



Uncertainty propagation through integral inversion of satellite gradient data in regional gravity field recovery

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Abstract

The Gravity field and steady-state Ocean Circulation Explorer (GOCE) mission, launched by the European Space Agency, provided high-quality gravitational gradient data with near-global coverage, excluding polar regions. These data have been instrumental in regional gravity field modelling through various methods. One approach involves a mathematical model based on Fredholm's integral equation of the first kind, which relates surface gravity anomalies to satellite gradient data. Solving this equation requires discretising a surface integral and applying further regularisation techniques to stabilise the numerical solution of a resulting system of linear equations. This study examines four methods for modifying the system of linear equations derived by discretising the Fredholm integral equation. The methods include direct inversion, remove-compute-restore, truncation reduction of the integral formula, and inversion of a modified integral for estimating surface gravity anomalies from satellite gradient data over a test area in Central Europe. Since the system of linear equations is ill-conditioned, the Tikhonov regularisation is applied to stabilise its numerical solution. To assess the precision and reliability of the estimated gravity anomalies, the study introduces mathematical models for estimation of biased and de-biased noise variance–covariance matrices of estimated surface gravity anomalies. The results indicate that the signal-to-noise ratio of reduced satellite gradient data in the remove-compute-restore method is smaller compared to other methods in the study, necessitating stronger stabilisation of the model to recover surface gravity anomalies. This, in turn, leads to a more optimistic uncertainty propagation than the other considered methods.

Keywords Fredholm's integral equation · Gravity anomaly · Regularisation bias · Satellite gradient data · Uncertainty estimation · Variance–covariance matrix

1 Introduction

The gravity field of the Earth together with its figure and dynamics represent three connected research areas of modern geodesy, e.g. (Angermann et al. 2022), as the figure of the Earth has evolved primarily under the effect of self-gravitation and rotation. The gravity field must be considered in e.g. realisation of geodetic reference systems, processing

geodetic data, satellite orbit integration, and geoid determination. The geoid represents an equipotential surface of the static Earth's gravity field approximated by the ocean surface at rest which is used in geodesy as a reference surface for physical heights. Thus, the knowledge of the precise geoid and the static Earth's gravity field is important for geodesists, geophysicists, glaciologists, geologists, oceanographers, and other users.

Over the past two decades, a considerable progress has been achieved in collecting gravity data by sensors mounted on low orbiting satellites. The Gravity field and steady-state Ocean Circulation Explorer (GOCE) was the first satellite mission dedicated to measuring components of the second-order gravitational tensor (in a Cartesian coordinate frame defined as second-order directional derivatives of the gravitational potential denoted herein as satellite gradients) along its orbital path (ESA 1999). Gradient data measured by the

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GOCE satellite in a local Cartesian coordinate frame surpassed the sensitivity of previous satellite gravity data in the medium-wavelength part of the gravity field frequency spectrum. This enhanced sensitivity enabled the determination of surface gravity anomalies with the 1 mGal accuracy level at the superior spatial resolution of 80 km (half wavelength at the equator). However, uncertainties of satellite gradients used for recovery of surface gravity anomalies are often disregarded in the inversion process. Therefore, it is crucial to address observation errors of satellite gradients, investigate their impact on estimated surface gravity anomalies, and to assess their quality when employing integral equations in regional gravity field modelling.

One of the pioneering works in inversion of satellite gradients was that of Reed (1973) who developed integral equations for second-order derivatives of the extended Stokes integral, aiming at recovering surface gravity anomalies from satellite gradients. His work represented the basis for other methods that refined and extended the application of integral equations for regional gravity field modelling. Subsequent developments of this method included least-squares collocation (Krarup 1969) that was applied by Tscherning (1988, 1989), Arabelos and Tscherning (1990, 1995). Least-squares collocation was another significant advancement, offering a robust statistical approach to interpolation and prediction of geodetic and geophysical quantities.

In the 1990s, Xu (1992, 1998) embarked on solving integral equations by using Tikhonov's regularisation method and truncated singular-value decomposition. These efforts were paralleled by Tscherning et al. (1990) who pioneered the direct integration method that integrated satellite gradients over the mean orbital sphere and continued them downward to the mean sea level (or the Earth's surface), a methodology further developed by Eshagh (2011a, 2012), and Sjöberg and Eshagh (2012). Tóth et al. (2004) investigated the concept of upward/downward continuation of satellite gradients to the mean orbital sphere. In addition, Kotsakis (2007) utilised Tikhonov's regularisation method with the covariance-adaptive approach, which represented another significant methodological advancement.

In the late 2000s and early 2010s, Xu (2009) proposed an iterative generalised cross-validation method for simultaneous estimation of regularisation parameters and variance components, which were applied for recovery of surface gravity anomalies from satellite gradient data. Kern and Haagmans (2005) and Janák et al. (2009) investigated the inversion of the full second-order gradient tensor formulated in the geocentric coordinate system to recover surface gravity anomalies, a complex and comprehensive approach to the problem. Eshagh (2011b) developed the inversion of stochastically modified surface integrals for surface gravity anomaly recovery from satellite gradient data, with Eshagh (2011c) further exploring the impact of spatial truncation

errors (STE) on their recovery. Eshagh and Sjöberg (2011) conducted a study on the inversion and combination of satellite gradients, employing the variance component estimation for their optimal weighting.

Pitoňák et al. (2017, 2020, 2023) and Saadat et al. (2019) contributed to the inversion of satellite gradient data. Concurrently, the application of radial basis functions gained attraction, with the seminal works by Schmidt et al. (2006), Eicker (2008), Eicker et al. (2013), followed by Naeimi and Bouman (2017) who examined the contribution of satellite gradients to regional gravity field modelling using radial basis functions. Eshagh et al. (2018) advanced the inversion of the diagonal elements of the gradient tensor and illustrated the ongoing refinement of inversion techniques and the integral role of satellite gradients for the regional gravity field modelling.

Parameter estimation and error analysis have been fundamental routines in geodesy since the advent of the least-squares adjustment (LSA) method, independently introduced by Legendre, Gauss and Laplace in the eighteenth and/or nineteenth century. Since then, the estimation of unknown parameters, along with their variances (mean quadratic errors) and covariances has been standardised across all sub-disciplines of geodesy. Whereas prior investigations into estimation of surface gravity anomalies from satellite gradients predominantly focused on the effective continuation of gradients, the present study turns its attention to propagation of satellite gradient errors into estimated gravity anomalies.

In many studies concerning the downward continuation of satellite gradients to the mean sea level, the primary emphasis has typically been on selecting an appropriate estimation method or formulating suitable solutions to systems of linear equations originating from the discretised integral equations. There are studies about error propagation in geoid/quasigeoid determination, e.g. (Featherstone et al. 2018; McCubbine et al. 2019; Slobbe et al. 2019; Ophaug and Gerlach 2020; Foroughi et al. 2023). Yet, the propagation of satellite gradient errors to estimates of surface gravity anomalies has been somewhat overlooked. For example, investigations by Eshagh and Sjöberg (2011) were strictly based on simulations, neglecting the STE in the estimated gravity anomalies and the subsequent error propagation. Later, Eshagh and Ghorbannia (2014) recognised the influence of the STE in joint inversion of GOCE orbital and gradient data for estimating surface gravity anomalies and their uncertainties. Error propagation in inversion of gradient data by integral transforms and integral equations was recently studied in Novák et al. (2024).

This study compares three modifications of the integral equation used for setting up a system of linear equations by discretisation of the integration domain linking radial gradients of the disturbing potential (derived from measured GOCE gradients) to surface gravity anomalies (at the mean

geocentric sphere). Moreover, we will also use the original form of the integral equation for comparison. Thus, we refer to four methods while we focus on assessing propagation of satellite gradient errors into unknown surface gravity anomalies. The system of linear equations is set up for the original integral equation and its three different modified versions, with respective methods called as follows:

- Direct inversion (DIR) of satellite gradients with no reduction applied.
- Remove-compute-restore (RCR), wherein the long-wavelength component of satellite gradients is assumed to be known through Earth gravitational models (EGMs) and removed from satellite gradients prior to solving the system of linear equations; the long-wavelength component is restored in estimated values of surface gravity anomalies.
- Truncation reduction (TR) based on estimation and subsequent removal of STE, i.e. considering the effect of far-zone surface gravity anomalies omitted in inversion of local data before solving a discretised integral equation (Pitoňák et al. 2016).
- Modified integral inversion (MII) based on solving a system of linear equations based on the surface integral modified through the least-squares approach as proposed by Sjöberg (1984).

This study also proposes a mathematical model aimed at reducing the regularisation bias in the estimated noise variance–covariance matrix (VCM) of surface gravity anomalies estimated by the regularised solution to the system of linear equations.

Note that we disregard gravitational effects of topographic and atmospheric masses on satellite gradients (see e.g. Novák and Grafarend 2006; Eshagh and Sjöberg 2009a,b), which must be applied to harmonise the disturbing potential and its functionals (including measured gradients and unknown gravity anomalies) in the space where the mathematical model is solved (i.e. outside the mean sea level). Consequently, our solutions include topographic and atmospheric biases which can be easily removed (Eshagh 2009b, a).

In each method, satellite gradients measured by GOCE are used to estimate unknown values of surface gravity anomalies over a test region in Central Europe. The study aims at uncertainty estimation for surface gravity anomalies recovered by the four methods, paying special attention to the gradient data error propagation in each method. It is known that the involved surface integral is more localised than the Poisson integral due to its sharper, well-behaving (i.e. attenuating with the spherical distance) and isotropic kernel function (Eshagh 2011a). Thus, the system of linear equations obtained by discretising the surface integral is more stable, and values of the STE are significantly smaller.

The structure of the text is as follows: Sect. 2 delineates the methodology, encompassing an introduction of the integral equation tailored to the problem at hand, and its four modifications. Subsequently, the Gauss-Helmert model is applied to solve the system of linear equations obtained by discretisation of the integral equation with four modifications and regularised by the Tikhonov method. Thereafter, mathematical models for the bias estimation of the noise VCM of estimated surface gravity anomalies are developed. Section 3 contains results of numerical experiments based on the four modification methods. Section 4 summarises results of the numerical experiments, and conclusions and summary can be found in Sect. 5.

2 Methodology

We consider the integral equation relating the second-order radial derivative of the disturbing potential T , denoted as T_{rr} , at the satellite orbit to the gravity anomaly Δg at mean sea level:

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

where R stands for the radius of the mean geocentric sphere approximating mean sea level, r is the geocentric radius of the computation point at the satellite orbit, the attenuation factor is defined as $t = R/r$, $\Omega = (\varphi, \lambda)$ represents the geocentric direction to the computation point defined by the spherical latitude φ and longitude λ , $\Omega' = (\varphi', \lambda')$ stands for the geocentric direction to the integration element, ψ is the spherical distance between the computation point and the integration element $d\Omega' = \cos \varphi' d\varphi' d\lambda'$. The second-order radial derivative of the extended Stokes function S_{rr} is defined as follows: e.g. Reed (1973):

$$S_{rr}(t, \psi) = \frac{t^3}{R^2} \left[(1 - tx) \left(\frac{3(1 - t^2)}{D^5} - \frac{4}{D^3} \right) - \frac{1 + t^2}{D^3} - \frac{10}{D} - 18D + 2 - 3tx \left(15 + 6 \ln \frac{1 - tx + D}{2} \right) \right], \quad (1b)$$

where the r -normalised Euclidean distance D between the computation point and the integration element is defined as $D = \sqrt{1 - 2tx + t^2}$ and $x = \cos \psi$. Equation (1a) represents Fredholm's integral equation of the first kind. In the regional gravity field modelling, the number of measured satellite gradients is larger than that of estimated gravity anomalies so the system of linear equations obtained by discretisation of the surface integral in Eq. (1a) is overdetermined and sought values of Δg can be estimated e.g. by the least-squares method.

Its solution must further be regularised as the system of linear equations is ill-conditioned. For estimating the noise VCM of the estimated gravity anomalies, different methods based on a posteriori variance factors or variance components have been developed (see e.g. Xu et al. (2006), Eshagh and Sjöberg (2011), or Eshagh and Ghorbannia (2014)).

In the DIR method, we solve the discretised integral Eq. (1a) over the limited computation area (spherical cap) without any reduction of satellite gradients for far-zone gravity anomaly data. However, the focus of the study is on the methods that apply different modifications of the integral equation for reduction of far-zone gravity anomalies.

2.1 Solving the discretised integral equation by the RCR method

The RCR method is widely used for the regional gravity field modelling (Vincent and Marsh 1974; Rapp and Rummel 1975). Its principle is to remove the long-wavelength component (synthesised from EGM at the satellite orbit) from measured satellite gradients, solve the discretised integral equation with residual (reduced) gradient data, and restore a long-wavelength component (synthesised from the same EGM at the mean sea level) in the estimated surface gravity anomaly. The principle of the method is given below. Consider Eq. (1a) but with the long-wavelength gradient component (synthesised from EGM) removed from observed satellite gradients T_{rr} :

$$\begin{aligned} \frac{R}{4\pi} \iint_{\Omega'} S_{rr}(t, \psi) \Delta g^L(R, \Omega') d\Omega' &= T_{rr}(r, \Omega) \\ &- \frac{R}{2} \sum_{n=2}^L \Gamma_n(r) \Delta g_n(\Omega) \\ &= T_{rr}^L(r, \Omega), \end{aligned} \quad (2a)$$

with coefficients

$$\Gamma_n(r) = \frac{2(n+1)(n+2)}{r^2(n-1)} t^{n+1}, \quad (2b)$$

and Laplace's harmonics of the gravity anomaly Δg_n . After discretisation of the surface integral on the left-hand side of Eq. (2a), a system of linear equations is obtained, the solution to which represents the residual surface gravity anomaly (reduced for the EGM-based long-wavelength component). Consequently, it is imperative to restore its long-wavelength component using the same EGM.

A critical consideration must be given to the integration domain and the kernel function. As demonstrated by Eq. (1a), the integration domain encompasses the full spatial angle Ω' (entire mean sphere). As regional gravity field modelling is discussed in this study, the integration domain is limited to

a spherical cap Ω_0 of a spherical radius ψ_0 . Spatial characteristics of the kernel function are equally significant, as they affect the effect of the far-zone gravity anomalies (gravity anomalies outside the spherical cap). The kernel function must be limited by the same minimum degree as the residual gradient data. Fortunately, the kernel function S_{rr} is a well-behaving function (Eshagh 2011a, b, c): its values decrease and approach the zero value as the spherical distance increases. This decay means that the effect of residual gravity anomalies in the far zone, i.e. outside the spherical cap, is substantially mitigated if this estimator is used for recovery of the unknown gravity anomalies.

2.2 Solving the discretised integral equation by the TR method

The truncation coefficients Q_n of the surface integral can be derived using the spectral representation of its kernel function for the given spherical cap Ω_0 . The truncation coefficients facilitate the calculation of the STEs (far-zone contributions) associated with spatially limited integration domains, which in our case represent the contribution of gravity anomalies outside the spherical cap that are not included in the surface integral. This error can be quantitatively derived in the spectral domain using truncation coefficients and Laplace's harmonics of the gravity anomaly. Pitoňák et al. (2016) employed this method to eliminate such an error from the satellite gradient data, thereby reducing the contribution of the far-zone gravity anomalies. This method, proposed originally by Molodensky et al. (1962) for Stokes's surface integral, results in the following expression when applied to satellite gradients and gravity anomalies:

$$\begin{aligned} T_{rr}(r, \Omega) &= \frac{R}{4\pi} \iint_{\Omega_0} S_{rr}(t, \psi) \Delta g(R, \Omega') d\Omega' \\ &+ \frac{R}{4\pi} \iint_{\Omega' - \Omega_0} S_{rr}(t, \psi) \Delta g(R, \Omega') d\Omega', \end{aligned} \quad (3a)$$

where Ω_0 stands for the spherical cap centred at the computation point with the spherical radius ψ_0 . The second integral on the right-hand side of Eq. (3a), i.e. the far-zone effect, has the following spectral form:

$$\begin{aligned} \frac{R}{4\pi} \iint_{\Omega' - \Omega_0} S_{rr}(t, \psi) \Delta g(R, \Omega') d\Omega' \\ \cong \frac{R}{2} \sum_{n=2}^L Q_n(r, \psi_0) \Delta g_n(\Omega). \end{aligned} \quad (3b)$$

The truncation coefficients can be estimated by a series:

$$Q_n(r, \psi_0) = \sum_{k=2}^{\infty} \Gamma_n(r) E_{nk}(\psi_0) \text{ with} \\ E_{nk}(\psi_0) = \frac{2n+1}{2} e_{nk}(\psi_0), \quad (3c)$$

and

$$e_{nk}(\psi_0) = \int_{\psi_0}^{\pi} P_n(\cos \psi) P_k(\cos \psi) \sin \psi d\psi, \quad (3d)$$

are coefficients which can be computed using recursive formulas provided by Paul (1973).

From Eqs. (2a), (3a) and (3b), the following integral equation can be written for recovering the gravity anomalies:

$$\frac{R}{4\pi} \iint_{\Omega_0} S_{rr}(t, \psi) \Delta g(R, \Omega') d\Omega' = T_{rr}(r, \Omega) \\ - \frac{R}{2} \sum_{n=2}^L Q_n(r, \psi_0) \Delta g_n(\Omega). \quad (3e)$$

For calculation of the truncation errors of the integral, the Laplace coefficients of the gravity anomaly are required as indicated on the right-hand side of Eq. (3e). The employment of the EGM for their computation introduces additional errors into the integral equation that are related to errors of EGM coefficients (commission errors) and truncating the series in Eq. (3b) to some maximum degree $L \ll \infty$ (omission errors). The quantification and analysis of these errors are explored later.

2.3 Solving the discretised integral equation by the MII method

Generally, modifying a surface integral involves altering the spatial behaviour of its kernel function in a manner that minimises the truncation error, i.e. the contribution of the far-zone gravity anomalies. The contribution of the far-zone gravity anomalies is partially replaced by the magnified effect of the local gravity data involved in the integration, so the sum of the near- and far-zone effects remains the same.

Various modification methods have been proposed, but it is crucial to ensure that any modification of the kernel function is compensated for in the result. Simply changing the kernel function without adjusting the corresponding far-zone effect is not correct. Furthermore, the extent of the modification is another critical factor that must be considered, alongside the size of the spherical cap (usually predetermined by an extent of available local gravity data). The maximum modification degree L is typically aligned with the maximum degree of

the available EGM. A modified integral formula is presented in the following generic form:

$$T_{rr}(r, \Omega) = \frac{R}{4\pi} \iint_{\Omega_0} S_{rr}^{*L}(t, \psi) \Delta g(R, \Omega') d\Omega' \\ + \frac{R}{2} \sum_{n=2}^L s_n(r, \psi_0) \Delta g_n(\Omega), \quad (4a)$$

where L is the maximum modification degree of the kernel function, s_n are the modification coefficients, and S_{rr}^{*L} is the modified second-order radial derivative of the extended Stokes function (see Eshagh 2011b):

$$S_{rr}^{*L}(t, \psi) = S_{rr}(t, \psi) - \sum_{n=2}^L \frac{2n+1}{2} s_n(r, \psi_0) P_n(\cos \psi). \quad (4b)$$

According to Molodensky (1962), the modification parameters are determined in a way that increases the weight of regional gravity data within the near zone (i.e. inside the spherical cap), thereby minimising the contribution of gravity data in the far zone (i.e. outside the spherical cap). Conversely, Sjöberg (1984) introduced the least-squares modification of the Stokes integral, which accounts for both truncation errors inherent in the integral formula, and errors associated with the EGM and regional gravity data. This approach has been successfully employed by Eshagh (2011b), and Eshagh and Romeshkani (2012) for computation of gravity gradients by applying second-order derivatives of the extended Stokes formula and facilitating the validation of satellite gradient data.

Based on the least-squares modification of the kernel function, the modification coefficients s_n are estimated by solving the following system of linear equations (see Eshagh 2011b):

$$\sum_{l=2}^L a_{kl}(\psi_0) s_l(r, \psi_0) = h_k(r, \psi_0), \quad (4d)$$

with

$$a_{kl}(\psi_0) = \left(\sigma_l^2 + d_{cl} \right) \delta_{kl} - E_{kl}(\psi_0) \sigma_l^2 - E_{lk}(\psi_0) \sigma_k^2 \\ + \sum_{n=2}^L E_{nl}(\psi_0) \\ E_{nk}(\psi_0) \left(\sigma_n^2 + c_n \right), \quad (4e)$$

$$h_k(r, \psi_0) = \{ \Gamma_k(r) - Q_k(r, \psi_0) \} \sigma_k^2 \\ + \sum_{n=2}^L \left\{ Q_k(r, \psi_0) \left(\sigma_n^2 + c_n \right) - \Gamma_k(r) \sigma_n^2 \right\} E_{nk}(\psi_0), \quad (4f)$$

where $\sigma_{i(k)}^2$, $c_{i(k)}$ and $dc_{i(k)}$ denote respectively the error degree variances of surface gravity anomalies, and signal and error degree variances of the employed EGM, with $i(k)$ representing either i or k .

The system of linear equations in Eq. (4d) is well-conditioned for the biased least-squares modification; however, the regularisation is required for unbiased and optimum modifications to stabilise estimation of the modification parameters as discussed e.g. by Ellmann (2005). For validation and inversion of satellite gradient data, the biased least-squares modification emerges as the most suitable method (Eshagh 2011b).

In Eq. (4a) the EGM is again required to compute Δg_n , which means that additional (commission) errors must be considered for reduced satellite gradient data on the right-hand side of Eq. (4a). Their behaviour and magnitude depend on the EGM errors and coefficients s_n .

2.4 Linear equations of Gauss-Helmert type and Tikhonov's regularisation

So far, three modification methods of the integral equation inverting satellite gradient data into surface gravity anomalies have been introduced and discussed. Equations (2a), (3e), and (4a) may be generalised in the following form:

$$\begin{aligned} \frac{R}{4\pi} \iint_{\Omega_0} K(t, \psi) G(R, \Omega') d\Omega' = T_{rr}(r, \Omega) \\ - \frac{R}{2} \sum_{n=2}^L M_n(r) \Delta g_n(\Omega), \end{aligned} \quad (5a)$$

with

$$M_n(r, \psi_0) = \begin{cases} 0, & K = S_{rr}, \quad G = \Delta g \text{ for the DIR method,} \\ \Gamma_n(r), & K = S_{rr}, \quad G = \Delta g^L \text{ for the RCR method} \\ Q_n(r, \psi_0) & K = S_{rr}, \quad G = \Delta g \text{ for the TR method,} \\ s_n(r, \psi_0) & K = S_{rr}^*, \quad G = \Delta g \text{ for the MII method.} \end{cases} \quad (5b)$$

M_n are in fact coefficients which control in the spectral domain how much the long-wavelength component of the sought surface gravity anomaly contributes to measured satellite gradients.

Equation (5a) represents a general integral equation for solving surface gravity anomalies using the four methods. The same kernel function is used in the DIR and TR methods. In the DIR method, no reduction is applied to satellite gradients prior their inversion, whereas in the RCR method, only frequencies higher than L are recovered through the integral inversion of residual satellite gradient data. From the perspective of the error propagation, it is

evident that uncertainties of the residual gradient data are greater than those of the measured gradient data. Consequently, any reduction applied to the gradient data introduces additional errors that must be accounted for in the observation equations, when applying the RCR, TR and MII methods.

Errors associated with reductions of gradient data depend directly on how errors of EGM-based long-wavelength surface gravity anomalies propagate to residual satellite gradients. In our study, we account for these errors and use the Gauss-Helmert model to emphasise that errors of the reductions are considered in addition to errors of measured gradient data. While one could apply the Gauss-Markov model, it is essential to incorporate errors of the reductions into the weight matrix for the residual gradients.

Let us write the discretised form of Eq. (5a) as the Gauss-Helmert model (matrices and vectors are typed in bold):

$$\begin{aligned} \mathbf{Ax} + \mathbf{B}(\mathbf{L} - \mathbf{e}) &= 0, \\ \text{with } E\{\mathbf{ee}^T\} &= \sigma_0^2 \mathbf{Q} = \sigma_1^2 \mathbf{Q}_1 + \sigma_2^2 \mathbf{Q}_2, \\ E\{\mathbf{e}\} &= 0, \end{aligned} \quad (6a)$$

where $\mathbf{A}$ is the design matrix derived after discretisation of the near-zone integration domain, $\mathbf{x}$ is the vector of the unknown gravity anomalies at mean sea level, $\mathbf{e}$ stands for the random observation error of the gradient data and $E\{\cdot\}$ is the statistical expectation operator. σ_0^2 is the a priori variance factor of the gradient data and $\mathbf{Q}$ is their co-factor matrix:

$$\mathbf{B} = [\mathbf{I}_{n'} \quad -\mathbf{I}_{n'}], \quad \mathbf{L} = [\mathbf{L}_1 \quad \mathbf{L}_2]^T \text{ and } \mathbf{w} = -\mathbf{BL}, \quad (6b)$$

where $\mathbf{L}_1$ is a vector of T_{rr} and $\mathbf{L}_2$ is a vector of $\frac{R}{2} \sum_{n=2}^L M_n(r, \psi_0) \Delta g_n(\Omega)$ computed from the EGM at the points where T_{rr} are observed. $\mathbf{I}_{n'}$ is an identity matrix with the size of n' (number of input gradients). In Eq. (6a), σ_1^2 and σ_2^2 are the variance components of satellite gradients and those synthesised from EGM, and $\mathbf{Q}_1$ and $\mathbf{Q}_2$ are their respective co-factor matrices.

Since the system of linear Eqs. (6a) is generally ill-conditioned, applying additional regularisation (beyond discretisation of the surface integral) of the mathematical model

is in our case required for obtaining its stable numerical solution. Here, we consider only Tikhonov's regularisation (parameters with the hat denote LSA estimates):

$$\hat{\mathbf{x}}_{\text{reg}} = \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{w}, \text{ with } \mathbf{N} = \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} + \alpha^2 \mathbf{I}_n \text{ and } \mathbf{C} = \mathbf{B} \mathbf{Q} \mathbf{B}^T \quad (6c)$$

If this estimator is used for estimating values of the unknown gravity anomalies, a bias due to regularisation is introduced in the solution which can be estimated by (Xu et al. 2006):

$$\text{bias}(\hat{\mathbf{x}}_{\text{reg}}) = -\alpha^2 \mathbf{N}^{-1} \mathbf{x}. \quad (6d)$$

The noise VCM of the estimated parameters reads then as follows:

$$\mathbf{C}_{\hat{\mathbf{x}}_{\text{reg}}} = \sigma_0^2 \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1}. \quad (6e)$$

In estimation of the noise VCM, the a posteriori variance factors, and even $\mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1}$, are affected by regularisation and contain the regularisation bias. In the following propositions, the bias of the noise VCM is formulated.

Proposition 1 *The regularisation bias of the estimated noise VCM of the estimated parameters from an ill-conditioned system of linear equations regularised by the Tikhonov method is:*

$$\text{bias}(\mathbf{C}_{\hat{\mathbf{x}}_{\text{reg}}}) = \alpha^2 \mathbf{N}^{-1} (-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1}) \mathbf{C}_{\mathbf{x}}.$$

See Appendix for the proof.

As it can be observed, the bias of the noise VCM of the estimated gravity anomalies depends on the true VCM, which is of course not known. However, the estimated noise VCM in Eq. (6e) can be used to approximate the bias. This regularisation bias is negative because $\mathbf{N}$ is positive-definite with positive diagonal elements so as $\mathbf{C}_{\mathbf{x}}$ and $-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1} < 0$. However, in some cases, the magnitude of the bias may be large so that the diagonal elements of $\mathbf{C}_{\mathbf{x}}$ become negative. In this case, another method must be used for estimating the noise VCM of the solution based on the system with the applied Tikhonov regularisation.

Proposition 2 *The de-biased noise VCM of the de-biased estimated parameters in a system of linear equations regularised by the Tikhonov method is:*

$$\mathbf{C}_{\hat{\mathbf{x}}_{\text{db}}} = \sigma_0^2 \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1} + \alpha^4 \mathbf{N}^{-1} \mathbf{C}_{\mathbf{x}} \mathbf{N}^{-1}.$$

Proof The estimated de-biased parameters are:

$$\hat{\mathbf{x}}_{\text{db}} = \hat{\mathbf{x}}_{\text{reg}} - \text{bias}(\hat{\mathbf{x}}_{\text{reg}}) = \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{w} - \alpha^2 \mathbf{N}^{-1} \mathbf{x}. \quad (7a)$$

Applying the error propagation law for uncorrelated $\mathbf{x}$ and $\mathbf{e}$, the proposition is proved.

The a posteriori variance factor is estimated for an ill-conditioned system of linear equations regularised with the Tikhonov method (Xu et al. 2006) as follows:

$$\hat{\sigma}_{\text{reg}}^2 = \frac{\mathbf{e}_{\text{reg}}^T \mathbf{C}^{-1} \mathbf{e}_{\text{reg}} - \alpha^4 \mathbf{x}^T (\mathbf{N}^{-1} - \alpha^2 \mathbf{N}^{-2}) \mathbf{x}}{n' - u + \alpha^2 \text{trace}(\mathbf{N}^{-2})}. \quad (7b)$$

The second term in the numerator of Eq. (7b) may be larger than the first term leading to a negative variance which is not acceptable. Therefore, the de-biased estimator of the variance factor can be applied (Xu et al. 2006) ($\mathbf{e}_{\text{reg}}$ residual vector of regularised solution.):

$$\hat{\sigma}_{\text{db}}^2 = \frac{(\mathbf{e}_{\text{reg}} + \alpha^2 \mathbf{A} \mathbf{N}^{-1} \mathbf{x})^T \mathbf{C}^{-1} (\mathbf{e}_{\text{reg}} + \alpha^2 \mathbf{A} \mathbf{N}^{-1} \mathbf{x})}{n' - u + \alpha^8 \text{trace}(\mathbf{N}^{-4})}. \quad (7c)$$

Now, by considering the estimated variances, the estimated noise VCM of the estimated parameters are computed by:

$$\hat{\mathbf{C}}_{\hat{\mathbf{x}}} = \mathbf{C}_{\hat{\mathbf{x}}_{\text{reg}}} - \alpha^2 \mathbf{N}^{-1} (-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1}) \mathbf{C}_{\mathbf{x}}, \quad (8a)$$

and in the case of using $\mathbf{C}_{\hat{\mathbf{x}}_{\text{reg}}}$ as an approximation to $\mathbf{C}_{\mathbf{x}}$, one obtains:

$$\hat{\mathbf{C}}_{\hat{\mathbf{x}}} \approx \sigma_0^2 \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1} - \sigma_0^2 \alpha^2 \mathbf{N}^{-1} (-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1}) \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1}. \quad (8b)$$

Therefore, by considering the a posteriori variance factor, the estimated noise VCM reads:

$$\hat{\mathbf{C}}_{\hat{\mathbf{x}}} = \sigma_i^2 \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1} - \sigma_i^2 \alpha^2 \mathbf{N}^{-1} (-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1}) \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1}, \quad i = \text{reg or db}. \quad (8c)$$

Similarly, the de-biased (db) noise VCM of the de-biased estimates considering the a posteriori variance factor reads:

$$\hat{\mathbf{C}}_{\hat{\mathbf{x}}_{\text{db}}} = \sigma_i^2 \mathbf{N}^{-1} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-1} + \sigma_i^2 \alpha^4 \mathbf{N}^{-2} \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A} \mathbf{N}^{-2}, \quad i = \text{reg or db} \quad (8d)$$

The noise VCM of the estimated gravity anomalies derived using Eq. (8d) depends on the a priori variance factor and the method used for its estimation. Both Eqs. (7b) and (7c) are applicable for this purpose. This point is also investigated numerically in this study.

3 Numerical experiments

In this section, the methods introduced in Sec. 2 are applied in the numerical experiments to study the propagation of gradient data errors while solving the discretised integral equations transforming satellite gradient data into gravity anomalies at mean sea level. For illustrative purposes, GOCE radial gradient data serve as an example. However, insights and conclusions obtained by the analyses are also relevant for integral inversion of other second-order gradient data.

We start with a detailed exposition and critical evaluation of the spatial behaviour of the kernel function within the considered integral equation. Subsequently, the test area and GOCE gradient data, along with associated errors, are introduced. The signal-to-noise ratio (SNR) of the gradient data is visually represented and thoroughly discussed. In the final stage of our analysis, we invert satellite gradient data to obtain gravity anomalies at mean sea level, investigating and statistically validating estimated uncertainties and biases.

3.1 Spatial behaviour of the kernel functions

The spatial behaviour of the kernel functions within the surface convolution integral reflects the contribution of gradient data across the entire integration domain. The kernel functions in our integrals are isotropic and exhibit well-behaving spatial characteristics as identified by Eshagh (2011c). Their maximum values are at the computation point and their values decay rapidly to zero as the spherical distance increases. Such attributes allow for greater weighing of gradient data near the computation point (centre of the spherical cap), with gradient data contribution diminishing with their increasing spherical distance from the central point. This characteristic spatial behaviour of kernel functions significantly influences results of the integral equation. It inherently shows the required integration domain and determines the magnitude of the STE associated with the surface integral. This relationship highlights the role of the spatial behaviour of the kernel function in optimising results of the integral equation by balancing the contribution of near- and far-zone gravity anomaly data within the integration domain.

Figure 1 illustrates the spatial behaviour of the kernel function S_{rr} and its modified version S_{rr}^{*L} based on application of the least-squares modification method as proposed by Sjöberg (1984). The modification employs the spherical cap with radius of $\psi_0 = 3$ arc-deg with the maximum modification degree set to $L = 100$ (see Eshagh (2011b)). Both kernel functions behave well in the spatial domain; however, in agreement with our expectations, the modified kernel approaches the zero value beyond the spherical distance of 3 arc-deg. It is important to note that the modification procedure does not account for observation errors in GOCE gradient data. Given the magnitude of EGM errors is small,

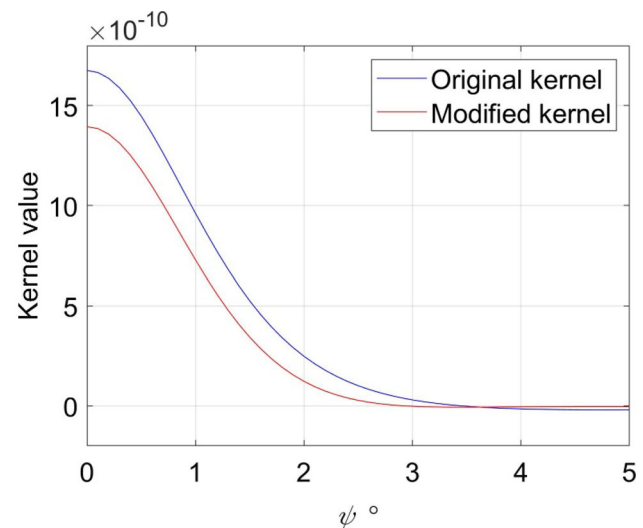


Fig. 1 Spatial behaviour of the original kernel function S_{rr} and its version S_{rr}^{*L} modified by the least-squares method to degree $L = 100$ for radius $\psi_0 = 3$ arc-deg (both are unitless). The horizontal axis represents the geocentric angle ψ (arc-deg)

the spatial behaviour of the modified kernel function remains unchanged, irrelevant of whether errors in the EGM are considered or not.

3.2 GOCE gradient data with reductions and the test area

The test area limited by the latitudes of 35 to 60 arc-deg N, and longitudes of 10 to 40 arc-deg E is selected. GOCE gradients from the product EGG_TRF_2 (EGG-C 2010) from August to September 2013, alongside their corresponding errors, are extracted for the test area with the temporal sampling rate of 10 s. The geodetic reference system GRS80 (Moritz 2000) is used for computing the contribution of the normal gravity field to the observed gradients, facilitating their conversion into the gradients of the disturbing potential (disturbing gradients). Figure 2a and b illustrates the disturbing gradients and their respective observation errors. Satellite disturbing gradients T_{rr} vary between -2 and 1 E (Eotvos = 10^{-9} s^{-2}), with positive values across Central and Southern Europe. Their errors, which do not show any spatial trend, range between 11 and 12 mE.

The ITSG-Grace2018s (Kvas et al. 2019), truncated to degree and order 100, is used as EGM for computation of the long-wavelength disturbing gradients at points where real GOCE gradient data are measured. Figure 3a and b show the long-wavelength disturbing gradients with their associated errors, which show the propagation of the EGM commission errors to the synthesised disturbing gradients. Their spatial patterns are similar, and their magnitudes are of the same order as those shown in Fig. 2a, which illustrates measured

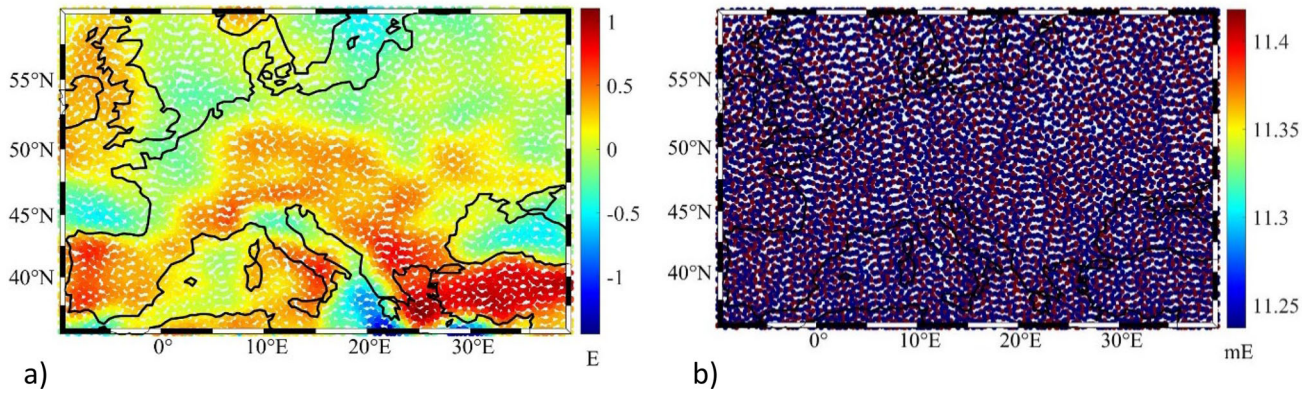


Fig. 2 **a** GOCE-based disturbing gradients T_{rr} , and **b** their errors $\sigma_{T_{rr}}$ (all values in mE)

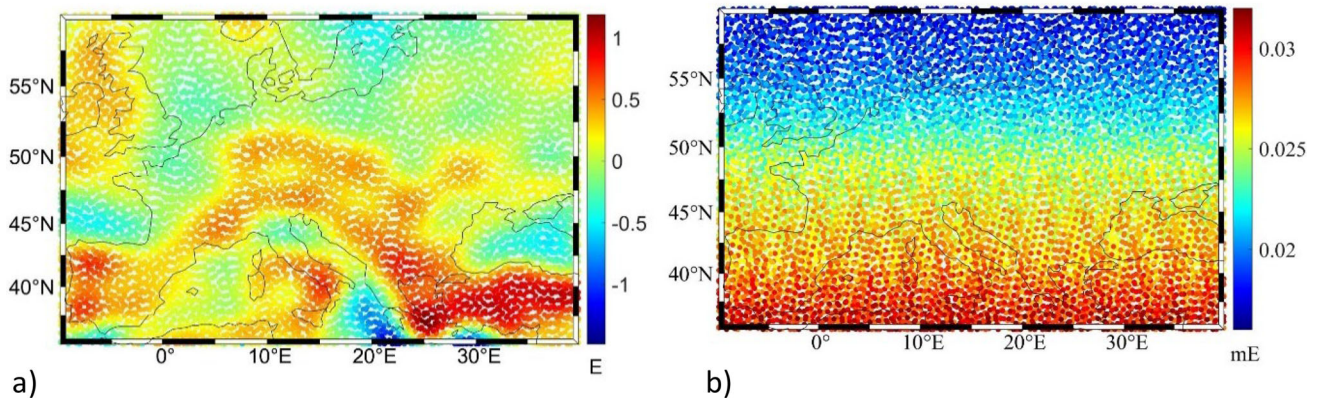


Fig. 3 **a** EGM-based long-wavelength disturbing gradients $\frac{R}{2} \sum_{n=2}^L \Gamma_n(r) \Delta g_n(\Omega)$ for $L = 100$, and **b** their estimated errors $\frac{R}{2} \sqrt{\sum_{n=2}^L \Gamma_n^2(r) \sigma_{\Delta g_n}^2}$ (all values in mE)

GOCE gradients. Thus, a considerable decrease of magnitude is expected when the EGM-based long-wavelength gradients are subtracted from the measured ones. Figure 3b depicts the errors propagated from EGM harmonic coefficients. Larger errors are primarily observed in the southern part of the test area, ranging from 0.016 to 0.032 mE, which are smaller than the observation errors of the measured GOCE data.

Figure 4 depicts truncation errors representing the contribution of gravity data outside the integration cap. Notably, their values are predominantly negative with positive magnitudes in the northeast part of the test area and augmenting in the inverse direction – markedly negative values – towards the southern part of the test area. Nonetheless, the recovery of the regional gravity field using integral equations is sensitive to any change in input data which influences the results. This aspect is further investigated below. As the propagated errors resulting from the truncation effects are close to zero, they are not presented herein.

Figures 5a and 5b represent the reduction of gradient data in the MII method, or the reduced satellite gradients generated using the modification parameters, alongside their errors propagated from the applied EGM. Their values across the

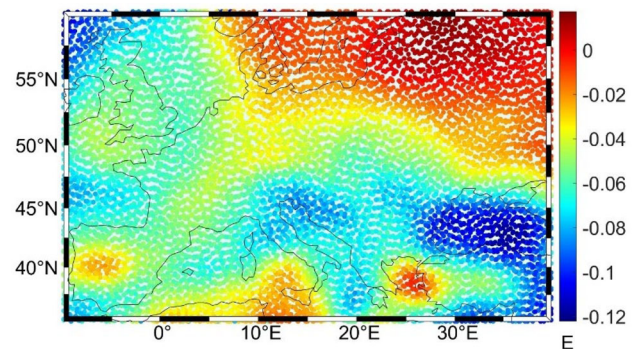


Fig. 4 Truncation errors $\frac{R}{2} \sum_{n=2}^L Q_n(r, \psi_0) \Delta g_n(\Omega)$ for $L = 100$ and $\psi_0 = 3$ arc-deg (units: E)

test area range from -0.15 to 0.04 E, with the estimated mean error of 0.01 mE. Notably, the most significant errors are observed in the southern part of the study area.

By comparing the map of gradients in Figs. 2a, 3a, 4 and 5a, we can see that the gradients generated from EGM have spatial patterns similar to those of measured gradients. This is expected because the gradients computed by the mentioned

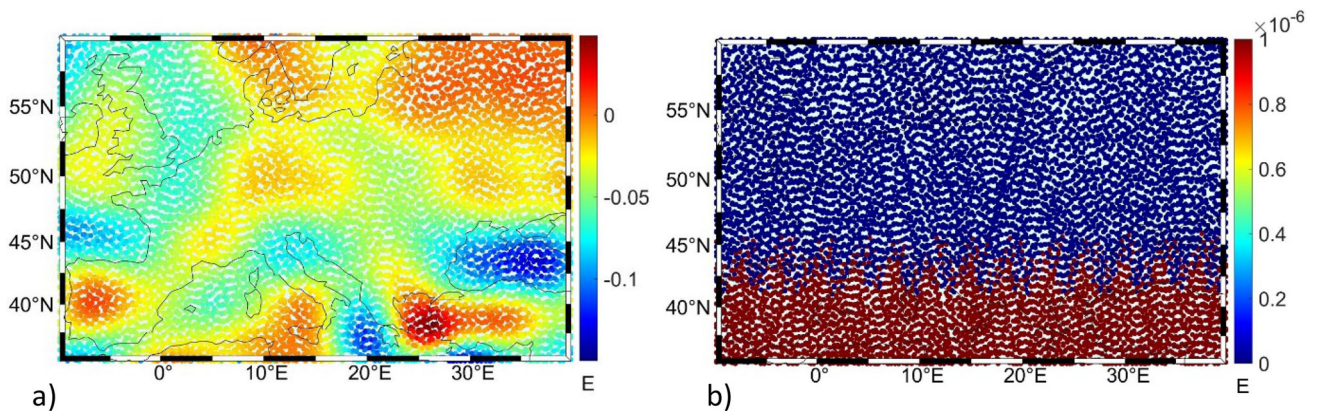


Fig. 5 **a** Reduction to T_{rr} generated using modification parameters $\frac{R}{2} \sum_{n=2}^L s_n(r) \Delta g_n(\Omega)$, and **b** its estimated errors $\frac{R}{2} \sqrt{\sum_{n=2}^L s_n^2(r, \psi_0) \sigma_{\Delta g_n}^2}$ for $L = 100$ (all values in E)

formulas are essentially a sort of measured gradients. This also ensures that the reduction is effective.

Generally, the largest and smallest reductions are observed in the RCR and TR methods, respectively. Consequently, it is expected that the respective systems of linear equations, even with the same coefficient matrix, will require different regularisation parameters. This aspect is also discussed later.

Regarding EGM errors propagated to the reductions in the RCR and TR methods, two main factors influence their magnitudes:

- Errors of EGM coefficients used to compute errors of synthesised long-wavelength gravity anomalies. In this study, the same EGM is used for all three modification methods which apply reductions of satellite gradients. Since errors of EGM coefficients are rather small, errors propagated to the reductions will also be small.
- Different mathematical models used for evaluation of the reductions are the primary reason for providing solutions with different noise levels.

From Figs. 2b, 3b, 4 and 5b, we can conclude that the errors of the reductions are significantly smaller than the observation noise of the GOCE gradient data. Consequently, errors of the reduced gradients do not substantially differ from each other. SNRs of the GOCE gradient data and their reductions for the RCR, TR and MII methods are analysed in the next section.

For estimating errors of estimated gravity anomalies from EGM, used in computing reductions, we do not consider the noise covariances of the EGM coefficients. This does not affect our numerical experiments as the same errors for gradient data were used consistently across all three modifications of the integral equation.

3.3 Signal-to-noise ratios of the reduced gradient data

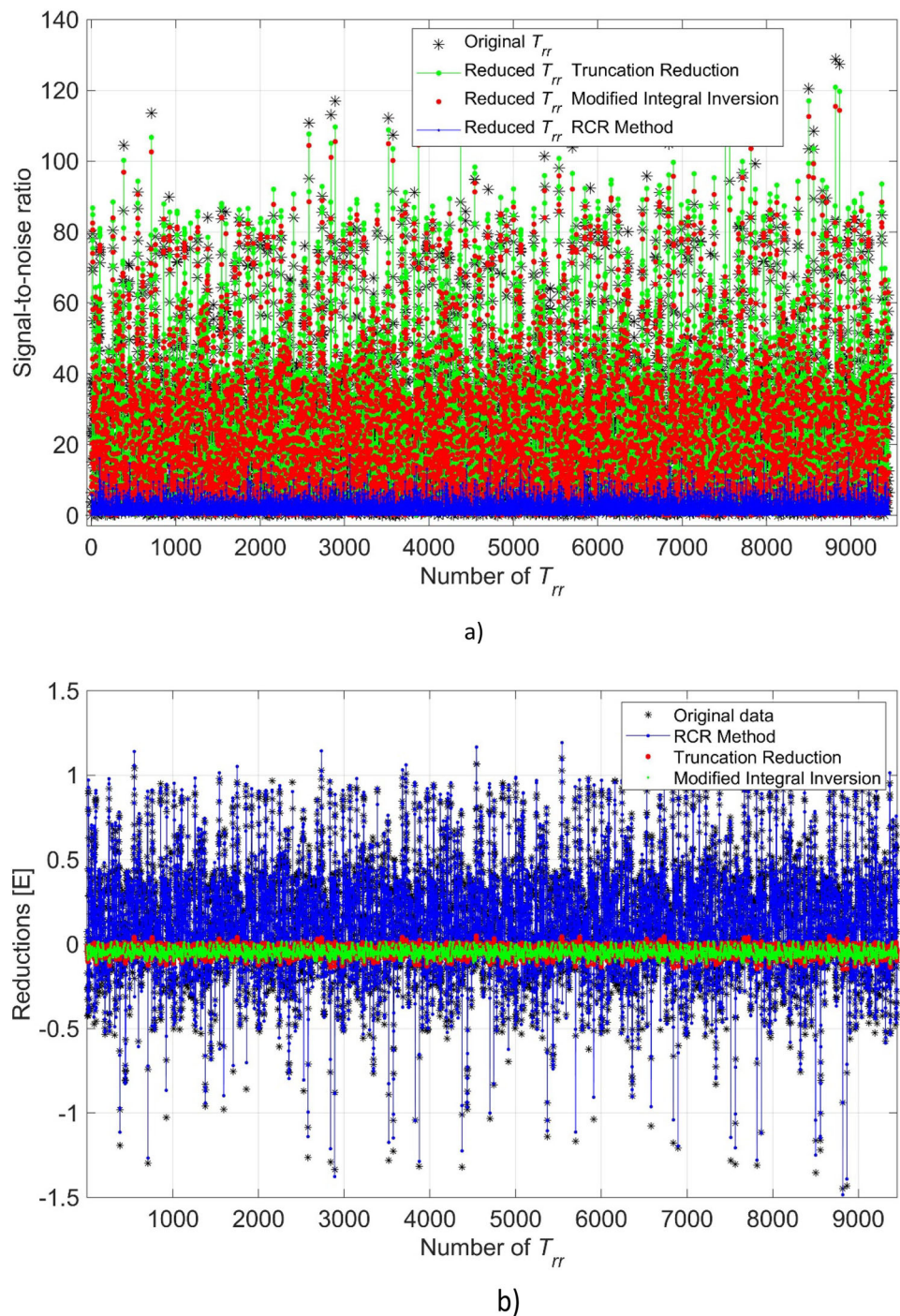
The system of linear equations based on discretised Fredholm's integral equations is ill-conditioned. As described in Secs. 2.1–2.3 concerning the RCR, TR and MII methods, the effect of the long-wavelength component of the gradient data is either considered or mitigated in satellite gradient data. This mitigation precipitates two primary issues: firstly, an increase of the noise level of the reduced gradient data and, secondly, a reduction of magnitude of the gradient data. This section discusses relative errors defined as signal-to-noise ratios (SNRs) of the reduced gradient data. The SNR is defined as follows:

$$\frac{\text{signal}}{\text{noise}} = \frac{\left| T_{rr}(r, \Omega) - \frac{R}{2} \sum_{n=2}^L M_n(r) \Delta g_n(\Omega) \right|}{\sqrt{\sigma_{T_{rr}}^2 + \frac{R^2}{4} \sum_{n=2}^L M_n^2(r) \sigma_{\Delta g_n}^2}}. \quad (9a)$$

Figure 6a depicts the SNRs for the gradient data reduced by the RCR, TR and MII methods as applied to satellite gradient data along real GOCE orbits over the test area. According to Fig. 6a, the SNR of the original GOCE gradient data is the highest, as expected since no reduction is applied. The TR method, having the smallest reduction effect compared to other methods, also has an extremely small uncertainty, resulting in the SNR value close to that of the original GOCE gradients. Although the reduction uncertainty in the RCR method is the largest among all three considered methods, it is still significantly smaller than the noise of the original GOCE gradients. Therefore, the smaller SNR in the RCR method is primarily due to the reduction of the gradient data.

We have already shown that the MII method has a slightly larger reduction than the TR method, but its uncertainty is larger than that in the TR method. For better clarity, values of all three reductions are presented in Fig. 6b. As shown, the RCR reduction is the largest compared to the TR and MII

Fig. 6 **a** SNRs of the reduced gradients over the test area, and **b** reductions computed in the RCR, TR and MII methods; original gradients are also plotted for comparison (note that in the DIR method, no reduction of the gradient data is applied)



reductions, with the TR method having the smallest reduction effect.

The statistics of the reductions in the TR, MII and RCR methods as well as the SNR of the original satellite gradients and gradients reduced by the three methods are presented in Table 1. The smallest SNR value is associated with the RCR method, while the largest is with the TR method. STDs of the SNRs in the TR and MII methods are closer to that of the original gradient data, indicating that the reductions have

not significantly altered the deviation from the mean SNR. However, the mean SNR value in the MII method is closer to that of the original gradients, suggesting that the result of the inversion of the original gradients and gradients reduced by the MII method should be closer when regularisation is applied.

Values of the gradient reductions computed over the test area by the RCR method are approximately one order of

Table 1 Statistics of gradient reductions computed by the TR, MII and RCR methods, and SNR of the original gradients and gradients reduced by the three methods

Reduction method	Max	Mean	Min	STD
TR	0.02	− 0.05	− 0.12	0.03
MI	0.05	− 0.04	0.15	0.03
RCR	1.19	0.12	− 1.48	0.30
SNR				
Original gradients	128.8	22.3	0.0	19.1
Gradients reduced by the TR method	120.9	24.2	0.0	20.1
Gradients reduced by the MI method	115.5	22.9	0.0	19.1
Gradient reduced by the RCR method	17.5	2.4	0.0	2.1

magnitude larger than those of the other two reduction methods. These statistics support the conclusion of the significant reduction of the gradient data in the RCR method, as observed in Figs. 6a and 6b.

3.4 Inversion of the reduced gradient data

To address challenges posed by solving the ill-conditioned system of linear equations, this study employs Tikhonov's regularisation method (Tikhonov 1963; Tikhonov and Arsenin 1977), wherein the regularisation parameter is determined using the L-curve criterion (Hansen 1998 and 2007). This approach is known for its simplicity and efficiency. Essentially, it aims at minimising the L2-norm of the estimated residuals, and the product of the estimates with a small positive scalar parameter, known as the regularisation parameter. In its most elementary form, Tikhonov's regularisation involves the addition of a small positive value to each diagonal element of the coefficient matrix of the normal equations to enhance the numerical stability of its inversion. A noteworthy attribute of this regularisation technique is its linearity, which facilitates the comparison of algebraic equations it generates with that employed in the least-squares adjustment method dominantly used in geodesy.

In this section, we introduce qualitative metrics for assessing surface gravity anomalies estimated from satellite gradient data, utilising the three modifications of the integral equation. This assessment aims at the efficiency and precision of the modification methods used for processing satellite gradient data.

3.4.1 Estimation of the a posteriori variance factor

The a posteriori variance factor is indispensable for uncertainty estimation based on least-squares methods. Based on the analysis of the estimated residuals, this parameter serves as an authoritative indicator of error estimates based on the least-squares adjustment. Ideally, given a stable system of linear equations, rigorous mathematical modelling, and realistically predicted data uncertainties, the a posteriori variance

factor should be equal to one. Nevertheless, our system of linear equations significantly differs from this ideal case.

As the system of linear equations for our problem is generally ill-conditioned, the application of regularisation techniques for its solution is required. Additionally, the mathematical model is obtained by discretising the surface integral, introducing complexity related to the spatial resolution and spherical approximation of mean sea level. Another consideration must be given to validation of assumed gradient data errors against estimated residuals, despite the presumed reliability of GOCE gradient data and their associated errors.

It is important to note that, within the framework of the conventional least-squares adjustment, the selection of an a priori variance factor does not affect estimated values of the unknown parameters. Conversely, in the context of ill-conditioned systems of linear equations, addressed herein by Tikhonov's regularisation, the choice of the a priori variance factor significantly influences the estimation of the regularisation parameter. This intricacy underscores a nuanced interplay between the model conditionality, data uncertainty, and the regularisation approach in the quest for a stable numerical solution.

In this section, we examine the estimated a posteriori variance factor in various scenarios. Initially, it is estimated using the same formula employed for the ordinary least-squares problem i.e. as the L2-norm of the residuals normalised by the degree of freedom of the mathematical model. In the second case, the unbiased estimation of the variance factor is applied, and later, the unbiased estimation of the variance factor based on the de-biased residuals is used. The primary objective of using the four methods is to evaluate how regularisation of the mathematical model influences the a posteriori variance factor and uncertainty estimation.

Table 2 presents the a posteriori variance factor estimates, derived through the application of explained variance factor estimators using the four methods. The a posteriori variance factor, unadjusted for regularisation, $\hat{\sigma}_0^2$, is 2.8 for both the RCR and TR methods, and slightly smaller at 2.7 for the MI method. Given that both $\hat{\sigma}_{\text{reg}}^2$ and $\hat{\sigma}_{\text{db}}^2$ require the a priori knowledge of the unknown values, this analysis utilises

Table 2 Estimated (a posteriori) variance factors $\hat{\sigma}_0^2$ without applying any regularisation, $\hat{\sigma}_{\text{reg}}^2$ estimated for the regularised system of linear equations, and $\hat{\sigma}_{\text{db}}^2$ for the de-biased estimates. $\hat{\Delta g}$ and $\hat{\Delta g}_{\text{db}}$ mean that both solutions are used as true values in estimating the a posteriori variance factors. α^2 is the estimated value of the regularisation parameter

Method	DIR		RCR		TR		MII	
$\alpha^2 \times 10^{-4}$	8.3		32		7.4		8.2	
Variance	$\hat{\Delta g}$	$\hat{\Delta g}_{\text{db}}$	$\hat{\Delta g}$	$\hat{\Delta g}_{\text{db}}$	$\hat{\Delta g}$	$\hat{\Delta g}_{\text{db}}$	$\hat{\Delta g}$	$\hat{\Delta g}_{\text{db}}$
$\hat{\sigma}_0^2$	2.8	2.8	2.8	2.8	2.8	2.8	2.7	2.7
$\hat{\sigma}_{\text{reg}}^2 \times 10^3$	2.3	2.3	8.5	8.4	2.2	2.1	2.2	2.2
$\hat{\sigma}_{\text{db}}^2$	1.4	1.3	1.3	1.3	1.4	1.4	1.3	1.3

both the estimated gravity anomalies $\hat{\Delta g}$ and the de-biased (db) gravity anomalies $\hat{\Delta g}_{\text{db}}$ used for their computation. The variance factor estimates exhibit marginal variation when assessed through $\hat{\Delta g}$ and $\hat{\Delta g}_{\text{db}}$, suggesting that this metric is suitable for the purpose of the variance estimation. Notwithstanding, the magnitude of the second term in Eq. (8b) is significantly reduced in comparison to the other variances, a notable discrepancy that does not render the variance negative. This reduction is attributed to the influence of the second term within the estimator, which diminishes the norm of the residual vector, albeit insufficiently to invert the sign of the variance. Despite this, the de-biased variance factor, Eq. (7b), is appropriately close to one. Consequently, in the progressive phases of our investigations, this a posteriori variance factor is selected to scale the estimated noise VCM of the estimated parameter.

Table 2 shows the regularisation parameter α^2 estimated by the L-curve method which can provide some information about the solved systems of linear equations. Since they are ill-conditioned, any minor change in observed gradients can lead to large changes in estimated values of the surface gravity anomaly. It should be noted that the DIR, RCR and TR methods have the same coefficient matrix of normal equations. Therefore, any change in the solution is solely due to the reductions applied to the gradient data. As Table 2 shows, for the DIR method, which uses the measured gradients without any reduction, α^2 came out 8.3×10^{-4} which is relatively small. This value is even smaller for the TR method; however, it is one order of magnitude larger for the RCR method. It can be expected, as its reduction is significantly larger than for the rest of the methods, that the system of linear equations needs to be more regularised to get a stable solution despite having the same coefficient matrix as the DIR and TR methods. The value of α^2 is slightly smaller than the one estimated by the DIR method; however, in this case, both the coefficients matrix and gradients are reduced. The condition number of the coefficient matrix of the MII method is 5.1×10^{-9} while in the rest of the methods it is 5.3×10^{-9} i.e. slightly larger meaning that the system of linear equations obtained after

discretisation of the modified integral equation is somewhat more stable.

3.4.2 Estimated uncertainties of the estimated gravity anomalies

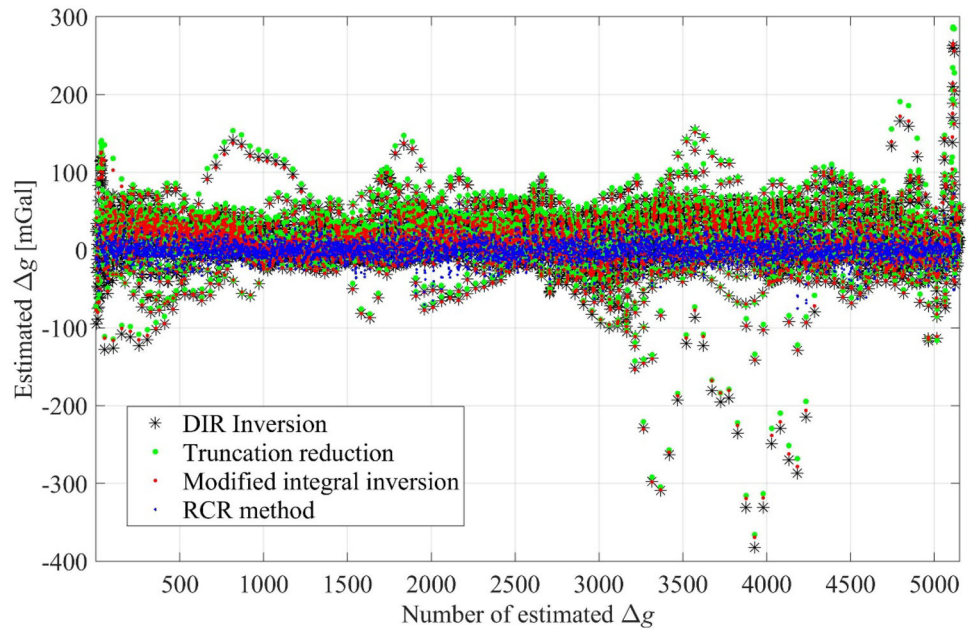
In this section, we present the estimated gravity anomalies employing the DIR, RCR, TR and MII methods. Our focus is primarily on surface gravity anomalies estimated directly from the system of linear equations based on the discretised integral equations, deliberately neglecting STE and restoring the long-wavelength component of the estimated gravity anomaly from EGM.

Figure 7a illustrates gravity anomalies estimated at mean sea level using discretised and regularised integral equations. Gravity anomalies estimated by the DIR, TR and MII methods exhibit a notable agreement. Conversely, the integral inversion of the reduced gradients in the RCR method yields attenuated surface gravity anomalies that can be attributed to removal of the long-wavelength component from the input gradient data. Hence, the estimated surface gravity anomalies represent only residual gravity anomalies that predominantly correspond to degrees above 100.

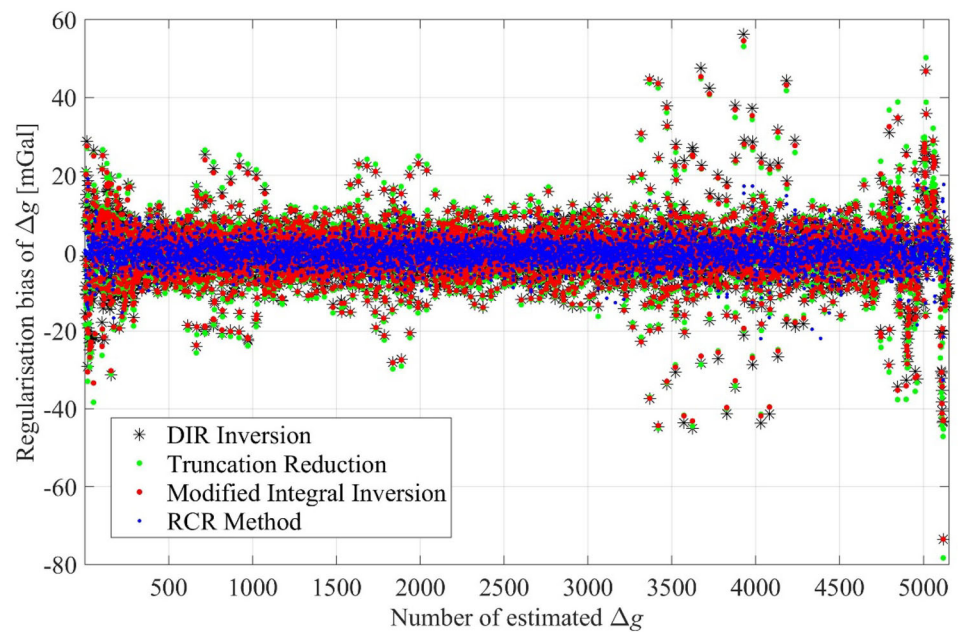
Figure 7b shows the estimated regularisation bias associated with the estimated gravity anomalies. The assessment of this bias requires the knowledge of the true gravity anomalies. The gravity anomalies, estimated by the systems of linear equations, are only their approximation. Figure 7b reveals that, in the context of STE, values of the bias range between -80 and 60 mGal. Once again, smaller values of the bias are detected in the RCR method; however, this reduction stems from the application of the residual gravity anomalies, which inherently have smaller magnitudes than their full values in context of the bias estimation.

Figure 7c presents the estimated uncertainties of the gravity anomalies, calculated using the de-biased a posteriori variance factor. The presence of the larger uncertainties in the gravity anomalies recovered over marginal areas introduced notable spikes within the plot and the trend is visible

Fig. 7 **a** Estimated surface gravity anomalies, **b** estimated regularisation bias, **c** estimated errors of the estimated surface gravity anomalies, and **d** de-biased errors of the estimated surface gravity anomalies (all values in mGal)



a)

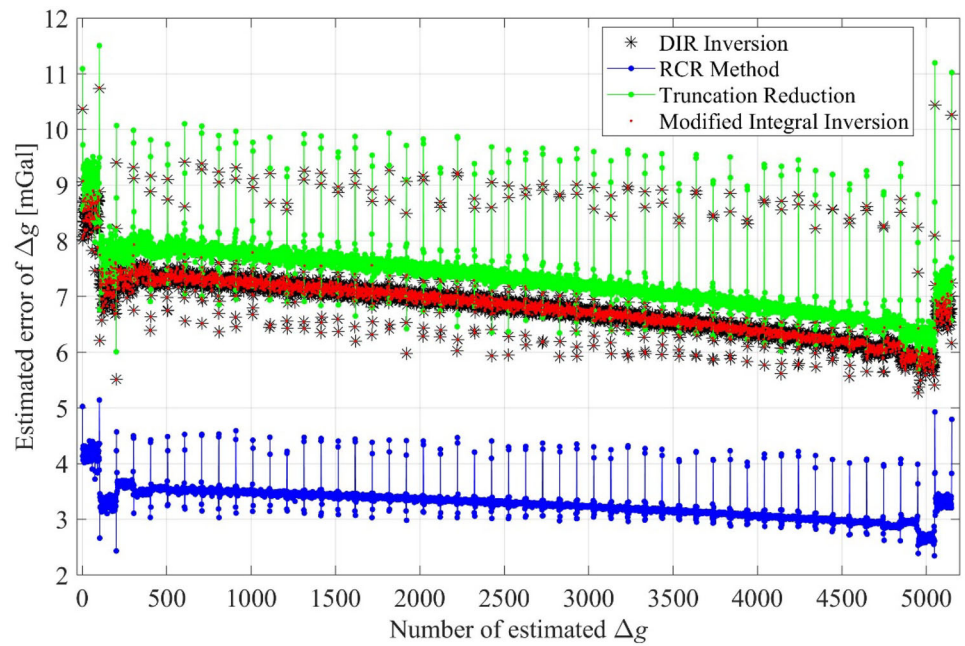


b)

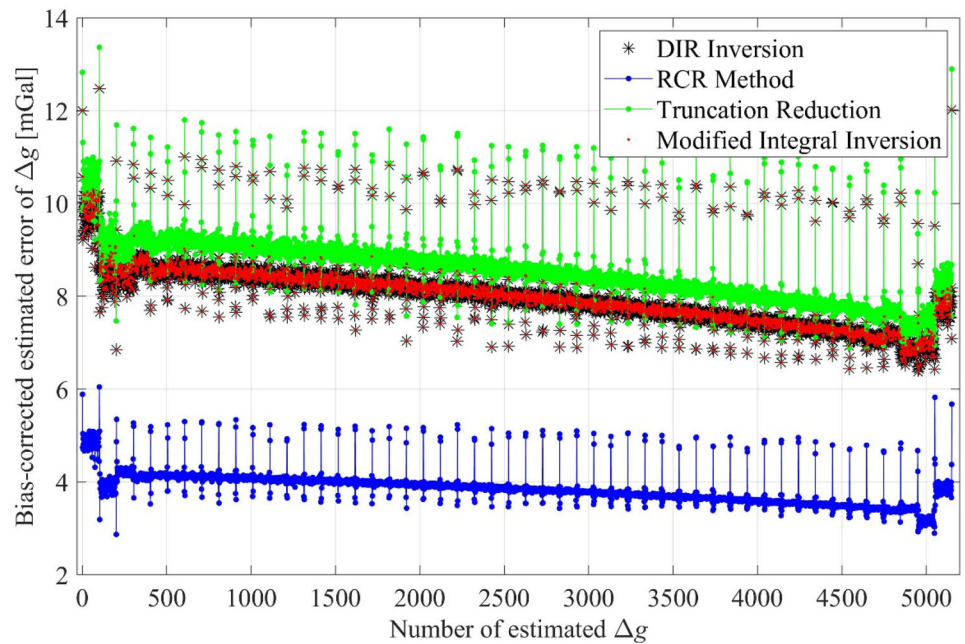
from the error assessment. For instance, uncertainties associated with the RCR method range from 3.0 to 3.5 mGal, while those based on the TR method vary between 6 and 8 mGal, and errors based on the MII method range between 5.5 and 7.5 mGal, i.e. in the same order of magnitude as in the DIR method. It is critical to recognise that relatively smaller uncertainties, identified for gravity anomalies estimated by the RCR method, are due to the omission of the long-wavelength

component of the GOCE gradients. This suggests that errors are likely to increase if the long-wavelength contributions are restored. However, the question is how significant this really is. Consider that (a) the error in the observed gradients is around 11 mE, while the long wavelengths below $L = 100$ contribute only 0.03 mE (just 0.3% of the total error), and (b) the formal and empirical errors of estimated gravity anomalies derived by RCR method are approximately

Fig. 7 continued



c)



d)

4 and 8 mGal, respectively, while the ITSG errors contribute just 0.006 mGal (about 0.1% of the total signal) to the gravity anomaly up to $L = 100$. However, in the DIR, RT and MII methods, there is no need to restore the long-wavelength portion of the gravity anomaly.

The coefficient matrices of the system of linear equations obtained by discretisation of the integral equations are the same across all methods, except for the MII method for which

it slightly differs. Applying the error propagation law for estimating the noise VCM of the estimated parameters, the uncertainty pattern arises directly from the structure of $\mathbf{C}_x$ which does not depend on any reduction. The role of the a posteriori variance factors are to scale the noise VCMs, but they do not alter their structures.

In our study, the uncertainties of the EGM, used for computing the reductions and restoring the long wavelengths,

are very small (relative to errors of the measured gradients). This is the main reason why these uncertainties do not significantly influence the propagation of uncertainties for the reduced GOCE data. Obviously, if an EGM with larger uncertainties is applied, results would differ. However, the primary assumption in the RCR method is that a significant part of the signal is known, resulting in residual gradients that are relatively small and closer to the noise level. This is one of the main challenges when applying the RCR method. When the system of equations is ill-conditioned, the SNR of gradient data plays more significant role in stabilising the solution of the system of linear equations. This causes that a larger regularisation parameter is estimated, and this affects the propagation of uncertainty through the inversion process.

Figure 7d depicts values of the de-biased error, which are noticeably larger due to re-inclusion of the estimated uncertainties of gravity anomalies after the elimination of the regularisation bias. In this context, errors associated with the RCR method vary from 3 to 4 mGal, errors of the TR method range from 7 to 9 mGal, and errors of the MII method range between 7 and 8.5 mGal as in the DIR inversion method.

Table 3 shows different types of errors (see the caption of the table). Smaller average errors are observed for the RCR method, but it should be emphasised that they are specifically related to the residual gradient data limited spectrally by the degree 100. The errors are smaller for the MII method than for the TR method. The three types of relative uncertainties are also presented in Table 3. The symbol $|\cdot|$ represents the absolute value. The uncertainties are relatively close to each other for the TR and MII methods, while they are more than 5% larger for the RCR method, because the residual gradients have smaller magnitudes than the full signal. However, since the uncertainties of GOCE gradient data are dominant comparing to their reduced values evaluated in the three methods, the larger uncertainty of reduction in the RCR method cannot be the main reason of the larger relative uncertainty.

3.4.3 Comparison of estimated surface gravity anomalies with reference (EGM-based) values

To evaluate our results, we employed the model WHU-SWPU-GOGR2022S (Zhao et al. 2023), the satellite-only EGM calculated to degree and order 300. Throughout this study, this EGM is referred to as WHU. Although the construction of WHU utilised data from both GRACE and GOCE satellite missions, it is imperative to recognise that our results cannot be deemed completely independent thereof. This limitation arises from the use of the GRACE-based EGM in the RCR method to diminish the effect of the GOCE data, given that both datasets contributed to estimation of WHU. Similarly, the truncation errors in the TR and MII methods were determined using the GRACE-based EGM, with the degree

variance of the same EGM being used to calculate the modification parameters and the errors associated with the reduction of the gradient data. Furthermore, satellite gradient data constitute the primary data source for all three methods that apply reductions.

The model ITSG-GRACE2018s (Kvas et al. 2019), the GRACE-only EGM limited to degree and order 200, is denoted as ITSG within this study. ITSG serves for evaluation of errors introduced by reducing satellite gradients up to degree 100. Within the context of the MII method, the corresponding degree of ITSG is applied to amend the integral formula.

Given that WHU is postulated to represent well the gravitational field in the test area, and ITSG is utilised for reducing the long-wavelength component of satellite gradients (and restoring the same component in the estimated surface gravity anomalies), it becomes imperative to examine their discrepancies. Figure 8a shows the signal and error degree variances of the two EGMs. Their signal patterns are nearly identical, with the error spectra having comparable magnitudes. Furthermore, Fig. 8a depicts the signal and error degree variances for WHU up to degree 300. It is evident that beyond degree 280, the error spectrum surpasses the signal spectrum in magnitude. This implies that the resolution of WHU is effective only up to degree 280, beyond which the information is statistically irrelevant.

To show the differences between the two EGMs, spherical harmonic coefficients of ITSG are subtracted from those of WHU, followed by the calculation of the harmonic spectrum of the differences. The corresponding error spectrum is derived by applying the error propagation law to the differences between the spherical harmonic coefficients. The results shown in Fig. 8b indicate that the spectrum of the differences exceed that of the propagated errors, suggesting that the differences between the two EGMs are statistically significant. This may be attributed either to considerable differences in the coefficients themselves or to unrealistic errors of the coefficients.

In evaluating the differences between ITSG and WHU, the gravity anomalies across the test area are computed from their differences. Figure 9a shows gravity anomalies derived from the differences, while Fig. 9b displays uncertainties associated with the differences, which are notably small. Consequently, despite the statistical significance of the differences, they are practically negligible at the level of gravity anomalies. Hence, it can be deduced that for low degrees (below 100), the two EGMs are identical in practical applications concerning gravity anomalies.

Since the RCR method removes the long-wavelength component from satellite gradients (utilising ITSG up to degree 100), the objective of inverting the reduced gradient data is to restore residual surface gravity anomalies with frequencies

Table 3 Average value of the estimated error ($\hat{\sigma}_{\Delta g}$), estimated

Method/parameter	DIR	RCR	TR	MII	
de-biased error $\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)_{\text{db}}$,	$\widehat{\sigma}_{\widehat{\Delta g}}$	6.9	3.3	7.3	6.8
removed bias error	$\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)_{\text{db}}$	8.1	3.8	8.6	8.0
$\widehat{\sigma}_{\widehat{\Delta g}} - \text{bias}\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)$, absolute value	$\widehat{\sigma}_{\widehat{\Delta g}} - \text{bias}\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)$	9.0	4.3	9.6	8.9
of the regularisation bias					
$ \text{bias}(\widehat{\Delta g}) $, and RMS($\widehat{\Delta g}$)– all	$ \text{bias}(\widehat{\Delta g}) $	4.8	2.4	5.1	4.6
values in mGal, and ratio of the	RMS($\widehat{\Delta g}$)	9.1	4.3	9.6	9.0
estimated error and estimated					
gravity anomaly $\frac{\widehat{\sigma}_{\widehat{\Delta g}}}{ \widehat{\Delta g} }$, estimated	$\frac{\widehat{\sigma}_{\widehat{\Delta g}}}{ \widehat{\Delta g} } [\%]$	27.4	34.1	26.8	27.4
de-biased error and					
bias-corrected gravity anomaly,	$\frac{\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)_{\text{db}}}{ \widehat{\Delta g} - \text{bias}(\widehat{\Delta g}) } [\%]$	29.8	34.5	29.3	29.7
$\frac{\left(\widehat{\sigma}_{\widehat{\Delta g}}\right)_{\text{db}}}{ \widehat{\Delta g} - \text{bias}(\widehat{\Delta g}) }$, and the ratio of	$\frac{\text{RMS}(\widehat{\Delta g})}{ \widehat{\Delta g} - \text{bias}(\widehat{\Delta g}) } [\%]$	33.7	39.0	32.8	33.5
RMS and estimated de-biased					
gravity anomaly $\frac{\text{RMS}(\widehat{\Delta g})}{ \widehat{\Delta g} - \text{bias}(\widehat{\Delta g}) }$					
(in %)					

beyond degree 100. Consequently, for a more refined comparison of the RCR method, we estimate the gravity anomalies over the degree band of 100 to 300 using WHU; they are shown in Fig. 10c. Their values exhibit large fluctuations, descending to -100 mGal in some parts of the test area and ascending to 80 mGal in others.

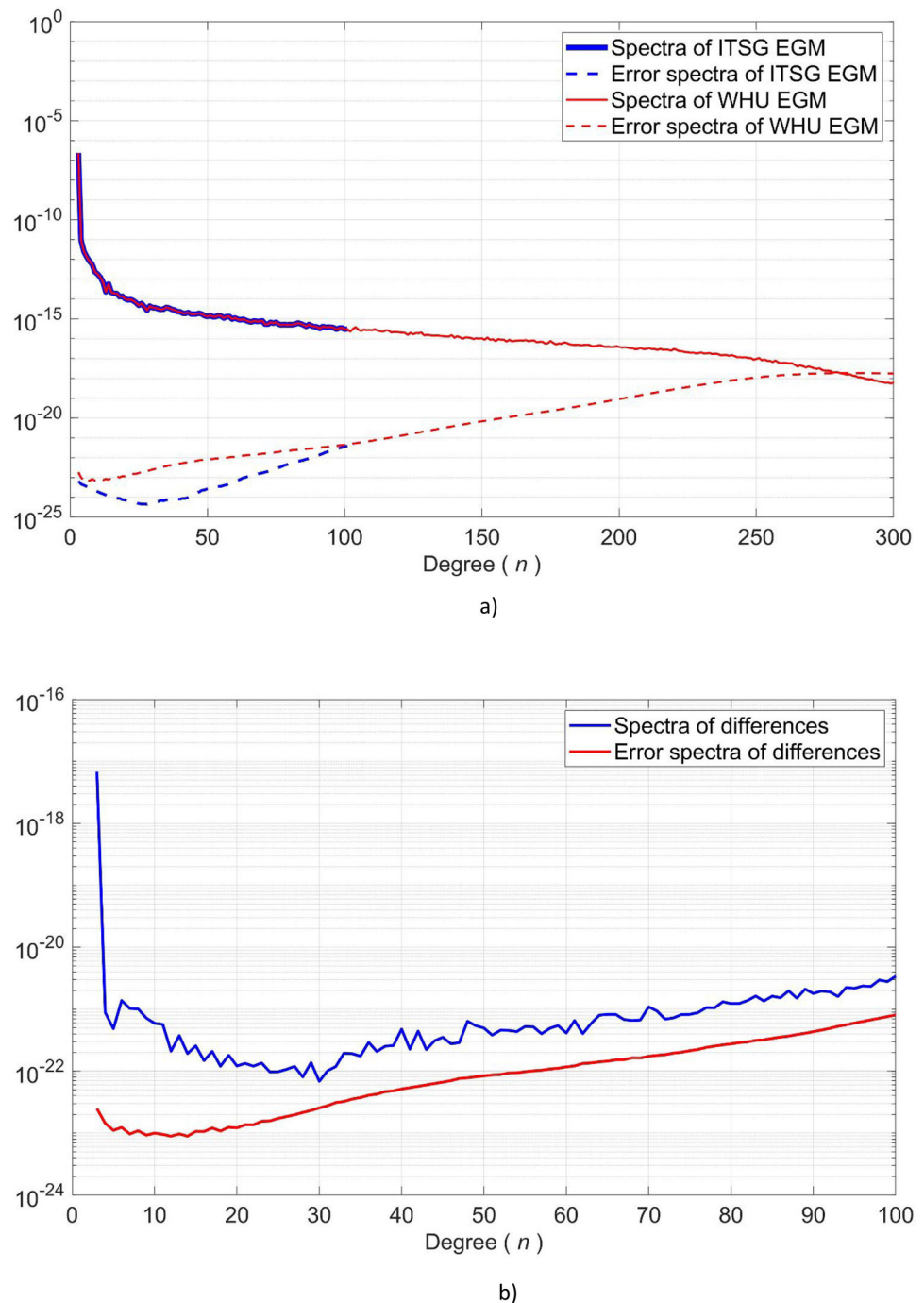
In the RCR method, long-wavelength gravity anomalies must be restored into the estimated residual surface gravity anomalies. This means that the long-wavelength component of the gradient data (employing ITSG up to degree 100) is removed from satellite gradients. This long-wavelength component must be restored into the estimated surface gravity anomalies. As the long-wavelength component of the gradient data is substantial, it contributes significantly to the estimated gravity anomalies. This procedure results in the solution that is more aligned with the gravity anomalies estimated directly using ITSG. Figure 10d shows errors of the surface gravity anomalies synthesised from WHU up to degree and order 300. Their values range up to approximately 2 mGal over the test area, with errors predominantly originating from the higher degrees, where the uncertainties increase simultaneously; refer to Fig. 8a.

Table 4 presents statistics of the degree-limited gravity anomalies derived from ITSG and WHU, specifically WHU for the degree band of 100 – 300 , and delineates differences among surface gravity anomalies estimated using the DIR, RCR, TR, and MII methods. Both EGMs provide surface gravity anomalies with the mean value of approximately 11 mGal across the test area. Nonetheless, the mean value approaches zero when employing WHU limited to the degree band of 100 – 300 . Given the sensitivity of the integral equations to STE, we present gravity anomalies under two scenarios, considering STE for the 3 and 5 arc-deg cap radii.

Statistics of the differences between the estimated gravity anomalies and their counterparts from WHU, considered as a reference for evaluating the performance of the methods, are presented in Table 4. The goal of this study is not to determine which method performs better but to assess how realistic are the errors they provide. Two sets of statistics are presented for the surface gravity anomalies estimated by each method; those in parentheses relate to the de-biased estimated gravity anomalies. The long-wavelength signal, applied for reduction of the satellite gradients by the ITSG model, is restored in the estimated surface gravity anomalies before comparison with the reference WHU-based gravity anomalies. According to Table 4, de-biasing increases statistics of the differences for the RCR method, unlike the other methods. This may be caused by the fact that the residual gravity anomalies require a larger value of the regularisation parameter to stabilise the solution to the system of linear equations.

The RMS of the differences for the DIR method is 9.1 mGal. When the de-biased gravity anomalies are considered, the respective RMS is 8.4 mGal. For surface gravity anomalies estimated by the RCR method, the RMS of the differences is 7.9 mGal. Increasing the radius of the spherical cap to 5 arc-deg does not significantly affect the results. The TR method results in the RMS of approximately 11.1 mGal, while increasing the spherical cap has only a marginal effect. The larger mean value of the differences may be due to the long-wavelength truncation errors over the test area. Reducing the truncation error is mainly effective for mitigating the effect of the far-zone gravity anomalies not included in spatially limited integration. Eshagh (2011b) noted that for integral inversion, the effect of gravity data outside the integration domain should be computed using EGM based on integration. The MII method results in the RMS of 8.3 mGal

Fig. 8 **a** Signal and error spectra of the ITSG and WHU models to degree 300, **b** signal and error spectra of the differences between ITSG and WHU



for the spherical cap of 3 arc-deg that slightly decreases to 8.2 mGal when the spherical cap extends to 5 arc-deg.

As shown in Table 4, the residual surface gravity anomaly, limited to the degree band of 100–300, has the mean value of 0.1 mGal over the test area, while the gravity anomaly limited by degree 300 has the mean value of 10.9 mGal. This indicates that the long-wavelength component of the gravity anomaly significantly contributes to their mean value.

Among the surface gravity anomalies recovered from satellite gradients, the residual gravity anomaly obtained by the discretised integral equation in the RCR method has the smallest mean value of the differences with WHU. However, this does not imply that the reduced satellite gradients in the RCR method have a smaller bias or are superior to other methods; rather, the residual satellite gradients lacking the long-wavelength component do not contribute to the

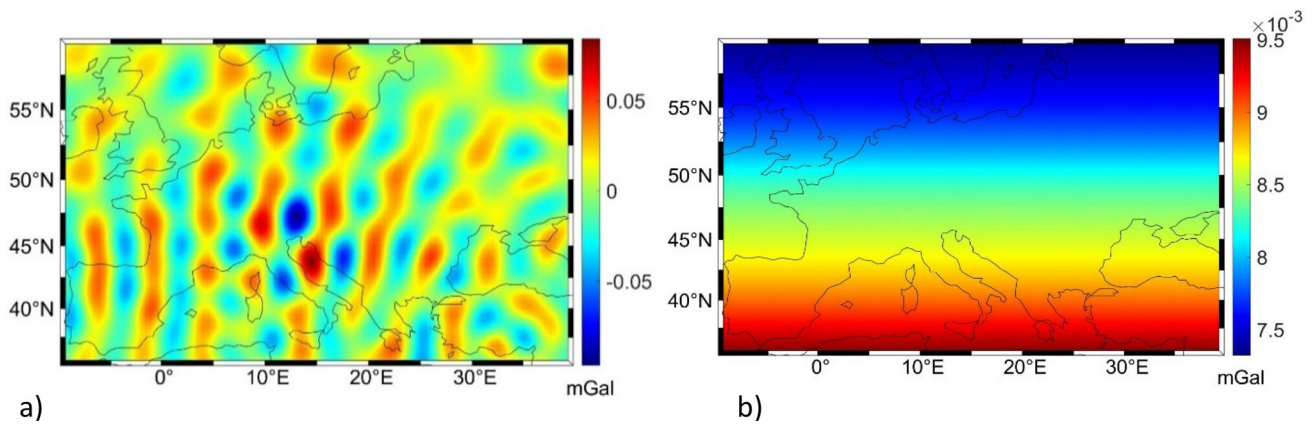


Fig. 9 **a** Δg computed using differences between ITSG and WHU, and **b** their uncertainties (mGal)

mean value of the surface gravity anomaly. After restoring the long-wavelength component in the estimated surface gravity anomaly, its mean value is closer to values synthesised from WHU. In contrast, other methods considered in this study recover the long-wavelength component of the gravity anomaly directly through integral inversion, resulting in nonzero mean value differences. Recovering long wavelengths of the surface gravity anomaly requires satellite gradient data with global or much larger integration area than used in our study.

Results obtained by the DIR and MII methods are similar. The mean difference with respect to the reference WHU-based gravity anomaly is 2.7 mGal for the MII method, 0.3 mGal smaller than that of the DIR method, although their RMS values remain the same. Considering the larger integration area (spherical cap of 5 arc-deg) slightly reduces values of RMS.

In this study, the maximum degree of the EGM used for modification of the surface integral and reduction of gradient data is 100. Increasing this degree increases the EGM contribution to the solution. The RCR method performs better than the TR method (Pitoňák et al. 2016) due to the higher degree of reduction. In this case, the significant part of the gradient data is removed, i.e. smaller residuals are used in solving the integral equation followed by restoring a significant long-wavelength component of the estimated gravity anomalies. This means that the contribution of the inverted residual gradients to the estimated surface gravity anomaly is relatively small.

3.5 Statistical analyses

To enhance the visual representation of estimated uncertainties, normalised differences defined as ratios of the differences between the gravity anomalies estimated by each method and their reference values calculated using WHU

alongside their propagated errors, are computed as follows:

$$\frac{w}{\sigma_w} = \frac{\hat{\Delta g} - \Delta g}{\sqrt{\hat{\sigma}_{\Delta g}^2 + \sigma_{\Delta g}^2}}. \quad (9b)$$

Figure 11a shows values of the normalised differences between the gravity anomalies estimated by each method and their reference values computed using WHU. Figure 11b presents a similar plot but in this case the de-biased surface gravity anomalies and their de-biased uncertainties are used. The uncertainties of the reference gravity anomalies computed using WHU ($\sigma_{\Delta g}$) are relatively small. Therefore, the de-biased uncertainties estimated by solving the discretised integral equations contribute most to the uncertainty of the differences w . Statistically, values of the ratio in Eq. (9b) should follow the normal distribution, meaning they should primarily fall within the confidence interval of -1.96 to 1.96 that corresponds to the 95% significance level. It is important to note that the STE of 3 arc-deg was applied prior to computing values of the ratio.

The normalised differences for the RCR method significantly exceed those of the other methods. This suggests that the differences between the surface gravity anomalies estimated by the RCR method, and their WHU-based reference values are larger than the corresponding uncertainties. In other words, the estimated uncertainties are too optimistic and smaller than the actual differences. This discrepancy is due to larger values of the regularisation parameter used in solving the discretised integral equation with the reduced satellite gradients. Nevertheless, the value of the de-biased a posteriori variance factor is nearly the same as those of the other methods, and the coefficient matrix is the same as for the DIR and TR methods, with only minor differences to the coefficient matrix of the MII method.

Conversely, values of the ratio to the MII method are within a more acceptable range, with most values within the 99.7% confidence interval of -3 to 3 . This indicates that

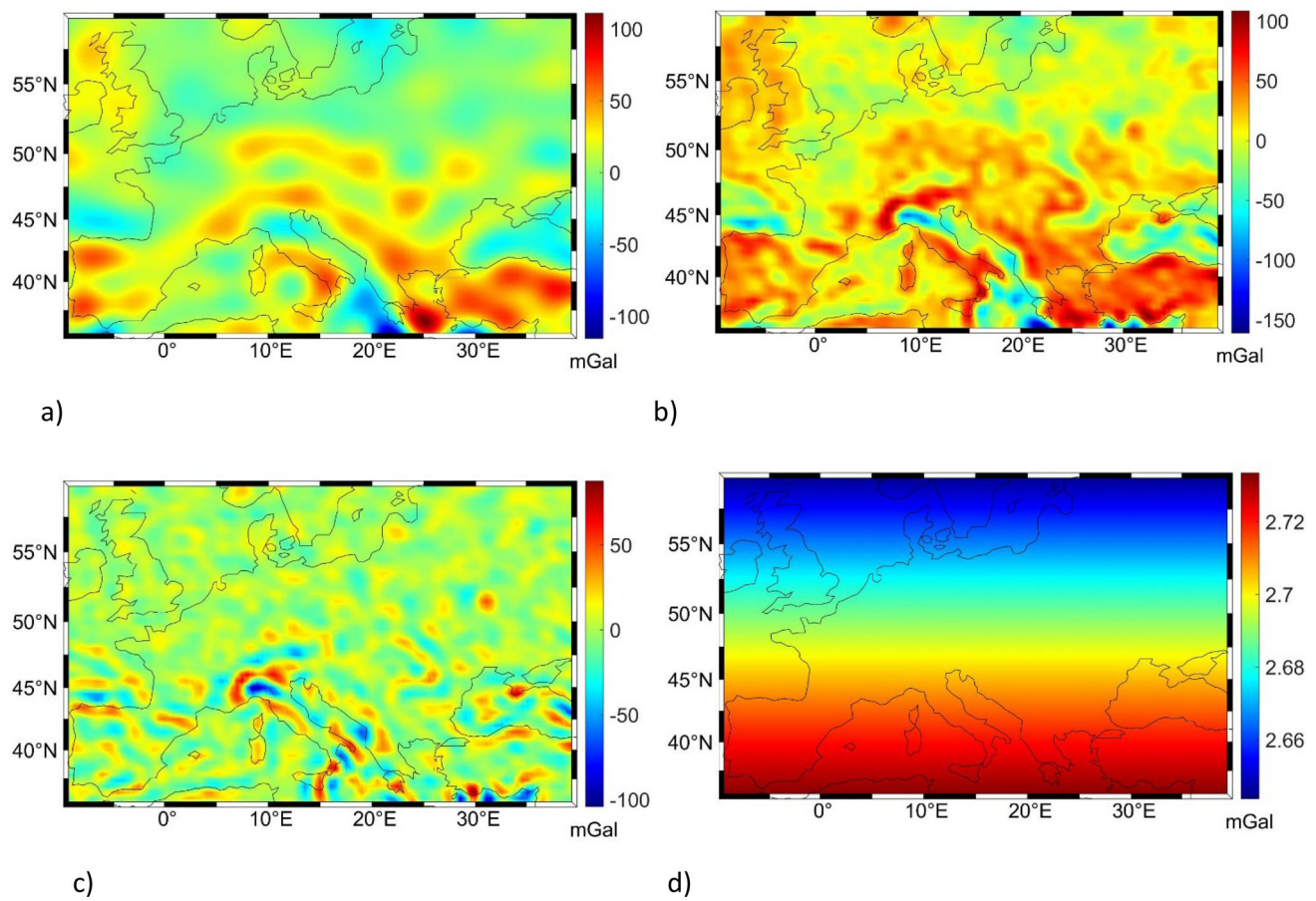
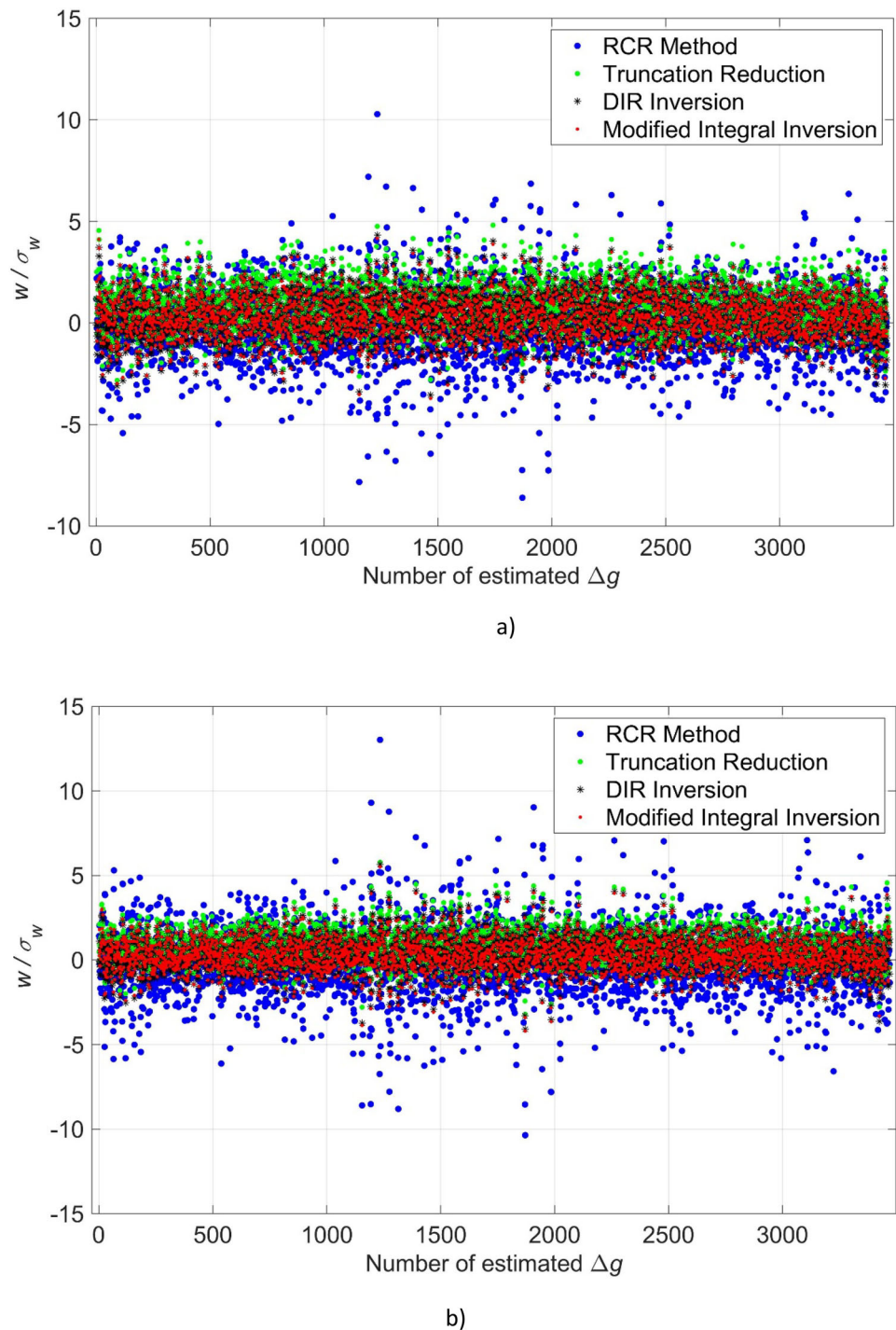


Fig. 10 Gravity anomalies based on **a** ITSG to degree 100, **b** WHU to degree 300, **c** WHU for the degree band of 100–300, and **d** uncertainties of surface gravity anomalies based on WHU to degree and order 300 (all values in mGal)

Table 4 Statistics of the EGM-based gravity anomalies, and their differences from gravity anomalies estimated by each method, de-biased solutions are in the brackets (in mGal)

	STE of 3 arc-deg					STE of 5 arc-deg				
	Min	Mean	Max	STD	RMS	Min	Mean	Max	STD	RMS
ITSG / 100	– 54.9	10.8	77.3	19.8		– 33.9	10.9	72.1	18.1	
WHU / 300	– 102.3	10.9	101.3	25.1		– 102.3	10.9	101.3	24.3	
WHU / 100–300	– 104.3	0.1	74.7	15.4		– 104.3	– 0.0	74.7	16.0	
DIR	– 30.7 (– 36.7)	2.6 (2.7)	36.6 (47.9)	8.7 (8.0)	9.1 (8.4)	– 30.7 (– 31.5)	3.0 (3.0)	36.6 (47.9)	8.8 (7.8)	9.3 (8.3)
RCR	– 42.3 (– 50.9)	– 0.1 (– 0.1)	48.8 (61.9)	7.9 (8.8)	7.9 (8.8)	– 37.1 (– 42.4)	0.0 (0.0)	48.8 (61.9)	7.9 (8.8)	7.9 (8.8)
TR	– 24.5 (– 30.7)	7.4 (7.4)	42.1 (52.1)	9.2 (8.2)	11.8 (11.1)	– 24.5 (– 25.1)	8.1 (8.1)	42.1 (52.1)	9.2 (8.0)	12.3 (11.4)
MII	– 32.1 (– 37.7)	2.3 (2.4)	35.3 (46.7)	8.7 (7.9)	9.0 (8.3)	– 32.1 (– 32.7)	2.5 (2.5)	35.3 (46.7)	8.7 (7.8)	9.2 (8.2)

Fig. 11 Normalised differences between **a** estimated surface gravity anomalies, **b** de-biased gravity anomalies estimated by each method and WHU-based reference gravity anomalies to degree 300



the uncertainties are at the order of differences for the MII method. The normalised differences of the surface gravity anomalies derived using the TR and DIR inversion methods are larger than that of the MII method and smaller than that of the RCR method.

In this study, we rely on formal uncertainties provided for satellite gradients and EGMs and apply the error propagation law in all methods to study how they propagate them into the

estimated gravity anomalies. Since in our uncertainty estimation, the a posteriori variance factors are estimated and applied to scale the noise VCMs of the estimated gravity anomalies, the estimated uncertainties of the estimated gravity anomalies are scaled with the quality of least-squares fitting of the gradient data. This means that the uncertainties are somewhat internally calibrated. Realistic calibration of errors of the estimated gravity anomalies would require

comparison with reference high-quality surface gravity data which is beyond the scope of this study.

Figure 12a shows values of surface gravity anomalies estimated by the MII method across the test area, while Fig. 12b illustrates the estimated de-biased errors of the estimated gravity anomalies, which display a slope from 7 to 9 mGal in the north–south direction. As highlighted in Table 4, the STD of the surface gravity anomalies estimated by this method is 8 mGal that is close to the magnitude of the estimated uncertainty presented in Fig. 12b.

4 Discussion

Our study shows that the reduction of gradient data in the RCR method is larger than in the TR and MII methods but it has the largest uncertainty. In this reduction method, the long-wavelength component of the gravity field, which is removed from satellite gradients, plays a significant role. Given this component contains the substantial portion of the signal, results of the RCR method are considerably influenced by the choice of used EGM. The long-wavelength component removed from satellite gradient data must be restored into the estimated surface gravity anomalies. Consequently, significant efforts in regional gravity field modelling must focus on selecting such an EGM that realistically describes the gravity field over a specific area. Upon selection and application of EGM for computation of the long-wavelength component of gravity gradients, reduced satellite gradient data composed of higher frequencies has a smaller average SNR for multiple reasons. Primarily, the uncertainty of the used EGM will contribute to the uncertainty of the reduced gradient data in addition to the gradient uncertainties. Thus, uncertainties of the reduced gradient data are larger than those of observed gradients. Furthermore, the reduction of satellite gradients for the long-wavelength component, as is done in the RCR method, results in small values of residual gradients, thereby diminishing their SNR, even if the EGM errors are small relatively to observation errors of gradient data. In other words, the ITSG errors affect the reduced gradient data more in the RCR method than in the other methods, because here the gradient reduction has the largest magnitude and therefore also the corresponding error contribution is largest.

The determination of the optimal degree for reduction of satellite gradients for the long-wavelength component is critical. Selecting a higher degree further reduces the magnitude of the residual gradient data that leads to their smaller SNRs. For instance, Pitoňák et al. (2017) adopted the maximum degrees of 180 and 250 that resulted in the compromised reliability of the estimated surface gravity anomalies and their uncertainties. However, in our study we used the maximum degree of 100, aiming to retain the more significant signal in

the satellite gradient data used for recovery of surface gravity anomalies.

Additional investigations concerned reduction of satellite gradient data for topographic and atmospheric effects (Eshagh and Sjöberg 2009a,b). Eshagh and Bagherbandi (2011) demonstrated that applying topographic effects on satellite gradient data could improve the accuracy of estimated surface gravity anomalies. However, the main purpose of this reduction is to guarantee that the gravitational potential and all functionals (such as gravity gradients or gravity anomalies in our study) are harmonic functions of 3D position in space where the problem is solved (i.e. outside the mean sea level). This process involves reduction of residual gradient data for high-frequency gravitational effects of the topographic and atmospheric masses, pending topographic heights and mass densities are known. However, this reduction introduces further errors to the residual gradient data, increasing their overall uncertainty.

Moreover, some studies have proposed to eliminate both long- and short-wavelength components of the gradient data before estimation of surface gravity anomalies (see e.g. (Yildiz et al. 2012)). Here, errors associated with topographic heights and mass densities, and errors in EGM used for the long-wavelength component estimation propagate to the residual gradient data. This reduction further decreases magnitude of the residual satellite gradient data even if errors of topographic heights, mass densities, and EGM are small. Consequently, estimated errors of estimated surface gravity anomalies significantly surpass their values, sometimes mirroring the order of magnitude of their estimated errors. By restoring both long- and short-wavelength components of the gravity anomalies into the solution of the discretised integral equation, estimated gravity anomalies are close to those based on EGM.

Our investigations also reveal that employing the least-squares modification of the surface integral, i.e. the MII method, provides a slightly better solution to the discretised integral equation than other two modification methods. Even when employing EGM for computing modification parameters, as evidenced by Eshagh (2009b) in his modification of Stokes's kernel function, the choice of EGM proved to be non-critical. The well-known Tscherning-Rapp empirical model for the harmonic spectrum of the Earth's gravitational field can be used for modification of the surface integral.

Eshagh and Ghorbannia (2014) conducted joint inversion of GOCE orbital and gradient data, incorporating the variance component estimation for optimal data weighting. They also devised a method to reduce STE from the estimated variances. However, we do not apply this method in this study to weigh contributions based on EGM and regional satellite gradient data due to their different frequency contents. EGM lacks high frequencies that are mistakenly interpreted as its

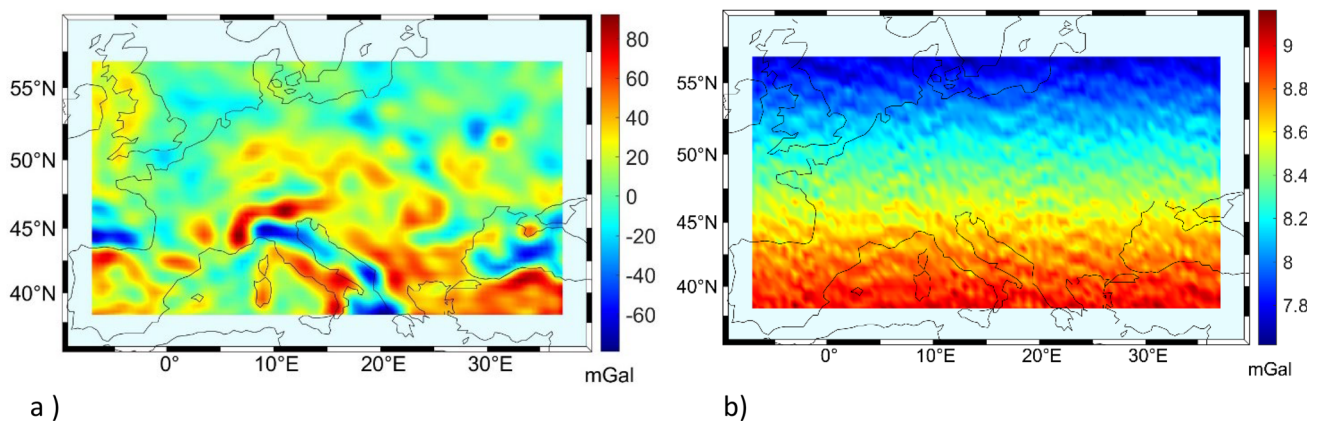


Fig. 12 **a** Surface gravity anomalies estimated by the MII method, and **b** their estimated de-biased uncertainties (in mGal)

random noise. Eshagh and Romeshkani (2011) indicated significant noise variances for EGM under such circumstances in the context of solving the upward continuation problem. Nonetheless, the underlying principle of variance component estimation remains consistent.

5 Conclusions

Four methods are investigated for studying the error propagation through integral-based inversion of gradient data measured by the GOCE satellite mission to recover 30 arc-min surface gravity anomalies over the test area in Central Europe: direct inversion (DIR), remove-compute-restore (RCR), truncation reduction (TR), and modified integral inversion (MII).

Our analysis indicates that the RCR method produced the lowest SNR among the four methods. This was because surface gravity anomalies estimated by the RCR method do not contain the long-wavelength component of the gravity signal. The reduction generated from EGM to remove the long-wavelength portion of the gradient data has the largest uncertainty compared to reductions applied in the TR and MII methods. However, since uncertainties of the reductions are significantly smaller than the uncertainties of GOCE gradient data, they do not significantly affect the uncertainty of the residual gradient data.

Both the RCR and TR methods remove some parts of the signal from the GOCE gradients. The former is based on the maximum spectral frequency (or harmonic degree) of EGM, while the latter is based on splitting the integration domain into two zones. In contrast, the MII method optimises the solution by linking the size of the integration domain of the surface integral with the maximum degree of the used EGM.

Mathematical models for estimating the biased and de-biased VCMs of the estimated gravity anomalies, modified by Tikhonov's regularisation, are formulated and employed

to estimate surface gravity anomalies from satellite gradient data. In all four methods of the integral inversion, the de-biased a posteriori variance factors have almost the same value. However, the propagated and de-biased errors in the solution of the discretised integral equation by the RCR method are the smallest compared to those obtained by the other methods. This is because the largest reduction in the RCR method reduces the SNR of the residual satellite gradients. Even if the coefficients matrix of the system of linear equations obtained by discretisation of the integral equation is the same as that of the DIR and TR methods, the system of linear equations needs more regularisation to recover meaningful gravity anomalies. Consequently, the estimated regularisation parameter is one order of magnitude larger than that in the other methods, resulting in smaller diagonal elements of the estimated noise VCM of the estimated gravity anomalies.

In the analysis of the differences between the estimated gravity anomalies and those synthesised from EGM, all the methods perform equally well in terms of RMS of the differences between the estimated and reference values. However, the mean value of the differences is the largest for the TR method and the smallest for the RCR method. The largest normalised differences are obtained in the RCR method and the smallest with the MII method. This is due to the optimistic estimation of uncertainties in the surface gravity anomalies estimated by the RCR method, not magnitude of the differences. From the statistical point of view and in terms of uncertainty propagation through discretised integral equations, the DIR, TR and MII methods propagate the GOCE gradient errors more realistically than the RCR method.

Appendix A

Proof of Proposition 1

Since the matrix $\mathbf{A}$ in Eq. (6a) has a full-column rank, the noise VCM of the unknown gravity anomalies can be estimated by:

$$\mathbf{C}_x = \sigma_0^2 (\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A})^{-1}. \quad (\text{A1})$$

Equation (A1) can be re-written as

$$(\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}) \mathbf{C}_x (\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}) = \sigma_0^2 \mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}, \quad (\text{A2})$$

and by inserting it into Eq. (6e), the relation between $\mathbf{C}_{\hat{x}_{\text{reg}}}$ and $\mathbf{C}_x$ is obtained:

$$\mathbf{C}_{\hat{x}_{\text{reg}}} = \mathbf{N}^{-1} (\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}) \mathbf{C}_x (\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}) \mathbf{N}^{-1}. \quad (\text{A3})$$

Further simplifications and considering $\mathbf{N}^{-1} (\mathbf{A}^T \mathbf{C}^{-1} \mathbf{A}) = \mathbf{I} - \alpha^2 \mathbf{N}^{-1}$ yields

$$\mathbf{C}_{\hat{x}_{\text{reg}}} = \mathbf{C}_x + \alpha^2 \mathbf{N}^{-1} (-2\mathbf{I} + \alpha^2 \mathbf{N}^{-1}) \mathbf{C}_x. \quad (\text{A4})$$

Taking $\mathbf{C}_x$ to the left-hand side of Eq. (A4) proves the proposition.

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Data availability The product EGG_TRF_2 is freely available via https://goce-s.eo.esa.int/oads/access/collection/GOCE_Level_2/tree after free registration. GGMs used within this study are available via ICGEM.

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