The use of Least-Squares Collocation for the processing of GOCE data

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Kurzfassung

Die Methode der Kollokation nach Kleinsten Quadraten (engl. LSC) basiert auf Überlegungen, die von H.Moritz für optimale Schwerefeldinterpolation, Prädiktion, Filterung und Parameterschätzung entwickelt wurde. Die Methode wurde von T. Krarup zur Lösung von partiellen Differentialgleichungen weiterentwickelt, wie z.B. die Laplace-Gleichung zur Verarbeitung heterogener Daten, sowohl im Randbereich als auch im Raum. Diese Methode ist daher auch sehr gut für die Bearbeitung jener Messdaten geeignet, die im Rahmen der ESA-Mission Gravity and Ocean Circulation Explorer (GOCE) anfallen. Die mittels GPS bestimmten Bahnparameter wären für die Berechnung der langwelligen Anteile des Schwerefeldes geeignet, während Bandbreiten-limitierte Gradiometer-Daten zur Bestimmung kurzer Wellenlängen bis hinunter zu 100 km genutzt werden könnten. Da erwartet wird, dass bei dieser Satellitenmission Millionen von Daten anfallen werden, ist die Nutzung von LSC nicht möglich, da LSC gleichviele Gleichungen wie Beobachtungen bedingt. Jedoch kann LSC zur Grid-Erstellung durch Prädiktion in kleinräumigen Bereichen herangezogen werden, wobei die interpolierten Daten Gleichungssysteme ergeben, die mit schnellen Methoden gelöst werden können. Leider müssen die in den interpolierten Daten (Grid-Daten) enthaltenen Fehler als unkorreliert angenommen werden. Bei kleinen Grids mit 20000 Beobachtungen haben numerische Simulationen gezeigt, dass die Fehler-Korrelationen der berechneten sphärischen harmonischen Koeffizienten bis zu einem Ausmaß von 40 % als zu gering ausfallen, unter der Annahme von unkorrelierten Fehlern in den Grid-Daten. Andere Anwendungen von LSC werden für die GOCE Kalibrierung herangezogen, wobei bodenbezogene Daten hoher Qualität für die Prädiktion von GOCE Messungen in Satellitenhöhe herangezogen werden.

Schlüsselwörter: Schwerefeld, Kollokation nach Kleinsten Quadraten, GOCE, Kalibrierung

Abstract

The method of Least-Squares Collocation (LSC) is based on ideas developed by H. Moritz for optimal gravity field interpolation, prediction, filtering and parameter estimation. The method was further developed by T. Krarup, for the use of solving partial differential equations, like the Laplace equation, using heterogeneous data both at the boundary and in space. The method is therefore well suited to handle data to be measured by ESA's Gravity and Ocean Circulation Explorer (GOCE) mission. Orbit data observed by GPS may be used to determine the long-wavelength part of the gravity field while the band-limited gradiometer data may be used to determine shorter wavelengths down to 100 km. The satellite is expected to collect millions of data, and this makes it impossible to use LSC which requires as many equations to be solved as the number of observations. However, LSC may be used to grid the data by prediction on local areas, and the gridded data results in systems of equations which can be solved by fast methods. Unfortunately the gridded data has to be considered as having uncorrelated errors. For small grids with 20000 observations numerical simulations have shown that error-correlations of computed spherical harmonic coefficients may be up to 40 % too small under this assumption of uncorrelated errors of the gridded data. Other applications of LSC are in the use for GOCE calibration, where high quality ground data are used to predict GOCE measurements at satellite altitude.

Keywords: Gravity field, Least-Squares Collocation, Gravity and Ocean Circulation Explorer Mission (GOCE), Calibration

1. Introduction

The anomalous gravity potential, T, is a harmonic function, i.e. it fulfills a partial differential equation, the Laplace equation. This property permits us to use the Stoke's equation for geoid determination and the representation of the function through the coefficients of a series of spherical harmonics. Its determination requires gravity anomaly data distributed globally and with a homogeneous distribution. This required the interpolation and extrapolation of existing scattered gravity anomaly data. Furthermore, it is important to be able to calculate errors and error-correlations of these quantities.

A solution was found in the sixties in the method of Least Squares Prediction, see Moritz (1965) and Heiskanen and Moritz (1967, Section 7-6). Simultaneously a method for solving ordinary and partial differential equations called collocation was developed by mathematicians. This method has the property (when applied to the modeling of T) that more general classes of data (not necessarily associated with the surface of the Earth), could be used.

The connection between the collocation method and the method of Least Squares Prediction method was recognized by T. Krarup (1969), and lead to the development of the method called Least-Squares Collocation (LSC), which merged statistical and purely mathematical tools.

The relationship between the methods is most clearly illustrated by the fact that a covariance function (of the anomalous potential T) simultaneously is a reproducing kernel in a Hilbert space of harmonic functions.

When applying Least Squares Prediction, the covariance function is empirically estimated, and its use leads to predictions which are the "best" in a least-squares global sense. If the reproducing kernel is selected so that it approximates the covariance function, then the use of the collocation method will also lead to a solution which is the "best".

The method has been widely used for many gravity field applications: geoid determination, prediction of deflections of the vertical (see e.g. Heitz and Tscherning (1972)), gravity anomaly prediction and computation of spherical harmonic coefficients (Howe et al. 2003). Also the ability to compute error-estimates and error-correlations have been utilized, see e.g. Arabelos et al. (2007) and Arabelos and Tscherning (2008).

A limitation, however, has been that there has to be solved as many equations as the number of data. Different procedures have been proposed to circumvent this problem (Moritz, 1973, Tscherning, 1974). But if the data are gridded to form a grid of data distributed equidistantly in longitude, symmetries arise in the normal-equations, which may be taken advantage of. Based on ideas by Colombo (1979) a general procedure called Fast Spherical Collocation (FSC) was developed by Sansò and Tscherning (2003).

The planned use of LSC for processing data from the Gravity and Ocean Circulation Explorer Satellite (GOCE), Johannesen et al.,(2003) will be described in the following. It is very much due to the results achieved in the research of H. Moritz that LSC has matured so much that it has been accepted as a valid tool for the processing of data from the GOCE mission.

2. Processing of GOCE data

GOCE was launched 17 March, 2009 by ESA. The satellite carries GPS receivers which permit the precise determination of the position and velocity. The main gravity instrument is the 3 axis gradiometer, which will determine the gravity gradients, i.e. the second order derivatives of the potential V. The derivatives will be determined in a frame determined by star-trackers. Furthermore, in order to increase the sensitivity, the measurements will be restricted to the so-called measurement band-width, corresponding to wavelengths in the range from 100 km to 1200 km.

The data will initially be processed by the so-called High-Level Processing Facility (HPF) and subsequently made available for processing by groups approved by ESA. The HPF is composed of scientists from 10 European institutions, including TU Graz and the University of Copenhagen, who collaborate on producing the best possible results from GOCE.

There will be used 3 main processing schemes:

- the direct method, which use the basic observation equations and least-squares adjustment
- the time-wise method which takes advantage of the time-wise sampling of the data
- the space-wise method which take advantage of the spatial correlation of the data

Besides this the HPF will determine fast (using parts of the data) spherical harmonic solutions with the purpose of continuously checking the state of the satellite. A further task is the determination of possible outliers and the filling of data-gaps.

The satellite is expected to collect data in at least 2 years. The instruments will collect data with a 1 Hz sampling rate, so the amount of data will be very large.

The main products by the HPF will be spherical harmonic coefficients and associated error-covariances up to a maximum degree of about 250, (i.e. 62500 coefficients) and gravity gradients given in a North-West-Up (NWU) frame.

3. The use of LSC

3.1 Gridding and interpolating

The basic equations of LSC are shown in the Appendix. Here we see that in order to determine an approximation to T, a number of equations equal to the number of observations must be solved. This makes it impossible to use all data simultaneously.

However, LSC will be used to grid (interpolate) data, making the foundation for using numerical integration procedures to determine coefficients of a spherical harmonic expansion.

Initially the energy-balance method is used to produce values of V from the velocity vector converted to kinetic energy and corrected for time-varying phenomena. This gives us values of T at orbit altitude which using LSC will produce values in a grid equidistant in longitude at mean satellite altitude (as well as error-estimates). From these data spherical harmonic coefficients up to a maximal degree 100 may be determined. Both numerical integration and Fast Spherical Collocation may be used to estimate these coefficients. The use of FSC, however, requires that the errors of the interpolated data are uncorrelated – which is not the case. Consequently the error-estimates and error-correlations of the coefficients will be under-estimated, see Arabelos and Tscherning (2008).

The availability of a low-degree and order spherical harmonic solution makes it possible to restitute the gravity gradients to their full power and have them represented in an NWU frame. Here again LSC will be used to produce several new grids equidistant in longitude on parallels at the same distance from the center of the Earth. As an example let us regard the second order radial derivative.

$$\frac{\partial^2 T}{\partial r^2} = \frac{GM}{r^3}\sum_{i=2}^{\infty}\left(\frac{a}{r}\right)^i \sum_{j=-i}^{i}(i+1)(i+2)C_{ij}S_{ij}(\overline{\varphi},\lambda)$$

(see Appendix for the meaning of the different quantities). Consequently a spherical harmonic analysis will determine coefficients multiplied by $(i+1)(i+2)/r^2$ from which we obviously can find the coefficients C_{ij}.

This gravity gradient may be used together with other components in a weighted numerical integration procedure, see Migliaccio et al. (2004, 2005, 2007). The use of FSC has also been investigated, but it resulted in coefficient estimates which were inferior to those obtained by numerical integration. Here it is appropriate to mention that the GOCE orbit inclination leaves two gaps at the poles, with no data. If these gaps are filled in with values computed from an existing spherical harmonic solution, the result will improve.

3.2 Calibration of gravity gradients

As mentioned above the gravity gradients will have values given with the highest precision in the measurement band-width. In order to extract these precise data Fourier analysis is applied in order to obtain data in the band. A similar analysis is made of data computed from a spherical harmonic model, and the values corresponding to the measurement band-width are removed. The two time series are added, and we have "full" gravity gradients. These values are calibrated as described in Arabelos et al. (2007), Boumann et al. (2004 and 2008). In this calibration process LSC is applied in order to compute precise reference values over 5 selected areas, where the gravity field is smooth. The Fourier analysis is then applied on a time-series here with the enhanced values in the 5 areas and values derived from a spherical harmonic expansion outside the areas. Inside the areas the filtered calibrated values are compared to the filtered "enhanced" values. The comparison is done for each track which crosses the area, and it is checked that the two time-series have the same scale, see Bouman et al. (2008).

3.3 Gross-error detection and frame-transformation

The calibrated gravity gradients must be checked for gross-errors and converted from the instrument reference frame to the NWU frame.

The check for gross-errors may be done by predicting a gradient value from values nearby on the same track and comparing the difference to the error-estimate, see Tscherning (1991). The frame-transformation is simply done by selecting a local window, and then predicting the data in the NWU frame from the data in the instrument frame, see Tscherning (2004).

4. Outlook

The procedures for processing GOCE data by the HPF are "frozen" after having been checked in detail by ESA through simulations. The satellite should have been launched several years ago, and meanwhile computers have become faster and have facilities for multiprocessing (see e.g. Tscherning and Veicherts, 2007). If one considers that one of the main goals is the estimation of less than 70 000 numbers – coefficients – , then one may ask how much data are really needed, if one could select (cf. Arabelos and Tscherning, 2007) the "best" data from all the data collected during the expected 2 year lifetime of the satellite. A good guess is 10 times the number of coefficients, if one is able to select data which have uncorrelated noise, e.g. due to the fact that they have been measured at times a year or more apart. Also one may using LSC include precise ground data collected at the poles, so that one in the end have a dataset with 1 000 000 observations. The use of LSC with so many data will be a big but not impossible task.

Appendix: Basic equations (cf. Heiskanen and Moritz, 1967 and Moritz 1980).

The gravity potential W, is the sum of the potential V due to the attraction of the masses and the centrifugal potential. The anomalous potential is the difference between W and the normal potential U. In space quantities related to V are measured, while at the surface of the Earth W is the important quantity. T is however the same everywhere, because the centrifugal part is eliminated.

T may be represented by a series in spherical harmonics

$$T(\bar{\varphi},\lambda,r) = \frac{GM}{r}\sum_{i=2}^{\infty}\left(\frac{a}{r}\right)^{i}\sum_{j=-i}^{i}C_{ij}S_{ij}(\bar{\varphi},\lambda)$$

where r is the radial distance, λ the longitude, $\bar{\varphi}$ the geocentric latitude, S_{ij} the surface spherical harmonics and GM the product of the mass of the Earth and the gravitational constant and a is a scale-factor generally close to the semi-major axis of the earth's ellipsoid and C_{ij} the spherical harmonic coefficients.

The basic observation equation for LSC is

$y_i = L_i(T_{LSC}) + e_i + A_i^T X$, where

X are contingent parameters, A_i is a vector connecting parameters and the observations y_i, e_i is the error contribution.

Here the contribution from a contingent datum-transformation and a Earth Gravity Model must have been subtracted.

The estimate of T_{LSC} is obtained by

$\tilde{T}_{LSC}(P) = \left\{C_{Pi}\right\}^T \bar{C}^{-1}\left\{y - A^T X\right\}$, where

$\bar{C} = \left\{C_{ij} + \sigma_{ij}\right\}$, and

σ_{ij} is the variance-covariances of the errors.

The estimate of the (M) parameters are obtained by

$$\tilde{X} = \left(A^T\bar{C}^{-1}A + W\right)^{-1}\left(A^T\bar{C}^{-1}y\right)$$

The error-estimates and error-covariances, ec_{kl} are found with:

$$H_k = \left\{COV(L_k, L_i)\right\}^T \bar{C}^{-1}, \quad MxN\ matrix$$

$$m_X^2 = \left(A^T\bar{C}^{-1}A + W\right)^{-1}$$

$$\left\{ec_{kl}\right\} = \left\{\sigma_{kl}\right\} - H_k\left\{cov(L_j, L_l)\right\} + H_k A M_X (H_l A)^T$$

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