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Fast Variance Component Estimation in GOCE Data Processing

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Abstract. For the processing of GOCE (Gravity Field and steady-state Ocean Circulation Explorer) data the program system `pcgma` (Preconditioned Conjugate Gradient Multiple Adjustment) was designed as a tailored solution strategy for the determination of the Earth's gravity field in terms of a spherical harmonic analysis. Within GOCE-HPF (High Level Processing Facility) the `pcgma` algorithm works with the purpose of a tuning machine in that it is used to optimize the filter design and to determine optimal variance components with respect to the combination of satellite-to-satellite tracking (sst) data, satellite gravity gradiometry (sgg) data and additional prior information about the smoothness of the gravity field (the latter especially with regard to the polar regions). `pcgma` is based on an extended version of the iterative conjugate gradient (CG) algorithm, which allows for data combination in terms of observation and normal equations. A basic prerequisite for handling the nesting of the two iterative methods (variance component estimation (VCE) and parameter estimation using CG) is an efficient and fast implementation, because the VCE requires a repeated solution of the system. In this paper we will show how the nesting can be organized in an optimal way. We will concentrate on the reduction of CG iteration steps.

Keywords. GOCE, variance component estimation, conjugate gradients, data combination

1 Introduction

Starting from the linear normal equation system in terms of a least squares adjustment, the GOCE observations could be combined by summation of the normal equations of each observation group. Assuming the groups to be uncorrelated, the system reads

$$\left(\omega_{\text{sgg}}\mathbf{A}_{\text{sgg}}^T\mathbf{P}_{\text{sgg}}\mathbf{A}_{\text{sgg}} + \omega_{\text{sst}}\mathbf{N}_{\text{sst}} + \omega_{\text{reg}}\mathbf{P}_{\text{reg}}\right)\mathbf{x} = \omega_{\text{sgg}}\mathbf{A}_{\text{sgg}}^T\mathbf{P}_{\text{sgg}}\mathbf{l}_{\text{sgg}} + \omega_{\text{sst}}\mathbf{n}_{\text{sst}} + \omega_{\text{reg}}\mathbf{n}_{\text{reg}} \quad (1)$$

where

$\mathbf{A}_{\text{sgg}}$ ... decorrelated design matrix (sgg group),
$\mathbf{l}_{\text{sgg}}$ ... decorrelated observations (sgg group),
$\mathbf{P}_{\text{sgg}}$ ... weight matrix (sgg group),
$\mathbf{N}_{\text{sst}}$ ... normal equation matrix (sst group),
$\mathbf{n}_{\text{sst}}$ ... right hand side (sst group),
$\mathbf{P}_{\text{reg}}$ ... regularization matrix, inverse covariance matrix of prior information,
$\mathbf{n}_{\text{reg}}$ ... prior information of parameter values,
ω_i ... unknown weight factor, $i \in \{\text{sgg, sst, reg}\}$ (inverse variance components),
$\mathbf{x}$ ... unknown parameters, $\{c_{lm}\ s_{lm}\}$.

The sgg observation equations are decorrelated by applying digital autoregressive-moving average filters (cf. Siemes (2008), Schuh (2003)) estimated from the residuals. Since we estimate independent filters for the three tensor components V_{xx}, V_{yy} and V_{zz} correlations between the observations along on axes are modelled, but correlations between the three gradients are neglected. Then, after filtering the observation equations, $\mathbf{l}_{\text{sgg}}$ and $\mathbf{A}_{\text{sgg}}$ emerge as the decorrelated observation vector and design matrix, and $\mathbf{P}_{\text{sgg}} = \mathbf{I}$. We did not compute the sst observation equations, but we used the sst normal equations as they have been preprocessed by the HPF. Mainly there are two alternative ways of solving eq. (1),

1. Compute the joint normal equation matrix $\mathbf{N}$ as left hand side of eq. (1) and solve $\mathbf{N}\mathbf{x} = \mathbf{n}$.
2. Avoid computing $\mathbf{N}$ (especially the large scaled product $\mathbf{A}_{\text{sgg}}^T\mathbf{P}_{\text{sgg}}\mathbf{A}_{\text{sgg}}$), by using a tailored iterative solution strategy for eq. (1) (in our case `pcgma`, Schuh (1996)).

The general equation to determine the variance components σ_i^2 for observation group i (e.g. Koch (2007)) can be written as

$$\sigma_i^2 = \frac{\Omega_i}{n_i - u_i} = \frac{\Omega_i}{r_i} = \frac{1}{\omega_i}, \quad (2)$$

where

n_i ... # of observations in group i,
u_i ... # of parameters determined by group i,
r_i ... partial redundancy of observation group i,
ω_i ... weight factor of observation group i.

Ω_i is weighted squared sum of residuals and equals

$$\Omega_i = \mathbf{v}_i^T \mathbf{P}_i \mathbf{v}_i \text{ or}$$
$$\Omega_i = \mathbf{x}^T \mathbf{N}_i \mathbf{x} - 2\mathbf{x}^T \mathbf{n}_i + \mathbf{l}_i^T \mathbf{P}_i \mathbf{l}_i$$

depending on whether the observation groups are available as observation or as normal equations (assuming the constant $\mathbf{l}_i^T \mathbf{P}_i \mathbf{l}_i$ to be known).

Starting with initial weights $\omega_i^{(0)}$, new weight factors $\omega_i^{(\iota)}$ could be determined as inverse variance components using the squared sum of residuals and the partial redundancy for each observation group $i \in \{\text{sgg, sst, reg}\}$ after parameter estimation. With these new weight factors eq. (1) is then solved again using the iterative CG algorithm. Due to the nesting of a second iterative method in the processing chain and the fact that the normal equation matrix of the parameters is not explicitly computed, the algorithm for VCE must be modified. The whole strategy is briefly summarized by Fig. 1.

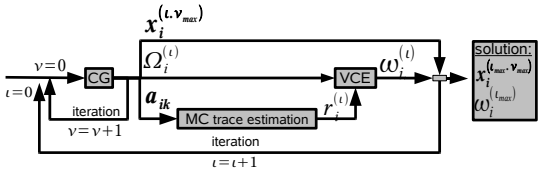


Fig. 1 Flowchart of the nested processing strategy.

In this paper we will concentrate upon three parts:

1. Integration of a Monte-Carlo based trace estimator into the VCE algorithm (cf. Koch and Kusche (2001)) combined with iterative CG.

2. Quality requirement for weight factors ω_i to get an optimal solution (Brockmann (2008)).

3. Convergence of VCE, with regard to trace and squared sum of residuals in the iterative solver.

The paper is organized in the following way. Section 2 shows how the VCE suggested by Koch and Kusche (2001) is applied in an iterative parameter estimation procedure (Alkhatib (2007)). In Section 3 the effect of errors in the weight determination in the case of GOCE data processing is analyzed. In Section 4 numerical simulations are used to analyze the convergence of VCE. Using these results, we present an optimized nesting of the iterative methods with the goal of minimizing the number of CG steps necessary to obtain convergence of weights. This paper ends with a summary and an outlook in Section 5.

2 VCE as part of an iterative solver

Starting from eq. (2) to determine σ_i^2 and replacing the partial redundancy by (e.g. Alkhatib (2007))

$$r_i = n_i - \frac{1}{\sigma_i^2} \text{trace}\left(\mathbf{A}_i^T \mathbf{P}_i \mathbf{A}_i \mathbf{N}^{-1}\right) \quad (3)$$

$$r_i = n_i - \frac{1}{\sigma_i^2} \text{trace}\left(\mathbf{N}_i \mathbf{N}^{-1}\right) \quad (4)$$

depending on whether the observation groups are available as observation or as normal equations, two facts become apparent: The procedure

(i) is iterative, because initial values for σ_i^2 are needed (cf. eq. (3)), and the computation of σ_i^2 is based upon residuals, which change after parameter estimation with updated VCE (cf. eq. (2)).

(ii) requires the combined normal equation matrix and $\mathbf{A}_i^T \mathbf{P}_i \mathbf{A}_i$, whose computation is avoided using CG.

Introducing the stochastic trace estimator for estimating the trace in eq. (3) and (4) as presented in Hutchinson (1990) and as suggested by Koch and Kusche (2001) in the context of GOCE data analysis, and noting the fact that the matrix in the trace term must be symmetric (cf. Hutchinson (1990)), we can reformulate the computation of the partial redundancy as

$$r_i = n_i - \frac{1}{\sigma_i^2} E\{\boldsymbol{\mathcal{P}}_i^T \mathbf{R}_i \mathbf{A}_i \mathbf{N}^{-1} \mathbf{A}_i^T \mathbf{R}_i^T \boldsymbol{\mathcal{P}}_i\} \quad (5)$$

$$r_i = n_i - \frac{1}{\sigma_i^2} E\{\boldsymbol{\mathcal{P}}_i^T \mathbf{G}_i \mathbf{N}^{-1} \mathbf{G}_i^T \boldsymbol{\mathcal{P}}_i\} \quad (6)$$

using the Cholesky decompositions $\mathbf{P}_i = \mathbf{R}_i^T \mathbf{R}_i$ and $\mathbf{N}_i = \mathbf{G}_i^T \mathbf{G}_i$ respectively. In these equations the random vectors $\boldsymbol{\mathcal{P}}_i$ follow a discrete uniform distribution taking the values ± 1 with probability 0.5.

Replacing the random variable $\boldsymbol{\mathcal{P}}_i$ with one of $k \in \{1 \dots K\}$ realizations named as $\mathbf{p}_{ik}$, for each observation group i and each realization k, and introducing the transformed realizations of the random vector, $\bar{\mathbf{p}}_{ik} = \mathbf{A}_i^T \mathbf{R}_i^T \mathbf{p}_{ik}$ and $\bar{\mathbf{p}}_{ik} = \mathbf{G}_i^T \mathbf{p}_{ik}$ respectively, eq. (5) and (6) can be written for a single realization as

$$r_{ik} = n_i - \frac{1}{\sigma_i^2} \bar{\mathbf{p}}_{ik}^T \mathbf{N}^{-1} \bar{\mathbf{p}}_{ik}. \quad (7)$$

This equation can now be evaluated by applying the iterative solver `pcgma` to additional right hand sides $\bar{\mathbf{p}}_{ik}$ for each realization k of each observation group i. In other words, `pcgma` is used to solve the system of equations $\mathbf{N}\mathbf{a}_{ik} = \bar{\mathbf{p}}_{ik}$ to compute the product

$\mathbf{a}_{ik} = \mathbf{N}^{-1}\bar{\mathbf{p}}_{ik}$. With the estimated parameters $\mathbf{a}_{ik}$ we are now able to compute the partial redundancy using the mean values of all realizations from each observation group by

$$r_i = n_i - \frac{1}{\sigma_i^2}\frac{1}{K}\sum_{k=1}^{K}\bar{\mathbf{p}}_{ik}^T\mathbf{a}_{ik}. \tag{8}$$

3 Effect of inaccuracies in the weights

When estimating new weight factors two elements could be erroneous, as we can see from eq. (2). First, the partial redundancy due to a random error of the stochastic trace estimator and systematic error caused by insufficient CG convergence in the additional trace parameters; second, the squared sum of residuals due to insufficient CG convergence in the estimation of the primary parameters ($\{c_{lm}\ s_{lm}\}$).

3.1 Effect of a trace error on the weights

Introducing an error into the trace estimation (number of parameters determined by group i) in eq. (5) and (6), the erroneous weights follow to be (cf. (2))

$$\begin{aligned}\tilde{\omega}_i &= \frac{n_i - (u_i + \Delta u_i)}{\Omega_i} = \frac{n_i - u_i}{\Omega_i} - \frac{\Delta u_i}{\Omega_i} \\ &= \omega_i - \Delta\omega_i.\end{aligned}$$

The relative weight error may then be written as a function of the relative error in the trace estimation,

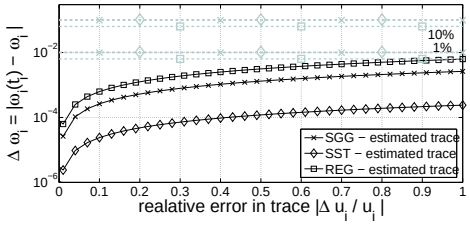
$$\frac{\Delta\omega_i}{\omega_i} = \frac{\frac{\Delta u_i}{\Omega_i}}{\frac{n_i - u_i}{\Omega_i}} = \frac{\Delta u_i}{n_i - u_i} = \frac{1}{\frac{n_i}{u_i} - 1}\frac{\Delta u_i}{u_i}, \tag{9}$$

demonstrating a linear dependence (with factor $a_i = \frac{1}{\frac{n_i}{u_i}-1}$) on the relative trace error. Evaluating the number of unknowns u_i and the number of observations n_i in the context of GOCE data processing (and taking into account the realistic resolutions), the factor a_i has the magnitude as shown in Table 1 for the different observation groups.

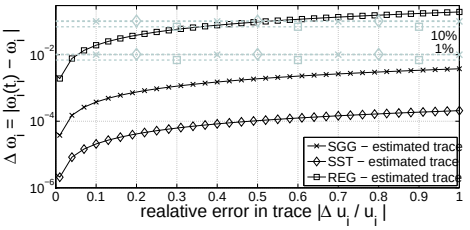
Table 1 Scaling factor of relative trace error on weights.

i	$\mathbf{n_i}$	$\mathbf{u_i}$	$\mathbf{a_i}$
sgg	$> 10^7$	$< 10^5$	$< 10^{-2}$
sst	$3 \cdot 10^6$	$< 10^4$	$< 3 \cdot 10^{-3}$
reg	$< 10^5$	$10^2 \ldots 10^5$	$10^{-3} \ldots 1$

Realizing that we can always limit the trace error to 100% (replacing the trace estimation by the assumption $u_i = 0$) the resulting weight errors for sgg and sst are limited to less than 1%. The strict estimation of the trace turns out to be unnecessary for these two observation groups. By introducing additional assumptions (all low frequency parameters are determined by sst and all high frequency parameters are determined by sgg) about u_{sst} and u_{sgg}, the resulting error could be reduced to about 0.1%.



(a) For model up to d/o 200.



(b) For model up to d/o 270.

Fig. 2 Absolute weight error due to a relative trace error.

If we take a look at the regularization group, we see a generally greater influence up to $a_{\text{reg}} = 1.0$. Inserting the optimal values for trace estimation and squared sum of residuals from a reference solution for two different resolutions (d/o 200 and d/o 270) we see the resulting weight error caused by a relative trace error in Fig. 2.

We may draw the following three conclusions:

1. The effect of a trace error is highly resolution dependent.
2. The effect of a trace error on sgg and sst is negligible for all realistic resolutions.
3. The quality in the trace estimation for the regularization group becomes more and more important with increasing resolution.

3.2 Effect of insufficiently converged residuals on the weights

An error $\Delta\Omega_i$ in the squared sum of residuals caused for example by insufficient convergence of the CG algorithm for the primary parameter estimation, could be introduced as

$$\tilde{\omega}_i = \frac{n_i - u_i}{\Omega_i + \Delta\Omega_i}. \tag{10}$$

Linearization according to Taylor implies

$$\Delta\omega_i \approx -\frac{n_i - u_i}{\Omega_i^2}\Delta\Omega_i + \frac{n_i - u_i}{\Omega_i^3}\Delta\Omega_i^2 \mp \mathcal{O}(\Delta\Omega_i^3)$$

as an error in the weights. A relative weight error as a function of the relative error in Ω_i can be written as

$$\frac{\Delta\omega_i}{\omega_i} \approx -\frac{\Delta\Omega_i}{\Omega_i} + \left(\frac{\Delta\Omega_i}{\Omega_i}\right)^2 \mp \mathcal{O}\Big(\big(\tfrac{\Delta\Omega_i}{\Omega_i}\big)^3\Big). \quad (11)$$

As can be seen in eq. (11) a relative error of insufficiently converged residuals in the first approximation causes an error scaled by 1 in the weights. In contrast to the trace estimator, the absolute error in $\Delta\Omega_i$ can be larger than Ω_i. Therefore, the relative error is not limited. But we have to keep in mind that an update of the weights has only a small influence on the parameters and therefore the iterative process (CG) can be restarted with more precise initial values. In addition we can take advantage of the typical behavior of the CG algorithm where the major part of the residuals is minimized in the first iteration steps.

3.3 Effect of weight errors on the final solution

As already mentioned in Section 3.1 and as will be seen in Fig. 5, the convergence of the weight for the regularization group is most critical. To investigate the behavior in detail we introduce an error in ω_{reg} to simulate the convergence of ω_{reg}. If convergence of the regularization group is reached we could assume that the sst and sgg weights have reached convergence up to higher digits. The error $\Delta\omega_{\text{reg}}$ is applied to the optimal estimation of ω_{reg}. With this weight and the optimal estimation of ω_{sst} and ω_{sgg} a complete CG iteration is performed to estimate an optimal solution for the potential coefficients $\mathbf{x}$ using the constant weight factors. Table 2 shows the results when a weight error of $\Delta\omega_{\text{reg}} = 0.1$ and 0.01, respectively, is added. With these errors the convergence of the weights up to the first and second digit is simulated. The differences are shown in terms of geoid heights with reference to the optimal solution for which all weights reached convergence (the model was resolved up to d/o 270).

Convergence of ω_{reg} up to the second digit (error $\approx 1.5\%$) causes a maximal error in terms of geoid heights with regard to the optimal solution of less than $1\,cm$, which is about one magnitude smaller than the mean error that the optimal solution of this test data set reaches with respect to the "true" model (ESA-AR3 data, EGM96 true model in closed loop simulation). As a conclusion we can say that the convergence of ω_{reg} up to the second digit leads to an insignificant error in the geoid, whereas the error caused by convergence up to the first digit ($\Delta\omega_{\text{reg}} = 0.1$) is one magnitude larger and thus exactly of the same magnitude as the outer accuracy, resulting in significant geoid errors.

4 Numerical Simulations

The following simulations are closed-loop simulations, i.e. the observations were created by using the EGM96 as input and adding a realistic GOCE noise; thus we have the advantage of knowing the true solution. We created a reference solution with simulated GOCE observations (60 days, $15\,000\,000$ sgg observations, sst normal equation matrix up to d/o 90), where a sufficient number of CG iteration steps were performed within each VCE iteration. As the regularization model we used Kaula's rule of thumb, introducing stochastic prior information assuming the spherical harmonic coefficients to be zero with a variance given by Kaula's rule ($\mathbf{P}_{\text{reg}}$). We computed the trace, squared sum of residuals and estimates for the weights within each CG iteration (step) ν of VCE iteration ι (named $\iota.\nu$) to see how the estimation performs. For this simulation $\nu_{\max}$ is fixed by 20 (d/o 200) and 10/20 (d/o 270) iterations for deriving a solution with 6 to 10 digits accuracy with respect to ω_i (see Fig. 5). The goal of this simulation is to determine where the main estimation effort takes place and to see where wasted CG iterations are done with respect to VCE. It will be seen that the main minimization in the CG algorithm is done in the first iterations. After this first steps, there is slow convergence to the optimal solution, which are wasted iterations in the context of VCE and for the parameter estimation, because the target function is, due to the non-optimal weights, wrong.

Table 2 Effect of an error in ω_{reg} on geoid heights [m], as difference to solution with optimal weights.

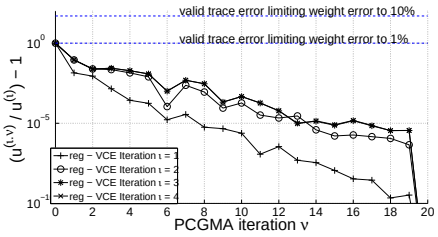
$\Delta\omega_{\text{reg}}$	**Sector**	**min/max**	**mean**	**rms**
0.1	$\pm 84°$	-0.075 / 0.091	0.000	0.009
0.1	$\pm 90°$	-0.127 / 0.112	0.000	0.012
0.01	$\pm 84°$	-0.007 / 0.009	0.000	0.001
0.01	$\pm 90°$	-0.012 / 0.014	0.000	0.001

In a first simulation the model is resolved up to d/o 200, in a second up to d/o 270. The reference solution for the d/o 200 model consists of 4 VCE iterations with 20 CG iterations each. For the d/o 270 model, 8 VCE iterations with 10 CG iterations each were required (the last VCE iteration was performed

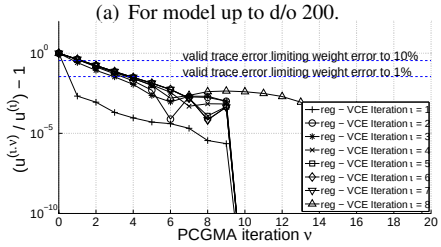
with 20 CG iterations to make sure CG reached convergence). The initial weights were chosen so that $\omega_{\text{sst}} = \omega_{\text{sgg}} = 1.0$ and $\omega_{\text{reg}} = 10^{-12}$ (i.e. assuming no regularization is needed). The initial values for the parameters were set to $\mathbf{x} = \mathbf{0}$.

4.1 Convergence of the trace estimation

As explained in Section 3.1, the trace estimation for the regularization group is the most critical issue. We have shown in Section 3.3 that we have to make sure that an error in the weight estimation is limited to 1%. If we assume the last trace estimation in each VCE iteration to be optimal, Fig. 3 shows the remaining error after each CG iteration for both models.



(a) For model up to d/o 200.



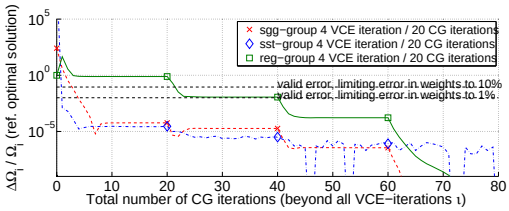
(b) For model up to d/o 270.

Fig. 3 Remaining relative trace error regarding trace estimation $u^{(\iota)}$, the estimation at the last CG iteration of the ι-th VCE iteration.

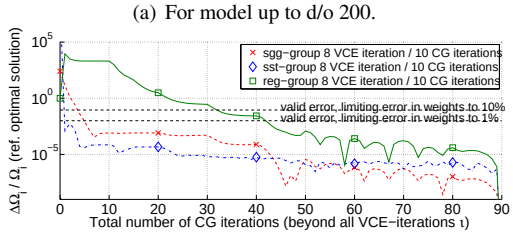
Using eq. (9) we can calculate the trace error which limits the weight error to 1%. We see that in the lower resolution model this threshold is immediately reached, but regarding the higher resolution model we see that the trace estimation needs at least 4 CG iterations to ensure that the weight error is limited to 1% (in a strict sense the 1% line in Fig. 3 is only valid for the final VCE iteration step where the trace and Ω_i assume realistic values).

4.2 Convergency of residuals

After applying the tailored preconditioner (cf. Boxhammer and Schuh (2006), Boxhammer (2006)) the convergence of the CG algorithm is very fast. Assuming the Ω_i to be minimal after the final CG iteration step of the last VCE iteration Fig. 4 shows the remaining errors over all CG iteration steps.



(a) For model up to d/o 200.



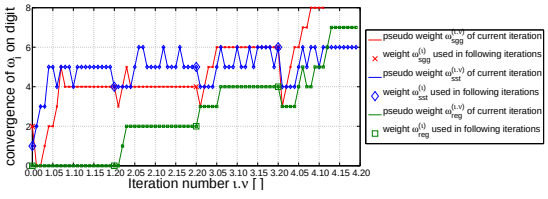
(b) For model up to d/o 270.

Fig. 4 Relative error in Ω_i with respect to the final value Ω_i of the last VCE iteration.

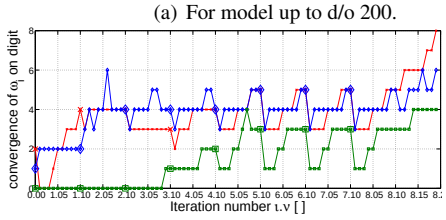
We can notice two important facts: the convergence of residuals is highly dependent on the resolution, and the main advance in each VCE step occurs in the first few CG steps. Counting the steps where Ω_{reg} is significantly reduced we obtain for the d/o 200 model about 5–7 iterations and for the d/o 270 model about 35 iterations.

4.3 Overall weight convergence

Starting from the trace estimation and the squared sum of residuals, the weights $\omega^{(\iota.\nu)}$ may be computed in each CG step (without applying them to eq. (1), which is why they will be called pseudo weights in the following figures). Assuming the ultimate weight estimation to be optimal, Fig. 5 shows the number of correct digits of weights in each CG step $\iota.\nu$.



(a) For model up to d/o 200.



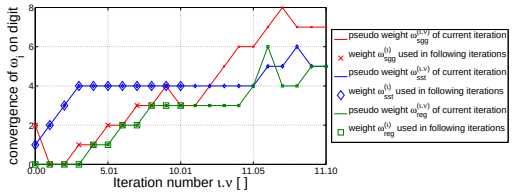
(b) For model up to d/o 270.

Fig. 5 Number of correct weight digits in each CG iteration ν of every VCE iteration ι. Ref.: last estimation.

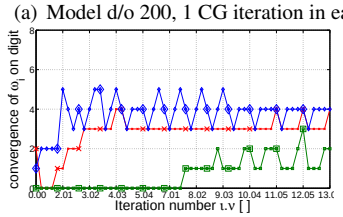
Although sgg and sst weights start with accurate values, the first estimations lose in accuracy (as a consequence of large Ω_i), but reach the convergence of the second digit after at most 5 steps. The convergence of the regularization group is thus limiting the overall convergence rate. For the d/o 270 model the effect on trace estimation is strong (starting at iteration 5.10). Because the additional parameters start from zero at each VCE step, 4 CG steps are always required to reach the second correct digit, and 6 CG steps are required to reach the third digit.

4.4 Optimized solution strategy

First of all, it is important to remark that for general parameter convergence it is not crucial how many CG iterations are done consecutively. The rate of convergence will not decrease if CG is restarted after only a few steps. It makes therefore sense to update the weights after as many CG steps the trace needs to be estimated correctly in each VCE iteration. This results in a sequence of 1 CG iteration in each VCE iteration for the d/o 200 model. Applying this strategy to the d/o 270 model 4 CG steps are necessary for the trace to converge. Fig. 6 shows the number of correct digits of the weights computed in this optimized strategy using the same reference of Fig. 5.



(a) Model d/o 200, 1 CG iteration in each VCE iteration.



(b) Model d/o 270, 4 CG iteration in each VCE iteration.

Fig. 6 Number of correct weight digits in each CG iteration ν of every VCE iteration ι for the optimized strategy.

5 Summary and outlook

In this paper we showed how VCE may be integrated into an iterative solution method for large scaled estimation problems. Starting from numerical simulations it was demonstrated how the VCE and especially the required trace estimation and the squared sum of residuals converge in two typical data sets of GOCE processing, limiting the expected resolution.

In this investigation we assumed the optimal decorrelation filter to be known. However, in the real GOCE data processing chain the iterative procedures considered in this paper are complemented by the iterative decorrelation filter estimation (Siemes (2008)). An interesting investigation would be how the filter estimation influences the VCE and vice versa. Another interesting investigation would be to integrate an additional data group, e.g. polar gap regularization (Metzler and Pail (2005)) or gridded surface gravity anomalies, and to analyse how this additional information influences the weight estimation.

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