On the accuracy assessment of input gravity data in local gravity field modeling

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A bstract: The subject of this study is an assessment of the accuracy of gravity data used in local gravity field modeling when the a priori standard deviations of input gravity data are not available. To assess the accuracy of gravity data sets, Variance Component Estimation (VCE) technique for the observation group weighting is applied. The parameterization of gravity field is realized in terms of the spherical radial basis functions (SRBF). The unknown parameters are estimated by a least-squares technique. The performance of VCE technique for the observation group weighting is demonstrated using real data, providing that the parameterization of gravity field is chosen optimally by means of modeling the gravity signal and not the observation data noise.

Key words: local gravity field modeling, penalized least-squares technique, spherical radial basis functions, variance component estimation

1. Introduction

Various types of the spherical radial basis functions were utilized for parameterization of the Earth's gravity field such as the point mass kernel (Weightmann, 1965), the radial multipoles of different orders (Marchenko, 1998), Poisson wavelets of different orders (Holschneider et al., 2003), and the Poisson kernel. In Tenzer and Klees (2007) we demonstrated that almost the same accuracy of gravity field modeling can be achieved for different types of the SRBFs if the bandwidth of the SRBFs is chosen optimally. In Klees et al. (2007) we developed a data-driven approach for the local gravity field modeling using various least-squares techniques. After finding an optimal configuration of the SRBFs by applying Generalized Cross Validation

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(GCV) technique, VCE technique for the observation group weighting is implemented to estimate the variance factors of the observation data sets used for the SRBF analysis. These estimated variance factors are then adopted as the a priory information of accuracy in the least-squares adjustment. Following principles of the methodology developed by *Klees et al. (2007)*, VCE technique for the observation group weighting is utilized in this study to assess the accuracy of input gravity data. The functional model, the estimation principle and VCE technique for the observation group weighting are briefly recapitulated through sections 2-4. The optimal configuration of the SRBFs and the performance of VCE for an objective assessment of the accuracy of gravity data are investigated in section 5 and the results of the numerical experiment are summarized in section 6.

2. Functional model

Let us consider a residual gravity field of which the quantities are obtained after subtracting the contribution of the global gravity field. The corresponding residual disturbing gravity potential T at a point \mathbf{r} can be expressed as a linear combination of I spherical radial basis functions { $\Psi(\mathbf{r}, \mathbf{r}'_i)$: $i = 1 \dots I$ }. Hence

$$T(\mathbf{x}) = \sum_{i=1}^{I} \beta_i \Psi(\mathbf{r}, \mathbf{r}'_i), \qquad (1)$$

where the coefficients $\{\beta_i : i = 1 \dots I\}$ parameterize gravity field at the positions \mathbf{r}'_i of the SRBFs. The objective of local gravity field modeling is to determine the unknown parameters $\{\beta_i : i = 1 \dots I\}$ from various types of gravity observables, such as the gravity anomalies and/or the gravity disturbances. After linearization and spherical approximation, the residual gravity anomalies Δg and the residual gravity disturbances δg are related to the residual disturbing gravity potential according to well-known formulae

$$\Delta g(\mathbf{r}) = -\frac{2}{|\mathbf{r}|} T(\mathbf{x}) - \frac{\partial T(\mathbf{r})}{\partial |\mathbf{r}|}, \qquad \delta g(\mathbf{r}) = -\frac{\partial T(\mathbf{r})}{\partial |\mathbf{r}|}.$$
(2)

In this study we consider the parameterization of gravity field in terms of the Poisson kernel. The Poisson kernel Ψ_{pk} is defined by (see e.g. Heiskanen and Moritz, 1967)

$$\Psi_{pk}(\mathbf{r},\mathbf{r}') = \sum_{n=0}^{\infty} (2n+1) \left(\frac{|\mathbf{r}'|}{|\mathbf{r}|}\right)^{n+1} P_n\left(\hat{\mathbf{r}}^T \, \hat{\mathbf{r}}'\right), \qquad (3)$$

where P_n is the Legendre polynomial of degree n for the argument $\mathbf{\hat{r}}^T \mathbf{\hat{r}}'$; $\mathbf{\hat{r}} = \mathbf{r}/|\mathbf{r}|$ and $\mathbf{\hat{r}}' = \mathbf{r}'/|\mathbf{r}'|$. The corresponding spatial representation of the Poisson kernel Ψ_{pk} reads

$$\Psi_{pk}\left(\mathbf{r},\mathbf{r}'\right) = |\mathbf{r}'|\frac{|\mathbf{r}|^2 - |\mathbf{r}'|^2}{|\mathbf{r} - \mathbf{r}'|^3},\tag{4}$$

where $|\mathbf{r} - \mathbf{r}'|$ is the Euclidean spatial distance. To implement the Poisson kernel from eqn. (4) for the gravity observables δg and Δg , the linear observation operators $D_{\delta g}$ and $D_{\Delta g}$ are applied. The operator $D_{\delta g}$ is defined as $D_{\delta g} = -\partial/\partial |\mathbf{r}|$, and $D_{\Delta g} = D_{\delta g} - 2|\mathbf{r}|^{-1}\Im$, where \Im denotes the identity operator.

3. Estimation principle

The observation data of different quality are separated into the individual observation groups for which the variance factors are estimated using VCE technique (see the next section). The observation equations are then formed for P observation groups (cf. *Klees et al.*, 2007),

$$\mathbf{l}_p + \boldsymbol{\varepsilon}_p = \mathbf{A}_p \mathbf{x}, \quad p = 1 \dots P, \tag{5}$$

where \mathbf{l}_p is the observation vector of observation group p, \mathbf{A}_p the corresponding design matrix, and \mathbf{x} the vector of gravity field parameters $\{\beta_i : i = 1 \dots I\}$. Assuming that the observation noise is white Gaussian with zero mean, the variance-covariance matrix $\boldsymbol{\Sigma}_p$ of the stochastic observation noise vector $\boldsymbol{\varepsilon}_p$ is a diagonal matrix. Moreover, it is assumed that the noise variance is the same for the data within each observation group. Therefore, the noise variance-covariance matrix $\boldsymbol{\Sigma}_p$ of observation group p is

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$$\Sigma_p = \sigma_p^2 \mathbf{I}_p, \quad p = 1 \dots P, \tag{6}$$

where \mathbf{I}_p is the $J_p \times J_p$ identity matrix; and σ_p^2 the variance factor of observation group p.

A penalized least-squares estimation principle is chosen, i.e. for a given regularization parameter α the quadratic objective function Φ is minimized *(ibid.)*

$$\Phi(\mathbf{x}) = \sum_{p=1}^{P} ||\boldsymbol{\varepsilon}_p||_{\boldsymbol{\Sigma}_p^{-1}}^2 + \alpha ||\mathbf{x}||_{\mathbf{R}}^2, \qquad (7)$$

where **R** is the (positive definite) regularization matrix. The regularization matrix is the identity matrix; i.e., $\mathbf{R} \equiv \mathbf{I}$. For a given regularization parameter α and known variance factors $\{\sigma_p^2 : p = 1...P\}$, the minimum of the quadratic objective function $\Phi(\mathbf{x})$ is attained for

$$\hat{\mathbf{x}} = \mathbf{N}^{-1} \, \mathbf{h},\tag{8}$$

where the normal matrix ${\bf N}$ reads

$$\mathbf{N} = \sum_{p=1}^{P} \mathbf{N}_{p} + \alpha \,\mathbf{R} \,, \quad \mathbf{N}_{p} = \mathbf{A}_{p}^{\mathrm{T}} \,\boldsymbol{\Sigma}_{p}^{-1} \,\mathbf{A}_{p} \,.$$
(9)

The right-hand side vector of the system of normal equations is given by

$$\mathbf{h} = \sum_{p=1}^{P} \mathbf{h}_{p}, \quad \mathbf{h}_{p} = \mathbf{A}_{p}^{\mathrm{T}} \boldsymbol{\Sigma}_{p}^{-1} \mathbf{l}_{p}.$$
(10)

Once the definite variance factors and the associated least-squares solution have been found, the accuracy of estimated parameters and adjusted observations can be computed from the error propagation. The noise variance-covariance matrix $\Sigma_{\hat{\mathbf{x}}}$ of the estimated parameters reads

$$\boldsymbol{\Sigma}_{\hat{\mathbf{x}}} = \left(\sum_{p=1}^{P} \mathbf{A}_{p}^{\mathrm{T}} \boldsymbol{\Sigma}_{p}^{-1} \mathbf{A}_{p} + \alpha \, \mathbf{R}\right)^{-1} \,. \tag{11}$$

4. Observation group weighting

To assess the accuracy of input gravity data, VCE technique is used to estimate the unknown variance factors σ_p^2 of all observation groups used for the SRBF analysis. The estimated variance factors obtained from applying VCE technique are then used as the a priori information about the accuracy of input gravity data. The VCE technique can also be applied in order to determine the regularization parameter α . To do that, the quadratic objective function $\Phi(\mathbf{x})$ from eqn. (7) is rewritten as (*Klees et al., 2007*)

$$\Phi(\mathbf{x}) = \sum_{p=1}^{P} ||\boldsymbol{\varepsilon}_{p}||_{\boldsymbol{\Sigma}_{p}^{-1}}^{2} + \alpha||\boldsymbol{\varepsilon}_{P+1}||_{\boldsymbol{\Sigma}_{P+1}^{-1}}^{2},$$
$$\boldsymbol{\varepsilon}_{P+1} = \mathbf{I} \mathbf{x}, \qquad (12)$$

$$\mathcal{D}\{\boldsymbol{\varepsilon}_{P+1}\} = \boldsymbol{\Sigma}_{P+1} = \alpha^{-1} \mathbf{I},$$

where \mathcal{D} is the dispersion operator. The minimization of the quadratic objective function $\Phi(\mathbf{x})$ of eqn. (12) is then given by the unconstraint leastsquares solution for P+1 observation groups with the additional observation group $\mathbf{l}_{P+1} = \mathbf{0}$. The determination of the regularization parameter α is thus treated as a determination of the variance factor of an additional observation group; i.e., $\mathbf{\Sigma}_{P+1} \equiv \alpha^{-1} \mathbf{R}^{-1}$ and $\alpha^{-1} \equiv \sigma_{P+1}^2$. The variance factors σ_p^2 can be estimated by the Almost Unbiased Estimator (cf. *Förstner*, 1979);

$$\hat{\sigma}_p^2 = \frac{\hat{\varepsilon}_p^{\mathrm{T}} \mathbf{W}_p \,\hat{\varepsilon}_p}{r_p}, \quad \sigma_p^2 \,\mathbf{W}_p^{-1} = \mathbf{\Sigma}_p, \quad p = 1 \dots P + 1\,, \tag{13}$$

where $\hat{\boldsymbol{\varepsilon}}_p$ is the vector of residuals $\left\{ \hat{\varepsilon}_j = \hat{l}_j - l_j : j = 1 \dots J_p \right\}$ of observation group p, and the group redundancy number r_p is defined as a difference of the number of observations J_p in the group and the trace of the observation group influence matrix $\mathbf{N}^{-1} \mathbf{N}_p$; i.e.,

$$r_p = J_p - \text{trace}\left(\mathbf{N}^{-1} \ \mathbf{N}_p\right). \tag{14}$$

The trace of the observation group influence matrix is a measure of the influence of the particular observation group p on the least-squares solution $\hat{\mathbf{x}}$.

The estimation of the variance factors is carried out iteratively, starting with some a priori values $\left\{ \hat{\sigma}_{p,0}^2 : p = 1 \dots P + 1 \right\}$. The initial least-squares solution is computed according to eqn. (8) using $\hat{\sigma}_{p,0}^2$. From the residuals of the initial solution, the improved values of the variance factors are obtained according to eqn. (13). Improved variance factors are used in the next iteration to define new noise variance-covariance matrices Σ_p in order to form the system of normal equations. The procedure is repeated until some chosen criterion of convergence is achieved. The criterion of convergence $\max_{p=1...P+1} \left(\hat{\sigma}_{p,\mathbf{k}}^2 / \hat{\sigma}_{p,\mathbf{k}-1}^2 \right) \leq \tau, \text{ where } \tau \text{ is the}$ can be chosen for instance as: threshold, and $\hat{\sigma}_{p,\mathbf{k}}^2$ is the variance factor of observation group p after k-th iteration. If the iteration converges, the almost unbiased estimator is equal to the maximum likelihood estimator. The original idea of this algorithm is given by $F\ddot{o}rstner$ (1979) and a modified version in which the Monte Carlo VCE technique was utilized was introduced by Koch and Kusche (2002), see also Kusche (2003).

5. Numerical study

The data used for the numerical analysis consist of the 30178 free air gravity anomalies which cover the computation area bounded by the parallels of 50° and 54° arc-deg northern geodetic latitude and the meridians of 3° and 8° arc-deg eastern geodetic longitude (see Fig. 1). The residual free-air gravity anomalies over the computation area were separated into 7 observation groups, depending on a priori information about the expected accuracy, the data type (point or grid values) and the location. Among the input data sets, the data over the target area (the territory of the Netherlands) were assigned into 3 observation groups (Holland data set of observed ground gravity anomalies, Holland-Ÿsselmeer data sets 1 and 2 of the seaborn gravity anomalies of different quality). Within the target area, 653 control points were further selected randomly to verify a performance of least-squares techniques applied to the optimal parameterization of gravity field (by GCV) and the observation group weighting (by VCE).



Fig. 1. The residual free-air gravity anomalies used for the SRBF analysis. For the Netherlands, the residual gravity anomalies range from -28.7 to 15.0 mGal; the mean value is -5.9 mGal, and the standard deviation is 7.4 mGal.

To assess objectively the accuracy of gravity data, the optimal parameterization of gravity field should be realized in prior of applying the VCE to the observation group weighting. The main reason is due to the requirement of modeling the real gravity signal and not the data noise at the level of a stochastic significance.

For finding an optimal parameterization of the gravity field, the first experiment was carried out in order to form the horizontal configuration of the coarse-grid SRBFs. Particularly, the correlation between the accuracy of least-squares approximation of gravity field and the number of the coarsegrid SRBFs was investigated. The parameterization of gravity field in terms of the different number of the coarse-grid SRBFs used for the numerical experiment is summarized in Table 1.

Equal-angular step of	Number
the coarse-grid SRBFs	of SRBFs
$0.10 [\mathrm{deg}]$	2000
$0.09 [\mathrm{deg}]$	2520
$0.08 [\mathrm{deg}]$	3213
$0.07 [\mathrm{deg}]$	4176
$0.06 [\mathrm{deg}]$	5628
$0.05 [\mathrm{deg}]$	8000
$0.04 [\mathrm{deg}]$	12726
$0.03 [\mathrm{deg}]$	22378

Table 1. The coarse-grid SRBFs used for a parameterization of the gravity field

As follows from the results shown in Figs. 2 and 3, the sufficient number of the coarse-grid SRBFs is about 18 - 30% of the total number of observations used for the SRBF analysis. The accuracy of the SRBF analysis (provided in terms of the RMS of least-squares residuals) does not increase significantly with the number of SRBFs. Moreover, the use of large number of SRBFs can yield the over-fitting. As a consequence, too many SRBFs model not only the gravity signal but also the data noise. The over-fitting is particularly evident from the SRBF synthesis at the control points (Fig. 3). Whereas the least-squares approximation of the gravity signal at the observation data points for the SRBF analysis improves with increasing number of the SRBFs, the accuracy of a prediction at the control points (provided in terms of the RMS of differences between observed and predicted residual gravity anomalies) remains almost unchanged despite more SRBFs were used for the parameterization.

After forming an appropriate horizontal configuration of the coarse-grid SRBFs, the selection of the optimal depth of the coarse-grid SRBFs was realized. The accuracy of least-squares approximation of the gravity signal at the observation data points with respect to the depth of the coarse-grid SRBFs is shown in Fig. 4. The corresponding correlation between the accuracy of prediction at the control points and the depth of the coarse-grid SRBFs is shown in Fig. 5. As follows from the results, the gravity field



Fig. 2. RMS of least-squares residuals for different steps of the coarse-grid SRBFs. The depth of the coarse-grid SRBFs is 13.5 km.



Fig. 3. RMS of differences between observed and predicted residual gravity anomalies at the control points for different steps of the coarse-grid SRBFs. The depth of the coarse-grid SRBFs is 13.5 km.



Fig. 4. RMS of least-squares residuals for different depths of the coarse-grid SRBFs. Search interval between 2 and 25 km with the step of 1 km.



Fig. 5. RMS of differences between observed and predicted residual gravity anomalies at the control points for different depths of the coarse-grid SRBFs. Search interval between 2 and 25 km with the step of 1 km.

solution is somehow robust with respect to the choice of the depth; fixing the depth with an accuracy of a few kilometers is sufficient for the data set used in this study.

From the above results, the optimal parameterization of gravity field comprises 5628 coarse-grid SRBFs (about 19% of the number of observations) of which the optimal depth below the Bjerhammar sphere is 13.5 km. The optimal depth 13.5 km of the coarse-grid SRBFs was selected by GCV (cf. *Klees et al., 2007*). The mean distance between the SRBFs is about 4.3 km. The accuracy of least-squares approximation of the gravity signal at the observation data points and the accuracy of prediction at the control points after the parameterization of gravity field by the coarse-grid SRBFs are shown in Figs. 6 and 7 and summarized in Table 2.

Table 2. RMS of least-squares residuals and RMS of differences between observed and predicted residual gravity anomalies after the parameterization of gravity field by the coarse-grid SRBFs

	RMS [mGal]		
	Holland	Holland-Ÿsselmeer data set 1	$\begin{array}{c} \text{Holland-} \ddot{\text{Y}} \text{sselmeer} \\ \text{data set } 2 \end{array}$
SRBF analysis	0.53	0.41	1.31
SRBF synthesis	0.60	0.48	1.94

To reveal a possible presence of the remaining un-modeled gravity signal after the parameterization by the coarse-grid SRBFs, the local refinement procedure was implemented by means of adding additional local-refinement SRBFs bellow the observation data points according to the pre-defined criteria. The selection criteria for locating the additional SRBFs were defined as follows: The threshold for the absolute value of least-squares residual at a candidate point for the local refinement should be at least 3 times larger than the RMS of coarse-grid solution. To avoid local over-fitting, the minimum spherical distance between two SRBFs was set up to be at least 0.01 deg. To avoid modeling of large isolated residuals which are more likely outliers and not the real gravity signal, the additional threshold criteria for the average RMS of residuals and the minimum number of observations within the area of local refinement were specified. The average RMS threshold was set up to be 3 times larger than the RMS of coarse-grid solution, providing



Fig. 6. Least-squares residuals at observation points after the parameterization of gravity field by the coarse-grid SRBFs (statistics: min = -4.83 mGal, max = 4.98 mGal, mean = 0.01 mGal, RMS = 0.53 mGal).



Fig. 7. Differences between observed and predicted residual gravity anomalies at the control points after the parameterization of gravity field by the coarse-grid SRBFs (statistics: min = -5.44 mGal, max = 3.86 mGal, mean = 0.04 mGal, RMS = 0.70 mGal).

that at least 30 data points were located within the area of local refinement. The GCV was applied individually for each local-refinement SRBF to find its optimal depth at the search interval between 0.1 and 13.5 km with the step of 0.2 km. The accuracy of least-squares approximation and prediction after complete parameterization of gravity field by the coarse-grid and local-refinement SRBFs are summarized in Table 3.

Table 3. RMS of least-squares residuals and RMS of differences between observed and predicted residual gravity anomalies after complete parameterization of gravity field by the coarse-grid and local refinement SRBFs

	RMS [mGal]		
	Holland	Holland-Ÿsselmeer data set 1	Holland-Ÿsselmeer data set 2
SRBF analysis	0.46	0.41	1.30
SRBF synthesis	0.60	0.48	1.93

From comparison of the accuracy in Tables 2 and 3, the 52 selected localrefinement SRBFs improve the accuracy of the least-squares approximation within the target area less than 0.1 mGal which is bellow a stochastic significance. Hence, the parameterization of gravity field by the coarse-grid SRBFs is sufficient and VCE for the observation groups weighting can be applied to assess the accuracy of gravity data.

As follows from the experiment for finding the optimal 3-D configuration of the coarse-grid SRBFs, the accuracy of least-squares approximation is less correlated with the number of the SRBFs than with the depth of the SRBFs. Hence, the accuracy of least-squares approximation after applying VCE for the observation group weighting was further investigated only for different depths of the coarse-grid SRBFs. The result in terms of the RMS of leastsquares residuals for different depths of the coarse-grid SRBFs is shown in Fig. 8. The corresponding result in terms of the RMS of differences between observed and predicted residual gravity anomalies at the control points is shown in Fig. 9. From the depth of approximately 6 km, the results after applying VCE are very similar to the results obtained without applying VCE (cf. Figs. 4 and 5). The gravity field solution is again robust with respect to the choice of the depth. For the depth 13.5 km of the coarse-grid SRBFs, the results of the SRBF analysis and synthesis are summarized in Table 4.



Fig. 8. RMS of least-squares residuals for different depths of the coarse-grid SRBFs after applying VCE for the observation group weighting. Search interval between 2 and 25 km with the step of 1 km.



Fig. 9. RMS of differences between observed and predicted residual gravity anomalies at the control points for different depths of the coarse-grid SRBFs after applying VCE for the observation group weighting. Search interval between 2 and 25 km with the step of 1 km.

The estimated standard deviations obtained from VCE are summarized in Table 5.

From comparison of the results in Tables 2 and 4, VCE improved the quality of least-squares approximation of the gravity signal by means of better fitting within the data sets of the higher accuracy while decreasing the accuracy within the data sets with the larger data noise.

Table 4. RMS of least-squares residuals and RMS of differences between observed and predicted residual gravity anomalies after applying VCE for the observation group weighting

	RMS [mGal]		
	Holland	Holland-Ÿsselmeer data set 1	$\begin{array}{c} \mbox{Holland-}\ddot{\rm Y}\mbox{sselmeer}\\ \mbox{data set } 2 \end{array}$
SRBF analysis	0.46	0.41	1.30
SRBF synthesis	0.60	0.46	2.14

Table 5. The estimated standard deviations from VCE

	Holland	Holland-Ÿsselmeer data set 1	Holland-Ÿsselmeer data set 2
Standard deviation	0.60	0.36	1.48

The procedure of assessing the accuracy of gravity data is realized iteratively. After finding the initial variance factors of the observation data sets according to the method described above, the outlier detection is applied. The new variance factors are then estimated from VCE using the initial parameterization of gravity field. The reason of using the same parameterization is due to the fact that an elimination of the outliers cannot affect the configuration of SRBFs which is formed so that the real gravity signal is modeled and not the data noise.

6. Conclusions

To assess the accuracy of the input gravity data in the local and regional gravity field modeling, the parameterization of gravity field should be realized so that it models the gravity signal and not the data noise.

Homogeneously distributed gravity data over a flat area were used in our numerical experiment. As consequence, a simple parameterization scheme was chosen. The equal-angular coarse grid of the SRBFs with the constant depth bellow the Bjerhammar sphere used in this study represents one example of forming a simple parameterization model, providing that the data coverage and the horizontal distribution of the SRBFs should extend the target area at least 3 times of the correlation length of the SRBFs. The correlation length of a SRBF is defined as the spherical distance for which the value of the SRBF has dropped to 50% of its maximal value.

To find the optimal configuration of the SRBFs, we firstly investigated the accuracy of least-squares gravity field approximation with respect to the number of the coarse-grid SRBFs. After finding the sufficient horizontal configuration of the SRBFs, we applied GCV technique for finding the optimal depth of the coarse-grid SRBFs. Results of GCV indicate that the gravity field solution is robust with respect to the depth of the coarse-grid SRBFs.

After finding the optimal 3-D configuration of the coarse-grid SRBFs, the local refinement procedure was applied for modeling the remaining gravity signal. The parameterization was realized by adding additional localrefinement SRBFs below the selected observation data points. The selection of candidate points for the local refinement was realized according to the pre-defined criteria in order to avoid the local over-fitting or modeling the large isolated residuals.

The accuracy of the least-squares approximation after the local refinement procedure has not improved significantly compared with the accuracy obtained after the parameterization by the course-grid SRBFs. This is due to the homogeneous distribution of gravity data and the small variation of the gravity signal. In this case, a simple parameterization by the coarsegrid SRBFs is sufficient. The additional local-refinement parameterization of gravity field is needed especially for regions with a large gravity signal variation and/or an inhomogeneous distribution of gravity data.

The VCE technique for the observation group weighting was applied to assess the accuracy of gravity data sets of different accuracy. Despite a very similar accuracy of the gravity data sets used in this study, the quality of least-squares approximation after applying VCE slightly improved by means of modeling the real gravity signal and not the data noise. The observation group weighting by VCE becomes essential for combined processing of the data sets of different accuracy (for instance in processing the terrestrial and satellite data).

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