Least-Squares Collocation.

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1. Introduction.

The difference *T=W-U* is denoted the anomalous gravity potential. *W* is the gravity potential and *U* is a suitable reference potential which include the same centrifugal potential as *W*. *T* therefore becomes a harmonic function, i.e. it satisfies the Laplace equation outside the masses of the Earth. (The contribution of the Moon and the planets, as well as of the atmosphere will not be discussed here). The determination of (approximations to) *T* is thus equivalent to the solution of a partial differential equation. The following discussion will be limited to the solution in 3 dimensions. For 2 dimensions see Forsberg(1984).

One of the methods for the solution of the partial differential equation in the form of an approximation to *T* is the method of Least-Squares Collocation (LSC). It was developed in the 1960'ties based on theoretical advances by T.Krarup (Krarup, 1969) and H.Moritz (1965, 1980). It gives an optimal (best) linear approximation in a reproducing kernel Hilbert-Space of harmonic functions or in an equivalent stochastic process (see Parzen (1959). The solution is „best" in the sense that a minimum norm solution is obtained.

The method may not only be used for the determination of approximations to *T*, T_{LSC}, but associated parameters like biases or tilts may also be estimated. Random or correlated noise may also be accounted for. All gravity field observables which may be related to *T* through a linear functional may be predicted and error-estimates computed. Examples are gravity anomalies, height anomalies, deflections of the vertical, gravity gradients and coefficients of spherical harmoninc series.

The convergence of the method (i.e. that the correct solution is obtained) has been proven in ideal situations for increasing number of globally distributed (contingently noisy) data, see Tscherning (1978), Sansò and Tscherning (1980).

The basic observation equation for LSC is

$$y_i = L_i(T_{LSC}) + e_i + A_i^T X, \qquad (1)$$

where y_i is a vector of *n* observations, L_i is a vector of functionals associating *T* with the observation, e_i is a vector of errors, *X* is a m-vector of parameters and A_i^T a nxm matrix relating the n observations and m parameters. Here the contribution from a contingent datum-transformation and an Earth Gravity Model (*U*) must have been subtracted.

Suppose the observation functionals are elements of the dual of a reproducing kernel Hilbert space or are stochastic variables with a finite variance within a stochastic process. The space will have a reproducing kernel, *K(P,Q)* equal to the inner product of the evaluation functionals in the points *P* and *Q*. In the stochastic process the corresponding stochastic variables will have a covariance, *C(P,Q)=K(P,Q)*. An arbitrary pair of linear functionals L_i, L_j will have an inner product equal to the value obtained by applying the functionals on the reproducing kernel or the value of the covariance in the stochastic process. We will denote the value C_{ij} or C_{Pi} if one of the functionals is the evaluation functional in the point *P*. Note that the functionals do not have to be associated with points on the boundary of the set of harmonicity, but could be any linear functional with finite norm (or variance). Hence LSC solves a more general problem than the traditional boundary value problem for a harmonic function.

The estimate of T_{LSC} in a point *P* is obtained by

$$\tilde{T}_{LSC}(P) = \{C_{Pi}\}^T \overline{C}^{-1}\{y - A^T X)\}, \qquad (2)$$

where $\overline{C} = \{C_{ij} + \sigma_{ij}\}$, and σ_{ij} is the variance-covariances of the errors.

The estimate of the (M) parameters are obtained by

$$\tilde{X} = (A^T \overline{C}^{-1} A + W)^{-1} (A^T \overline{C}^{-1} y) \qquad (3)$$

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

$$H_k = \{COV(L_k, L_i)\}^T \overline{C}^{-1}, \text{ mxn matrix}$$

$$m_X^2 = (A^T \overline{C}^{-1} A + W)^{-1} \tag{4}$$

$$\{ec_{kl}\} = \{\sigma_{kl}\} - H_k \{\text{cov}(L_j, L_l)\} + H_k A M_X (H_l A)^T \tag{5}$$

2. Solution of equations.

The equation system in its most general form is positive semi-definite, so the traditionally used method of Cholesky decomposition has been modified to take this into account, see e.g. Tscherning (1978).

The LSC 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 Kaas et al., 2013. In Table 1 is given an example of the time 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. Choice of reproducing kernel Hilbert space or or an equivalent stochastic process.

In the original work (Moritz, 1965) a method for least-squares (optimal) linear prediction was developed. The method would for noise-free data give predictions equal to the input data if such data were predicted. This is the property of collocation methods used to solved (ordinary or partial) differential equations and is the reson for the „C“ in the LSC.

Covariance functions were regarded as global functions depending on the spherical distance between the points associated with the functionals (stochastic variables). Such functions could be obtained using a development of T in spherical harmonics or by forming product sums of data located at distances within a certain interval (bin), see e.g. Tscherning and Rapp (1974). The (so-called empirical) covariance functions obtained using such procedures are similar to reproducing kernels of Hilbert spaces with inner-products of integrals of derivatives of harmonic functions. Consequently an inner product may be chosen so that the kernel approximates the empirically estimated covariance functions. If this procedure is followed, the approximation T_{LSC} is optimal in a least-squares sense and thereby the „LS“ in the name of the method is justified.

For a local area a similar procedure can be used. The local area must be considered as representing the whole Earth. This is naturally incorrect, but by removing the main part of the gravity field outside the local area, (by e.g. subtracting a global model and smoothing the field), reproducing kernels of local character may be determined, see Goad et al. (1984).

4. Covariance function representation.

The method has generally 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).

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. 1.

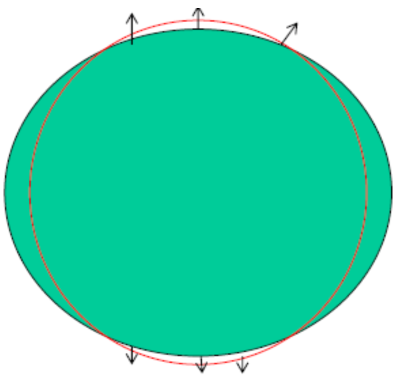

Fig. 1. Moving data at the poles outside the best fitting Bjerhammar sphere.

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 require 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).

6. Software.

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 as a part of the GRAVSOFT package (Forsberg and Tscherning, 2008). Programs have also been developed at TUGraz, POLIMI and UHannover.

7. A final remark.

One may ask whether LSC is « better » than other methods. It is for sure very flexible, but the correctness of the procedure for selecting the reproducing kernel still remains to be shown. When methods have been compared e.g. for height anomaly determination in areas with dense data coverage, the method gives results similar to other well founded methods, see e.g. Yldiz (2012).

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