Article

COVARIANCE FUNCTION MODELLING IN LOCAL GEODETIC APPLICATIONS USING THE SIMPLEX METHOD

Modelagem da função covariância em aplicações geodésicas locais utilizando o método simplex

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Abstract:

Collocation has been widely applied in geodesy for estimating the gravity field of the Earth both locally and globally. Particularly, this is the standard geodetic method used to combine all the available data to get an integrated estimate of any functional of the anomalous potential T. The key point of the method is the definition of proper covariance functions of the data. Covariance function models have been proposed by many authors together with the related software. In this paper a new method for finding suitable covariance models has been devised. The covariance fitting problem is reduced to an optimization problem in Linear Programming and solved by using the Simplex Method. The procedure has been implemented in a FORTRAN95 software and has been tested on simulated and real data sets. These first tests proved that the proposed method is a reliable tool for estimating proper covariance function models to be used in the collocation procedure.

Keywords: Local Disturbing Potential, Data Integration, Collocation, Covariance Functions, Linear Programming, Simplex Method

Resumo:

A técnica de Colocação tem sido bastante aplicada em Geodésia para estimação do campo da gravidade da Terra em ambos os aspectos, isto é, localmente e globalmente. Particularmente, este é o método geodésico padrão usado para combinar todos os dados disponíveis para se obter uma estimativa integrada de qualquer anomalia potencial T. A principal característica do método é a definição da função covariância dos dados. Diversas funções covariância tem sido propostas na literatura, juntamente, com o software relacionado. Neste trabalho, um novo método para

determinar funções covariância é proposto. O problema de ajustamento da covariância é reduzido para um problema de otimização em programação linear e solucionado pelo método conhecido como Simplex. O método proposto foi implementado em linguagem de programação FORTRAN95 e foi testado com dados simulados e reais. Os resultados obtidos mostraram que o método proposto é uma potente ferramenta para estimação de modelos da função covariância e pode ser empregado em técnicas de Colocação.

Palavras-chave: Potencial de Distúrbio Local; Integração de Dados; Colocação; Função Covariânica; Programação Linear; Método Simplex.

1. Introdução

One of the standard procedures for local gravity field modelling is based on the combination of the Remove-Restore technique (RR) (Sansò, 2013a) and Collocation method (Sansò, 2013b). The RR principle is one of the most well-known strategies used for regional and local gravity field determination. It is based on the assumption that gravity signals can be divided into long, medium and short wavelength components. The long wavelength component can be properly accounted for by Global Geopotential Models (GGM) that are estimated using satellite derived observations and ground based gravity data (Pavlis et al., 2012). Removing the effect of a GGM corresponds to a high-pass filtering of the data. In this reduction step, the gravity signals due to the mean crust, the upper mantle and the long wavelength topographic signal are removed from the observed values.

After reduction for a global model, in addition to medium frequencies, high frequency components are still present in the residual data. They are essentially due to the high frequency features of the topography which cannot be suitably described by global models (Forsberg, 1994). This residual topographic signal is then removed from the observed data by computing the so called Residual Terrain Correction (RTC) (Forsberg, 1994). The residual data obtained by applying both the reduction for the global model and the related RTC contain only the intermediate wavelengths to be used for local gravity field modelling. They usually have a mean value close to zero and a standard deviation that is remarkably smaller than the standard deviation of the unreduced data. Collocation can be suitably applied to these reduced data to get estimates of the local features of the gravity field (Tscherning, 2004). The final estimate is then obtained by restoring the geopotential model and RTC effects which are added to this local residual component in order to obtain the final full power estimate.

As mentioned, Collocation is applied to get the estimate of the residual local component of the gravity signal. Collocation is a statistical-mathematical theory applied to gravity field modelling problems (Heiskanen and Moritz, 1967; Moritz, 1980; Sansò, 2013b). It is based on the assumption that the gravity observations can be considered as a realization of a weakly stationary and ergodic stochastic process (Moritz, 1980, pp. 279-285). This theory has become more and more important because it allows combining different kinds of gravity field observables in order to obtain a better estimate of any linear functional of the anomalous potential $T(P)$. With the great amount of heterogeneous data nowadays available, this approach has been fully accepted as the standard methodology for integrated gravity field modelling. The key point in Collocation is the concept of spatial correlation which is described by the covariance function of the observations. Being all the observed geodetic quantities (as Δg, N or T_{rr}) linear(ized) functionals

of the anomalous gravity potential (T), it can be also proved (Moritz, 1980, pp. 86-87) that their covariance functions can be propagated one to each other by applying the proper linear operators to the well-known analytical model of covariance of the anomalous potential $T(P)$.

In local geodetic applications, this model (Knudsen, 1987) is given by

$$C\left(\psi_{PQ}\right) = \sum_{n=2}^{N_{red}} \alpha e_n^2(T)\left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n\left(\cos\psi_{PQ}\right) + \sum_{n=N_{red}+1}^{\infty} \sigma_n^2(T)\left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n\left(\cos\psi_{PQ}\right) \qquad (1)$$

where R is the radius of the Bjerhammar sphere, r_P and r_Q are the geocentric radii of points P and Q, σ_n^2 are the degree variances, e_n^2 are the error degree variances, α is a scale factor, P_n are the Legendre polynomials and ψ_{PQ} is the spherical distance between P and Q.

Such covariance model is the sum of two parts. The first comes from the commission error of the global model removed from observations. It is given in terms of the sum of the error degree variances e_n^2 up to the maximum degree of computation of the global model subtracted in the remove phase. e_n^2 are computed as the sum of the variances of the estimated spherical harmonic model coefficients, $\sigma^2(C_{nm})$ and $\sigma^2(S_{nm})$ (Pavlis et al., 2012):

$$e_n^2 = \sum_{m=0}^{n}\left[\sigma^2(C_{nm}) + \sigma^2(S_{nm})\right] \qquad (2)$$

So, error degree variances depend on the global model used and the coefficient α in (1) allows weighting their influence. The second part is related to the residual part of the signal. Suitable models for $\sigma_n^2(T)$ in (1) were proposed by Tscherning and Rapp (Tscherning and Rapp, 1974; Tscherning, 2004)

$$\sigma_n^2(T) = \frac{A}{(n-1)(n-2)}$$
$$\sigma_n^2(T) = \frac{A}{(n-1)(n-2)(n+B)} \qquad (3)$$

where A and B are model constants to be estimated. As stated, using covariance propagation, these covariance models of the anomalous potential T can be used to get models for any functional of T. By tuning the model constants (i.e. A, α, R and B), these model functions can be used to properly fit the empirical covariances of the available data.

In turn, the empirical covariance function of the observed data can be estimated using the formula (Mussio, 1984):

$$C(\psi) = C\left(k\frac{\Delta\psi}{2}\right) = \frac{1}{m}\sum_{i=1}^{m}\frac{1}{n}\sum_{j=1}^{n} l_i l_j' \qquad (4)$$

where m is the number of l_i observations and n is the number of l_j' observations at spherical distance ψ_{ij} from l_i so that

$$(k-1)\Delta\psi \le \psi_{ij} \le k\Delta\psi, \quad k = 1,...,k \qquad (5)$$

for a suitable $\Delta\psi$ value.

If homogeneous data are considered, formula (4) gives the empirical estimate of the auto-covariance of these data. In case l and l' are different functionals of T (e.g. Δg and N), (4) is the empirical estimate of the cross-covariance between l and l'.

Once the covariance functions of the observed data are properly modeled, Collocation formula can be applied to get the estimate of any functional of the anomalous potential T. As it is well known, the general formula of Least Squares Collocation (LSC) giving the estimate is (Moritz, 1980, pp. 84-87; Sansò, 2013):

$$\hat{L}_P(T) = \sum_{i,j=1}^{N} \left[L_i L_P C_{T_i T_P} \right] \left[L_i L_j C_{T_i T_j} + \sigma_v^2 I \right]^{-1} \left[L_i(T) + v_i \right] \tag{6}$$

where L_i is the observed linear(ized) functional of T in P_i, $L_i L_j C_{T_i T_j}$ is the covariance matrix of observations, σ_v^2 is the variance of the observation noise v, L_P is the estimated linear functional of T in P and I is the identity matrix.

This is the usual procedure for covariance function modelling and collocation estimate computation. As it is evident, the covariance structure of the data plays a fundamental role in getting the solution in equation (6). Thus, the correct modelling of the covariance functions is a critical point in computing a reliable estimate.

The proposed models are sometimes unable to properly fit the empirical covariances, particularly when different functionals are considered. In a previously proposed approach (Tselfes, 2008; Barzaghi et al., 2009) regularized least squares adjustment have been applied for integrated covariance function modelling which, however, can lead to negative $\sigma_n^2(T)$ values that must be rejected. Hence, this procedure must be iterated to get a final set of suitable $\sigma_n^2(T)$. In the next section, a new covariance modelling procedure solving this problem will be described.

2. A new procedure for covariance modelling based on Linear Programming

In order to overcome some limits of the method presented in Barzaghi et al. (2009), a covariance fitting method based on linear programming is proposed.

Considering a system of linear inequalities of the following form (see also Figure 1):

$$
\begin{cases}
a_{11}x_1 + a_{12}x_2 + ... + a_{1n}x_n \le b_1 \\
a_{21}x_1 + a_{22}x_2 + ... + a_{2n}x_n \le b_2 \\
\quad M \\
a_{m1}x_1 + a_{m2}x_2 + ... + a_{mn}x_n \le b_m \\
x_1 \ge 0 \\
x_2 \ge 0 \\
\quad M \\
x_n \ge 0
\end{cases}
\tag{7}
$$

there are several sets of values $(x_1, x_2, ... x_n)$ that are solutions to (7). Finding one of particular interest is an *optimization process* (Press et al., 1989). When this solution is the one minimizing (or maximizing) a given linear combination of the variables (called *objective function*)

$$
c_1x_1 + c_2x_2 + ... + c_nx_n = \min \tag{8}
$$

subject to constraints expressed as (7), the optimization process is called *Linear Programming* (LP) (Chvatal et al., 1983).

Figure 1: Graphical sketch of a system of linear inequalities in two dimensions. P is a possible solution.

Each of the inequalities of (7) cuts the hyperspace $(x_1, x_2, ... x_n)$ into two parts. So, it is possible to identify the region containing all the sets of values $(x_1, x_2, ... x_n)$ satisfying all the inequalities. Outside this region, at least one of the constraints is not satisfied. This region, called *feasible region*, contains all the possible solution (*feasible solution*s) expressed in the constraints system (Figure 2). One of them is the *optimal solution* that solve the LP problem. Fundamental theorems of linear programming prove that, if a solution does exist, it occurs on one of the vertex of the feasible region.
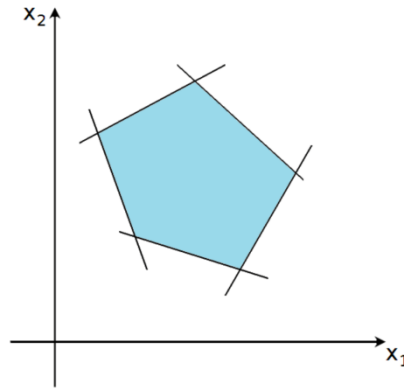
Figure 2: Example of two-dimensional feasible region of constraints

For applications involving a large number of constraints or variables, numerical methods must be applied. One of them is the *Simplex Method* (Ficken, 1961). It provides a systematic way of examining the vertices of the feasible region to determine the optimal value of the objective function. The simplex method consists in elementary row operations on a particular matrix corresponding to the LP problem called *tableau*. The initial version of the tableau changes its form through iterative optimality checks. This operation is called *pivoting*. To form the improved solution, Gauss-Jordan elimination is applied with the pivot (crossing pivot row and column) to the column pivot. After improving the solution, the simplex algorithm starts a new iteration checking for further improvements. The tableau changes at each iteration and the conditions of optimality or unfeasibility of the solution to the proposed LP problem stop the algorithm. Based on fundamental theorem of linear programming, simplex method is able to verify the existence of at least one solution to the proposed LP problem. If this exists, the algorithm is also able to find the best numerical solution in a finite amount of time.

Using this principle, a new covariance fitting procedure based on the simplex method and the analytical covariance function model (1) has been devised. It applies simplex method for estimating some suitable parameters of the model covariance function (1) in order to fit simultaneously the empirical covariances of all the available data. One possible way of doing so using the simplex method is to assume as a model covariance for the anomalous potential T a slightly modified version of (1), i.e.

$$C\left(\psi_{PQ}\right) = \sum_{n=2}^{N_{red}} \alpha \tilde{e}_n^2(T) \left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n\left(\cos\psi_{PQ}\right) + \sum_{n=N_{red}+1}^{N_{\max}} \beta \tilde{\sigma}_n^2(T) \left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n\left(\cos\psi_{PQ}\right) \qquad (9)$$

where $\tilde{e}_n^2$, are the error degree variances of the model used for reducing the data in the remove step and $\tilde{\sigma}_n^2$ are some guess values for the degree variances. $\tilde{\sigma}_n^2$ can be computed by using again the applied geopotential model (in case $N_{red} < N_{\max}$) or by describing them according to some general rule, e.g. the Kaula's rule (Kaula, 2000). The fitting procedure is then implemented through the following conditions that allow estimating suitable values for α and β

$$\alpha + \beta = \min \qquad (10)$$

$$\begin{cases} \alpha > 0 \\ \beta > 0 \\ C_{L(T)L'(T)}(\psi_i, \alpha, \beta) \leq C^{emp}_{L(T)L'(T)}(\psi_i) + \Delta C^+_{L(T)L'(T)} \\ C_{L(T)L'(T)}(\psi_i, \alpha, \beta) \geq C^{emp}_{L(T)L'(T)}(\psi_i) + \Delta C^-_{L(T)L'(T)} \end{cases} \qquad (11)$$

where $C^{emp}_{L(T)L'(T)}(\psi_i)$ and $C_{L(T)L'(T)}(\psi_i)$ are, respectively, the empirical and the model covariances related to the $L(T)$ and $L'(T)$ functionals.

Thus, we minimize the discrepancy between the model covariance and the empirical covariance values through some tolerance levels $\Delta C^+_{L(T)L'(T)}$ and $\Delta C^-_{L(T)L'(T)}$ (Figure 3).

Figure 3: Constraints applied on model covariance function (in red)

The conditions (11) can be applied for all the given empirical (auto and cross) covariance functions, i.e. for all the observed functionals $L(T)$ that are available in the area under investigation. With these constraints on the estimated covariance functions, simplex method is forced to find a unique suitable set of estimated α and β values for all the given empirical covariances (Figure 4).
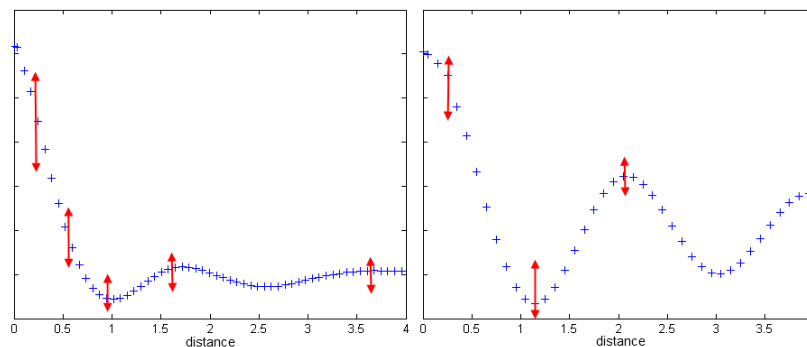

Figure 4: Multiple constraints on model covariance functions

This covariance fitting methodology is numerically implemented through an iterative procedure. While objective condition (10) is fixed, conditions (11) are tuned in order to get the best possible fit with empirical covariance values. Referring to the feasible region, this procedure identifies an initial large feasible region (soft constraints, poor fit) and reduces this hyperspace until the vertex of optimality solution practically coincide one to each other (strongest constraints, best fit). In Figure 5, this process is sketched.
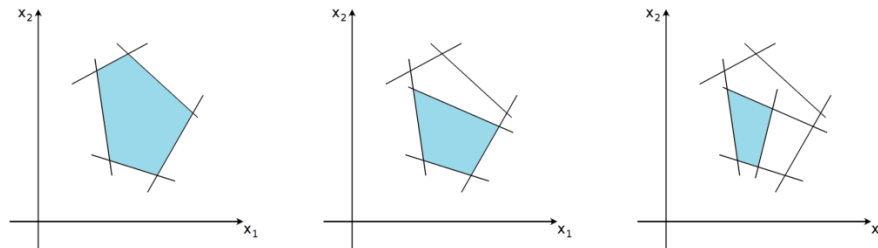

Figure 5: Impact of iterative constraints adjustment on the feasible region

Thus in this procedure, simplex method has been applied in a quite different way with respect to standard applications of linear programming. While in the usual application of simplex algorithm the focus is on the objective function and the constraints are fixed, the devised procedure is applied in a reverse way. As a matter of facts, the focus of the method is less on the objective function than on suitable constraints allowing the best possible agreement between model covariance functions and empirical values.

3. Some tests based on simulated and real data

Covariance function estimate and modelling with simplex method has been implemented through a FORTRAN95 software, named SIMPLEXCOV, based on the concepts explained before. This procedure is basically composed by three steps (De Gaetani, 2012):

1. analysis of input data for assessment of the best sampling of empirical covariance functions;
2. computation of empirical auto- and cross- covariances;
3. iterative computation of the best fit model of auto- and cross-covariance functions with the simplex method.

The third step is composed by two nested loops. In the external loop a set of suitable constraints on empirical covariance functions are defined. Based on these constraints, in the internal loop many optimization problems are generated and solved by the simplex method. In each of them, the starting $\tilde{e}_n^2$ derived from a global model are step by step shifted and a simplex algorithm solution is searched for. If more than one set of error degree/degree variances is able to satisfy the constraints, an improved fit can be obtained modifying the constraints in the external loop and so on. On the contrary, if all the LP problems have no feasible solution in the internal loop, constraints are softened in the external loop. The final solution corresponds to a unique

combination of shifted error degree variances $\tilde{e}_n^2$, α and β values that allow to obtain the best possible fit between empirical covariances and the model covariance functions.

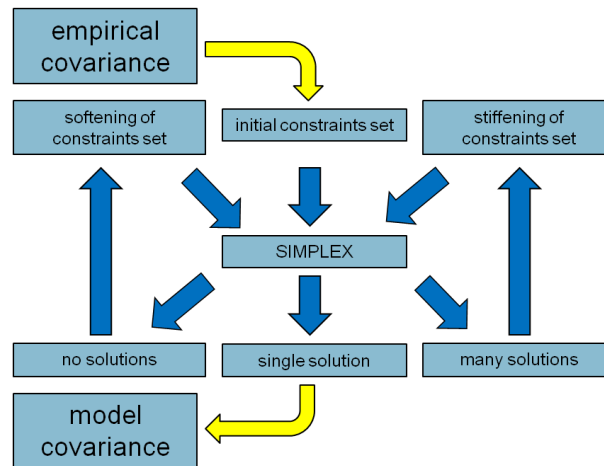The scheme of the implemented procedure is sketched in Figure 6.

Figure 6: Iterative covariance function modelling process with the simplex method

The proposed fitting procedure has been initially tested with simulated data in the North-Western part of Italy, in the area $40° \leq \varphi \leq 49°$; $5° \leq \lambda \leq 14°$ (Figure 7).

In this test, 24328 points quite homogeneously distributed in that $9°×9°$ area have been considered. Data distribution is obtained by selecting real data positions belonging to the Italian gravity database (Barzaghi et al., 2007). The final database has a mean density of 3'.

Free air gravity anomalies Δg_{FA} and geoid undulations N on these points have been synthetized by the EGM2008 global model up to degree 2190 (Pavlis et al., 2012).
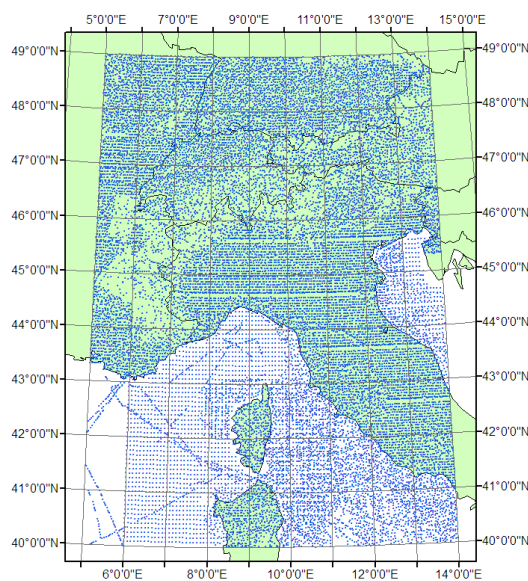

Figure 7: The distribution of the simulation points

Then, the data have been reduced for the long wavelength component removing the same global model EGM2008, synthesized up to degree 1500 (which allows a suitable reduction of the low-frequency component of the data given the mean 3' data density). Statistics of the "observed" and reduced data are summarized in Table 1.

Table 1: Statistics of simulated and reduced data (E: average, σ: standard deviation)

	E	**σ**	**max**	**min**
Δg_{obs} [mGal]	11.151	50.680	232.790	-156.341
Δg_{res} [mGal]	-0.843	11.203	74.646	-94.160
N_{obs} [m]	47.779	2.942	55.921	39.294
N_{res} [m]	-0.003	0.041	0.276	-0.332

Empirical covariance functions of both functionals are computed and suitable model covariance functions are estimated so to represent at best the spatial correlation given by the empirical values. In a first computation, the empirical covariance values of residual gravity and geoid have been fitted separately adopting the new procedure. In this test, the error degree variances $\tilde{e}_n^2$ (with n up to 1500) and the degree-variances $\tilde{\sigma}_n^2$ (with $1501 \leq n \leq 2190$) were derived from the EGM2008 model.

The results are plotted in Fig. 8 and 9, where it is possible to see that the agreement between model and empirical covariance values is remarkable: considering the differences between model and empirical values, for Δg_{res} the average and the standard deviation are respectively 1.1^{-10} m^2/s^4 and 1.2^{-10} m^2/s^4, while they are 1.4^{-5} m^2 and 1.5^{-5} m^2 for N_{res}.
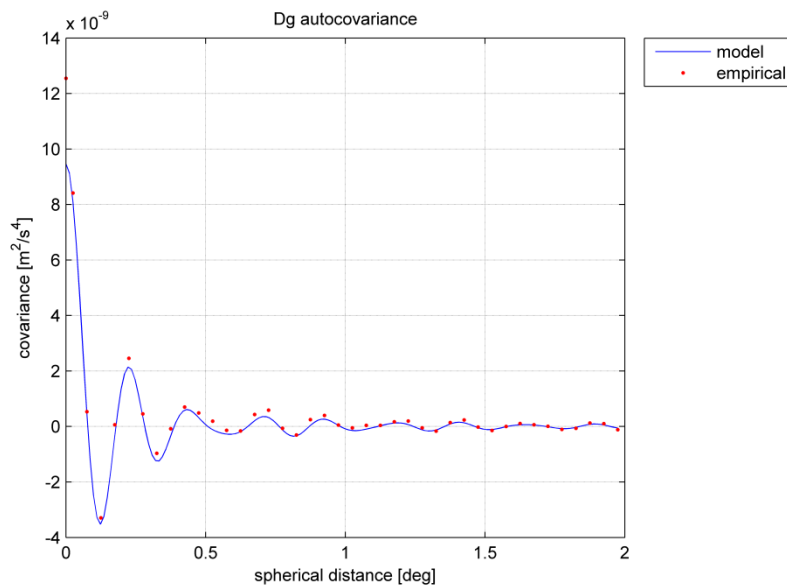

Figure 8: Model auto-covariance obtained by fitting the empirical function of Δg_{res}
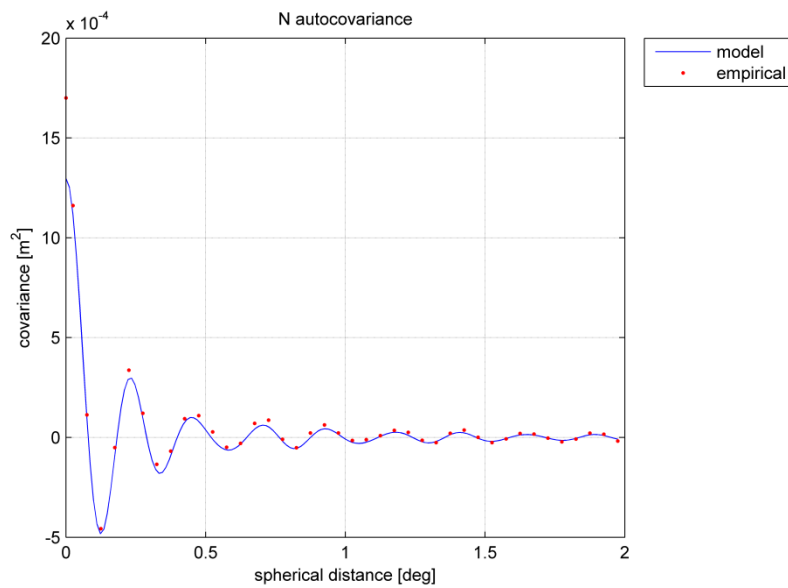
Figure 9: Model auto-covariance obtained by fitting the empirical function of N_{res}

In Figure 10, the comparison between the original EGM2008 error degree/degree variances and the final scaled obtained solution is shown. As can be seen, in order to properly fit the empirical values, larger degree variances must be considered for the higher degrees. On the other hand, the error degree variances have to be zero because the removed model is the same of that used for data simulation, so the commission error is null.
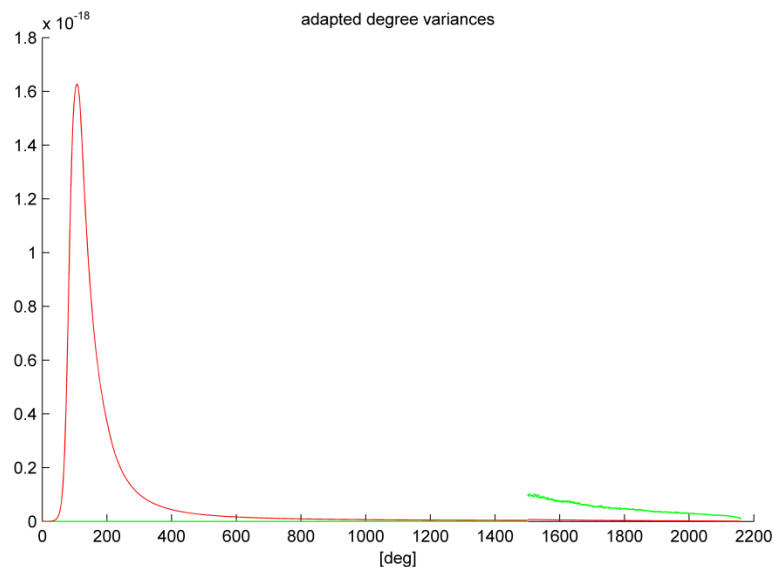

Figure 10: In green, the adapted error degree variances (up to $n = 1500$) and the adapted degree variances ($1501 \leq n \leq 2190$) obtained from the simplex method. In red, the starting EGM2008 error degree/degree variances

Moreover, with the proposed method it is possible to estimate the optimal solution considering simultaneously both the functionals. The simplex method has been then applied to both empirical covariances in order to get a set of scaled error degree/degree variances allowing a common improved fit. Thus, both empirical auto-covariances of residual undulation and residual gravity anomalies have been considered in the fitting procedure. The results are nearly identical to those previously obtained. By using the estimated parameters in the model covariances one can also define the model cross-covariance between Δg_{res} and N_{res}. The differences between this cross-covariance model and the empirical cross-covariance values have average -3.6^{-8} m^2/s^2 and standard deviation 5.6^{-7} m^2/s^2 (see Figure 11). Thus, despite the fact that the empirical cross-covariance values were not included in the fitting procedure, the obtained cross-covariance model properly interpolates the corresponding empirical function proving the numerical stability of the devised method[1].
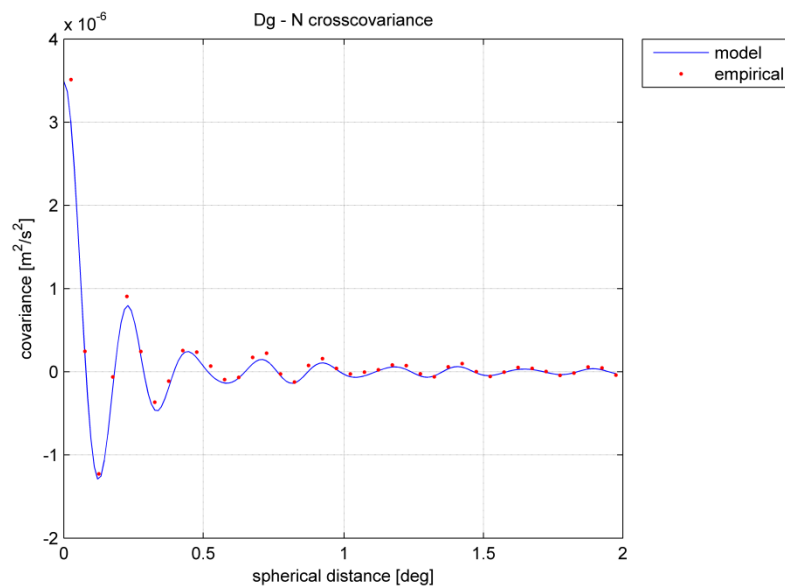

Figure 11: The empirical cross-covariance $C^{emp}_{\Delta g_{res}N_{res}}$ and the model cross-covariance $C_{\Delta g_{res}N_{res}}$ obtained by simultaneously fitting the empirical covariance functions of N_{res} and Δg_{res}

In the same points where simulated data were generated, real observations of free-air gravity anomalies have been then considered. The simplex method has been applied to them in order to check for the new approach with real data too.

The adopted procedure is the classical remove technique (Forsberg, 1994). The free-air anomalies have been reduced for the long wavelength component in the same way of the simulated data, i.e. removing the global model EGM2008 up to degree 1500, while for the short wavelengths the residual terrain correction (RTC) has been performed considering the detailed DTM (pixel size: 3"×3") already used for evaluating the Italian geoid model Italgeo05 (Barzaghi et al, 2007; Borghi et al., 2007). The reference altimetry grid for the RTC computation has been

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[1] However, it must be underlined that the procedure can be run also considering the empirical cross-covariance values.

obtained filtering the DTM with a moving average window sized 5'×5'. The size of the moving window has been chosen according to the statistical properties of the residuals (minimization of their root mean squared error). The RTC, both for gravity and height anomaly, has been evaluated up to 120 km from each computation point. The program used in this computation is TC from the GRAVSOFT package (Tscherning, 2004). Statistics of the observed and reduced data are summarized in Table 2.

Table 2: Statistics of observed and reduced free-air gravity anomalies

	E	**σ**	**max**	**min**
Δg_{obs} [mGal]	0.105	47.618	212.511	-162.22
Δg_{res} [mGal]	-0.236	9.210	94.649	-97.310

Then the simplex method has been applied to them. Again, as done in the simulations, the error degree variances $\tilde{e}_n^2$ (with n up to 1500) and the degree-variances $\tilde{\sigma}_n^2$ (with $1501 \leq n \leq 2190$) have been derived from the EGM2008 model.

Despite the noise present in real data that drives to a poorer fitting with respect to the simulation, it is possible to see (Figure 12) that the agreement between empirical and covariance function is still good, especially considering the main correlation length: average of differences between model and empirical values is 1.5^{-10} m^2/s^4 and the standard deviation 2.2^{-10} m^2/s^4 (comparable to the accuracy achieved in the simulation).
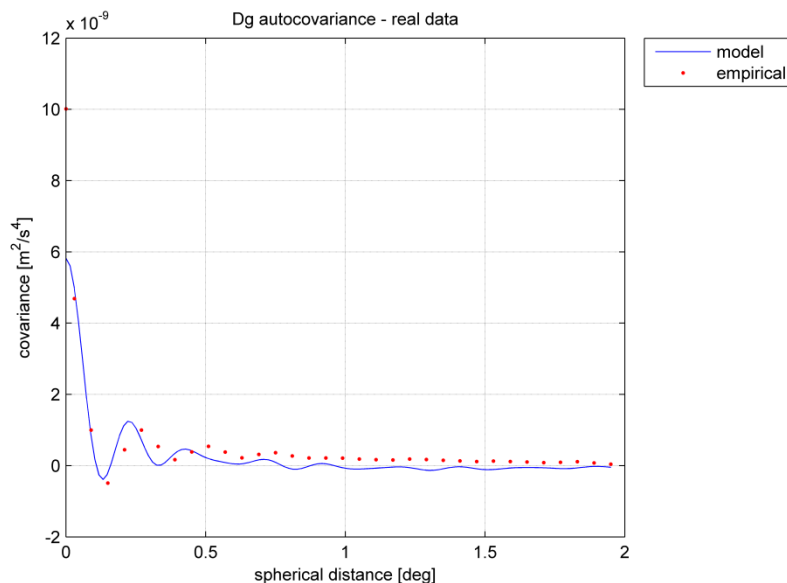

Figure 12: Model autocovariance obtained by fitting the empirical function of Δg_{res}

To be thorough, in Figure 13 the adapted degree variances obtained using the reduced free-air gravity anomalies are represented.
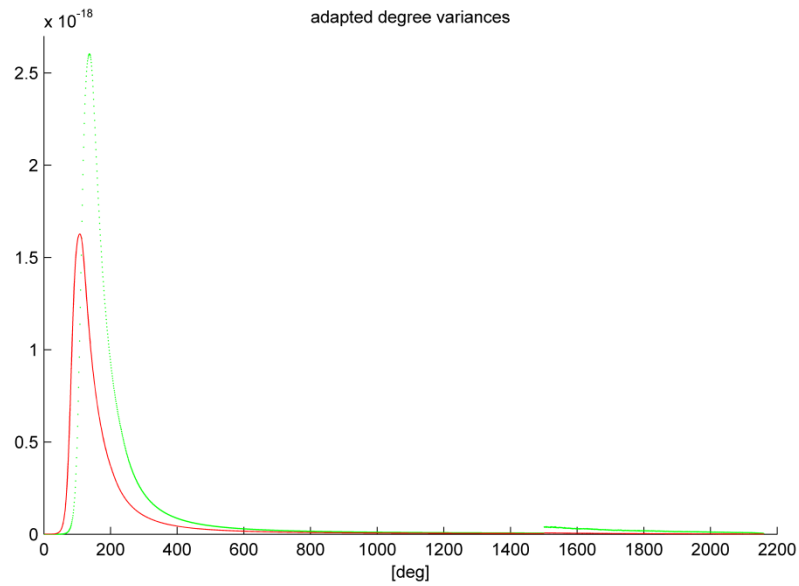
Figure 13: In green, the adapted error degree variances (up to degree 1500) and degree variances (from degree 1501) obtained from the simplex method. In red, the EGM2008 degree/error degree variances

4. Conclusions

The new methodology for covariance modelling based on Linear Programming and Simplex Method proved to be flexible and able to properly reproduce all the main features of the given empirical covariances. The simulated and real data tests in the NW part of Italy based on gravity anomaly and geoid undulation data led to proper covariance models.

The simulated test was based on the EGM2008 global geopotential model. Either gravity and geoid undulation values were computed from the model in the frequency band $1501 \leq n \leq 2190$ over a set of points selected by the Italian gravity database. The fitting procedure of the empirical covariances of these simulated data gave good results according to the statistics of the residuals between model and empirical values. At first, the empirical auto-covariances of the simulated residual gravity and geoid undulation values were fitted separately with the respective model covariances. The final coherence between the model covariance functions and the empirical covariance estimates is suitable since the most relevant features of the empirical values are properly fitted by the model covariances.

The same valuable results were obtained when model estimates were derived by jointly using the available empirical auto-covariance estimates, $C_{N_{res}N_{res}}^{emp}$ and $C_{\Delta g_{res}\Delta g_{res}}^{emp}$.

Real gravity data were then used having the same distribution of the simulated ones. They were reduced for the long-wavelength components using EGM2008 to degree 1500, as done in the simulated test. In this case, RTC effect was also estimated and subtracted from the data. As for the simulated test, the empirical function of residual gravity was properly fitted by the model covariance obtained by applying the new proposed procedure.

Thus, the new method for covariance fitting based on Linear Programming and Simplex Method is effective and gives estimated model covariances which allow a suitable fitting to the empirical values. Therefore, this procedure can be considered as a valuable tool in further developments and applications of collocation.

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