors of DWC for the CGLS and Landweber iterative methods with respect to the number of iterations.

Results of applying the proposed criterion to stop DWC in Table 4 indicate that DP works fine particularly for the Landweber method when the input data noise is estimated by the proposed LOOCV method. Its values of RMS are comparable with those based on the residual L-curve rule in Table 2.

6. Conclusions

The discrete DWC of surface gravity anomalies was investigated in this contribution. Based on the presented results it was concluded that DWC of surface gravity anomalies with angular resolutions at the level of 1 arc-min and higher represents an ill-posed problem in a sense of the discrete Picard condition. Two iterative methods, namely Landweber's and CGLS, were used for solving the discrete DWC of surface gravity anomalies synthesized from EGM2008 over the mountainous test area in Colorado, USA. It was shown that both iterative methods suffered from the semi-convergence property which caused premature stopping of both iterative methods. The Landweber method needs more iterations to achieve the desired solution compared to the CGLS method. In contrary, the semi-convergence property of the CGLS method is more significant than in case of the Landweber method. Input data noise statistics are important for finding an optimal number of iterations in both iterative

1 methods but their knowledge is more vital for the CGLS method than for the Landweber
2 method. Results presented in Tables 2, 3 and 4 also indicate that results based on the
3 Landweber method are superior to those based on the CGLS iterative method for all blocks.
4 Five common stopping rules were applied to find an optimal number of iterations for the
5 CGLS and Landweber iterative methods. All stopping rules, except residual L-curve, failed to
6 stop the iterative processes in the appropriate moment due to data border effects.
7 Numerical investigations also showed that the residual L-curve rule can stop the iterative
8 process within 1-2 iterations from the best approximation of the reasonable solution. In
9 addition, we propose an algorithm to estimate data noise statistics using the LOOCV
10 procedure. Estimated data noise statistics were used to stop the iterative process using the
11 DP rule. Results based on simulated surface gravity data show that this rule can be used for
12 DWC of Helmert's gravity anomalies using both the Landweber and CGLS iterative methods.
13 The efficiency of this rule is comparable with that based on the residual L-curve.

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Table Captions:

Table 1: Five stopping rules applied in iterative methods

Table 2: Results of the five stopping rules applied to the Landweber iterative method. RMS is in mGal, k_e is the reasonable iteration number, $\overline{\text{RMS}}$ is the mean RMS and $\text{RMS of } k_i =$

$$\sqrt{\frac{\Sigma(k_c - k_e)^2}{8}}$$

Table 3: Results of the five stopping rules applied to the CGLS iterative method. RMS is in mGal, k_e is the reasonable iteration number, $\overline{\text{RMS}}$ is the mean RMS and $\text{RMS of } k_i =$

$$\sqrt{\frac{\Sigma(k_c - k_e)^2}{8}}$$

Table 4: Results of the DP stopping rule (using LOOCV estimated noise) applied to the Landweber and CGLS methods. RMS is in mGal. k_e is the reasonable iteration number, $\overline{\text{RMS}}$

is the mean of RMS and $\text{RMS of } k_i = \sqrt{\frac{\Sigma(k_c - k_e)^2}{8}}$

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Figure Captions

Figure 1: Topographic heights over the test area in Colorado (m).
Min = 1500.0, max = 4070.5, mean=2407.1 and STD= 498.9 m

Figure 2: EGM2008 Helmert’s surface gravity anomalies of the harmonic degree 361-2190 over the test area in Colorado (mGal).
Min = -85.28, max = 122.92, mean = -0.79, STD = 31.23 mGal

Figure 3: Singular values of the matrix **A** and DPC of 5 (a), 2 (b) and 1 arc-min (c) surface gravity anomalies

Figure 4: Errors of DWC for the CGLS and Landweber iterative methods with respect to the number of iterations.

Tables

Table 1: Five stopping rules applied in the iterative methods

Rule	Description
Rule 1: L-Curve (Hansen, 1998)	Corner of the plot $(\log\ \mathbf{x}_k\ , \log\ \mathbf{r}_k\)$
Rule 2: Residual L-curve Reichel and Sadok (2008)	Corner of the plot $(k, \log\ \mathbf{r}_k\)$
Rule 3: Reginska's method (Reginska, 1996)	$\min_k (\ \mathbf{r}_k\ \ \mathbf{x}_k\ ^v)$
Rule 4: Extrapolation method (Bauer and Lukas, 2011)	$\min_k \left(\frac{\ \mathbf{r}_k\ ^2}{\ \mathbf{A}\mathbf{r}_k\ } \right)$
Rule 5: GCV (Kilmer and O'Leary, 2001)	$\min_k \left(\frac{\ \mathbf{r}_k\ ^2}{(n-k)^2} \right)$

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8 **Table 2:** Results of the five stopping rules applied to the Landweber iterative method. RMS
9 is in mGal, k_e is the reasonable iteration number, $\overline{RMS}$ is the mean RMS and $RMS\ of\ k_i =$

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$$\sqrt{\frac{\Sigma(k_c - k_e)^2}{8}}$$

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Block	$H_{\max}$ (meter)	reasonable solution		Rule 1		Rule 2		Rule 3		Rule 4		Rule 5	
		k_e		k_c	RMS	k_c	RMS	k_c	RMS	k_c	RMS	k_c	RMS
			RMS										
1	4031	9	3.58	27	3.83	8	3.60	-	fail	5	4.08	1	9
2	3996	7	3.07	27	3.39	7	3.07	-	fail	5	3.29	2	7
3	4070	8	4.15	23	4.22	7	4.16	-	fail	5	4.31	3	8
4	2395	4	0.90	2	1.07	3	0.92	-	fail	4	0.90	4	4
5	3364	6	2.18	2	3.55	5	2.25	-	fail	5	2.25	5	6
6	3791	6	3.20	2	6.07	8	3.25	-	fail	5	3.27	6	6
7	3257	4	1.33	4	1.33	3	1.45	-	fail	2	1.66	7	4
8	3322	6	1.53	4	1.57	4	1.57	-	fail	4	1.57	8	6
9	3716	7	1.74	4	2.06	5	1.83	-	fail	4	2.06	9	7
$\overline{RMS}$			2.41		3.01		2.46		NA		2.60		
$RMS\ of\ k_i$		NA		10		1.37		NA		2.30			NA

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Table 3: Results of the five stopping rules applied to the CGLS iterative method. RMS is in mGal, k_e is the reasonable iteration number, $\overline{\text{RMS}}$ is the mean RMS and $\text{RMS of } k_i =$

$$\sqrt{\frac{\sum (k_c - k_e)^2}{8}}$$

Block	H_max (meter)	reasonable solution k_e RMS		Rule 1 k_c RMS		Rule 2 k_c RMS		Rule 3 k_c RMS		Rule 4 k_c RMS		Rule 5 k_c RMS	
1	4031	12	3.85	36	6.76	6	3.91	-	fail	45	8.30	-	fail
2	3996	11	3.29	37	6.39	6	3.54	-	fail	48	8.25	-	fail
3	4070	10	4.18	36	7.25	10	4.18	-	fail	46	9.16	-	fail
4	2395	6	0.95	29	5.51	3	1.19	-	fail	47	9.51	-	fail
5	3364	8	2.25	38	6.86	6	2.30	-	fail	-	Fail	-	fail
6	3791	9	3.47	36	6.95	6	3.74	-	fail	47	9.05	-	fail
7	3257	6	1.32	29	5.76	3	1.54	-	fail	48	10.00	-	fail
8	3322	7	1.48	29	5.91	5	1.66	-	fail	-	Fail	-	fail
9	3716	8	1.98	31	6.02	5	2.13	-	fail	-	Fail	-	fail
$\overline{\text{RMS}}$			2.53		6.37		2.68				NA		NA
$\text{RMS of } k_i$		NA		25		3.41		NA	NA	NA		NA	

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Table 4: Results of the DP stopping rule (using LOOCV estimated noise) applied to the Landweber and CGLS methods. RMS is in mGal. k_e is the reasonable iteration number, $\overline{RMS}$

is the mean of RMS and $RMS\ of\ k_i = \sqrt{\frac{\sum(k_c - k_e)^2}{8}}$

Block	H_max (meter)	reasonable solution		Estimated noise	Landweber		CGLS	
		k_e	RMS		k_c	RMS	k_c	RMS
1	4031	12	3.85	0.73	8	3.60	6	3.90
2	3996	11	3.29	0.66	8	3.08	7	3.54
3	4070	10	4.18	0.77	8	4.15	7	4.35
4	2395	6	0.95	0.58	3	0.92	5	0.99
5	3364	8	2.25	0.60	6	2.18	6	2.30
6	3791	9	3.47	0.68	8	3.25	7	3.57
7	3257	6	1.32	0.58	4	1.33	5	1.43
8	3322	7	1.48	0.64	4	1.57	5	1.66
9	3716	8	1.98	0.63	6	1.74	6	2.04
$\overline{RMS}$			2.53			2.42		2.65
RMS of k_i		NA			1.1		2.9	

Figures

Figure 1: Topographic heights over the test area in Colorado (m).

Min = 1500.0, max = 4070.5, mean=2407.1 and STD= 498.9 m

Figure 2: EGM2008-synthesized Helmert’s surface gravity anomalies of the degree 361-2190 over the test area in Colorado (mGal).

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