



Iterative Regularisation and Uncertainty Propagation in Solving Ill-Posed Problems: A GOCE-Based Regional Gravity Field Modelling

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Abstract—Inverse problems are fundamental in geoscience, enabling estimation of Earth’s physical properties that cannot be measured directly. These problems are typically ill-posed, meaning their solutions are highly sensitive to noise and variability in observational data, and thus require regularisation to ensure stability. Both direct and iterative regularisation methods have been extensively studied across geoscientific applications. However, accurately quantifying uncertainty—particularly for iterative regularisation—remains a major challenge, as uncertainty estimation in these methods is less well understood. This study examines the performance and uncertainty characteristics of four iterative regularisation techniques—conjugate gradient least-squares (CGLS), minimum residual 2 (MR2), algebraic reconstruction technique (ART), and the ν -method (Nu). Here, a comprehensive conceptual overview of these methods is provided, along with an evaluation of two internal uncertainty quantification approaches: (a) the error propagation using numerical Jacobians, and (b) the Monte Carlo method. Although computationally demanding, these techniques offer valuable insights into how observational errors propagate through nonlinear iterative processes. The methods are applied to the regional recovery of gravity anomalies at sea level from the Gravity field and steady-state Ocean Circulation Explorer (GOCE) 2nd-order radial gradients over Alpine and surrounding south-central European region as a case study. Results demonstrate that different iterative techniques yield distinct solutions even under identical regularisation criteria (e.g., the L-curve), and that the magnitude of propagated error alone is not a reliable indicator of solution quality. The estimated gravity anomalies and their uncertainties by the MR2 and ART are close to each other. Nu provides faster, smoother solutions with lower uncertainties, while the CGLS preserves more high-frequency geophysical signals at the cost of higher propagated errors. Error propagation with numerical Jacobians produces smaller error estimates compared to with the Monte Carlo method, which consistently reports larger uncertainties, reflecting its ability to account for both random noise and nonlinear effects. The difference between the estimated uncertainties by these methods over the study area are around 2 mGal or less.

Keywords: Error propagation, gravity field modelling, ill-conditioning, ill-posed problems, iterative regularisation, Monte Carlo method, numerical Jacobian, satellite gradiometry, variance-covariance analysis.

1. Introduction

Understanding the physical properties of the Earth’s interior is a central objective in geoscience. However, many of these properties—such as subsurface density, elasticity, or gravitational potential—cannot be measured directly. Instead, geoscientists rely on *inverse problems*, where mathematical models are used to infer unobservable parameters from measurements such as satellite observations, seismic waves, or gravitational gradients. Inverse problems are inherently *ill-posed*, meaning that small errors or noise in the data can lead to large uncertainties or instability in the solution. To address this, regularisation techniques are employed to stabilise the inversion process and yield geophysically meaningful results. While both direct and iterative regularisation methods have been widely studied and applied in the geosciences, a significant challenge remains in understanding how observational errors propagate through these inversion schemes—particularly for iterative methods. Despite their computational advantages and flexibility, iterative approaches often lack robust frameworks for uncertainty quantification. Iterative regularisations are often used in geophysical applications due to their computational efficiency and flexibility. However, the lack of well-established frameworks for uncertainty quantification in these methods poses a critical gap. This study focuses on evaluating four iterative regularisation techniques and explores two approaches for uncertainty estimation for determination of gravity anomalies at sea level

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from using gradiometric data from the Gravity field and steady-state Ocean Circulation Explorer (GOCE, ESA, 1999) data by integral inversion over Alpine and surrounding south-central European region. Our approach and finding can also be applicable for inversion of other geophysical data for uncertainty quantification.

Over the past two decades, significant advancements have been made in collecting gravity data via sensors onboard low-orbiting satellites. The GOCE mission was the first dedicated to measuring components of the 2nd-order gravitational tensor (ESA, 1999). The GOCE gradient data, measured in a local Cartesian coordinate frame, significantly surpassed the sensitivity of previous satellite missions in the medium-wavelength range of the gravity field spectrum. This increased sensitivity allowed for surface gravity anomalies to be determined with an accuracy of 1 mGal at 80 km spatial resolution (half-wavelength at the equator). However, in many studies, uncertainties of satellite gradients have been overlooked in the inversion process. It is therefore necessary to investigate the impact of observation errors on estimated surface gravity anomalies and evaluate their influence when employing integral equations in regional gravity field modelling.

The inversion of satellite gradients was first explored by Reed (1973), who developed integral equations for 2nd-order derivatives of the extended Stokes integral, aiming to recover surface gravity anomalies from satellite gradient data. In the 1990s, Xu (1992, 1998) introduced the Tikhonov regularisation (Tikhonov et al., 1963; Tikhonov & Arsenin, 1977) method and truncated singular-value decomposition for solving such integral equations. Additional contributions included the work of Tóth et al. (2004), who studied upward/downward continuation of satellite gradients, and Kotsakis (2007), who employed the Tikhonov regularisation with a covariance-adaptive approach, further refining of the recovered smoothed gravity anomalies.

By the late 2000s and early 2010s, Xu (2009) proposed an iterative generalised cross-validation method to estimate regularisation parameters and variance components, which was subsequently

applied to recover surface gravity anomalies from satellite gradient data. Other notable contributions include the work of Kern and Haagmans (2005) and Janák et al. (2009), who formulated full 2nd-order gradient tensor inversion in the geocentric coordinate system. Eshagh (2011a, 2011b) developed stochastically modified surface integral inversions, investigating the impact of spatial truncation errors (STE) on gravity anomaly recovery. Eshagh and Sjöberg (2011) further expanded this work by incorporating variance component estimation for optimal weighting of satellite gradients. Yildiz (2012) studied the problem of determination of gravity anomalies from the GOCE data using least-squares collocation in a combination with remove-compute-restore scheme. Janák et al. (2014) combined GOCE-derived gravity anomalies on the Earth's surface with terrestrial or marine gravity data at sea level, yielding a solution largely independent of high-degree global gravity models and achieving a 10 cm standard deviation in comparison against global navigation satellite systems (GNSS)/levelling data in the Auvergne region. Sebera et al. (2014) presented an iterative method based on the Poisson integral and Fourier transforms to downward continue satellite magnetic and gravitational potential data from orbital altitudes to a reference surface. Later in another study, Sebera et al. (2015) studied downward continuation of gravity or magnetic potentials to enhance source interpretation by applying three Poisson-integral-based methods and four integration schemes to GOCE-derived second vertical derivatives over Central Europe. They concluded that the Tikhonov regularisation performs best when prior information is included while the iterative approach is most effective without prior information. Furthermore, Pitoňák et al., (2016, 2017, 2018, 2020, 2023) and Saadat et al. (2019) contributed to refining satellite gradient inversion techniques, while the radial basis function approach gained traction through the works of Schmidt et al. (2006), Eicker (2008), and Eicker et al. (2013). Also, Naeimi and Bouman (2017) examined the contribution of satellite gradients to regional gravity field modelling using the radial basis function, and Eshagh et al. (2018) developed

inversion methods for the diagonal elements of the gradient tensor, further refining regional gravity field solutions.

Existing research has often prioritised estimation techniques and solutions to linear equation systems derived from integral equations, but fewer studies have addressed error propagation (Ku, 1966) in surface gravity anomaly estimates. Eshagh and Sjöberg (2011) examined this issue but relied on simulated data, omitting the STE effects. Later, Eshagh and Ghorbannia (2014) acknowledged the role of the STE in joint inversion of the GOCE orbital and gradient data for error estimation. Novák et al. (2024) investigated error propagation in integral transform-based inversions for 1st, 2nd and 3rd -order derivatives of gravitational potential. Eshagh et al. (2025) studied uncertainty propagation through integral inversion of the GOCE data to gravity anomalies at sea level using the Tikhonov regularisation and three scenarios of inversion.

This study builds upon the work of Eshagh et al. (2025) on error propagation, with a key distinction: the focus here is on the quality of *iterative regularisation methods* rather than *direct methods*. They applied Tikhonov regularisation, a well-established direct method supported by a comprehensive theoretical foundation and mature techniques for variance estimation and bias correction. Their objective was to compare a range of regional gravity field recovery strategies—including remove-compute-restore, direct integral inversion, truncation error removal, and inversion of modified integral formulae—and to analyse how uncertainty propagates through each method. In all these gravity field recovery approaches, Tikhonov regularisation served as the primary stabilisation tool. In contrast, the present study concentrates on uncertainty propagation when solving ill-conditioned systems using iterative approaches. Iterative methods are computationally more efficient and often faster and are particularly suitable for a large and/or ill-conditioned system they avoid explicit formation or inversion of the system's coefficient matrix. However, they are inherently nonlinear, and unlike direct methods, they lack a straightforward analytical relationship between the solution and the observations. As a result, uncertainty propagation is more complex than in direct methods such as the Tikhonov regularisation (Tikhonov et al., 1963),

where the Jacobian matrix explicitly links the solution to the unknown parameters. Moreover, applying direct regularisation becomes impractical when dealing with a vast number of observations. In such cases, iterative regularisation methods are typically preferred; however, propagating errors from observations to unknowns remains a significant challenge. Here, we investigate two classes of iterative regularisation methods: classical iterative methods and Krylov subspace-based methods. We evaluate the quality of the recovered gravity anomalies at sea level using the GOCE data over the Alpine and surrounding south-central European region. To estimate the uncertainties of the retrieved gravity anomalies, we apply both the Monte Carlo method (MC, Metropolis & Ulam, 1949) and error propagation with numerical Jacobian (EPNJ).

Although these techniques are applied here in the context of gravity field modelling, they are broadly applicable to any iterative method used for solving systems of equations. For example, in seismology, MC have been applied to mapping earthquake locations (Fuggi et al., 2024) and analysing travel times (Sun & Williamson, 2025). In engineering, they enable fast predictions of how materials respond under stress (Degenhardt et al., 2025; Pasparakis et al., 2025). In hydrology and medical imaging, these methods support the estimation of water content in soils (Minsley et al., 2025) and the reconstruction of high-quality medical images (Huang et al., 2025). However, applying MC and EPNJ for uncertainty estimation by iterative regularisation for regional gravity field modelling is the novelty of this study.

In Sect. 2, the integral equation relating GOCE data to gravity anomalies is presented. Section 3 introduces the iterative regularisation methods, divided into classical iterative and Krylov-space-based approaches in SubSects. 3.1 and 3.2, respectively. Two well-known classical iterative methods, the v-method (Nu) and the algebraic reconstruction technique (ART), are discussed in SubSect. 3.1.1, while conjugate gradient least-squares (CGLS) and minimum residual 2 (MR2) are presented in SubSect. 3.1.2. Section 4 addresses uncertainty propagation, with EPNJ described in SubSect. 4.1 and MC methods in SubSect. 4.2. Section 5 presents a numerical experiment, including the experiment

setup, estimation of gravity anomalies from GOCE data, application of error propagation, and discussion of the results in SubSects. 5.1–5.4. Conclusions are provided in Sect. 6.

2. The Integral Relation between GOCE Data and Gravity Anomaly

The integral equation connecting the 2nd -order radial derivative of the disturbing gravitational potential T , denoted as T_{rr} , at the satellite orbit to the gravity anomaly (Δg) at mean sea level is (Reed, 1973):

$$T_{rr}(r, \Omega) = \frac{R}{4\pi} \iint_{\Omega_0} S_{rr}(t, \Omega, \Omega') \Delta g(R, \Omega') d\Omega' \quad (1a)$$

where $t = R / r$ with R as the radius of the spherical Earth approximating the mean sea level, and r the geocentric distance of satellite. $\Omega = (\theta, \lambda)$ and $\Omega' = (\theta', \lambda')$ with the spherical co-latitude θ and longitude λ of the computation point, θ' and λ' are the corresponding ones for the integration point. The surface integration element is $d\Omega' = \sin\theta' d\theta' d\lambda'$. Ω_0 is the unit sphere on which the integration is taken. The 2nd-order radial derivative of the extended Stokes function S_{rr} is defined as follows, e.g., Reed (1973):

$$S_{rr}(t, \Omega, \Omega') = \frac{t^3}{R^2} \left[(1 - tx) \left(\frac{3(1 - t^2)}{D^5} - \frac{4}{D^3} \right) - \frac{1 + t^2}{D^3} - \frac{10}{D} - 18D + 2 - 3tx \left(15 + 6 \ln \frac{1 - tx + D}{2} \right) \right] \quad (1b)$$

where $D = \sqrt{1 - 2tx + t^2}$ and $x = \cos\psi$, with ψ is the spherical geocentric distance between the computation point and the integration element or in other words, a function of $\Omega = (\theta, \lambda)$ and $\Omega' = (\theta', \lambda')$.

The number of observed T_{rr} are much larger than those of Δg . The number of Δg depends also on the resolution of the grid at the surface of that part of the spherical Earth fitted to the study area. This resolution plays an important role in conditionality of the coefficient matrix derived after discretisation of the integral (1a) considering higher resolutions lead to more unstable system of equations and stronger regularisation methods should be applied to control the

instability. Let us write this discretised integral in the following Gauss-Markov form:

$$\mathbf{Ax} = \mathbf{L} - \epsilon, \text{ with } E\{\epsilon\epsilon^T\} = \sigma_0^2 \mathbf{Q}, E\{\epsilon\} = 0 \quad (1c)$$

where $\mathbf{A}$ is the design matrix derived after discretisation of the near-zone integration domain, $\mathbf{x}$ is the vector of the unknown values of Δg at mean sea level, ϵ stands for the vector random error of T_{rr} in the column vector $\mathbf{L}$, and $E\{\cdot\}$ is the statistical expectation operator. σ_0^2 is the a priori variance factor of T_{rr} , $()^T$ stands for transposition operator and $\mathbf{Q}$ is their co-factor matrix.

Equation (1c) is overdetermined and solved through the following minimisation problem:

$$\min_{\mathbf{x}} \|\mathbf{Ax} - \mathbf{L}\|_2 \quad (1d)$$

Since $\epsilon = \mathbf{Ax} - \mathbf{L}$ and $\|\cdot\|_2$ is the L_2 -norm, then the minimisation problem means minimising the following quadratic form:

$$\epsilon^T \mathbf{Q}^{-1} \epsilon = \mathbf{x}^T (\mathbf{A}^T \mathbf{Q}^{-1} \mathbf{A}) \mathbf{x} - \mathbf{L}^T \mathbf{Q}^{-1} \mathbf{Ax} - \mathbf{x}^T \mathbf{A}^T \mathbf{Q}^{-1} \mathbf{L} + \mathbf{L}^T \mathbf{Q}^{-1} \mathbf{L} \quad (1e)$$

Taking derivative with respect to $\mathbf{x}$ leads the following system, which is known as normal equations:

$$(\mathbf{A}^T \mathbf{Q}^{-1} \mathbf{A}) \mathbf{x} = \mathbf{A}^T \mathbf{Q}^{-1} \mathbf{L} \quad (1f)$$

Both coefficient matrices of the Gauss-Markov model (1c) and the normal Eqs. (1f) are ill-conditioned, meaning that the solution is extremely sensitive to noise of the data. Any small change in the data can lead to drastic changes in the solution. Therefore, the standard least-squares (LS) method cannot be applied, and the system should be regularised on such a way that stable solution is obtained; see, e.g. Eshagh and Sjöberg (2011), or Eshagh and Ghorbannia (2014), Eshagh et al. (2025).

Various methods exist for solving such unstable systems, which are generally categorised into two main classes: direct and iterative methods. Direct methods are those in which the solution is obtained in a single step, without the need for repeated updates or iterative refinement. The Tikhonov regularisation is one of the most well-known direct regularisation techniques. Due to its similarity to the standard LS approach, it is widely used, and it also offers the

advantage of enabling direct estimation of the variance of unit weight and the uncertainty of the solution. As a result, uncertainty propagation in ill-conditioned systems solved by the Tikhonov regularisation is well-established. In the remainder of this paper, we shift our focus to iterative regularisation methods, evaluating their efficiency, solution quality, and their capability to propagate uncertainties from observations to final estimates.

3. Iterative Regularisation Methods

Generally, iterative methods are divided in two categories of classical iterative and the Krylov space-based methods. Two examples of the first group are the ν -method (Nu, Brakhage, 1987) and the algebraic reconstruction technique (ART) (Kaczmarz, 1937), and in the second one, the conjugate gradients least-squares (CGLS, Hestenes & Stiefel, 1952), the minimum residual (MR, Hanke, 1995; Paige & Saunders, 1973) techniques. These methods are briefly reviewed in this section.

3.1. Classical Iterative Methods

In this section, Nu and ART the two well-known classical iterative solvers of system of equations, are reviewed conceptually. A classical iterative method has the form, which is in fact, known the classical Landweber iterative method (Landweber, 1951):

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \omega \mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{L}) \quad (2a)$$

where k is iterative number, of ω is step-size showing that of convergence to the solution.

Equation (2a) means that the previous approximate solution $\mathbf{x}^k$ is transformed to observation space by $\mathbf{A}$, i.e. $\mathbf{A} \mathbf{x}^k$, which should reproduce the observation $\mathbf{L}$ if $\mathbf{x}^k$ is a good approximation or close to the true solution. In fact, $\mathbf{A} \mathbf{x}^k - \mathbf{L}$ is the difference between the reproduced and real observations in the observation space and to transform it back to solution space, $\mathbf{A}^T$ should be multiplied to it. ω is the step-size towards the solution. Based on the choice of ω different types of iterative Landweber method are derived. It can be a scalar value or even a matrix like e.g. $\omega = (\mathbf{A}^T \mathbf{A})^{-1}$, then the iterative LS estimation is

derived. If $\omega = (\mathbf{A}^T \mathbf{A} + \alpha \mathbf{I})^{-1}$ with $\alpha > 0$ as regularisation parameter and $\mathbf{I}$ as an identity matrix, then the iterative Tikhonov regularisation is obtained.

The iteration should be performed until the solution converges, i.e., the difference between the last two solutions becomes $|\mathbf{x}^{k+1} - \mathbf{x}^k| < \varepsilon$ with ε a pre-defined threshold for stopping iteration and considering convergence of solution.

In the following two subsections, we will explain how Nu is developed from the general Landweber iterative form (2a).

3.1.1 The ν Method

The ν method (Nu) enhances the Landweber iterative form (2a) by introducing two key modifications. First, updating solution based solely on the previous one i.e. $\mathbf{x}^k$, it incorporates a weighted average of two past iterates, i.e. $\mathbf{x}^{k+1}$ and $\mathbf{x}^k$. This helps to stabilise the solution and reduce oscillations. Second, it allows the step-size ω to vary at each iteration ω_k , adapting dynamically to improve convergence behaviour, allowing it to dynamically transform residuals from observation space into parameter space with an adaptive weight. These modifications make Nu more robust for solving ill-conditioned problems, as it achieves faster convergence, improved stability, and better handling of noise and numerical errors, making it a valuable extension of the Landweber method in inverse problem-solving.

Brakhage (1987) developed this idea as

$$\mathbf{x}^{k+1} = \mu_k \mathbf{x}^k + (1 - \mu_k) \mathbf{x}^{k-1} + \omega_k \mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{L}) \quad (2b)$$

Brakhage (1987) introduced a weighting factor, μ_k which is a function of both ν and k , to refine the estimation of $\mathbf{x}^k$. This method can be interpreted as a weighted average of the last two iterates, with an adjustment derived from the observational data. Hansen (2007) demonstrated that this modification enhances stability and improves the convergence behaviour of the iterative process. The coefficients μ_k and ω_k are computed by:

$$\mu_k = \frac{(k + \nu)(k + 1)(k + 0.5)}{(k + 2\nu)(k + 2\nu + 0.5)(k + \nu + 1)} \quad (2c)$$

$$\omega_k = \frac{4(k+v)(k+v-0.5)}{(k+2v)(k+2v-0.5)} \quad (2d)$$

with $0 < v < 1$ it is evident that μ_k and ω_k depend solely on v and k , meaning that neither the observations nor the design matrix $\mathbf{A}$ directly influence their values. Instead, the contribution of the observations and the role of $\mathbf{A}$ become apparent in the third term of the equation. It is important to note that the observations and the design matrix have already influenced the solution through the last two estimates, as they were incorporated in the previous iterations. Thus, while μ_k and ω_k remain independent of the data at each step, the iterative process ensures that the observations and system dynamics are continuously reflected in the updated solution. Normally $v = 0.755$ and μ_k and ω_k are generated from $k = 0$.

3.1.2 Algebraic Reconstruction Technique

The algebraic reconstruction technique (ART) is also an iterative method for solving systems of linear equations, based on the classical Landweber method, and particularly useful in applications such as tomographic image reconstruction and geodesy. In ART the solution is updated sequentially, incorporating one equation at a time rather than solving the entire system simultaneously. The fundamental update formula for ART is given by

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \delta \frac{l_i - \mathbf{a}_i \mathbf{x}^k}{\|\mathbf{a}_i\|^2} \mathbf{a}_i^T \quad (2e)$$

where $\mathbf{a}_i$ and l_i are the i^{th} row of $\mathbf{A}$ and $\mathbf{L}$. The term $l_i - \mathbf{a}_i \mathbf{x}^k$ represents the residual error, indicating how far the current estimate deviates from satisfying equation i . This residual is normalised by $\|\mathbf{a}_i\|$, where $\|\cdot\|$ stands for the L_2 -norm, to ensure proper scaling and then projected in the direction of $\mathbf{a}_i$, ensuring that the correction is applied along the correct axis. The relaxation parameter δ (typically between 0 and 1) controls the step size, allowing for more stable updates when dealing with noisy or inconsistent systems. In comparison to the classical Landweber for we can say that $\omega = \frac{\delta}{\|\mathbf{a}_i\|^2}$.

ART is an iterative method that solves a system of equations by sequentially projecting the current estimate onto hyperplanes defined by individual

equations. This row-wise, incremental approach contrasts with traditional methods that process the entire system simultaneously, making ART particularly effective for large, sparse, or ill-posed systems. Each equation is treated as a geometric constraint in an n -dimensional space, and the solution is refined step-by-step towards the intersection of all hyperplanes. ART is valued for its adaptability to noisy or incomplete data and its ability to incorporate new information immediately, enabling real-time updates and efficient computation—especially in applications such as medical imaging, geophysical modelling, and geodesy. A key feature of ART is the relaxation parameter δ , which controls the step size of updates. While a full projection ($\delta = 1$) can accelerate convergence, it may lead to instability in noisy conditions. Therefore, a damped relaxation ($0 < \delta < 10$) is often used to enhance stability at the expense of slower convergence. The choice of δ is critical in balancing convergence speed and robustness. In this study we considered $\delta = 0.5$.

3.2. Krylov Space-Based Methods

Krylov subspace-based methods offer a powerful, efficient way to solve large systems of linear equations by projecting the problem onto a smaller subspace. These methods balance computational efficiency, memory usage, and numerical stability, making them essential tools in scientific computing and numerical linear algebra. Their flexibility and adaptability to different types of matrices have made the Krylov subspace-based methods indispensable in real-world applications.

In solving ill-posed systems, noise in observations can cause large errors in the solution due to ill-conditioning of the coefficient matrix of the system. The Krylov subspace-based methods can act as implicit regularisers by reducing the solution's sensitivity to noise. The initial steps tend to approximate the solution in low-frequency components of the spectrum of $\mathbf{A}$. Higher-frequency components, which are more prone to noise, are introduced more slowly. In early iterations, these methods focus on minimising large, dominant eigenvalues, leading to smoother and more stable solutions and based on a suitable stopping criterion it can prevent the solution

from overfitting noise. This implicit filtering effect mimics explicit regularisation techniques by naturally damping unstable, noise-sensitive components.

In all Krylov subspace-based methods, the following optimisation problem is solved:

$$\min_{\mathbf{x} \in K_k} \|\mathbf{A}\mathbf{x} - \mathbf{L}\|_2 \quad (3a)$$

This means that the solution $\mathbf{x}$ is sought in the Krylov subspaces in such a way that the norm of residuals is minimised. A Krylov space of order k is a linear space spanned by the images of $\mathbf{L}$ under the first k powers of $\mathbf{A}$.

$$\mathbf{x} \in K_k(\mathbf{A}, \mathbf{r}^0) = \text{span}\{\mathbf{r}^0, \mathbf{A}\mathbf{r}^0, \mathbf{A}^2\mathbf{r}^0, \dots, \mathbf{A}^{k-1}\mathbf{r}^0\} \quad (3b)$$

where $\mathbf{r}^0$ stands for residual of the system. This means that the solution is a linear combination of these Krylov subspace basis vectors

$$\mathbf{x}^k = \mathbf{x}^0 + \alpha_0\mathbf{r}^0 + \alpha_1\mathbf{A}\mathbf{r}^0 + \alpha_2\mathbf{A}^2\mathbf{r}^0 + \dots + \alpha_{k-1}\mathbf{A}^{k-1}\mathbf{r}^0 \quad (3c)$$

where are α_i , $i = 1, 2, \dots, k-1$ coefficients of the polynomial. The generic solution for $\mathbf{x}$ based on a Krylov subspaces is (Jensen & Hansen, 2007):

$$\mathbf{x}_k = \Phi_k(\mathbf{B})\mathbf{B}'\mathbf{L} \quad (3d)$$

where $\Phi_k(\mathbf{B})$ is a polynomial of degree k with $\mathbf{B}$. $\mathbf{B}$ and $\mathbf{B}'$ are defined based the chosen Krylov subspace-based method. $\mathbf{x}^k$ similar to the other method is the k^{th} iterated solution. The Krylov subspaces are presented for the solution as

$$\mathbf{x} \in K_k(\mathbf{B}, \mathbf{B}'\mathbf{L}) = \text{span}\{\mathbf{B}'\mathbf{L}, \mathbf{B}\mathbf{B}'\mathbf{L}, \dots, \mathbf{B}^{k-1}\mathbf{B}'\mathbf{L}\} \quad (3e)$$

Equation (3e) says that $\{\mathbf{B}'\mathbf{L}, \mathbf{B}\mathbf{B}'\mathbf{L}, \dots, \mathbf{B}^{k-1}\mathbf{B}'\mathbf{L}\}$ are basis vectors for the Krylov subspaces, which the solution is built as a combination of these vectors. However, they are not generally orthonormal, but by applying e.g. the Gram-Schmit method can be orthonormalised.

In the following subsection, we will explain how $\mathbf{B}$ and $\mathbf{B}'$ are chosen based on the selected method.

3.2.1 Conjugate Gradient Least-Squares Method

The conjugate gradient least-squares method (CGLS) is an iterative algorithm designed to solve large, sparse, and potentially ill-conditioned linear systems particularly when the system is overdetermined or inconsistent. Instead of solving this system directly, the CGLS tackles the associated normal equations; see Eq. (1f) for $\mathbf{Q} = \mathbf{I}$, so that it can have LS property. The CGLS applies the conjugate gradient method to the symmetric and positive semi-definite matrix $\mathbf{A}^T\mathbf{A}$, using $\mathbf{A}^T\mathbf{L}$ as the right-hand side. One of its key advantages is that it only requires matrix-vector products with $\mathbf{A}$ and $\mathbf{A}^T$, making it well-suited for large-scale problems where inverting $\mathbf{A}^T\mathbf{A}$ explicitly is impractical. Importantly, the CGLS also exhibits intrinsic regularisation properties when applied to ill-conditioned systems. Early iterations of the CGLS tend to reconstruct the dominant, stable components of the solution, while suppressing the influence of noise and instability associated with the small singular values of $\mathbf{A}$. This behaviour is known as semi-convergence; the solution improves initially but deteriorates if the iteration continues too far. As such, the iteration count itself can act as a regularisation parameter, with a suitable stopping criterion playing a role analogous to classical regularisation methods. In fact, the components of the solution related to the large singular values converges faster than those with small ones (Hansen, 2007). Geometrically, the minimisation problem creates concentric ellipse passing from the iterative solution is generated towards the final solution (Bouman, 1998) so that the gradient is orthogonal to all previous ones.

If we select $\mathbf{B} = \mathbf{A}^T\mathbf{A}$ and $\mathbf{B}' = \mathbf{A}^T$ in Eq. (3d), we can see that

$$\begin{aligned} K_k(\mathbf{A}^T\mathbf{A}, \mathbf{A}^T\mathbf{L}) \\ = \text{span}\{\mathbf{A}^T\mathbf{L}, \mathbf{A}^T\mathbf{A}\mathbf{A}^T\mathbf{L}, (\mathbf{A}^T\mathbf{A})^2\mathbf{A}^T\mathbf{L}, \dots, (\mathbf{A}^T\mathbf{A})^{k-1}\mathbf{A}^T\mathbf{L}\} \end{aligned} \quad (3f)$$

Such Krylov subspace solution means that instead of solving the system of normal equations directly, the solution is built up step by step by combining a few directions that bring the solution closer to the true solution. Being conjugate means that two vectors

are orthogonal with respect to the inner product. Consider $\mathbf{p}_k$ as the sequence of orthogonal directions, the iterative solution to the system of equations is:

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \frac{\mathbf{p}_k^T \mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{L})}{\mathbf{p}_k^T \mathbf{A}^T \mathbf{A} \mathbf{p}_k} \mathbf{p}_k \quad (3g)$$

The details about derivation of Eq. (3g) and $\mathbf{p}_k$ are available in Appendix A. In order to use the CGLS, some initial values are needed. Normally, we consider $\mathbf{x}^0 = 0$, $\mathbf{r}^0 = -\mathbf{L}$, and the initial search direction $\mathbf{p}_0 = \mathbf{A}^T \mathbf{r}^0$.

Now, let us compare the CGLS solution with the standard Landweber iterative generic form in Eq. (2a). As we observe in both cases, the former solution $\mathbf{x}^k$ is updated by adding a term in which involves $\mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{L})$. In the Landweber method, we observe that $\mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{L})$ is projected on the direction of $\mathbf{p}_k$, or in other words, the contribution to the solution in the direction of $\mathbf{p}_k$ Eq. (3g) means that $(\mathbf{A} \mathbf{x}^k - \mathbf{L})$ is projected on to an orthonormalised vector along $\mathbf{p}_k$. In other words, the residuals are transformed based to the unknown space in the direction $\mathbf{p}_k$.

3.2.2 Minimum Residual 2 Method

The minimum residual 2 method (MR2) is an iterative algorithm designed for solving systems of linear equations, particularly those that are symmetric but not necessarily positive definite. It is a refinement of the original minimum residual method, which is known for its efficiency in minimising the residual error in each iteration.

In this method, the key idea is to iteratively approximate the solution by minimising the residual norm. This is done through a combination of the Krylov subspaces, which ensures that the error is minimised at each iteration. For overdetermined systems, the system should be augmented. The MR2 should not be applied on the normal equations as the condition numbers will be squared, and the normal equations becomes more ill-conditioned than the original system. In this case this method provided significantly over-smooth solution. Let us show the augmented system by:

$$\begin{bmatrix} \mathbf{0} & \mathbf{A} \\ \mathbf{A}^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \lambda \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{L} \\ \mathbf{0} \end{bmatrix} \text{ or } \tilde{\mathbf{A}} \mathbf{x} = \tilde{\mathbf{L}} \quad (4a)$$

where λ is a help vector.

The MR2 is a variant of that algorithm for symmetric indefinite linear systems starting with vector $\tilde{\mathbf{A}}^T \tilde{\mathbf{L}}$ instead of $\tilde{\mathbf{L}}$ as in the other minimum residual methods. Unlike the CGLS, the MR2 does not require $\tilde{\mathbf{A}}$ to be positive definite, making it more versatile. At each iteration, the MR2 updates the solution vector in such a way that the residual is reduced as much as possible in the least-squares sense.

The algorithm is efficient in terms of computational resources, particularly when dealing with large, sparse systems, as it avoids storing or manipulating $\tilde{\mathbf{A}}$ directly. Instead, it relies on matrix-vector products, which are often more feasible in practice for large systems. In this method the Lanczos transformation is used:

$$\tilde{\mathbf{A}} \mathbf{V}_k \approx \mathbf{V}_k \mathbf{T}_k \quad (4b)$$

where $\mathbf{V}_k = [\mathbf{v}_0 \ \mathbf{v}_1 \ \dots \ \mathbf{v}_k]$, a matrix with orthogonal columns, $\mathbf{v}_i$, $i = 0, 1, 2, \dots, k$, and $\mathbf{T}_k$ is tridiagonal matrix. The goal is to minimise the norm of the residuals namely

$$\min_{\tilde{\mathbf{x}}^k} \|\tilde{\mathbf{A}} \tilde{\mathbf{x}}^k - \tilde{\mathbf{L}}\|_2 = \min_{\tilde{\mathbf{y}}^k} \|\mathbf{T}_k \tilde{\mathbf{y}}^k - \mathbf{V}_k^T \tilde{\mathbf{L}}\|_2 \quad (4c)$$

The Krylov subspaces used in MR2 is:

$$\mathcal{K}_k(\tilde{\mathbf{A}}, \tilde{\mathbf{r}}^0) = \text{span}\{\tilde{\mathbf{r}}^0, \tilde{\mathbf{A}} \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^2 \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^3 \tilde{\mathbf{r}}^0, \dots, \tilde{\mathbf{A}}^{k-1} \tilde{\mathbf{r}}^0\} \quad (4d)$$

Once $\mathbf{y}^k$ is estimated, $\tilde{\mathbf{x}}^0$ can be obtained from it simple by

$$\tilde{\mathbf{x}}^k = \mathbf{V}_k \mathbf{y}^k \quad (4e)$$

The mathematical details of MR2 are provided in Appendix B.

The difference of the MR2 from the minimum residual method is due to considering $\mathbf{v}_0 = \tilde{\mathbf{A}} \tilde{\mathbf{r}}_0$ instead of $\tilde{\mathbf{r}}^0$ to improve the convergence. This has the effect of pre-filtering the error components in directions that correspond to the eigenvectors of $\tilde{\mathbf{A}}$ associated with small eigenvalues. These small eigenvalue directions are usually responsible for slow convergence and ill-

conditioning. Starting from $\tilde{\mathbf{A}}^T \tilde{\mathbf{L}}$ rather than $\tilde{\mathbf{L}}$ suppresses these problematic components early on. It effectively starts the iterative process from a direction already weighted by the spectrum of $\tilde{\mathbf{A}}$, giving preference to directions where $\tilde{\mathbf{A}}$ is well-behaved. This leads to faster decay of the residual norm in early iterations, especially in ill-posed or indefinite problems.

4. Uncertainty Propagation

Error/uncertainty propagation in computational models becomes particularly critical when dealing with ill-conditioned systems, where even small perturbations in input variables can result in large, unstable variations in the output. In such cases, understanding how uncertainty travels through the system are essential for producing reliable predictions. One widely used approach involves computing the Jacobian matrix, which captures local sensitivities of outputs to inputs and can be used to propagate uncertainty linearly. When analytical derivatives are unavailable, the Jacobian matrix is often approximated numerically using the central finite difference method, which offers a good balance between accuracy and simplicity. However, in ill-conditioned or nonlinear systems, numerical differentiation amplifies errors and may lead to unreliable uncertainty estimates. An alternative approach is the Monte Carlo method (MC), which bypasses the need for derivatives entirely by sampling inputs from their probability distributions and statistically analysing the spread in outputs. The following subsections explore these two techniques—finite difference—based Jacobian error propagation and the MC—in detail, highlighting their assumptions, strengths, and limitations in the context of uncertainty quantification.

4.1. Error Propagation with Numerical Jacobian

Applying error propagation law in explicit mathematical models is straightforward as a direct mathematical relation exists to obtain the solution from observations, for example, when the system is well-conditioned, the Cayley Inverse can be applied

to solve it and when the system is overdetermined, the LS method-the left generalised inverse- can be used. Even if the system is ill-conditioned the Tikhonov regularisation can be applied to find a stable solution. However, in iterative methods such a direct solution does not exist as the system cannot be solved in one step. Generally, iterative methods can be interpreted in such a way that each iteration is a step towards the solution, and each iterative method has its own number and size of steps towards the solution. For example, some may come closer to the final solution by low number of iterations, and some with higher. In this case, we should consider the solution after convergence as the final solution and numerically compute the Jacobian matrix for using the error propagation law, whilst in the direct methods this mathematical model exists, and differentiation can be done analytically.

Now consider the following generic formula for solution of a system of equations:

$$\mathbf{x}^k = \mathcal{F}(\mathbf{x}^0, \mathbf{A}, \mathbf{L}, \mathbf{k}) \quad (6a)$$

The error propagation of random errors says

$$\mathbf{C}_{\mathbf{x}^k} = \mathbf{J} \mathbf{C}_{\mathbf{L}} \mathbf{J}^T \quad (6b)$$

where $\mathbf{C}_{\mathbf{L}} = \sigma_0^2 \mathbf{Q}$ the VCM of the observations, $\mathbf{C}_{\mathbf{x}^k}$ that of the solution. $\mathbf{J}$ stands for the Jacobian matrix, which is interpreted as sensitivity of the solution to the observations. It can be derived analytically if we have a direct mathematical model, but in the case of applying iterative methods, we should numerically derive it. Let us consider the definition of central finite difference for numerical differentiation. Based on the VCM of observations, we know the uncertainty of each observation, then we can define

$$\mathbf{L}^- = -t_n \sigma_{\mathbf{L}} \quad (6c)$$

$$\mathbf{L}^+ = +t_n \sigma_{\mathbf{L}} \quad (6d)$$

where t_n is a constant selected based on the chosen confidence interval. $\sigma_{\mathbf{L}}$ are the square root of diagonal elements of $\mathbf{C}_{\mathbf{L}}$. However, we want to take derivative with respect to each observation separately to compute the sensitivity of the solution with respect to that single observation. The numerical differentiation can be done by element of $\mathbf{L}^-$ and $\mathbf{L}^+$

$$\frac{\partial \mathbf{x}^k}{\partial l_i} = \frac{\mathcal{F}(\mathbf{x}^0, \mathbf{A}, \mathbf{L} + \mathbf{e}_i \mathbf{L}^+, k) - \mathcal{F}(\mathbf{x}^0, \mathbf{A}, \mathbf{L} - \mathbf{e}_i \mathbf{L}^-, k)}{\mathbf{e}_i (\mathbf{L}^+ - \mathbf{L}^-)} \quad (6e)$$

where $\mathbf{e}_i = [0 \ 1 \ \dots \ 0]$, is a row vector with zero elements except for i^{th} which is 1. $\frac{\partial \mathbf{x}^{k-1}}{\partial l_i}$ is the derivative of the vector of solution with respect to i^{th} observation. Therefore, the numerical Jacobian matrix will be:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial \mathbf{x}^k}{\partial l_1} & \frac{\partial \mathbf{x}^k}{\partial l_2} & \frac{\partial \mathbf{x}^k}{\partial l_3} & \dots & \frac{\partial \mathbf{x}^k}{\partial l_n} \end{bmatrix}_{m \times n} \quad (6f)$$

After computing the Jacobian matrix, estimating the VCM of the solution using Eq. (6b) is straightforward.

4.2. Monte-Carlo Method

Monte Carlo method (MC) is a statistical technique that estimates how uncertainties in input variables affect the output of a model by simulating a large number of possible scenarios. Instead of relying on linear approximations or derivatives, this method samples input variables from their respective probability distributions—often Gaussian—and evaluates the model for each sampled input set. The resulting distribution of outputs captures the full effect of input variability, including nonlinear interactions and asymmetric uncertainty. By analysing this output distribution, one can compute key statistics such as the mean, standard deviation, and confidence intervals, offering a comprehensive view of the propagated uncertainty. The MC are especially valuable in complex or ill-conditioned systems, where traditional linear approaches like error propagation with numerical Jacobian (EPNJ) may fail due to instability or strong nonlinearities. Although computationally more expensive, this approach is highly flexible, as it requires only the ability to evaluate the model and does not assume differentiability or linearity. As such, the MC provides a robust alternative for uncertainty quantification in situations where analytical or numerical derivative-based methods may be unreliable.

The idea is that the noise of observations is Gaussian, therefore, for each observation a set of Gaussian errors are generated and added to the

observation. Let us say that we have generated W realisations of noise for each observation. Therefore, a matrix of $N \times W$ for noise is generated and each column (ϵ_w) of it is added to the observation vector $\mathbf{L}$, and the system is solved. Therefore, the solution of the system will be:

$$(\mathbf{x}^k)_w = \mathcal{F}(\mathbf{x}^0, \mathbf{A}, \tilde{\mathbf{L}}_w, k) \quad (7a)$$

where $\tilde{\mathbf{L}}_w = \mathbf{L} + \epsilon_w$, $w = 1, 2, \dots, W$, as noise realisation index.

This means the observation vector $\mathbf{L}$ is perturbed by noise W times, and each time it is used to solve the system. In other words, we obtain W solutions, which each one of them is the resulted solving the system with one perturbed observation.

In this case, we have W solutions for each element of the solution vector, and we can simply compute the VCM matrix of the solution by:

$$\mathbf{C}_{\mathbf{x}^k} = \frac{1}{W-1} \sum_{w=1}^W \left((\mathbf{x}^k)_w - E\{(\mathbf{x}^k)_w\} \right) \left((\mathbf{x}^k)_w - E\{(\mathbf{x}^k)_w\} \right)^T \quad (7b)$$

where

$$E\{(\mathbf{x}^k)_w\} = \frac{1}{W} \sum_{w=1}^W (\mathbf{x}^k)_w \quad (7c)$$

The VCM derived from the MC reflects not only the propagation of random errors but also the bias of the inversion method. In fact, it reveals the behaviour of the inversion method when applied to perturbed observations.

5. Numerical Experiment

In this section, we will apply the four iterative methods for solving the integral equation for recovering gravity anomaly at sea level from GOCE data. Later the error propagation with numerical Jacobian (EPNJ) and the MC are applied to the four solutions.

5.1. Experiment Set Up

The Alpine and surrounding south-central European region, limited by latitudes 35°N to 55°N and longitudes 0°E to 25°E was selected as the study

region. The GOCE 2nd-order radial gravity gradients from the product EGG_TRF_2 (EGG-C, 2010), collected from August to September 2013 at 10-s intervals, were reduced using the normal gravity field GRS80 (Moritz, 2000) to obtain T_{rr} . Figure 1a shows the spatial distribution of T_{rr} across the study area, with values ranging from approximately -1.5 E to 1 E. Positive values are concentrated over the Alpine region and southern Italy, while negative values are mainly observed in the north and southeast. Figure 1b presents the map of gravity anomaly (Δg) derived from the WHU-SWPU-GOGR2022S (Zhao et al., 2023) Earth's gravity model (EGM), to degree and order 200, with values ranging from approximately -150 to +100 mGal. While Δg represents broader-scale variations in the gravity field, T_{rr} highlight finer-scale features and localised changes. The maximum, mean, minimum and standard deviation of T_{rr} are, respectively, 1.10, 0.15, -1.32 and 0.29 E, and the equivalent statistics for Δg are 93.84, 10.8, -161.1 and 28.2 mGal.

5.2. Estimating Gravity Anomalies from GOCE Data

Now, the four iterative regularisation methods discussed in Sect. 3 are applied to invert in-orbit T_{rr}

of GOCE to Δg at sea level. As explained before, the system of equations organised after discretisation of the integral (1a) is ill-conditioned and regularisation is highly needed to obtain a stable solution. However, these iterative methods have different properties and do not behave similarly in practice. Therefore, their behaviour should be studied prior to doing any error propagation. One important factor in iterative regularisation is how many times the process should be iterated to obtain a regularised solution. Letting the iterative process go to convergence leads to the distorted solution of the system of equations, which is sensitive to the noise of data. Therefore, the iteration should be stopped before convergence to obtain a smoother solution. Here, we use the L-curve method (Hansen, 1998) to determine the optimal number of iterations in the iterative regularisation. The system is solved over a predefined iteration range (e.g., 1–50 iterations), and at each step, the norm of the solution and the norm of the residuals are recorded and plotted on a logarithmic scale, which appear like a L-shaped curve. The “corner” of the L-curve—representing the best trade-off between solution stability and residual minimisation—is identified using the maximum curvature criterion. The iteration corresponding to this

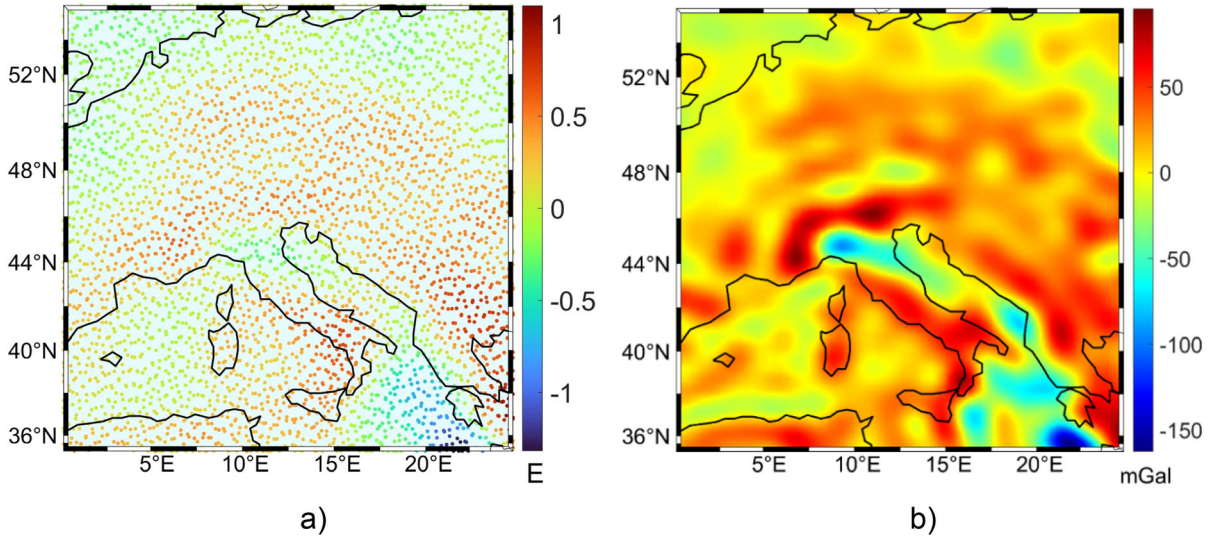


Figure 1

Map of **a** 2nd-order radial derivative of disturbing potential (T_{rr}) of GOCE [E] and **b** gravity anomalies at sea level (Δg) computed from the reference EGM [mGal]

corner is then selected as the optimal stopping point, ensuring a stable and accurate solution.

5.2.1 Norm of Residuals and Solutions

Figure 2 shows the evolution of the residual and solution norms during the iterations. As shown in Fig. 2a, the norm of the residual for the ν -method (Nu) begins to increase unboundedly after the fifth iteration, which suggests a divergence and limits its practical applicability. Additionally, although the solution norm for Nu initially aligns with that of the CGLS, it grows unboundedly thereafter. This is why we did not include more iterations in the plot—for better visual clarity. This unbounded behaviour indicates that Nu struggles to recover the high-frequency components of Δg . According to Fig. 2a, while the residual norm of the MR2 decreases with iterations, it does so less uniformly than in the CGLS. Moreover, the residual norms for the MR2 are consistently larger than those for both the CGLS and ART. The residuals of ART are relatively small during the early iterations and converge quickly to a steady value. Figure 2b shows that the solution norms of the MR2 remain smaller than those of the other methods, suggesting that the MR2 yields a smoother

solution. The solution norm for ART runs roughly parallel to that of the MR2, indicating similar behaviour between the two methods, though the difference appears as a vertical shift. The norm of the solution for the CGLS is initially close to that of the MR2 and then approaches ART's behaviour as iterations proceed—showing a trend somewhere between the MR2 and ART.

Having large or small norms for residuals and/or solutions alone does not necessarily indicate which method performs best. However, by using the L-curve method (Hansen, 1998), we can identify a solution that offers a good trade-off between the norm of the residuals and the norm of the solution. As shown in Figs. 2a and 2b, as the number of iterations increases, the norm of the solution tends to increase while the residual norm decreases. The L-curve provides a criterion to stop the iteration process at the point where these two norms are optimally balanced. This is particularly useful because, for example, ART yields the largest solution norm but the smallest residual norm, while the MR2 shows the opposite behaviour. The L-curve allows us to select a solution that balances these contrasting properties and offers a reasonable compromise.

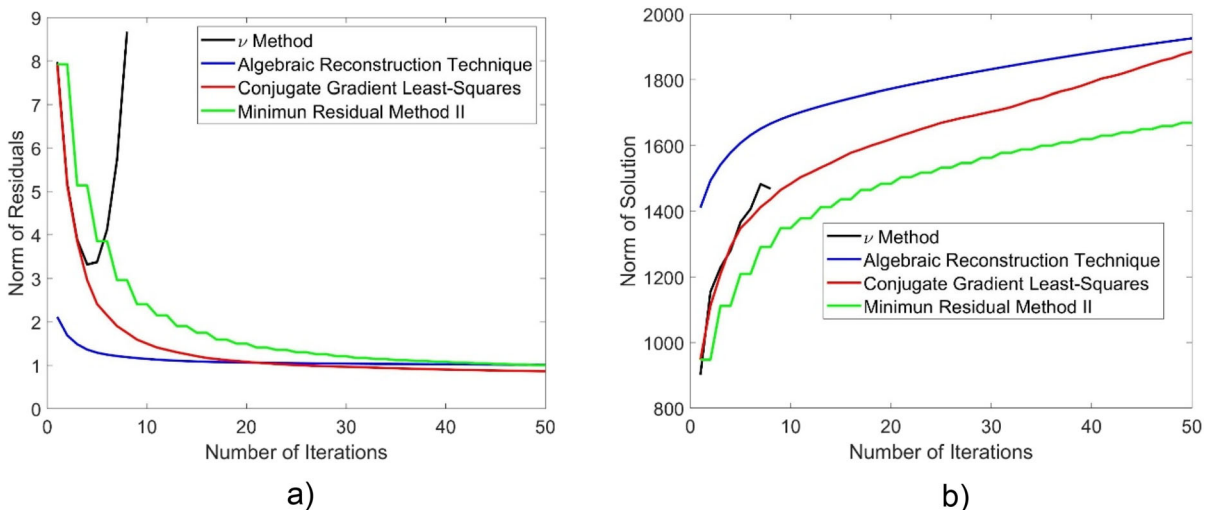


Figure 2

Norms of **a** residuals and **b** solutions during iterations for the iterative regularisation methods: conjugate gradient least-squares (CGLS), minimum residual 2 (MR2), algebraic reconstruction technique (ART), and ν -method (Nu)

5.2.2 Maximum Achievable Spatial Frequency

The next question is: *How good is the quality of the estimated Δg from these iterative regularisation methods when the stopping criterion is based on the L-curve?* This quality assessment is only possible by comparing the estimated Δg to an external reference. In this study, we use an EGM (WHU-SWPU-GOGR2022S, Zhao et al., 2023), which includes spherical harmonic coefficients up to a specified maximum degree 250 (note that the model is computed to degree and order 300), to generate Δg . We then compare the results to those derived from the inversion of GOCE T_{rr} . This comparison is not straightforward because each iterative method imposes its own regularisation characteristics. Therefore, using a fixed maximum degree for generating Δg from the EGM may not be a fair benchmark. To address this, we solve the system using each iterative method and stop the process according to the L-curve. Then, we compare the resulting solutions to Δg synthesised from the EGM at maximum degrees ranging from 1 to 250. In other words, we generate 250 sets of EGM-based Δg and compare them with the corresponding Δg derived from the GOCE data using each iterative method.

To reduce spatial truncation error (STE) and border effects, we retain only the central region of the estimated Δg field and discard a margin of 3° around the edges, based on the behaviour of the kernel of the integral formula; see e.g. Eshagh et al., (2025) for the plot of the kernel. The integral equation is formulated using the GOCE T_{rr} and Δg on a grid with a spatial resolution of $0.5^\circ \times 0.5^\circ$. After solving the system and recovering Δg on the full grid, we crop the outer boundary and keep only the interior portion that is reduced by 3° on each side. For this resolution, removing 3° corresponds to excluding six grid cells along each edge and retaining the central area where the solution is least affected by truncation artefacts.

Figure 3 shows the root mean squares (RMS) differences between those Δg derived from EGM and those estimated from GOCE data as a function of the EGM synthesis degree (1–250). Degree 250 was selected to examine the RMS behaviour beyond degree 200; however, practical comparisons of gravity anomalies are performed using the EGM truncated

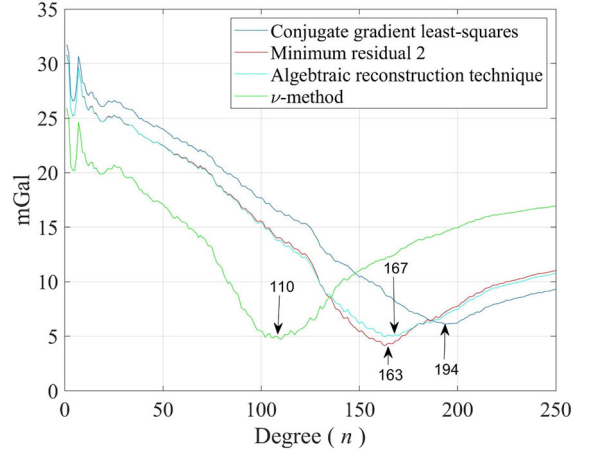


Figure 3

Plot of root mean square (RMS) differences between Δg estimated by iterative regularisation methods—conjugate gradient least-squares (CGLS), minimum residual 2 (MR2), algebraic reconstruction technique (ART), and ν -method (Nu)—and Δg generated from EGM, for spherical harmonic expansions truncated at maximum degrees from 1 to 250

at degree 200. Overall, Nu yields the lowest RMS values, with a minimum at around degree 110. This indicates that Δg estimated using this method contain meaningful spectral content primarily up to degree 110. ART and the MR2 exhibit similar behaviour, achieving their lowest RMS values around degrees 163 and 167, respectively. This suggests that these methods are capable of recovering higher-frequency components than Nu. Therefore, if the objective is to recover low-frequency components (up to degree 110), Nu is preferable. For mid-range frequencies (up to degree 163–167), ART and the MR2 are more suitable.

The CGLS achieves the lowest RMS values up to degree 194, extending to nearly degree 200. This makes the CGLS the best choice when the aim is to recover higher frequencies. Figure 3 can also be interpreted from another perspective: for degrees greater than 20, the differences in performance between the methods become more evident and method-specific characteristics start to dominate.

Table 1 presents the statistical comparison of differences between Δg recovered using the four inversion methods—CGLS, MR2, ART, and Nu—and the reference Δg derived from the EGM. The evaluation is performed at four maximum effective spherical harmonic degrees $L = 110, 163, 167$, and

Table 1

Statistics of differences between the recovered Δg by conjugate gradient least-squares (CGLS), minimum residual 2 (MR2), algebraic reconstruction technique (ART), and v-method (Nu) and Δg derived from EGM with the maximum effective degrees of $L = 110, 163, 167$ and 194 [mGal]

L	Method	Max	Mean	Min	STD	RMS
110	CGLS	58.3	1.8	− 68.4	16.4	16.5
	MR2	55.7	2.1	− 53.5	13.9	14.0
	ART	52.4	2.0	− 57.1	13.6	13.8
	Nu	15.6	0.6	− 14.4	4.7	4.7
163	CGLS	28.8	1.8	− 28.2	8.7	8.8
	MR2	25.3	2.1	− 10.2	3.6	4.1
	ART	23.3	2.0	− 11.4	4.5	4.9
	Nu	52.8	0.6	− 44.6	12.1	12.1
167	CGLS	28.4	1.8	− 25.2	8.2	8.4
	MR2	26.4	2.1	− 12.6	3.8	4.3
	ART	24.2	2.0	− 9.8	4.6	5.0
	Nu	54.4	0.6	− 47.4	12.4	12.4
194	CGLS	21.4	1.7	− 26.2	5.9	6.1
	MR2	25.7	2.0	− 18.1	7.0	7.3
	ART	30.2	1.9	− 18.6	6.7	7.0
	Nu	66.3	0.6	− 50.2	14.6	14.6

194. The statistics include maximum (Max), mean (Mean), minimum (Min), standard deviation (STD), and root mean square error (RMS), all expressed in mGal.

The results in Table 1 show that the MR2 and ART consistently achieve lower STD and RMS values for $L = 163$ and 167 . However, the CGLS demonstrates a unique strength, while it tends to have slightly higher STD and RMS values at lower degrees (e.g., $L = 110$), it recovers high-frequency Δg components more effectively than the other methods as the degree increases. This is especially evident at $L = 194$, where the RMS for the CGLS (6.1 mGal) is comparable to or better than that of the MR2 and ART, while also capturing more spatial detail. In contrast, Nu yields the lowest STD and RMS across for $L = 110$, reflecting the smoothest and most regularised solution. Although all methods report mean values of differences close to zero, suggesting an absence of significant systematic bias, the maximum and minimum values of the CGLS reveal the presence of localised extremes. These peaks reflect the method's ability to retain finer detail but also indicate greater sensitivity to noise in certain regions.

5.2.3 Maps of Recovered Gravity Anomalies and Comparisons

For a better visualisation of our recovered Δg based on our four inversion methods, their maps over the study area are presented. Δg of the recovered in the central area, smaller by $\frac{1}{3}$ from the area's margins, are selected to reduce the effect of the spatial truncation error (STE). In order to have a better visual comparison the same scale for the colourbar of the maps are chosen.

Figures 4a–d show the recovered Δg using the CGLS, MR2, ART, and v respectively, based on the L-curve criterion. The Δg recovered by CGLS (Fig. 4a) displays the strongest signal and the most details. Figures 4b and c are quite similar and appear slightly smoother than Fig. 4a, which is expected given that Δg from the MR2 and ART correspond more closely to the EGM at degrees 163 and 167, reflecting lower frequencies than CGLS (degree 194). Figure 4d, produced using Nu, is the smoothest of all, as anticipated.

While visual comparison of the Δg maps is necessary to evaluate the results of each method, it is not sufficient on its own. To provide a clearer assessment, we compare each set of recovered Δg with those derived from the EGM, using the maximum effective degree appropriate for each inversion method. Mapping the differences between these two sets offers a better indication of the error associated with the recovered Δg .

Figure 5a shows the difference map for Δg recovered from the GOCE data using the CGLS. Differences range from approximately -25 to 20 mGal but are mostly close to zero and slightly positive. Higher values appear along the margins, particularly in the eastern part of the central area, likely due to the STE.

Figures 5b and c show the difference maps for the MR2 and ART, respectively. Both are similar, with differences ranging from -25 to 25 mGal. The patterns appear mostly random. Figure 5b is smoother than Fig. 5c; in Fig. 5c, we observe two notably high values in the southeast of the central region, while several high negative values are scattered throughout the southern part of the area. This suggests that although the MR2 and ART

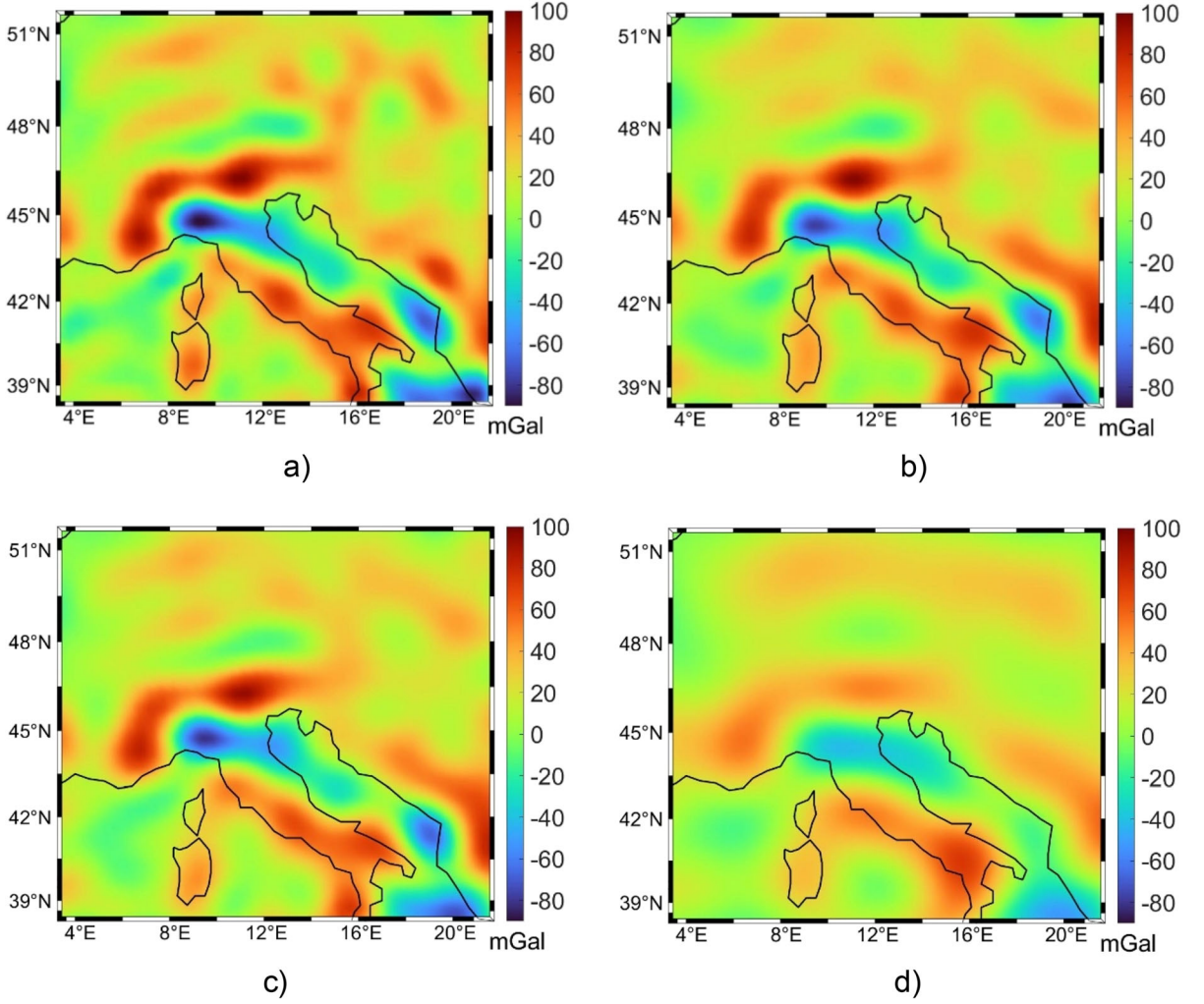


Figure 4

Maps of Δg estimated from GOCE data using four iterative inversion algorithms: **a** conjugate gradient least squares (CGLS), **b** minimum residual method 2 (MR2), **c** algebraic reconstruction technique (ART), and **d** v-method (Nu)

produced similar results in previous analyses, their errors—when compared to a reference model—differ more than initially expected.

Figure 5d presents the difference map for Nu. The differences here are smaller, ranging from -15 to 15 mGal. However, it is important to note that Nu yields the smoothest Δg , and these differences are compared against the EGM Δg truncated at degree $L = 110$. Using a higher degree would likely result in significantly larger differences.

Figure 6 presents histograms of the differences between Δg from EGM and GOCE using the selected

four iterative regularisation methods. The data exhibit an approximately normal (bell-shaped) distribution, as indicated by the red curve representing a theoretical normal distribution superimposed on each histogram. Figure 6a shows the histogram of differences when the GOCE data are inverted using the CGLS. The histogram closely follows the normal distribution curve, although some data points fall outside the curve, indicating the presence of outliers. Outliers are also observed in Figs. 6b and 6c, corresponding to the MR2 and ART methods, respectively. In contrast, Fig. 6d, which represents

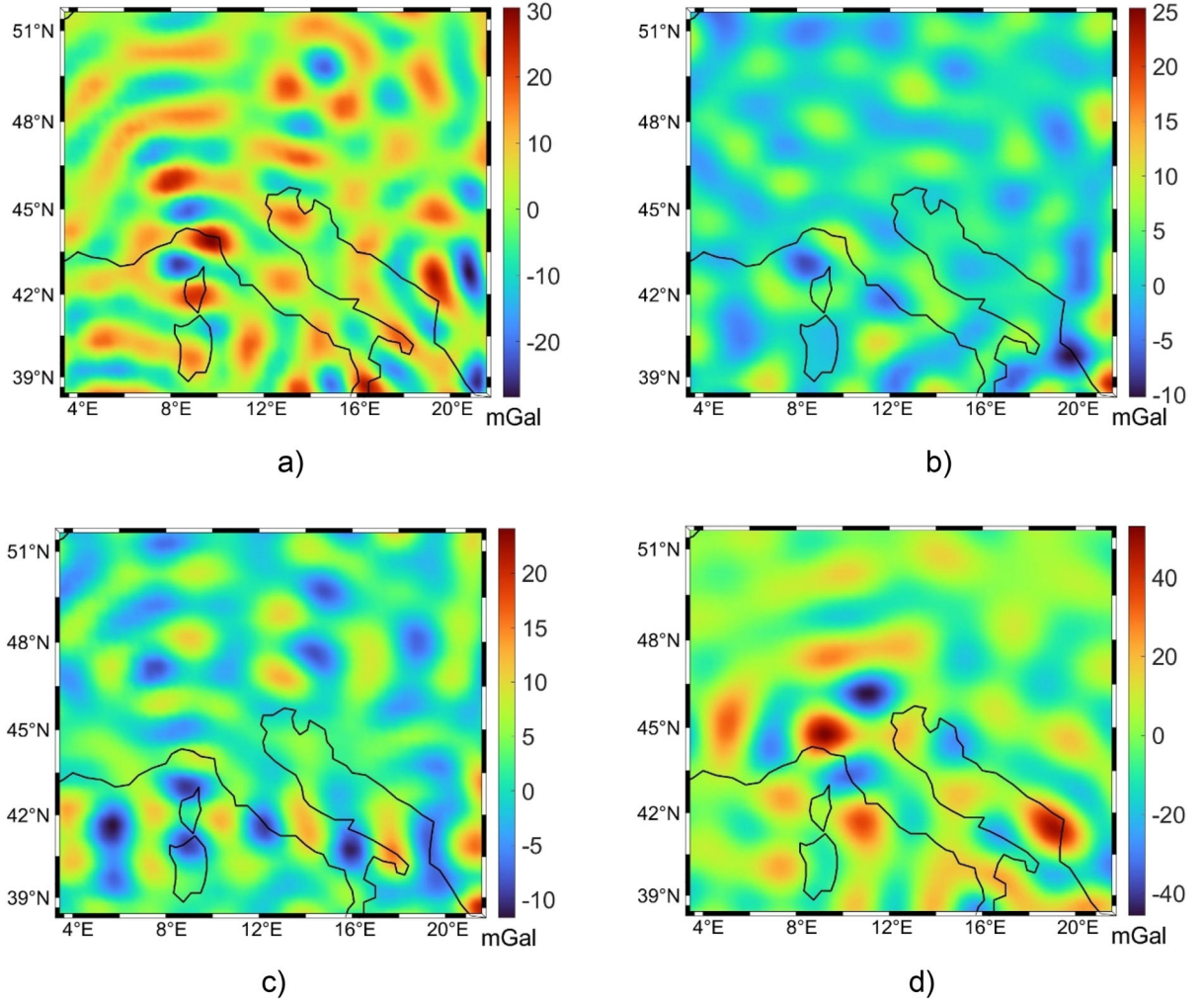


Figure 5

Maps of the differences between Δg estimated from GOCE data using four iterative inversion algorithms—**a** conjugate gradient least squares (CGLS), **b** minimum residual method 2 (MR2), **c** algebraic reconstruction technique (ART), and **d** v-method (Nu)—and the corresponding Δg from the reference EGM truncated to the best fit degree of each method

Nu, shows a histogram that fits the normal distribution curve quite well. It should be noted that the maximum effective degree of the EGM was used when computing the differences. Note that, the central area used in the analysis was reduced by 3° relative 5° to the inversion area to minimise the STE. To further investigate the source of the outliers, we reduced the size of the central area by 5° compared to the area. This adjustment led to a much better fit between the histograms and the normal distribution curve. Therefore, the primary cause of the observed outliers appears to be the STE, commonly referred to

as the edge effect or Gibbs phenomenon. We have previously observed that the CGLS produces Δg with stronger signals than the other methods, which may explain why it exhibits more pronounced edge-related outliers. In contrast, Nu provides the smoothest solution, and as a result, the influence of the STE is minimal or negligible.

5.3. Applying Error Propagation

In this section, we apply the error propagation with numerical Jacobian (EPNJ) and the Monte Carlo

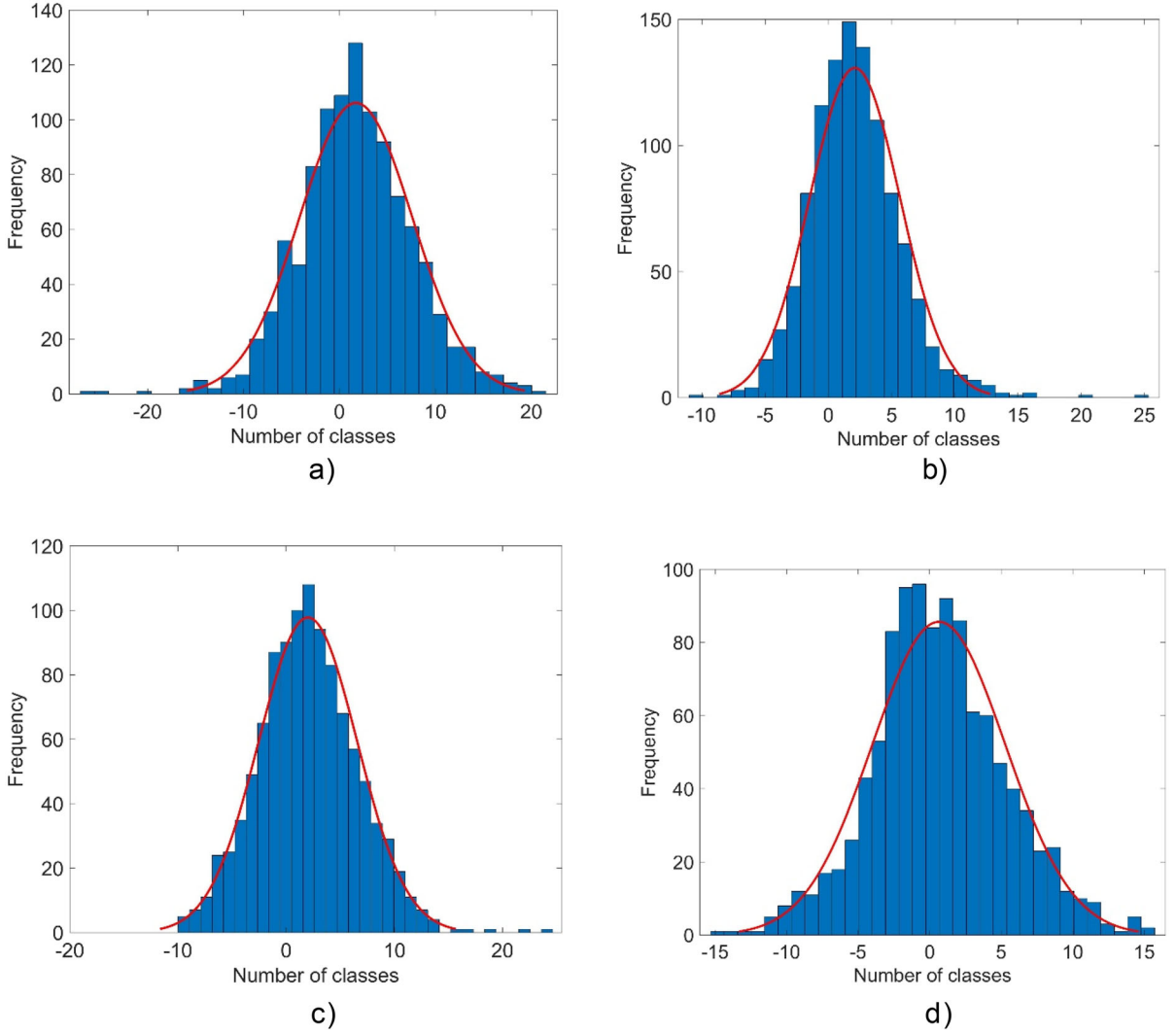


Figure 6

Histograms and corresponding fitted normal distributions of the differences between Δg estimated from GOCE data using for four iterative inversion algorithms: **a**) conjugate-gradient least squares (CGLS), **b**) minimum residual 2 (MR2), **c**) algebraic reconstruction technique (ART) and **d**) v-method (Nu) and those computed from the reference EGM

method (MC). The uncertainties of GOCE data over the study area are rather constant and about 11.4 mE. Here, we multiplied the errors by 1.96, equivalent to a confidence interval of 95%, and computed the Jacobian matrix and generated noise for the MC based on this interval. The perturbation size in numerical Jacobians is chosen as 1.96 as mentioned under the assumption of normally distributed uncertainties, ensuring that the finite differences capture the response of the system over the range of realistic

parameter variations. Using a value too small could lead to numerical errors due to machine precision, while too large a perturbation could exceed the linear regime and introduce nonlinearity effects. Therefore, 1.96 provides a practical balance, representing the typical uncertainty range while maintaining numerical stability in the Jacobian computation. In the following, section we explain how these processes have been performed.

5.3.1 Uncertainty based on Error Propagation with Numerical Jacobian

To estimate the uncertainties of the derived Δg using the error propagation law, the Jacobian matrix is required. However, since we employed iterative inversion methods, deriving the Jacobian analytically is not feasible. Therefore, we computed it numerically using the central finite difference method where each observation is treated as a central point. To compute the partial derivatives, we perturbed each observation by adding and subtracting 1.96 times the error to and from it, thereby obtaining the upper and lower limits needed for the derivative calculation with respect to each observation. This process requires repeating the differentiation N times, where N is the number of observations. In our case, with 3740 gradients, this means we need to compute 3740 derivatives. This requires solving the system of equations twice for each observation—once using the upper limit and once using the lower limit. Consequently, the system must be solved $2 \times 3740 = 7480$ times. Each solution of the system yields the derivatives of all estimated parameters with respect to a single observation. This process becomes time-consuming and computationally intensive, especially when dealing with large systems. It is important to note that the speed of convergence varies between iterative methods—some are fast, while others are significantly slower. For slower algorithms, performing numerical differentiation can be extremely time-consuming. To handle such computations efficiently, parallel programming is essential. Without it, the total computation time can extend to several hours, particularly for slow-converging iterative methods.

According to Eq. (6b), the variance–covariance matrix (VCM) of the estimated Δg is derived from the NPNJ. The square roots of the diagonal elements of the VCM represent the estimated errors or uncertainties of Δg . Figure 7 shows that the estimated errors obtained using the CGLS are approximately 3 mGal and are larger than those from the other methods. The spikes observed in the plot reflect increased errors near the boundaries of the area. The MR2 yields the smaller propagated errors, while ART results in intermediate error levels—around 2

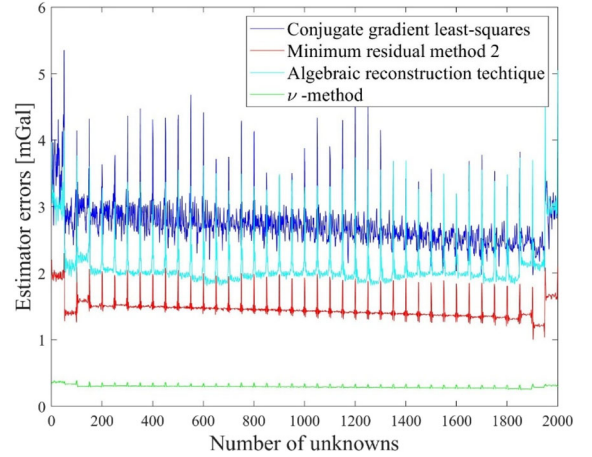


Figure 7

Estimated uncertainties of Δg recovered from GOCE data using four iterative inversion algorithms—conjugate gradient least squares (CGLS), minimum residual method 2 (MR2), algebraic reconstruction technique (ART), and ν -method (Nu)—as obtained through error propagation using the numerical Jacobian (EPNJ)

mGal—falling between those of the CGLS and MR2. This is expected, as those Δg derived from the MR2 and ART are smoother than those from the CGLS, and smoother solutions generally correspond to lower uncertainty. Based on Figs. 6b and 6c, it is evident that edge effects introduce more outliers when using the MR2 compared to ART. Additionally, those Δg obtained from ART contain slightly fewer high-frequency components than those from the MR2. As a result, the differences in propagated errors between ART and the MR2 are less than 1 mGal. Nu displays significantly smaller errors compared to all other methods. However, as seen in Fig. 7, this method fails to recover the high-frequency components of the solution. Consequently, the propagated errors appear small—not because of improved accuracy, but because the method does not capture the full spectral content of Δg .

5.3.2 Uncertainty based on Monte Carlo Method

To apply the Monte Carlo method (MC), we generated 3740 realisations of Gaussian noise and added them to the vector of observations (i.e., the GOCE T_{rr}). The number of MC realisations (3740) was chosen to match the number of observations available in our dataset, ensuring a one-to-one sampling of

observational uncertainty. Using 3740 realisations provides a direct correspondence with the observations and slightly improves statistical sampling without a significant increase in computational cost. Also, we have applied this as we used 3740 for computing the numerical Jacobian to have a fair comparison. Here, 50 iterations have been considered for each method, and the execution time of CGLS, MR2, ART and Nu have been, 1837, 2318, 2973 and 219 time-seconds, respectively. Meaning that Nu is the fastest, and ART the slowest, and CGLS faster than MR2.

The noise realisations were saved to ensure consistency across all regularisation methods, allowing for a fair comparison. For each noise realisation, the iterative solution was stopped based on the L-curve, which was used to select the optimal regularised solution. Because the system of equations is ill-conditioned and highly sensitive to observation noise, the inversion process using the L-curve was repeated 3740 times, once for each noise realisation.

The VCM of the estimated Δg is derived using Eq. (7b), and the uncertainties (errors) can be obtained by taking the square roots of its diagonal elements. Figure 8 presents the plots of the estimated errors of Δg using the MC for the four regularisation methods. As observed, the CGLS yields the largest

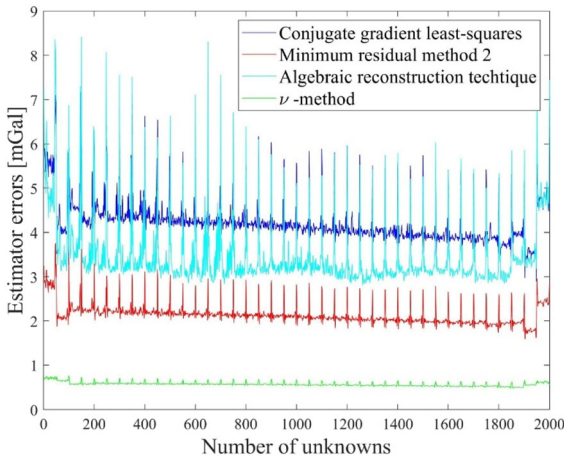


Figure 8

Estimated uncertainties of Δg recovered from GOCE data using four iterative inversion algorithms—conjugate gradient least squares (CGLS), minimum residual method 2 (MR2), algebraic reconstruction technique (ART), and ν -method (Nu)—as obtained through error propagation using the Monte Carlo method (MC)

errors, around 4.5 mGal, while ν (Nu) results in the smallest errors, less than 1 mGal. ART shows the second-largest errors at approximately 3.5 mGal, followed by the MR2 at around 2 mGal. The overall pattern of the plots in Fig. 8 closely resembles that of Fig. 7, which was based on the EPNJ. However, the errors estimated by this method are generally smaller—by about 1.5 mGal for the CGLS and ART, 1 mGal for the MR2, and less than 1 mGal for Nu. These differences will be discussed in more detail in the next section.

5.3.3 Error Propagation with Numerical Jacobian or Monte Carlo Method?

So far, we have demonstrated how the uncertainty in the estimated parameters can be quantified using both the error propagation with numerical Jacobian (EPNJ) and the Monte Carlo method (MC). However, each iterative method exhibits distinct characteristics in terms of how it propagates error. In general, we observe that the largest propagated errors occur with the CGLS under both approaches. This is followed by ART and the MR2, which produce intermediate error levels. Nu, while yielding the smallest errors, does not produce unrealistically low or non-physical values — its results remain within a plausible range. However, it should be mentioned that the larger error of the CGLS does not necessarily mean that this method is worse than the other methods, because those Δg derived by this method contain higher frequencies and stronger signal comparing to the rest of methods. In this section, we compare each error propagation method applied to iterative solutions to examine how the estimated errors differ. Figure 9 shows the propagated errors using the EPNJ and MC across the four iterative methods used.

As observed, the propagated errors using the MC are consistently larger, but they contain the full statistical response of the system to input noise, including nonlinearities and interactions, without relying on linear approximations—apart from the iterative solver used in both methods. Consequently, the MC may capture broader uncertainty and potential effects not accounted for in linearised methods. In contrast, the EPNJ is fundamentally linear. The Jacobian matrix, computed via central finite

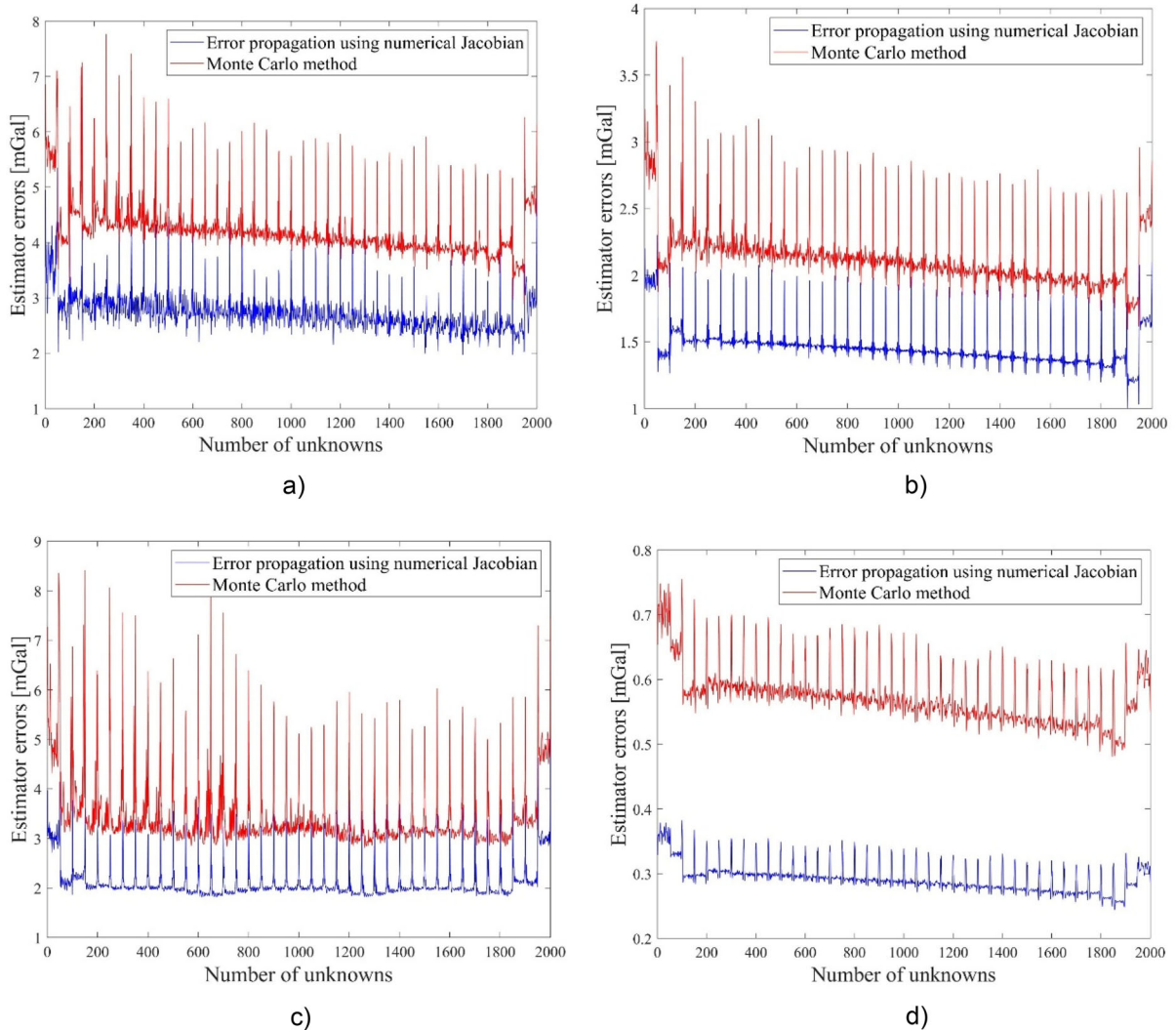


Figure 9

Estimated uncertainties of Δg recovered from GOCE data using two uncertainty assessment approaches—error propagation with the numerical Jacobian (EPNJ) and the Monte Carlo method (MC)—for four iterative inversion algorithms: **a** conjugate gradient least squares (CGLS), **b** minimum residual method 2 (MR2), **c** algebraic reconstruction technique (ART), and **d** v-method (Nu)

differences, is itself a local linearisation around each observation. Furthermore, the classical error propagation formula assumes linear propagation of small and random perturbations through this Jacobian. Therefore, it is not surprising that the errors estimated via the EPNJ are smaller. Figure 9a shows the error plots based on the two error propagation methods for the CGLS. On average, the errors are approximately 4 mGal using the MC and about 3 mGal using the EPNJ—resulting in a difference of roughly 1 mGal. Figure 9b presents a similar plot for the MR2, where

the errors are around 2 mGal with the MC and 1.5 mGal with the EPNJ, which is nearly half the error observed for the CGLS. According to Fig. 9c, the average errors for ART are approximately 3 mGal for the MC and 2 mGal for the EPNJ. Lastly, Fig. 9d shows that both methods yield errors smaller than 1 mGal for Nu.

From an execution-time perspective, the MC method is faster than EPNJ. If the number of noise realisations is taken to be equal to the number of observations (3740), the regularisation must be

repeated 3740 times. In the EPNJ approach, however, this number is approximately doubled because, for each observation, both upper and lower bounds must be considered, requiring two inversions per observation. Consequently, for 3740 observations, the total execution time of EPNJ is expected to be about twice that of the MC method.

5.4. Discussions

Inversion of satellite gradiometry data—specifically transforming 2nd-order radial derivatives of disturbing potential (T_{rr}) to Δg at sea level—is not a new topic. Reed (1973) was one of the pioneers in applying this approach for local gravity field modelling. One of the earliest studies to consider uncertainty in Δg during inversion was conducted by Xu (1992), who aimed to minimise the root mean square errors of the estimated Δg to determine the regularisation parameter in the Tikhonov regularisation.

Most early studies focused on identifying suitable inversion techniques, primarily the Tikhonov regularisation or truncated singular value decomposition (TSVD). For error estimation, recovered Δg was typically compared with external Δg derived from EGMs (e.g., Kern & Haagmans, 2005; Janák et al., 2009; Pitonak et al., 2016, 2017, 2018). Eshagh and Sjöberg (2011) further advanced the field by introducing variance-component estimation (VCE) for appropriately weighting all elements of the gradiometric tensor. Eshagh and Ghorbannia (2014) also focused on uncertainty estimation of Δg using both the GOCE gradiometric and orbital data using VCE. More recently, Novák et al. (2024) explored uncertainty estimation in integral transformations and regional gravity field recovery using the 1st-, 2nd-, and 3rd - order derivatives of the geopotential. Eshagh et al. (2025) applied three different methods for inverting the GOCE data and estimating Δg , along with error propagation using the Tikhonov regularisation, which is inherently a linear inversion technique. This method is particularly popular due to its resemblance to the standard adjustment model, making uncertainty estimation and error propagation relatively straightforward.

However, our approach in this paper diverges significantly from the mentioned studies above. We apply iterative regularisation for the inversion of the GOCE data—a topic that has been overlooked. Our results demonstrate that such methods follow distinct paths during the solution process, even when guided by the same criterion, such as the L-curve. Although Eshagh (2011c) showed that the sequential Tikhonov regularisation can compete with the CGLS, a key drawback is the accumulation of the STE during sequential inversion and quality of regularisation bias-correction, which can impact the accuracy of the uncertainty estimates for Δg . In this context, the CGLS is a promising alternative; however, a major challenge lies in propagating uncertainties from the observations to the estimated Δg .

Unlike most studies that estimate uncertainty solely through external validation against independent datasets, we applied two internal uncertainty propagation methods: the error propagation with numerical Jacobian (EPNJ) and the MC. Both methods are conceptually simple but computationally intensive, particularly for large systems. Calculating the Jacobian matrix requires deriving the sensitivity of each solution component with respect to each observation, which involves repeating the inversion process multiple times for every perturbed observation. Given that iterative methods themselves can be time-consuming, this makes the process even more demanding. For example, Nu is relatively fast, followed by the CGLS, while ART is considerably slower, as it solves the system row by row. The MC is similarly demanding, as it requires generating multiple noise realisations, perturbing the observations accordingly, and solving the system for each realisation. Therefore, uncertainty estimation in iterative inversion methods is generally less efficient than in direct regularisation methods such as the Tikhonov regularisation.

Another important point to highlight is that we cannot determine which iterative method is superior based solely on the magnitude of the propagated errors. For instance, we cannot conclude that Nu is the best simply because it results in the smallest propagated errors—this is primarily due to the fact that Nu naturally produces a significantly smoother solution. Similarly, we should not consider the CGLS

the worst merely because it yields the largest propagated errors, as those Δg that it produces contain more high-frequency information and gravitational signal content. In fact, one could argue that the CGLS offers a higher potential for recovering detailed features of the gravity field. On the other hand, if the objective is to obtain a smoother solution, then Nu would certainly be more appropriate.

The observation of larger errors using the MC is expected, as this technique does not rely on any assumptions or approximations such as linearisation. In this method, input data are perturbed according to a Gaussian distribution, and the system is repeatedly solved for each noise realisation. From the resulting ensemble of solutions, the variance–covariance matrix (VCM) of the estimated Δg can be determined. Unlike the EPNJ, the MC outputs reflect the natural behaviour of the inversion process and may incorporate not only random errors but also potential biases due to nonlinearity in the method. Furthermore, when upper and lower bounds are defined using a confidence interval (e.g., 95%) (see Eqs. 6c and 6d), and the data uncertainty is constant, and the numerical generation of the Jacobian matrix uses a limited range. However, when Gaussian noise is generated based on the same confidence interval, some values exceed the size of uncertainties. As a result, the uncertainty can be larger than that produced by the EPNJ for certain observations. This may partly explain why the MC yields larger estimated errors compared to the EPNJ. This behaviour is consistent with the broader uncertainty quantification literature, where MC are regarded as the most statistically complete approach to propagating uncertainty because they do not rely on linear approximations or small-perturbation assumptions (e.g. see Kager & Herwig, 2021). Consequently, MC captures nonlinear effects and parameter interactions that the linear method may suppress, leading to wider—but more realistic—uncertainty envelopes. However, the differences between the estimated uncertainties over the study area using EPNJ and MC will be around or less than 2 mGal.

While the MC can be applied to direct regularisation methods as well, it is often unnecessary. When the VCM, biases, and a posteriori variance can be derived analytically—as is the case for linear

methods like the Tikhonov regularisation—there is little justification for employing such a computationally intensive approach. The main challenge in the Tikhonov regularisation and uncertainty estimation is inverting large matrices for a huge number of data, whilst iterative methods avoid direct inversion of any matrix.

6. Conclusions

Iterative regularisation methods are computationally cheaper and faster than direct regularisation approaches, which require solving systems in a single, and often costly, step. They are particularly efficient for large and/or ill-conditioned systems because they avoid explicitly forming or inverting the system's coefficient matrix. As a result, they possess inherent regularisation properties by gradually refining the approximate solution, provided the iteration is terminated before full convergence. However, these methods are nonlinear in behaviour, and therefore propagating uncertainties from observations to estimates is not as straightforward as in direct methods. In this work, we investigated and recommended two practical strategies for uncertainty propagation through iterative schemes: (i) error propagation using numerical Jacobians (EPNJ), and (ii) Monte Carlo simulation (MC).

This study examined the performance of iterative regularisation methods for solving a system of equations arising from the discretisation of an integral transformation of the gravity field, specifically the transformation of the GOCE-derived T_{rr} component into gravity anomalies (Δg) at sea level. The methods evaluated include the ν -method (Nu), algebraic reconstruction technique (ART), conjugate gradient least-squares (CGLS), and the minimum residual 2 (MR2). These methods were conceptually reviewed and subsequently applied to determine Δg over a study area encompassing the Alpine and surrounding southern-central European region. The L-curve criterion was employed to terminate the iterations prior to full convergence. Our analysis revealed that Δg computed using Nu is significantly smoother, while results from the CGLS exhibit more pronounced short-wavelength gravity signal features compared with the other methods. Comparison with

that Δg derived from the WHU-SWPU-GOGR2022S Earth gravity model (EGM) indicates that Nu recovers the long-wavelength components of the gravity field up to degree 110. ART and the MR2 extend this recovery to degrees 163 and 167, respectively, while the CGLS achieves resolution up to degree 194 within the study area. These findings highlight the distinct characteristics of each iterative method. Nu is more suitable when the objective is to recover the long-wavelength portion of the gravity field, whereas the CGLS is preferable for resolving higher-frequency gravity signals.

By using EPNJ between T_{rr} and Δg and the MC, the variance–covariance matrix of Δg were estimated. Generally, the estimated error of Δg using the CGLS is largest and that of Nu is smallest based on both error propagation methods. This is expected as Δg of the CGLS has stronger signal than those of Nu. When Nu produces weaker signal, the error will be smaller. However, this does not mean that this method performs better, but we can say that it can recover long wavelengths better. Moreover, observing larger uncertainties based on the MC than the EPNJ is expected, because it reflects the iterative regularisation inherent capacity to capture both random variability and potential biases due to nonlinearity. The broader uncertainty range introduced by Gaussian noise realisation within a 95% confidence interval may lead the Monte Carlo method to over-estimate errors compared to the EPNJ method.

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I am the sole author of the paper

Author Contribution I am the sole author of the article meaning that the idea, theory, programming, setting up the experiment, results, discussion and writing up the paper were done by me.

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Data Availability

Data will be made available on reasonable request.

Declarations

Conflict of interest The authors declare no competing interests.

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Appendix A

Consider $\mathbf{p}_k$ as the sequence of orthogonal directions, therefore, they can play the role of base functions for the solution. In this case, the solution can be shown by:

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \gamma_k \mathbf{p}_k \quad (\text{A.1})$$

Since we want to apply conjugate gradient principle on the normal equations, let us multiply $\mathbf{A}^T \mathbf{A}$ to both sides of Eq. (A.1), and after subtracting $\mathbf{A}^T \mathbf{L}$ from both sides. Now, let us insert it in the normal equations,

$$\mathbf{A}^T \mathbf{r}^{k+1} = \mathbf{A}^T \mathbf{r}^k + \gamma_k \mathbf{A}^T \mathbf{A} \mathbf{p}_k \quad (\text{A.2})$$

Multiplying $\mathbf{p}_k^T$ to both sides, and considering conjugacy $\mathbf{p}_j^T \mathbf{A}^T \mathbf{A} \mathbf{p}_i = 0$ for $i \neq j$, then we can write

$$\gamma_k = - \frac{\mathbf{p}_k^T \mathbf{A}^T \mathbf{r}^k}{\mathbf{p}_k^T \mathbf{A}^T \mathbf{A} \mathbf{p}_k} \quad (\text{A.3})$$

γ_k is the contribution of the solution in the direction $\mathbf{p}_k$ and it is also known as step size.

As observed, $\mathbf{p}_k$, as the base function, plays a significant role for computing γ_k . Generally, the Gram-Schmit orthonormalisation is applied as the suitable orthogonal base functions. According to this method, $\mathbf{p}_{k+1}$ derived by:

$$\mathbf{p}_{k+1} = \mathbf{A}^T \mathbf{r}^{k+1} - \beta_k \mathbf{p}_k \quad (\text{A.4})$$

Now β_k should be derived in such a way that $\mathbf{p}_{k+1}$ is orthogonal to all former $\mathbf{p}_k$. After transposition of Eq. (A.4) and solving it for $(\mathbf{r}^{k+1})^T \mathbf{A}$ and multiplying $\mathbf{A}^T \mathbf{A}$ to both hand side from right and solving the result for β_k , we obtain

$$\beta_k = \frac{(\mathbf{r}^{k+1})^T \mathbf{A} \mathbf{A}^T \mathbf{A} \mathbf{p}_k}{\mathbf{p}_k^T \mathbf{A}^T \mathbf{A} \mathbf{p}_k} = \frac{(\mathbf{r}^{k+1})^T \mathbf{A} \mathbf{A}^T \mathbf{r}^{k+1}}{(\mathbf{r}^k)^T \mathbf{A} \mathbf{A}^T \mathbf{r}^k} \quad (\text{A.5})$$

In order to use the CGLS, some initial values are needed. Normally the initial solution $\mathbf{x}^0 = 0$, $\mathbf{r}^0 = -\mathbf{L}$, the initial search direction is $\mathbf{p}_0 = \mathbf{A}^T \mathbf{r}^0$.

Now, let us compare the CGLS solution with the standard Landweber iterative generic form in Eq. (2a). As we observe in both cases, the former solution $\mathbf{x}^k$ is updated by adding a term in which involves $\mathbf{A}^T(\mathbf{A}\mathbf{x}^k - \mathbf{L})$. In the Landweber method, we observe that $\mathbf{A}^T(\mathbf{A}\mathbf{x}^k - \mathbf{L})$ is projected on the direction of $\mathbf{p}_k$, or in other words, the contribution to the solution in the direction of $\mathbf{p}_k$

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \frac{\mathbf{p}_k^T \mathbf{A}^T (\mathbf{A}\mathbf{x}^k - \mathbf{L})}{\mathbf{p}_k^T \mathbf{A}^T \mathbf{A} \mathbf{p}_k} \mathbf{p}_k \quad (\text{A.6})$$

Equation (A.6) means that $(\mathbf{A}\mathbf{x}^k - \mathbf{L})$ is projected on to an orthonormalised vector along $\mathbf{p}_k$. In other words, the residuals are transformed based to the unknown space in the direction $\mathbf{p}_k$.

Appendix B

In order to solve the system of Eqs. (4b), consider

$$\tilde{\mathbf{x}}^k = \mathbf{V}_k \mathbf{y}^k \quad (\text{B.1})$$

and by inserting it into the system (4b), we obtain:

$$\tilde{\mathbf{A}} \mathbf{V}_k \mathbf{y}^k = \tilde{\mathbf{L}} \quad (\text{B.2})$$

Since $\mathbf{V}_k$ is orthogonal then $\mathbf{V}_k^T \mathbf{V}_k = \mathbf{I}$, therefore multiplying $\mathbf{V}_k^T$ from the left to both sides of Eq. (B.2) reads

$$\mathbf{T}_k \mathbf{y}^k = \mathbf{V}_k^T \tilde{\mathbf{L}} \quad (\text{B.3})$$

which is easier to solve than the system (4a) because of tridiagonality of the coefficient matrix $\mathbf{T}_k$.

The residual of the solution at k^{th} step will be:

$$\mathbf{r}^k = \tilde{\mathbf{A}} \tilde{\mathbf{x}}^k - \tilde{\mathbf{L}} = \mathbf{T}_k \mathbf{y}^k - \mathbf{V}_k^T \tilde{\mathbf{L}} \quad (\text{B.4})$$

and in the MR2 method the goal is to minimise the norm of this residual namely

$$\min_{\tilde{\mathbf{x}}^k} \|\tilde{\mathbf{A}} \tilde{\mathbf{x}}^k - \tilde{\mathbf{L}}\|_2 = \min_{\tilde{\mathbf{y}}^k} \|\mathbf{T}_k \mathbf{y}^k - \mathbf{V}_k^T \tilde{\mathbf{L}}\|_2 \quad (\text{B.5})$$

Once $\mathbf{y}^k$ is estimated, $\tilde{\mathbf{x}}^0$ can be obtained from it simply by Eq. (B.1).

The process begins with an initial guess for the solution, normally $\tilde{\mathbf{x}}^0 = 0$ and the residual vector is computed $\tilde{\mathbf{r}}^0 = \tilde{\mathbf{A}} \tilde{\mathbf{x}}^0 - \tilde{\mathbf{L}}$

Considering $\mathbf{v}_0 = \tilde{\mathbf{A}} \tilde{\mathbf{r}}^0$ instead of $\tilde{\mathbf{r}}^0$ to improve the convergence. It effectively starts the iterative process from a direction already weighted by the spectrum of $\tilde{\mathbf{A}}$, giving preference to directions where $\tilde{\mathbf{A}}$ is well-behaved. This leads to faster decay of the residual norm in early iterations, especially in ill-posed or indefinite problems.

The Krylov subspaces for MR2 are:

$$K_k(\tilde{\mathbf{A}}, \tilde{\mathbf{r}}^0) = \text{span}\{\tilde{\mathbf{r}}^0, \tilde{\mathbf{A}} \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^2 \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^3 \tilde{\mathbf{r}}^0, \dots, \tilde{\mathbf{A}}^{k-1} \tilde{\mathbf{r}}^0\} \quad (\text{B.6})$$

The algorithm searches for the solution based on the linear combination of the vectors $\{\tilde{\mathbf{r}}^0, \tilde{\mathbf{A}} \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^2 \tilde{\mathbf{r}}^0, \tilde{\mathbf{A}}^3 \tilde{\mathbf{r}}^0, \dots, \tilde{\mathbf{A}}^{k-1} \tilde{\mathbf{r}}^0\}$. In the following the algorithm, provided in Regularisation Toolbox 7.0 (Hansen, 2007) of Matlab is presented only for the case where no reorthogonalisation is applied.

Some initial values should be defined to start the algorithm, i.e. $\tilde{\mathbf{x}}^0 = 0$, there for $\tilde{\mathbf{r}}^0 = \tilde{\mathbf{L}}$ and later $\tilde{\mathbf{v}}^0 = \tilde{\mathbf{A}} \tilde{\mathbf{r}}^0$ with $\tilde{\mathbf{w}}^0 = \tilde{\mathbf{A}} \tilde{\mathbf{v}}^0$. Through the algorithm $\tilde{\mathbf{v}}^0$ and $\tilde{\mathbf{w}}^0$ should be normalised by $\beta = \|\tilde{\mathbf{w}}^0\|$, this means they should be divided by β before starting the iteration. The following formulae can be used for iterations. The solutions and residuals are updated by

$$\tilde{\mathbf{x}}^k = \tilde{\mathbf{x}}^{k-1} + \rho_k \tilde{\mathbf{v}}^k \quad (\text{B.7})$$

$$\tilde{\mathbf{r}}^k = \tilde{\mathbf{r}}^{k-1} - \rho_k \tilde{\mathbf{A}} \tilde{\mathbf{v}}^k \quad (\text{B.8})$$

where $\rho_k = \mathbf{r}_{k-1}^T \omega_{k-1}$ and

$$\tilde{\mathbf{v}}^k = \tilde{\mathbf{v}}^{k-1} - \alpha \tilde{\mathbf{v}}^{k-1} - \beta \tilde{\mathbf{v}}^{k-2} \quad (\text{B.9})$$

$$\tilde{\mathbf{w}}^k = \tilde{\mathbf{A}} \tilde{\mathbf{w}}^{k-1} - \alpha \tilde{\mathbf{w}}^{k-1} - \beta \tilde{\mathbf{w}}^{k-2} \quad (\text{B.10})$$

where

$$\alpha = (\tilde{\mathbf{w}}^{k-1})^T \tilde{\mathbf{A}} \tilde{\mathbf{w}}^{k-1} \quad (\text{B.11})$$

$$\beta = \|\tilde{\mathbf{w}}^{k-2}\| \quad (\text{B.12})$$

and again $\tilde{\mathbf{v}}^k$ and $\tilde{\mathbf{w}}^k$ should be normalised by $\beta = \|\tilde{\mathbf{w}}^k\|$ and the process is repeated.

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