Estimating signal loss in regularized GRACE gravity field solutions

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SUMMARY

Gravity field solutions produced using data from the Gravity Recovery and Climate Experiment (GRACE) satellite mission are subject to errors that increase as a function of increasing spatial resolution. Two commonly used techniques to improve the signal-to-noise ratio in the gravity field solutions are post-processing, via spectral filters, and regularization, which occurs within the least-squares inversion process used to create the solutions. One advantage of post-processing methods is the ability to easily estimate the signal loss resulting from the application of the spectral filter by applying the filter to synthetic gravity field coefficients derived from models of mass variation. This is a critical step in the construction of an accurate error budget. Estimating the amount of signal loss due to regularization, however, requires the execution of the full gravity field determination process to create synthetic instrument data; this leads to a significant cost in computation and expertise relative to post-processing techniques, and inhibits the rapid development of optimal regularization weighting schemes. Thus, while a number of studies have quantified the effects of spectral filtering, signal modification in regularized GRACE gravity field solutions has not yet been estimated.

In this study, we examine the effect of one regularization method. First, we demonstrate that regularization can in fact be performed as a post-processing step if the solution covariance matrix is available. Regularization then is applied as a post-processing step to unconstrained solutions from the Center for Space Research (CSR), using weights reported by the Centre National d’Etudes Spatiales/Groupe de Recherches de geodesie spatiale (CNES/GRGS). After regularization, the power spectra of the CSR solutions agree well with those of the CNES/GRGS solutions. Finally, regularization is performed on synthetic gravity field solutions derived from a land surface model, revealing that in some locations significant signal loss can result from regularization. This signal loss is similar in magnitude to estimated signal loss in post-filtered solutions. End-users of GRACE data can use this method to improve the error budgets of GRACE time-series, or to restore the power lost through regularization using a scaling technique.

Key words: Satellite geodesy; Time variable gravity; Hydrology.

1 INTRODUCTION

Time-varying gravity field solutions have been produced using data from the Gravity Recovery and Climate Experiment (GRACE) satellite mission since its launch in 2002. Solutions are often reported as sets of spherical harmonic coefficients, complete to degree, \( l \), and order, \( m \), up to some maximum value, for example, \( l_{\text{max}} = 60 \). These solutions contain both random errors that increase as a function of spectral degree (Wahr et al. 1998) and systematic errors that are correlated within a particular spectral order (Swenson & Wahr 2006). To reduce the effects of these errors, and thereby improve the signal-to-noise ratio of these data, two different methods are commonly employed. One method consists of applying spectral filters to the spherical harmonic coefficients comprising the gravity field solutions. From the general isotropic Gaussian filter (Wahr et al. 1998) to more complex filters that depend on degree, order and perhaps time (Swenson & Wahr 2002, 2006; Han et al. 2005; Seo & Wilson 2005; Werth et al. 2009), a menagerie of filters designed specifically for GRACE populate the literature. A second strategy utilizes damped least-squares algorithms to constrain the solution to be close to an a priori solution estimate (Lemoine et al. 2007; Save 2009). This is achieved by adding a penalty based on the weighted solution length to the least-squares cost function. This method has not been an option for most users, because it requires the model covariance matrix, which has not been a publically available product from the GRACE Project. It can be shown, however, that these two methods produce solutions having comparable power spectra.

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While the ideal error reduction strategy would increase the signal-to-noise ratio by selectively removing noise only, in practice both signal and noise are modified. A technique still may be judged to be effective if the reduction in noise greatly outweighs signal loss. Thus, to assess the effectiveness of an error reduction method, an estimate of the signal loss is required. Signal loss caused by the application of spectral filters to unconstrained GRACE gravity field solutions can be estimated by applying the filter to synthetic gravity field coefficients derived from simulations of surface mass variations produced by models of land and ocean water storage (Swenson et al. 2003; See & Wilson 2005; Werth et al. 2009). By comparing the original and filtered simulated mass estimates, a quantitative measure of the filter-induced signal loss can be obtained. A similar signal-loss estimate can be determined for regularization by applying the gravity field determination procedure to synthetic instrument data. The disadvantage in this case is that the expertise required and the computational cost of running such simulations is significantly greater than that incurred when generating the simulations for the spectral filtering techniques.

In this paper, we show that if the covariance matrix used in the unconstrained least-squares gravity field solution process is available, then it is possible to perform regularization as a post-processing step, rather than as an internal step in the solution process. In the following sections, after describing the GRACE data and the geophysical model output used to generate synthetic data, we relate the damped solution to the unconstrained solution through the covariance matrix, and apply the CNES/GRGS regularization weights to the Center for Space Research (CSR) solutions. The resulting regularized CSR solutions are compared to both the regularized GRGS solutions and the filtered CSR solutions. Finally, regularization is applied to models of surface mass variability to quantify the likely signal loss in the regularized GRACE solutions.

2 DATA

2.1 GRACE

2.1.1 CSR Solutions

As part of its participation in the GRACE Project, CSR provides one of the official GRACE Level-2 global gravity field products. The CSR gravity fields, which are provided as spherical harmonic coefficient sets complete to degree and order 60, are determined from Level-1 data produced by a suite of instruments aboard the twin GRACE satellites (Tapley et al. 2004). While all measurement types are necessary to produce accurate gravity fields, the most important observation is made by the K-band ranging system, from which the K-band range rates are determined (Case et al. 2010). These data are used in a least-squares inversion to estimate updates to a background gravity field model. This study uses CSR Release-4 (RL04) gravity global fields. The background gravity field model used for Release-4 includes the Gif/22A static gravity field, as well as models of tidal and non-tidal atmospheric and oceanic mass variability (Bettadpur 2007; Flechtner 2007). Because solutions incorporate approximately 30 days of data, they are referred to as monthly solutions. No constraints are applied during the least-squares inversion.

2.1.2 Groupe de Recherches de Geodesie Spatiale (GRGS) Solutions

This study uses Release 01 gravity field solutions produced by GRGS (Lemoine et al. 2007). The GRGS solutions also use the traditional method of dynamic least-squares parameter adjustment to determine time-variable corrections to a background gravity field model. However, the GRGS processing strategy differs in a number of ways. The background gravity model is EIGEN-GRACE-02S, complete to degree and order 150 (Reigber et al. 2005), and a barotropic ocean model, MOG2D, is used (Carrere & Lyard 2003). GRGS computes its own K-band range rates, rather than using those provided by the GRACE Project. To improve the lowest degrees, for example, degrees 2 to 4, data from LAGEOS-1 and -2 are included. Solutions are based on 30 days of data, but the 10 days in the middle of the time period are given double weights relative to the 10 day periods before and after. A solution centred on each 10-day period is then computed up to 50 degree. Perhaps the most important difference between the CSR and GRGS solutions is the use by GRGS of a damped least-squares inversion method. To reduce the amount of noise present in the GRGS solutions, the time-variable coefficients are damped toward the static field coefficients using weights described by the following equation

\[
\omega_n = \sqrt{2.5 e^{-\frac{91}{2n^2}}},
\]

where \(n\) refers to the degree.

2.2 The Community Land Model

The effect of regularization on the recovered signal can be estimated by applying the inversion process to a model of surface mass variability. By far the largest surface mass fluctuations come from changes in the distribution of water and snow stored on land. Here, we use the Community Land Model version 4 (CLM), which is the land component of the Community Climate System Model, to estimate terrestrial water storage variations. CLM simulates the partitioning of mass and energy from the atmosphere, the redistribution of mass and energy within the land surface, and the export of fresh water and heat to the oceans. To realistically simulate these interactions, CLM includes terrestrial hydrological processes such as interception of precipitation by the vegetation canopy, throughfall, infiltration, surface and subsurface run-off, snow and soil moisture evolution, evaporation from soil and vegetation and transpiration (Oleson et al. 2008).

Simulations of the global land surface state were produced by running the model at 2.5° longitude by 1.9° latitude spatial resolution using observed forcing data generated by the Global Land Data Assimilation System (GLDAS) (Rodell et al. 2004). GLDAS provides 1° by 1°, 3-hourly, near-surface meteorological data (precipitation, air temperature and pressure, specific humidity, short- and long-wave radiation and wind speed) for the period 2002 to the present. Land surface state variables were initialized from the land surface state at the end of a multidecade offline run. Surface water (i.e. river channel) storage, soil moisture, groundwater and snow mass from the CLM simulations were combined to construct a synthetic surface mass signal.

3 METHODS

3.1 Standard Least Squares

In the gravity field determination process, measurements made on the satellites are used to infer spherical harmonic coefficients of the gravity field. While the relationship between the data and model is generally non-linear, a linear approximation is valid when small updates to a reference gravity field model are made. In this case, the
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0
10
20
30
40
50
60
degree

10-13
10-12
10-11
10-10

GRACE CLM

CSR
GRGS

Figure 1. Left panel: GRACE degree amplitude spectra for CSR (solid line) and GRGS (dashed line) gravity fields; right panel: degree amplitude spectrum for the synthetic gravity field derived from a CLM simulation.

reference, or background, model is used to predict measurements, and the differences between these predictions and the data are used in a linear least-squares inversion process to estimate corrections to the background model. Thus, in the linear approximation,

\[ y = Hx, \]

where the vector \( y \) represents the data residuals (e.g. differences between the observed K-band range-rates and those predicted from the background gravity field model), the vector \( x \) represents the updates to the spherical harmonic coefficients of the reference gravity field, and the matrix \( H \) contains the partial derivatives relating changes in the model to changes in the data.

In standard least-squares, the cost function is defined as the square of the difference between the data and the predictions

\[ \epsilon = (y - Hx)^T(y - Hx), \]

and a solution is obtained by minimizing \( \epsilon \)

\[ \frac{\partial \epsilon}{\partial x} = 0. \]

This leads to a solution of the form (Menke 1989)

\[ x = [H^T H]^{-1} H^T y, \]

where \([H^T H]^{-1}\) is the model covariance matrix.

The gravity field determination process for GRACE has many more observations than model parameters, and therefore, in principle, is overdetermined. However, some model parameters are more poorly determined than others, leading to highly uncertain parameter estimates. This effect can be seen in the CSR RL04 solutions by plotting the degree amplitudes, defined as

\[ A_l = \frac{1}{N} \sum_{t=0}^{N-1} \sum_{m=0}^{l} (C_{lm}(t))^2 + (S_{lm}(t))^2 \frac{2l+1}{2l+1}, \]

where \( N \) is the total number of monthly solutions, \( C_{lm} \) and \( S_{lm} \) are the gravity field coefficients, and the temporal mean has been removed from each coefficient before computing \( A_l \). Fig. 1 compares the degree amplitude spectrum of the CSR RL04 gravity field solutions (left panel) to the spectrum derived from a CLM simulation (right panel). The CSR RL04 spectrum decreases until about degree 30, after which it increases, while the spectrum estimated from CLM decreases nearly monotonically. From this comparison, we infer that the large amplitudes of the high degree coefficients are largely the result of errors in the data propagating into the solution.

3.2 Damped Least Squares

In underdetermined or mixed-determined problems, the cost function (eq. 3) can be modified to include solution error in addition to prediction error (Menke 1989). Using solution length as an estimate of solution error, the cost function becomes

\[ \epsilon_{damped} = \epsilon + \alpha^T x^T x \alpha, \]

where \( \alpha \) is a factor that determines the relative weight of solution error relative to model error. Solutions based on the cost function (7) are called damped least squares, or regularized, solutions and have the form

\[ x_{\alpha} = [H^T H + \alpha^T x^T x \alpha]^{-1} H^T y. \]
where $\alpha$ is the weight matrix. Typically $\alpha$ is a diagonal matrix whose elements $\alpha_i^2$ vary; in this study $\alpha_i^2$ are given by eq. (1).

An example of a damped least-squares solution is shown in the left panel of Fig. 1 by the dashed line, which represents the degree amplitude spectrum of the GRGS solutions. Because large model parameter values are penalized by the modified cost function, the GRGS damped solution does not exhibit the increasing degree amplitudes seen in the CSR solutions above degree 30. Eq. (8) provides one way to calculate the damped least-squares solution. For users of GRACE data who wish to estimate the effect of regularization on the surface mass signal, this approach may be undesirable due to the need for sophisticated simulation software to create synthetic measurements, $y$, from land and ocean models. This is a reason that development of spectral filters designed for GRACE data has been an active area of research by the end-user community, while regularization methods have largely been feasible only to those with expertise in gravity field determination.

### 3.3 Filtering

Post-processing of the standard (i.e. unconstrained) GRACE solutions provides comparable results to regularization, but with substantially smaller computational burden. Furthermore, the effect of the filter on the signal can be estimated easily by applying the filter to synthetic solutions, which are obtained by converting gridded surface mass simulations (e.g. output from land and/or ocean models) to truncated spherical harmonic coefficient sets. In many cases, the effect of the filter on the mass estimate is small, but for other cases, the signal loss due to the filtering may be the dominant term in the error budget. For example, Velicogna & Wahr (2005) found that filtering (via an optimized averaging kernel) caused signal loss of $\sim 50$ per cent in their estimates of Greenland mass balance from GRACE, while Swenson & Wahr (2007) found a $\sim 60$ per cent reduction in the amplitude of mass variations of the Caspian Sea using GRACE data that had been processed using the decorrelation filter of Swenson & Wahr (2006). The left panel of Fig. 2 compares CSR RL04 standard solutions (solid line) to solutions that have been filtered using the decorrelation filter described in Swenson & Wahr (2006). The reduction in the magnitude of the degree amplitude spectrum for high degrees is similar to that obtained by regularization (Fig. 1). An estimate of the signal loss due to the application of the filters is shown in the right panel of Fig. 2. The solid line shows the original degree amplitude spectrum of the CLM simulation, while the dashed line shows that of the filtered spectrum. The magnitude of the signal estimate shows progressively larger reductions at higher degrees, implying that both signal and error are affected by the filtering process. This trade-off between error reduction and signal loss is a feature of all filters.

### 3.4 Regularization

If regularization could be applied to the standard unconstrained GRACE solutions, it would greatly facilitate the ability of a GRACE data user to assess the trade-off between error reduction and signal loss caused by regularization, and to create weighting schemes optimized for specific regions. In this section, we show that if the covariance matrix and solution from the standard least-squares case are available, regularization can be expressed in terms of a matrix

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Figure 2. Left panel: CSR GRACE degree amplitude spectra for standard (solid line) and filtered (dashed line) solutions; right panel: degree amplitude spectrum for a synthetic gravity field derived from CLM (solid line) and after filtering (dashed line).
Figure 3. GRACE degree-order amplitude spectra for original CSR (left panel), regularized CSR (middle panel), and GRGS (right panel) solutions. Even and odd degree coefficients are shown in blue and red, respectively. For each degree, the order increases from left to right.

Figure 4. Same as Fig. 3, except only degrees between 30 and 35 are plotted.
operation on the unconstrained solution. Then the regularization operator can be applied to synthetic gravity field coefficients derived from land models to estimate signal loss, as has been done with spectral filters (Swenson et al. 2003; Seo & Wilson 2005; Werth et al. 2009).

An expression relating the regularized solution to the unconstrained solution can be obtained by simply solving eq. (5) for $H^T y$ (i.e. using the original normal equations) and substituting this expression into eq. (8). This leads to the equation

$$x_{\alpha} = \left[ H^T H + \alpha^T \alpha \right]^{-1} [H^T H] x,$$

(9)

which requires the unconstrained solution, its covariance matrix, and a weight matrix. One can easily see that when $\alpha$ is zero, $x_{\alpha}$ and $x$ are equal.

4 RESULTS

4.1 CSR/GRGS comparison

In this section, we compare the GRGS Release 01 regularized fields to CSR Release 04 fields that have been regularized as a post-processing step using eq. (9). The damping weights are taken from Lemoine et al. (2007) and are given by eq. (1). Because of the exponential function in eq. (1), the damping applied to the coefficients increases rapidly with increasing degree. After applying this regularization scheme to the CSR solutions, the noise in the high degree region of the degree amplitude spectrum (Fig. 1) is greatly reduced. Fig. 3 compares the degree-order amplitude spectra, $A_{lm}$

$$A_{lm} = \frac{1}{N} \sum_{t=0}^{N} (C_{lm}(t))^2 + (S_{lm}(t))^2.$$

(10)

of the original, regularized CSR, and GRGS solutions. Even-degree coefficients are plotted in blue and odd-degree coefficients are plotted in red. For each degree $l$, all coefficients of order $m$ are plotted from $m = 0$ to $m = l$. The damping of the original CSR solutions (left panel) results in regularized solutions (middle panel) that exhibit the same general amplitude decrease as a function of degree seen in the GRGS solutions (right panel). In addition to having large values at high degrees, the original CSR gravity field coefficients typically increase with increasing order. This can be seen more clearly in Fig. 4, which focuses on degrees 30 through 35. The

![Figure 5](https://academic.oup.com/gji/article-abstract/185/2/693/673871)
order-dependence of the regularized CSR and GRGS coefficients is much less pronounced than that of the original CSR coefficients. While the near-sectorial (i.e. \( l \sim m \)) terms still have the largest coefficients within a particular degree-band, the low- and middle-order amplitudes tend to be more uniform. This indicates that the higher order coefficients are more heavily damped by the regularization than the lower order coefficients; because the orbit of the GRACE satellites is nearly polar, the sectorial coefficients are less-well determined than the near-zonal coefficients.

In the spatial domain, the GRGS and CSR regularized solutions also agree reasonably well. Fig. 5 compares these solutions, as well as the original and post-filtered CSR solutions. Each map represents a single monthly solution that has had the temporal mean removed. The regularized solutions have not been further post-filtered, and in each case the sum is complete to degree and order 50. All solutions are expressed as mass in units of centimetre equivalent water thickness. The map of the original CSR field (Fig. 5, lower left panel) is dominated by noise. When either filtering or regularization is applied, much of this noise is removed from the solution. The upper left panel of Fig. 5 shows the results of post-filtering the CSR solution, while the upper right panel shows the standard CSR solution after regularization. The lower right panel of Fig. 5 shows the GRGS regularized solution. In the latter three cases, the large signals associated with the seasonal cycle of water storage in tropical land areas are clearly evident. Over much of the ocean, the residual errors are still significant. The filtering process used to create the filtered CSR solution in the upper left panel is designed to remove north–south trending features, and thus the residual noise is generally patchy in nature. The regularization scheme does not target the stripe-like features explicitly, but rather preferentially damps higher degree terms. The residual noise in both regularized solutions therefore still exhibits north–south striping, but with considerably smaller magnitude than the original solutions. The greater damping of the high degree terms seen in the GRGS solution relative to the regularized CSR solution (Fig. 3) is manifested in residual noise characterized by longer-wavelength features in the GRGS solution and more prominent short-wavelength features in the regularized CSR solution. Fig. 6 shows the amplitude of the best-fitting mean annual cycle for the entire data span, for each of the cases shown in Fig. 5. Although in each case the presence of noise is greatly reduced compared to a single month of data, the annual cycle of the original CSR fields still contain significant noise, indicated by

Figure 6. Comparison of amplitude of mean annual cycle for original CSR solution (lower left), filtered CSR solution (upper left), regularized CSR solution (upper right) and GRGS solution (lower right). Maps are expressed in centimetre equivalent water thickness.
the north–south stripe-like features over the ocean. Some of these features are faintly visible in the filtered and regularized annual amplitude maps, but overall the maps agree quite well. The CSR regularized map shows larger features over the oceans than does the GRGS map. This may be caused by regularizing each month’s solution using the same covariance matrix. It is likely that the true covariance matrices are different for each month, due to differences in instrument data quality and orbit characteristics. Because we only had a single covariance matrix, we could not explore this issue, but it is likely that using covariance matrices specific to each month would lead to results that are as good or better than those shown in the upper-right panel of Fig. 6.

4.2 Signal loss estimate

Having shown that regularizing the standard CSR solution as a post-processing step leads to a reduction in noise that is comparable to the internally regularized GRGS solutions, we may now estimate the signal loss, if any, that occurs. A synthetic truth data set was created by constructing monthly spherical harmonic coefficients, truncated at degree 60, from the CLM simulation of terrestrial water storage. Each monthly solution was then regularized using the CSR covariance matrix, and a damped least-squares solution was obtained via equation (9). Fig. 7 shows maps of the amplitude of the mean annual cycle derived from the CLM truth solutions (left panel) and regularized solutions (right panel). Overall, the maps are similar, but one can see a reduction in the magnitude of the signal, for example, across Eurasia and North America. The modification of the signal by the regularization process can be seen clearly in regional time-series. Fig. 8 shows the time-series for three regions using the synthetic CLM fields. The blue line represents the original (truth) signal, the red line represents the regularized field, and the green line represents the field after filtering. In each case, the amplitude of the regularized and filtered solutions is reduced. The reduction can be quantified by comparing the root-mean-square (rms) variation in the time-series. For the Amazon River basin (top panel) the ratio of the regularized rms to the original rms is 0.91 and the ratio of the filtered rms to the original rms is 0.95. The ratios for the Fraser River basin, which is located near the west coast of Canada (238E, 52N), are 0.84 and 0.74. Time-series for the Caspian Sea give ratios of 0.41 and 0.42. These results show that regularization does modify the signal, and that the effects are similar to those due to filtering.

5 DISCUSSION

Beginning with the first release of GRACE data, there has been a debate within the GRACE community regarding the utility of
Figure 8. Regional average time-series for the Amazon River basin (upper panel), the Fraser River basin (middle panel) and the Caspian Sea (lower panel). Blue line is truth CLM surface-mass estimate, red line is regularized estimate and green line is filtered estimate. Results are expressed in centimetre equivalent water thickness.

regularized solutions. While regularized solutions offer a relatively noise-free product to the end-user, their usefulness may be compromised by the potential signal modification, which is unknown. For example, a user who wishes to validate model simulations of terrestrial water storage can not quantify the uncertainty bounds for the GRACE data. We hope that the results of this study will help resolve this question by clarifying the fact that the regularized solution can be expressed as a linear function of the unconstrained solution. This obviates the need to utilize gravity field determination software to construct synthetic instrument observations in the course of creating simulated regularized gravity field solutions, and makes it feasible for an end-user to quantify the effects of regularization on the signal of interest. Given an estimate of the effects of regularization, the error budget can be better constrained, or the signal amplitude can be restored using a scaling technique. This will also allow a more direct comparison of regularization and filtering schemes; in fact, the ability to regularize the standard solution as a post-processing step blurs the distinction between the two methods.

The goal of this study is not to assess whether filtering provides more accurate gravity field solutions than regularization (or vice versa). Rather, it is to demonstrate that regularized GRACE solutions, like filtered solutions, are subject to non-negligible signal suppression, and to provide users of GRACE data the means to estimate the amount of signal suppression, and therefore more robust error budgets.

The regularization scheme of GRGS was chosen simply because it has been described in the publically available literature. The results of this paper imply that the GRGS regularization scheme induces signal loss in the solutions, but these results should not be used quantitatively because the GRGS covariance matrices and unconstrained solutions were not used here. To quantify the actual amount of signal loss, if any, present in the GRGS regularized solutions (or any other regularized solutions) the specific covariance matrix and unconstrained solution should be used.

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