Developments in the implementation and use of Least-Squares Collocation.

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The method of Least-Squares Collocation (LSC) was developed in the 1960'ties based on theoretical advances by T.Krarup and H.Moritz. The method may be used for the determination of approximations to the anomalous gravity potential (T) and associated parameters like biases or tilts. All gravity field observabels which may be related T through a linear functional may be predicted and error-estimates computed. The method has primarily been used in local or regional applications, due to the fact that a system of equations with as many unknowns as the number of observations need to be established and solved. The problem has been solved due to the use of multiprocessing in the current GRAVSOFT implementation of GEOCOL.

The method has been implemented using isotropic reproducing kernels fitted to empirical covariance functions. The Kernels are harmonic outside a so-called Bjerhammar-sphere, which must be inside the volume bounded by the location of the used data. This problem has been overcome by initially lifting the data in Polar areas 20 km, thereby enabeling global LSC solutions in the form of spherical harmonic expansions.

The theoretical possibility of computing error-estimates does not give good results due to the isotropy of the kernels used. The error estimates primarily shows where good data are located or where data are missing. However due to the advent of global gravity gradients from the ESA Gravity and Ocean Circulation Explorer (GOCE) mission it is possible to compute nearly everywhere local signal variances which can be used to tune the otherwise uniform estimates.

Keywords : Gravity, least-squares collocation, reproducing kernels, error-estimates, GEOCOL program, GRAVSOFT package.

1. Introduction.

The method of Least-Squares Collocation (LSC) was developed in the 1960'ties based on theoretical advances by T.Krarup (Krarup, 1969) and H.Moritz (1965, 1980). It gives the optimal (best) linear approximation in a reproducing kernel Hilbert-Space of harmonic functions or in an equivalent stochastic process. A minimum norm solution is obtained.

LSC is optimal so it gives the best results using less data. An example is the comparison with reduced point masses (RPM, a Radial basis-function) and LSC used in GOCINA test area with GOCE T_{zz} data, see Herceg et al. (2012).

The method may be used for the determination of approximations to the anomalous gravity potential (T) and associated parameters like biases or tilts. All gravity field observables which may be related T through a linear functional may be predicted and error-estimates computed.

The convergence of the method has been proven for increasing number of (noisy) data, see Tscherning (1978), Sansò and Tscherning (1980), Sansò and Venuti (2012)..

Despite these positive properties, a number of problems had to be solved before an operational, effective, method was developed. In the following is discussed the most important of these developments, many of which are due to results or software developed by other scientists. See the acknowledgements below. The following discussion will be limited to the 3D-implementation. For 2D LSC see Forsberg(1984). For more details about applications and theory see Sansò and Sideris (2012).

2. Solution of equations.

The method has primarily been used in local or regional applications, due to the fact that a system of equations with as many unknowns as the number of observations need to be established and solved. The problem has been solved due to the use of multiprocessing in the current GRAVSOFT implementation of GEOCOL, Forsberg and Tscherning(2008), Kaas et al.,(2013). It is available from http://cct.gfy.ku.dk/software/geocol19.htm. In Table 1 is given an example of the time (in seconds) needed for solving a typical system of equations with N observations using a 2.40 GHz Intel® computer for a different number of processors.

N	37971	22464	22464
Processors	22	22	4
Time (s)	440	136	391

Table 1. Computation time for Cholesky reduction of normal equations with N unknows.

3. Covariance function representation.

The method has in GRAVSOFT been implemented using isotropic reproducing kernels fitted to empirical covariance functions (Tscherning, 1972, Knudsen, 1978). The Kernels are harmonic outside a so-called Bjerhammar-sphere, which must be inside the volume bounded by the location of the used data. If spherical approximation is used, then this causes no problem. But for global use the best fitting model has an associated radius smaller than the semi-major axis, see Tscherning and Rapp (1974). This old covariance function representation is surprisingly still valid despite it was estimated using very few data. The model fits very well the degree-variances computed from EGM2008 (Pavlis et. al, 2012), see Fig. 1.

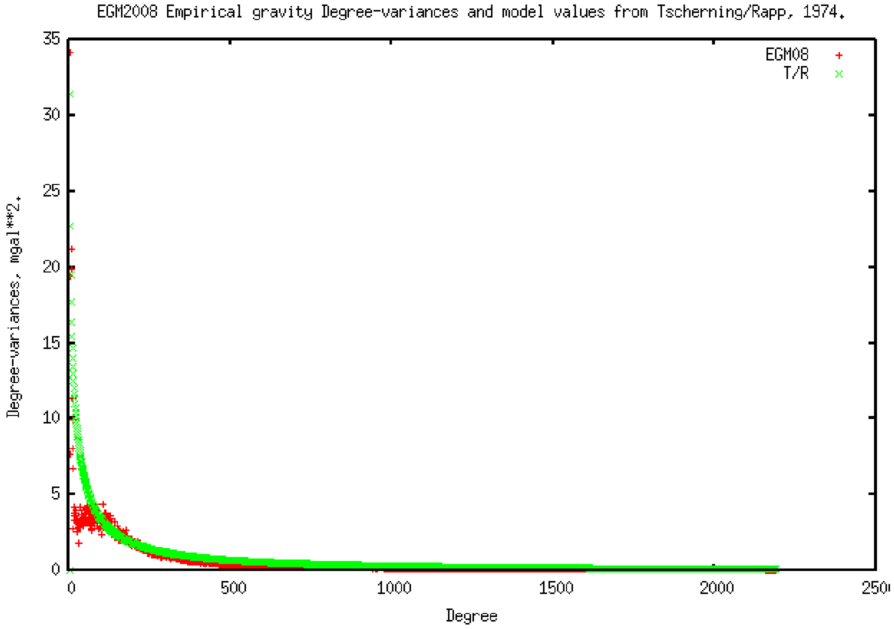


Fig. 1. EGM2008 and T/R degree-variances (mgal^2)

The Bjerhammar-sphere problem has been overcome by initially lifting the data in Polar areas 20 km, thereby enabeling global LSC solutions in the form of spherical harmonic expansions, as illustrated in Fig. 2, see the following section.

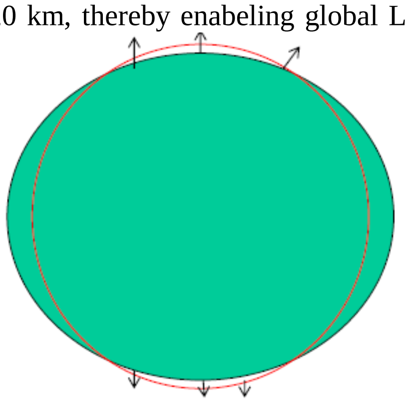


Fig. 2. Moving data at the poles outside the best fitting Bjerhammar sphere.

The basic model is isotropic, and this causes difficulties when LSC is applied in areas with a strongly non-isotropic gravity fiels such as along a mountain chain or a fault. However, the removal of the cause of an-isotropies – both in long and short wavelengths - has been succesful using the remove-restore method, Forsberg and Tscherning (1981), Migliaccio et al. (2005). But this obviously requires that reliable topographis data are available.

Recent development using an-isotropic functions are described in Petrusini et al., (2007) and in Reguzzoni and Gatti (2013).

Another difficult situation arizes if the ground data is un-reliable which for example may be detected using a simple tool as a histogram, or if data does not exist. The last excuse is happily not applicble anymore, due to the advent of global data especially from GOCE. This is illustrated in Fig. 3, where a covariance model has been estimated using ground data and GOCE T_{zz} data.

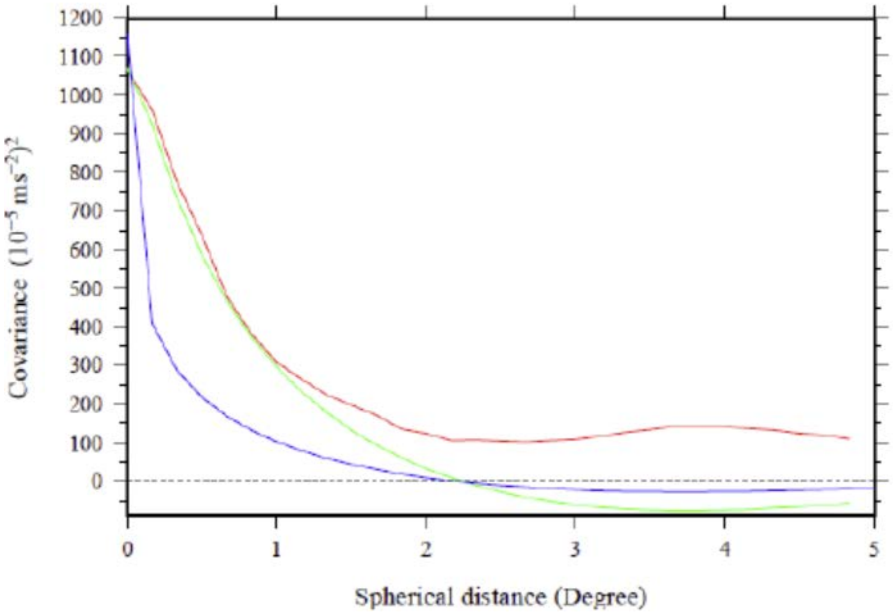


Fig. 3. Disagreement between the analytic models determined from the data, blue: T_{zz}, red: empirical Δg , green analytic from gravity. (Arabelos et al., 2013).

4. Applications of LSC.

4.1 Regional or local applications.

The method has been used extensively for regional geoid (height anomaly) determination. It is not possible to list all the references here. A good example is the computation of the geoid of Pakistan (Sadiq et al,2010). A comparison of LSC with other regional procedures is published in Yldiz et al (2012). Other important applications have been the use for the gridding and calibration of GOCE data Bouman et al (2005), Pail et al (2011) and the prediction of gravity anomalies from satellite altimeter data (Andersen et al, 1996).

4.2.Global LSC.

A recent development is the use LSC globally for the estimation of spherical harmonic coefficients (Tscherning, 2001) using GOCE Terrestrial Reference Frame (TRF) T_{zz} data (HPF, 2010) and gravity anomalies at the poles. The results are shown in Table 2 for various global gravity field models.

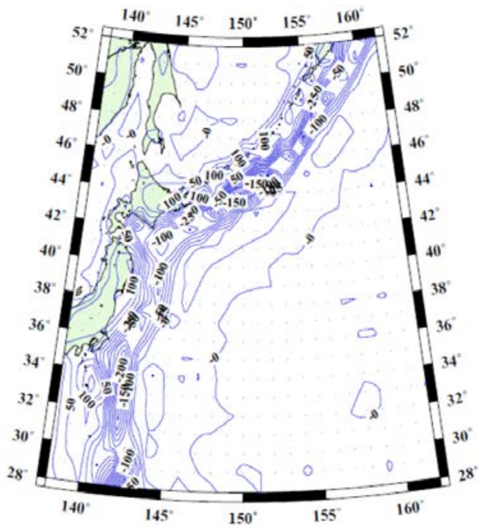
Model	N, Number of observations	Estimate	Error-estimate
EGM96		0.111	0.036
EGM2008		0.100	0.012
GOCE TIM2	➢ 10000000	0.105	0.015
LSC 1^o grid	42219	0.120	0.054
LSC 0.5^o grid	164212	0.106	0.028
LSC 0.25^o grid	~650000	?	0.014

Table 2. Unitless estimate and error estimate for coefficient $\bar{C}(100,100)*10^8$. Data distributed in the LSC solutions in an approximate equal-area grid.

Considering the associated error-estimates it should be possible to use LSC in order to obtain an error similar to the one obtained using many more data.

5. Computation of error estimates.

The theoretical possibility of computing error-estimates does not give good results due to the isotropy of the kernels used. The error estimates primarily shows where good data are located or where data are missing (see for example Fig. 8). However due to the advent of global gravity gradient from the ESA GOCE mission is is possible to compute local signal variances (see Fig. 8) where no ground data are available, which can be used to tune the otherwise uniform estimates. An example is the use of this method (still being developed) for the improvement of error-estimates of grids of gravity anomalies computed from GOCE T_{zz} data in the trench area south of Japan, see Fig. 4-9.



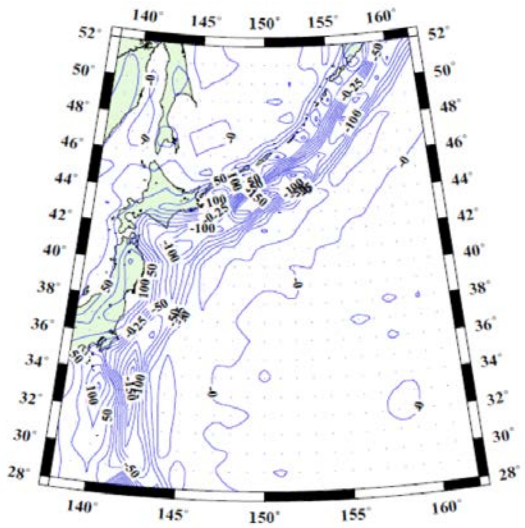
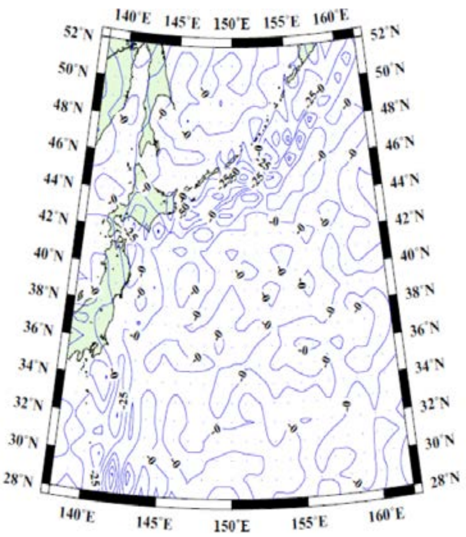


Fig. 4 and 5. Gravity anomalies from GOCE T_{zz} & EGM2008 to 512. (ITG-Grace2010c, Mayer-Guerr, 2010) to 36 subtracted everywhere), units: mgal.



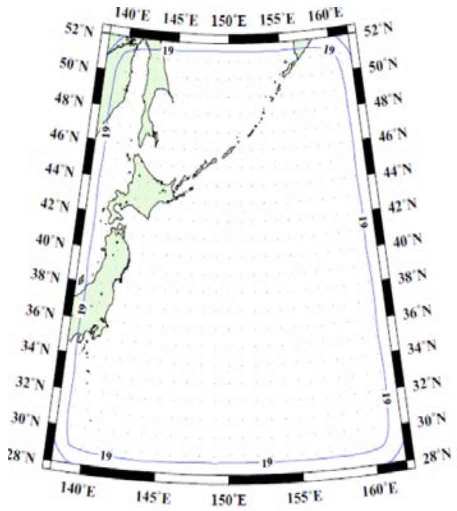


Fig. 6 and 7. Differences gravity (mgal) from GOCE T_{zz}- EGM2008 to 512 and LSC error estimates.

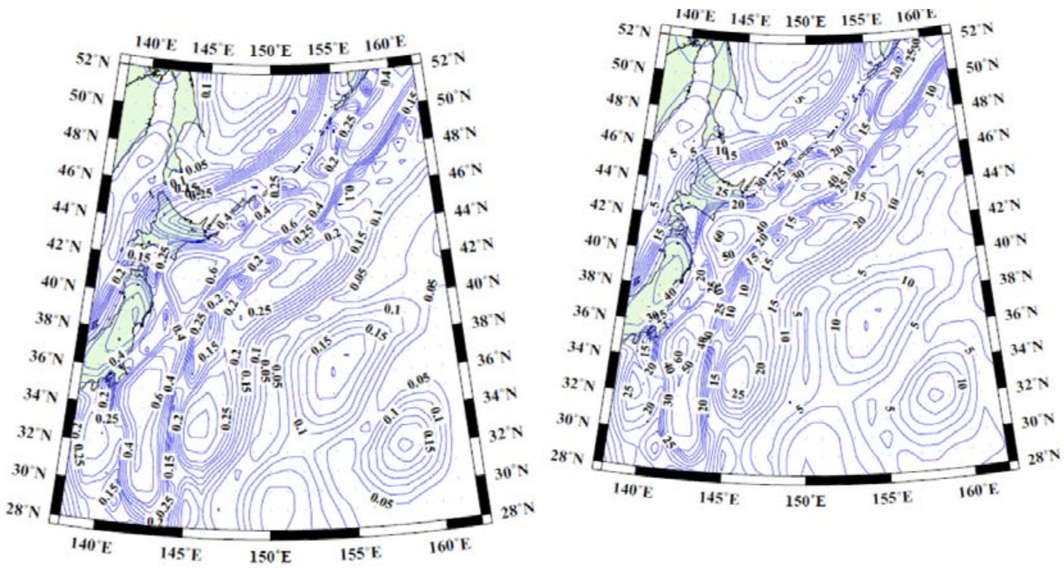


Fig. 8 and 9. T_{zz} RMS (E.U.) and scaled error estimates (mgal).

It is obvious (comparing Fig. 6 and Fig. 9) that the scaled error-estimates improves the reliability of the estimates. However, the procedure is still under development. More details are found in Tscherning(2013).

6. Software development.

The first general program was written in Algol in 1972 (Tscherning, 1972). A general FORTRAN program was written in 1974 for 3D LSC (Tscherning, 1974), geocol, now geocol19. A 2D LSC program, gpcol, was developen by R.Forsberg. Both programs are available for scientific or teaching purpose free of charge.

Programs have also been developed at TUGraz, POLIMI and UHannover.

7. Conclusion.

LSC is not anymore restricted due to large number of observations if multiprocessing can be used. Analytic ellipsoidal or anisotropic kernels are under development or already developed. Software is available in the GRAVSOFT package. The scaling of LSC derived error-estimates improves the error estimates, so that the variation of the error due to changing local signal standard deviation is seen. The development and use have involved many colleagues, whom the author is grateful to acknowledge, see the incomplete list below.

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