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Computation of spherical harmonic coefficients and their error estimates using least-squares collocation

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Abstract. Equations expressing the covariances between spherical harmonic coefficients and linear functionals applied on the anomalous gravity potential, T, are derived. The functionals are the evaluation functionals, and those associated with first- and second-order derivatives of T. These equations form the basis for the prediction of spherical harmonic coefficients using least-squares collocation (LSC). The equations were implemented in the GRAVSOFT program GEOCOL. Initially, tests using EGM96 were performed using global and regional sets of geoid heights, gravity anomalies and second-order vertical gravity gradients at ground level and at altitude. The global tests confirm that coefficients may be estimated consistently using LSC while the error estimates are much too large for the lower-order coefficients. The validity of an error estimate calculated using LSC with an isotropic covariance function is based on a hypothesis that the coefficients of a specific degree all belong to the same normal distribution. However, the coefficients of lower degree do not fulfil this, and this seems to be the reason for the too-pessimistic error estimates. In order to test this the coefficients of EGM96 were perturbed, so that the pertubations for a specific degree all belonged to a normal distribution with the variance equal to the mean error variance of the coefficients. The pertubations were used to generate residual geoid heights, gravity anomalies and second-order vertical gravity gradients. These data were then used to calculate estimates of the perturbed coefficients as well as error estimates of the quantities, which now have a very good agreement with the errors computed from the simulated observed minus calculated coefficients. Tests with regionally distributed data showed that long-wavelength information is lost, but also that it seems to be recovered for specific coefficients depending on where the data are located.

Key words: Spherical harmonic coefficients – Error estimation – Least-squares collocation

1 Introduction

When using least-squares collocation (LSC), available information about the spherical harmonic coefficients of the anomalous gravity potential, T, can be used directly as observations, or in a remove–restore procedure, see Forsberg and Tscherning (1981). However, if coefficients are to be predicted, we need the explicit covariances [or values of functionals applied on a reproducing kernel; see Tscherning (1974, Sect. 2.2) and Tscherning (1993)]. As shown in Sect. 2, the covariances are simply the observation functionals applied on the solid spherical harmonic function of a specific degree and order, multiplied by a constant which is dependent on the degree.

The equations have been implemented in the form of new versions of the subroutines COVAX, COVBX and COVCX (Tscherning 1976) in the program COVFIT (Knudsen 1987).

The equations to be used for the calculation of the estimates of the coefficients and their error estimates are derived in Sect. 3. They are implemented in a new version of the GRAVSOFT program (Tscherning et al. 1992) GEOCOL.

In Sect. 4 the results of coefficient prediction tests are described initially using the EGM96 (Lemoine et al. 1996) coefficients from degree 8 to 180. The coefficients were used as control data and to generate control data sets of geoid heights, gravity anomalies and second-order radial derivatives. The error estimates of the coefficients were compared to the differences between 'observed' and predicted coefficients, and it was found that the errors were too large for the low-degree coefficients. This seemed to be caused by the non-normal distribution of the low-degree coefficients.

The computational experiment was repeated, now using as coefficients from degree 2 to 180 pertubations of EGM96 generated using a random number generator so that they had a normal distribution with a variance which for a given degree was equal to the error degree variance of the EGM96 coefficients. Using the original EGM96 coefficients as a reference field, this resulted in error estimates which were in a very good agreement with the errors obtained in the calculations.

All derivations and tests have been carried out in spherical approximation. In order not to use this, the geodetic latitude must be changed to the geocentric latitude. Furthermore, the value of the radius vector (r), which is now calculated as $R + h$, where R is the mean radius of the Earth, must be computed rigorously from the Cartesian coordinates.

2 Covariances between spherical harmonic coefficients and point-related quantities

Let P, Q be two points with coordinates (latitude, longitude, r) (φ, λ, r), (φ', λ', r'), respectively, and having the spherical distance ψ. Y_{ij} are the surface spherical harmonics, P_i the Legendre polynomials and σ_i^2 the degree variances. Then, following the (non-stochastic) covariance definition of Heiskanen and Moritz (1967, Chap. 7), the covariance between the values of the anomalous potential T in P, Q is

$$\begin{aligned}\operatorname{cov}(P,Q) &= \sum_{i=2}^{\infty} \sigma_i^2 \left(\frac{R^2}{rr'}\right)^{i+1} P_i(\cos\psi) \\ &= \sum_{i=2}^{\infty} \frac{\sigma_i^2}{2i+1} R^2 \sum_{j=-i}^{i} \frac{R^i}{r^{i+1}} Y_{ij}(\varphi,\lambda) \\ &\quad \cdot \frac{R^i}{(r')^{i+1}} Y_{ij}(\varphi',\lambda') \end{aligned} \tag{1}$$

The covariance between the coefficient $GM\ C_{ij}/R$ and the anomalous potential is obtained by applying the functional L_{ij} on the covariance function, where

$$\begin{aligned} L_{ij}(T) &= \frac{1}{4\pi R^2} \int_\sigma \left(\frac{GM}{R} \cdot \sum_{n=2}^{\infty} \left(\frac{R}{r}\right)^{n+1} \sum_{m=-n}^{m=n} \right. \\ &\quad \left. \times C_{nm} Y_{nm}(\varphi,\lambda) \cdot \left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda) \right) \\ &\quad \times R^2 \cos\varphi \, d\varphi \, d\lambda = \frac{GM}{R} C_{ij} \end{aligned} \tag{2}$$

(units of m^2/s^2; the subscript σ at the integral sign signifies the mean Earth's surface).

Then we have

$$\begin{aligned} L_{ij}(\operatorname{cov}(P,Q)) &= \frac{1}{4\pi R^2} \int_\sigma \sum_{n=2}^{\infty} \frac{\sigma_n^2}{2n+1} \sum_{m=-n}^{n} \left(\frac{R}{r}\right)^{n+1} \\ &\quad \times Y_{nm}(\varphi,\lambda) \left(\frac{R}{r'}\right)^{n+1} \cdot Y_{nm}(\varphi',\lambda') \\ &\quad \times \left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda) R^2 \cos\varphi \, d\varphi \, d\lambda \\ &= \frac{\sigma_i^2}{2i+1} \left(\frac{R}{r'}\right)^{i+1} Y_{ij}(\varphi',\lambda') \end{aligned} \tag{3}$$

When applying the functional twice we obtain its norm, squared,

$$\begin{aligned} L_{ij}\ L_{ij}(\operatorname{cov}(P,Q)) &= \frac{1}{4\pi} \int_\sigma \frac{\sigma_i^2}{(2i+1)} \left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda) \\ &\quad \times \left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda) \cos\varphi \, d\varphi \, d\lambda \\ &= \frac{\sigma_i^2}{(2i+1)} = \|L_{ij}\|^2 \end{aligned} \tag{4}$$

or

$$\|L_{ij}\| = \frac{\sigma_i}{\sqrt{(2i+1)}} \tag{5}$$

The covariance with an arbitrary functional L_k is then

$$L_k\ L_{ij}(\operatorname{cov}(P,Q)) = \frac{\sigma_i^2}{2i+1} \cdot L_k\left(\frac{R^i}{r^{i+1}} Y_{ij}(\varphi,\lambda)\right) \tag{6}$$

Example

$$\begin{aligned} L_k &= -\frac{\partial}{\partial r} \rightarrow L_k\ L_{ij}(\operatorname{cov}(P,Q)) \\ &= (i+1)\left(\frac{\sigma_i^2}{(2i+1)R}\right)\left(\frac{R}{r}\right)^{i+2} Y_{ij}(\varphi,\lambda) \end{aligned}$$

$$\begin{aligned} L_k &= \frac{\partial^2}{\partial r^2} \rightarrow \frac{(i+1)(i+2)}{(2i+1)R}\ \sigma_i^2 \left(\frac{R}{r}\right)^{i+2} \frac{1}{r} Y_{ij}(\varphi,\lambda) \\ &= \frac{(i+1)(i+2)}{(2i+1)R^2}\ \sigma_i^2 \left(\frac{R}{r}\right)^{i+3} Y_{ij}(\varphi,\lambda) \end{aligned}$$

The correlation can also be calculated between, for example, the value of T in a point P and the i,jth coefficient $[ev_P(T) = T(P)]$

$$\rho(ev_P, L_{ij}) = \frac{\frac{\sigma_i^2}{2i+1}\left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda)}{\frac{\sigma_i}{\sqrt{2i+1}}\left(\sum_{i=2}^{\infty}\sigma_i^2\right)^{\frac{1}{2}}} \tag{7}$$

[Note that several of the above-derived equations may be found in a slightly different notation in Tscherning (1974).].

3 Prediction of spherical harmonic coefficients – theory

An approximation to T determined using LSC will have the form

$$\begin{aligned} \tilde{T}(P) &= \sum_{n=1}^{N} b_n \cdot \operatorname{cov}(P, L_n) \\ \{b_n\} &= \{C_{nm}\}^{-1}\{x_m\} \end{aligned} \tag{8}$$

with

$$\begin{aligned} &\operatorname{cov}(P, L_n) = L_n(\operatorname{cov}(P,Q)), \\ &C_{nm} = \operatorname{cov}(L_m, L_n) = L_m L_n(\operatorname{cov}(P,Q)) \end{aligned}$$

where b_n are the solutions of the normal equations, L_n are the observation functionals and N is the number of observations. If the data contain errors, the variance–covariance of the noise is added to the normal-equation matrix, $\{C_{nm}\}$.

The value of a predicted quantity is obtained by applying the associated functional to this expression. For the spherical harmonic coefficients we then have

$$\begin{aligned}\frac{GM}{R}C_{ij} &= \sum_{n=1}^{N} b_n \cdot \mathrm{cov}(L_{ij}, L_n) \\ &= \sum_{n=1}^{N} b_n \cdot \frac{\sigma_i^2}{2i+1} \cdot L_n\left(\left(\frac{R}{r}\right)^{i+1} Y_{ij}(\varphi,\lambda)\right) \qquad (9)\end{aligned}$$

The calculation of the observation functional applied to the solid spherical harmonic function is generally done by recursion, starting with the (0,0) term. This means that a better computational strategy would be to calculate all coefficients simultaneously up to and including degree i. However, this strategy should generally not be used when we want to calculate the error estimates

$$\begin{aligned}E(L_{ij}(T) - L_{ij}(\overline{T}))^2 &= \mathrm{cov}(L_{ij}, L_{ij}) - \{\mathrm{cov}(L_n, L_{ij})\}^T \\ &\quad \times C^{-1}\{\mathrm{cov}(L_{ij}, L_n)\} \qquad (10)\end{aligned}$$

because we must then store all the quantities $\mathrm{cov}(L_n, L_{ij})$ in the expression of Eq. (10) simultaneously, and subsequently evaluate the expressions for all degrees up to and including degree i.

At this point it is worth recalling that since we use an isotropic covariance function (kernel), cf. Eq. (1), the error estimate is an estimate of the error in a mean-square (MS) sense, which only can be interpreted in a standard manner if we deal with quantities associated with point or mean value functionals. This interpretation is independent of any assumed underlying stochastic model of the gravity field. For sets of coefficients of a given degree, an interpretation of the error as an MS error is possible if they all belong to the same normal distribution, and having the variance given by Eq. (4).

Finally, a remark on the computational procedures. If the coefficients have a normal distribution with the same variance for each degree, then we may compute error estimates by generating data from randomly generated normally distributed perturbed sets of coefficients. We may then calculate the difference between 'observed' coefficients and predicted values using Eq. (9). The MS difference should then give a correct estimate of the error which otherwise should have been calculated using Eq. (10), which is very demanding numerically.

4 Numerical tests of coefficient prediction and error estimation

LSC estimation of coefficients and of the corresponding error estimates should, according to theory, work. But will it work in practice? There are two reasons why this is now being tested.

First, computers have recently (i.e. 25 years after the equations were first derived) become so large that it would be numerically feasible to use the 100 000 observations needed to determine a global gravity field approximation corresponding to, for example, a set of spherical harmonic coefficients complete to degree 200. LSC has until now primarily been used successfully for local and regional gravity field approximation.

Second, the up-coming satellite gravity missions will produce data of mixed types (e.g. several of the second-order derivatives), a situation which LSC is especially well suited to handle.

Therefore, as mentioned in the Introduction, the GEOCOL program (Tscherning 1974) was upgraded to permit coefficient prediction implementing the equations given in Sects. 2 and 3.

Initially numerical test data were generated using EGM96 from degree 8 to 180. Here the results will be illustrated using two point configurations: (1) 400 points distributed in the centre of equal-area blocks having 10° latitude extent; and (2) 1600 additional points distributed with 5° spacing; 2000 points in total.

Three data types were generated: geoid heights, gravity anomalies and vertical gravity gradients, located either at zero altitude or at varying altitudes; see Table 1, in which selected results are presented. The covariance function used was the one generated from the EGM96 coefficients (the 'true' one). A signal to noise ratio of 10^3 was used throughout, since the investigation was not aimed at studying the influence of any noise.

Table1 shows – as expected – that the result improves with more gravity data and with a higher altitude. It is remarkable that, for this low degree, the second-order vertical gradient, T_{zz}, gives results which are nearly as good as those obtained when gravity was used. From Fig. 1 we see the expected result, namely that geoid heights and gravity give better results for lower degrees than T_{zz}. Figure 1 also shows that the main contributions to the coefficients are in the degrees below 40, corresponding very well to the data spacing of 5 degrees.

The root mean square (RMS) differences between predicted and 'observed' coefficients per degree are shown in Figs. 2–4. Two thousand values of each of the three data types at an altitude of 300 km have been used. The figures also show the root-mean collocation error estimates [Eq. (10)] and the coefficient root variances per degree. These figures show, as could be observed in Table 1, that the error estimates are too large. The largest discrepancy occurs for the case where geoid heights were used, and the smallest where vertical gravity gradients were used.

It might be supposed that the discrepancy was due to a program error. However, prediction tests using the same (global) data configurations (Sanso et al. 2000) showed an agreement between the MS differences between predicted and observed values and the LSC error estimate, Eq. (10). But since the prediction results were also excellent it was believed that the software used in the test was correct, so that the discrepancy must be caused by something else.

Table 1. Prediction of EGM96 spherical harmonic coefficients of degree 9 and order 9 to 0[1]

Order	Data type Height Number of observations	Gravity 0 m 400	Gravity 50 km 400	Gravity 300 km 400	Gravity 300 km 2000	T_{zz} 300 km 2000
m	EGM96					
9	−0.48	−0.02	−0.28	−0.63	−0.44	−0.39
8	1.88	0.76	1.29	1.84	1.82	1.82
7	−1.18	−0.24	−0.37	−0.84	−1.18	−1.26
6	0.63	0.58	0.75	0.80	0.59	0.48
5	−0.17	0.27	0.08	−0.13	−0.14	−0.04
4	−0.09	−0.08	−0.19	−0.23	−0.06	0.04
3	−1.70	−0.31	−0.80	−1.50	−1.53	−1.51
2	0.22	−0.63	−0.31	0.24	0.21	0.14
1	1.43	0.81	1.00	1.12	1.34	1.22
0	0.28	0.46	0.50	0.32	0.31	0.45
EGM96 − predicted	Mean	−0.18	−0.08	−0.02	−0.01	−0.01
	Standard deviation	0.64	0.40	0.18	0.07	0.14
	Estimat. error	0.79	0.60	0.34	0.29	0.32

[1] In column 2 are given the 'true' values, and in the following columns the estimated values for different altitudes and observation types. At the base of the table are given the mean and the standard deviation of the differences (ERM96 − predicted). In the last row the square root of the value calculated using Eq. (10), divided by GM/R, i.e. unitless, is given. Note that this value is much larger than the standard deviation in the second-last row. All values have been multiplied by 10^6

Recalling the final remarks of the previous section, an investigation was carried out to see whether the EGM96 coefficients had a normal distribution for each degree. Histograms per degree were formed; see Fig. 5. On inspecting the histograms, it immediately becomes clear that the lower-degree coefficients do not follow a normal distribution. [This fact has been conjectured by Jekeli(1991), based on certain theoretical considerations.] This also explains why the discrepancies were largest for geoid heights (which have the largest correlation with the lower-order coefficients) and smallest for the vertical gravity gradient.

In order to verify that we would be able to obtain valid error estimates for normally distributed coefficients, the following computational experiment was carried out. A random generator of data with a normal distribution with a given variance and zero mean was used to generate perturbed EGM96 coefficients. The program HARMEXG was used; see details in Tscherning et al. (1999). The variance of the normal distribution was set equal to the mean variance per degree of the EGM96 errors.

The perturbed coefficients were used to generate residual geoid heights, gravity anomalies and vertical

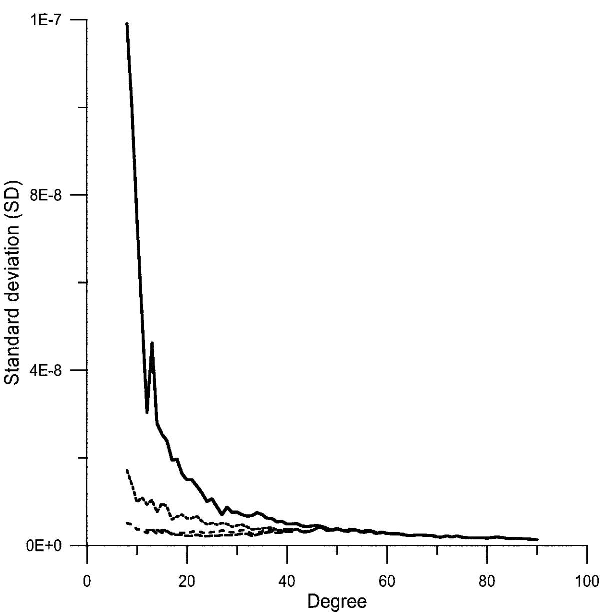

Fig. 1. Results of prediction of coefficients from degree 8 to 90. Data generated using EGM96 degree 8 to 180 ——— SD of coefficients; ······ SD of (obs.−pred.) coeff. from T_{zz}; - - - - - SD (obs.−pred.) coeff. from gravity; — — —— SD (obs.−pred.) coefficients from geoid

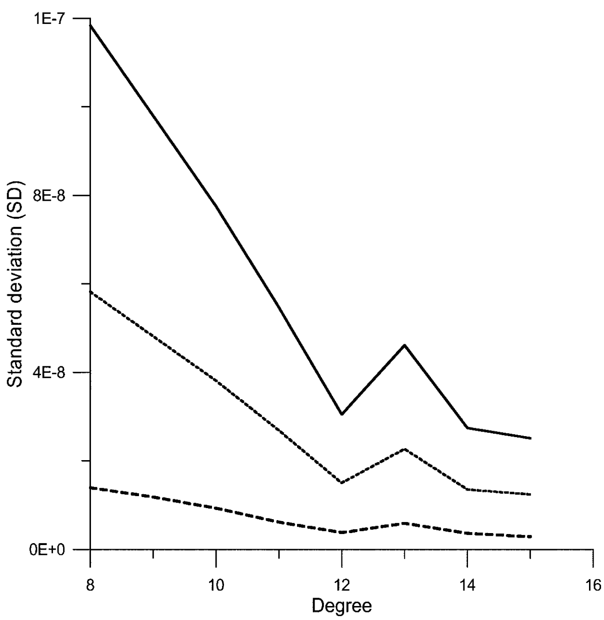

Fig. 2. Results of prediction of coefficients from degree 8 to 15 using geoid generated using EGM96 from degree 8 to 180 ——— SD of coefficients per degree; — — —— SD of (obs.−comp.); ······ Mean SD of collocation error estimates

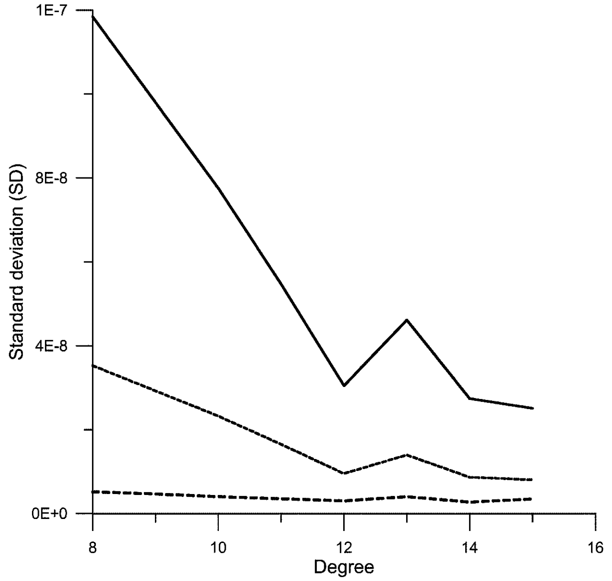

Fig. 3. Results of prediction of coefficients from degree 8 to 15 using gravity generated using EGM96 from degree 8 to 180 ——— SD of coefficients per degree; – – – – SD of (obs.–comp.); · · · · · · Mean SD of collocation error estimates

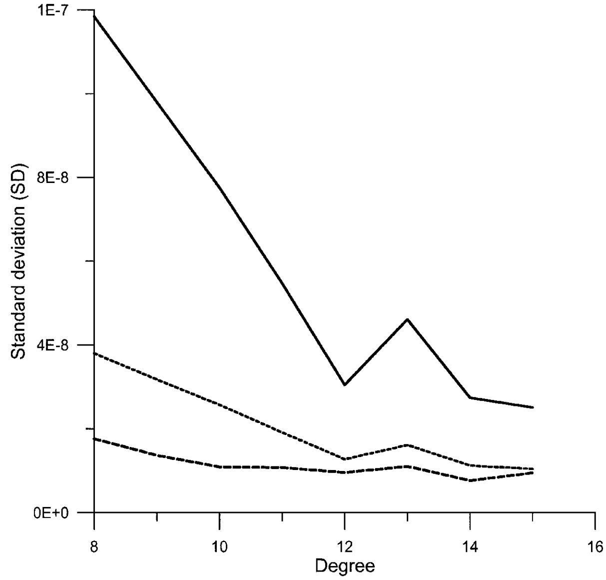

Fig. 4. Results of prediction of coefficients from degree 8 to 15 using T_{zz} generated using EGM96 from degree 8 to 180 ——— SD of coefficients per degree; – – – – SD of (obs.–comp.); · · · · · · Mean SD of collocation error estimates

gravity gradients at 300 km altitude, as in the first experiment. EGM96 itself was used as a reference field, and the perturbed coefficients were predicted. The results are shown in Figs. 6–9; it can be seen that the error estimates obtained from comparing observed and predicted values now agree well with the collocation error estimates. A small discrepancy is found for the lowest degrees, which is due to the fact that it is difficult to form a normally distributed set of numbers from very few values. Furthermore, we see that the second-order radial derivative contributes very little to the (perturbed) coefficients of the lowest degree.

5 Prediction of coefficients from a regional data distribution

The prediction of spherical harmonic coefficients will only be good when it is based on a global data coverage. We know that the estimate of the coefficients will degrade if, for example, we do not have data at the caps at the south and the north pole. But how much will the estimate degrade if the data only covers a part of the globe ?

Using the error-estimation capability of LSC we are able to study this. A small example is given here in Table 2, where we have used a subset of 678 of the 2000 gravity values used above at 300-km altitude with a distribution limited by $-45°$, $45°$ in latitude and $-90°$, $90°$ in longitude. The LSC estimated error which, as seen in Table 1, bottom row, was 0.29×10^6, changed to the values shown in Table 2.

It is interesting to see that the prediction of some coefficients becomes only slightly worse than when the full data set of 2000 values was used. This confirms the conjecture that regional gravity models may contain much correct information even at the longer wavelengths.

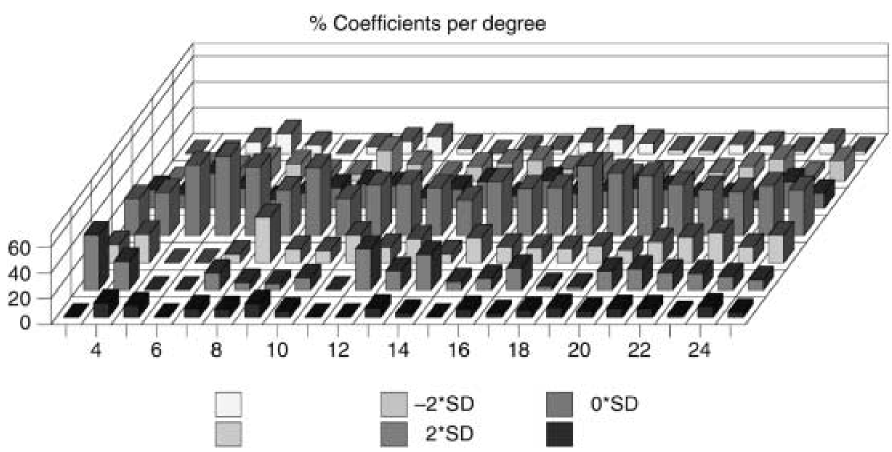

Fig. 5. X-axis is the degree, and the Y-axis is the percentage of the coefficients within bins of half the size of the standard deviation for the degree

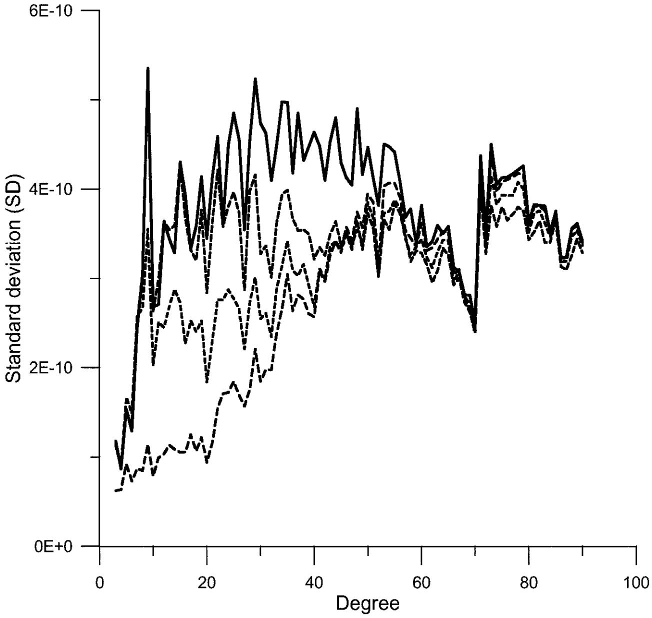

Fig. 6. Results of prediction of coefficients from degree 8 to 90. Data generated using EGM96 error degree variances to degree 180 ——— SD of coefficients; — — —— SD (obs.−pred.) coeff. from geoid; - - - - SD (obs.−pred.) coeff. from gravity; - - - -· SD (obs.−pred.) coefficients from T_{zz}

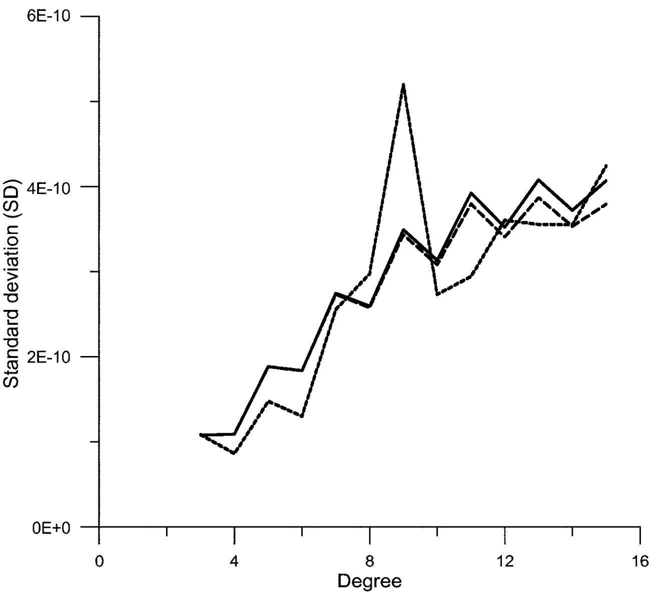

Fig. 7. Results of prediction of coefficients from degree 3 to 15 using T_{zz} generated using EGM96 error degree variances to degree 180 ——— SD of coefficients per degree; ······· SD of (obs.−comp.); — — — — — Mean SD of collocation error estimates

6 Conclusion

It has been demonstrated that it is numerically feasible to use LSC for the prediction of spherical harmonic coefficients. Meaningful error estimates can be calculated if we use the remove–restore method where an a priori gravity field is first subtracted and later added, so

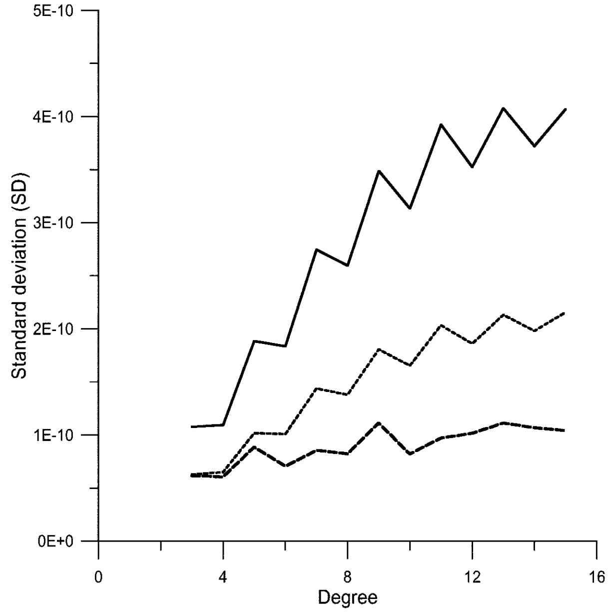

Fig. 8. Results of prediction of coefficients from degree 3 to 15 using geoid generated using EGM96 error degree variances to degree 180 ——— SD of coefficients per degree; — — — — — SD of (obs.−comp.); ········ Mean SD of collocation error estimates

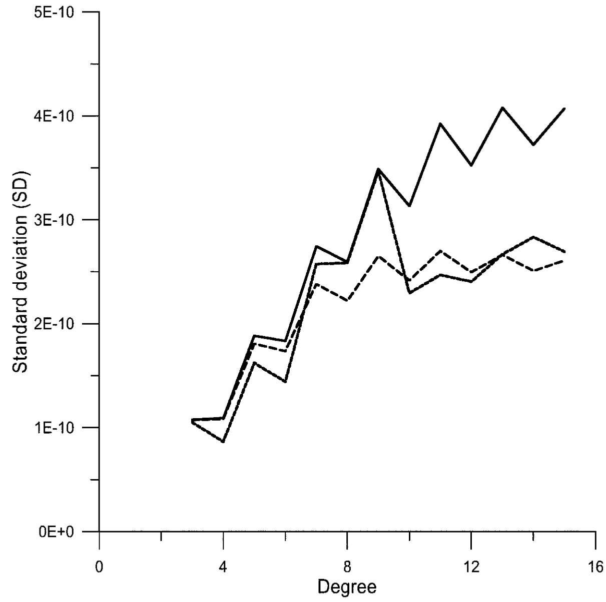

Fig. 9. Results of prediction of coefficients from degree 3 to 5 using gravity generated using EGM96 error degree variances to degree 180 ——— SD of coefficients per degree; ······· SD of (obs.−comp.); — — — — — Mean SD of collocation error estimates

Table 2. LSC error estimates of spherical harmonic coefficients of degree 9 calculated from 678 gravity values. Unitless and multiplied by 10^6

Order	9	8	7	6	5	4	3	2	1	0
Error estimate	0.48	0.54	0.56	0.62	0.72	0.71	0.76	0.75	0.79	0.76

that improvements to the set of coefficients and not the total quantity are determined using LSC. The same situation occurs in a network adjustment, where the object is to find not the coordinates, but improvements to the coordinates.

This will be important in simulation studies, where we try to understand the influence of various data types and data distribution on coefficient estimation. The use of the procedures for much larger data sets (simulations with sets corresponding to a 1° equal-area data distribution have already been carried out) will be possible using sparse matrix techniques, a topic where much progress recently has been made see Moraux et al. (1999).

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