Least-Squares collocation and its smoothing effect

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Abstract

An optimal modification of the least-squares collocation (LSC) method is presented in this paper, aiming to remove its inherent smoothing effect while sustaining most of its local prediction accuracy at each computation point. Our "de-smoothing" approach is based on a covariance-matching constraint that is imposed on a linear transform of the LSC solution so that the final predicted signal reproduces the spatial variation implied by an a-priori covariance (CV) function model. Concurrently, an optimal criterion is evoked which minimizes the loss in local prediction accuracy (in the mean squared sense) that occurs from the linear transformation of the original LSC solution to its CV-matching counterpart. The merit and the theoretical principles of this signal filtering technique are analytically explained and a comparative example with the usual LSC prediction method is also given.

1. Introduction

The prediction of the stochastic behavior of a continuous spatial random field (SRF) using a set of observed values of the same and/or other SRFs is a fundamental inverse problem in geosciences. The mathematical model that is commonly used for the solution of this problem can be formulated in terms of the generalized observation equation:

$$y_i = L_i(u) + v_i \ , \quad i = 1, 2, \ldots, n \tag{1}$$

where $u(P)$ denotes the primary random field of interest ($P \in D$, with D being a bounded or unbounded spatial domain) that needs to be determined, at one or more points, using n discrete measurements taken on the same and/or other locations. The symbols $L_i(\cdot)$ correspond to bounded linear or linearized functionals of the unknown field and they are dictated by the particular physical model that relates the observable quantities with the underlying SRF itself. The additive terms $\{v_i\}$ represent the effect of measurement random noise in the available data.

The predominant approach that is followed in geodesy for solving such problems is the method of *least-squares collocation* (LSC) which was introduced by Krarup (1969) in a deterministic context as a rigorous framework for signal approximation problems in separable Hilbert spaces with reproducing kernels, and formulated in parallel by Moritz (1970) under a probabilistic setting as an optimal prediction technique for spatially correlated random variables and stochastic processes; see also Dermanis (1976) and Sanso (1986).

A critical aspect in LSC is the smoothing effect on the predicted signal which typically exhibits less spatial variability than the actual field $u(P)$ that needs to recovered from the available discrete data. As a result, small signal values are often overestimated and large signal values are underestimated, thus introducing a likely conditional bias in the final results. Such a smoothing effect is not solely associated with the LSC method and it occurs in most interpolation techniques aiming at the optimal approximation of a continuous function from a finite number of observed functionals. Note that signal smoothing should not be perceived as an entirely "harmful" interpolation effect since it ensures that the recovered field does not produce artificial details not inherent or proven by the actual data (a fact that is certainly a desirable characteristic for any signal interpolator).

However, the use of smoothed SRF images or maps generated by optimal techniques such as LSC provides a shortfall for applications sensitive to the presence of extreme signal values, patterns of field continuity and spatial correlation structure. While founded on "local" optimality criteria that minimize the mean squared error (MSE) at each prediction point, the LSC approach overlooks to some extent a feature of reality that is often important to capture, namely *spatial variability*. The latter can be considered a "global" field attribute since it only has meaning in the context of the relationship of all signal values (true or predicted) to one another in space. As a result of its inherent smoothing effect, the ordinary LSC solution does not reproduce the histogram of the underlying SRF and the spatial correlation structure that is implied by its covariance (CV) function.

In this paper we present an ad-hoc technique that enhances the LSC prediction by eliminating its smoothing effect, while preserving most of its local prediction accuracy. Our approach applies an optimal linear transformation to the result obtained by the LSC algorithm in a way that the transformed field matches the spatial correlation structure of the unknown SRF. The optimality of this signal transformation scheme is controlled through a criterion that minimizes the prediction accuracy loss (in the MSE sense) that inevitably occurs within the conversion of the original LSC solution to its CV-matching counterpart.

The structure of the paper is organized as follows: in section 2 a general overview of the classic LSC method for SRF prediction is presented, along with the most important mathematical formulae that are required for the development of our CV-matching technique which is presented in detail in section 3; in section 4 a numerical example is given to demonstrate the performance of the classic LSC solution compared to the CV-matching solution for a standard noise filtering problem; in section 5 some concluding remarks are finally drawn and a few related ideas for future work are also outlined.

2. The least-squares collocation solution

Denoting by $s_i = L_i(u)$ the signal part in the available data, the system of observation equations formed by (1) can be written in the following vector form:

$$\mathbf{y} = \mathbf{s} + \mathbf{v} \tag{2}$$

where $\mathbf{y}$, $\mathbf{s}$ and $\mathbf{v}$ are random vectors containing the given measurements and the unknown signal and noise values, respectively, at all observation points.

The signal and noise components in (2) are considered uncorrelated with each other (a crucial simplification that is regularly applied in practice) and with known second-order spatio-statistical properties in terms of their given expectations and co-variances.

Assuming that the spatial variability of the primary SRF is described by a covariance function model $C_u(P, Q)$, the elements of the CV matrix of the signal vector $\mathbf{s}$ are determined according to the propagation law (Moritz 1980)

$$\mathbf{C_s}[i,j] = L_i \, L_j \, C_u(P_i, P_j) \tag{3}$$

where L_i and L_j correspond to the functionals associated with the i^{th} and j^{th} observation, respectively. In the same way, the cross-CV matrix between the primary SRF values at the selected prediction points ($P_i' : i = 1, ..., m$) and the observed signal values at the available data points ($P_j : j = 1, ..., n$) is formed as follows:

$$\mathbf{C_{us}}[i,j] = L_j \, C_u(P_i', P_j) \tag{4}$$

For the purpose of this paper, the CV matrix $\mathbf{C_v}$ of the measurement noise is also considered known based on an appropriate stochastic model that describes the statistical behavior of the zero-mean measurement errors.

An additional postulate on the spatial trend of the primary SRF is often employed as an auxiliary hypothesis for the LSC inversion of (1) or (2). In fact, various LSC prediction algorithms may arise in practice, depending on the treatment of the signal de-trending problem. For the purpose of this paper and without any essential loss of generality, it will be assumed that we deal only with zero-mean signals, $E\{u\} = 0$, $E\{\mathbf{s}\} = \mathbf{0}$.

Based on the previous assumptions, the LSC predictor is given by the well known matrix formula:

$$\hat{\mathbf{u}} = \mathbf{C_{us}}(\mathbf{C_s} + \mathbf{C_v})^{-1}\, \mathbf{y} \tag{5}$$

which corresponds to the linear unbiased solution with minimum mean squared prediction error (Moritz 1980, Sanso 1986).

The inherent smoothing effect in LSC can be identified from the covariance structure of its optimal result. Indeed, if we apply CV propagation to the signal prediction formula in (5), we get the CV matrix

$$\mathbf{C}_{\hat{\mathbf{u}}} = \mathbf{C}_{\mathbf{us}}(\mathbf{C}_{\mathbf{s}} + \mathbf{C}_{\mathbf{v}})^{-1}\mathbf{C}_{\mathbf{us}}^{\mathrm{T}} \tag{6}$$

which describes the spatial variability of the recovered field and it generally differs from the CV matrix of the original SRF at the same points, i.e.

$$\mathbf{C}_{\mathbf{u}}[i,j] = C_u(P_i', P_j') \neq \mathbf{C}_{\hat{\mathbf{u}}}[i,j] \tag{7}$$

Moreover, if we consider the LSC prediction errors $\mathbf{e} = \hat{\mathbf{u}} - \mathbf{u}$, it is well known that

$$\mathbf{C}_{\hat{\mathbf{u}}} = \mathbf{C}_{\mathbf{u}} - \mathbf{C}_{\mathbf{e}} \tag{8}$$

where the error CV matrix is given by the equation (Moritz 1980)

$$\mathbf{C}_{\mathbf{e}} = \mathbf{C}_{\mathbf{u}} - \mathbf{C}_{\mathbf{us}}(\mathbf{C}_{\mathbf{s}} + \mathbf{C}_{\mathbf{v}})^{-1}\mathbf{C}_{\mathbf{us}}^{\mathrm{T}} \tag{9}$$

The fundamental "orthogonality" relation in (8) conveys the meaning of the smoothing effect within the LSC algorithm which essentially acts as an optimal low-pass filter (Wiener filter) to the input data. The spatial variability of the LSC prediction error, in terms of the error variances and co-variances at the computation points, is exactly equal to the deficit in spatial signal variability of the LSC predictor with respect to the original SRF.

3. Optimal "de-smoothing" of the LSC solution

Our objective is to develop a correction procedure that can be applied to the optimal result obtained by LSC for the purpose of removing its inherent smoothing effect, while sustaining most of its local prediction accuracy. In general terms, we seek a "de-smoothing" transformation to act upon the LSC predictor $\hat{\mathbf{u}}' = \Re(\hat{\mathbf{u}})$ in a way that the covariance structure of the primary SRF is recovered. This means that the transformation $\Re(\cdot)$ should guarantee that

$$\mathbf{C}_{\hat{\mathbf{u}}'} = \mathbf{C}_{\mathbf{u}} \tag{10}$$

where $\mathbf{C}_{\mathbf{u}}$ is the CV matrix formed through the covariance function $C_u(P, Q)$ of the primary SRF; see (7).

Moreover, the prediction error $\mathbf{e}' = \hat{\mathbf{u}}' - \mathbf{u}$ associated with the "corrected" field should remain small in some sense, so that the new solution provides not only a CV-matching representation of the original field, but also locally accurate predicted values on the basis of the given data. For this purpose, the formulation of the transformation operator $\Re(\cdot)$ should incorporate an additional optimality principle by minimizing, for example, the trace of the error CV matrix $\mathbf{C}_{\mathbf{e}'}$.

Let us adopt a straightforward linear approach to transform the original LSC predictor in the following way

$$\hat{\mathbf{u}}' = \mathbf{R}\,\hat{\mathbf{u}} \tag{11}$$

where $\mathbf{R}$ is a square filtering matrix that needs to be determined according to some optimal criteria for the new predictor $\hat{\mathbf{u}}'$.

The transformed signal obtained from (11) should reproduce the spatial covariance structure of the primary SRF, in the sense that $\mathbf{C}_{\hat{\mathbf{u}}'} = \mathbf{C}_{\mathbf{u}}$ <u>for the given spatial distribution of all prediction points</u>. Hence, the matrix $\mathbf{R}$ has to satisfy the constraint

$$\mathbf{R}\mathbf{C}_{\hat{\mathbf{u}}}\mathbf{R}^{\mathrm{T}} = \mathbf{C}_{\mathbf{u}} \tag{12}$$

where $\mathbf{C}_{\mathbf{u}}$ and $\mathbf{C}_{\hat{\mathbf{u}}}$ correspond to the CV matrices of the primary and the LSC-predicted SRFs, respectively.

The accuracy assessment of the CV-matching predicted field should be based on the error CV matrix

$$\mathbf{C}_{\mathbf{e}'} = E\{(\hat{\mathbf{u}}' - \mathbf{u})\,(\hat{\mathbf{u}}' - \mathbf{u})^{\mathrm{T}}\} \tag{13}$$

which, taking into account (11), is reduced to the form

$$\mathbf{C}_{\mathbf{e}'} = \mathbf{R}\mathbf{C}_{\hat{\mathbf{u}}}\mathbf{R}^{\mathrm{T}} + \mathbf{C}_{\mathbf{u}} - \mathbf{R}\mathbf{C}_{\hat{\mathbf{u}}\mathbf{u}} - \mathbf{C}_{\mathbf{u}\hat{\mathbf{u}}}\mathbf{R}^{\mathrm{T}} \tag{14}$$

Using the orthogonality relation (8) and also the following equation that is always valid for the LSC predictor (assuming that there is zero correlation between the observed signals **s** and the measurement noise **v**)

$$\mathbf{C}_{\hat{\mathbf{u}}\mathbf{u}} = \mathbf{C}_{\hat{\mathbf{u}}} \tag{15}$$

the new error CV matrix can be finally expressed as

$$\mathbf{C}_{\mathbf{e}'} = \mathbf{C}_{\mathbf{e}} + (\mathbf{I} - \mathbf{R})\mathbf{C}_{\hat{\mathbf{u}}}(\mathbf{I} - \mathbf{R})^{\mathrm{T}} \tag{16}$$

where $\mathbf{C}_{\mathbf{e}}$ is the error CV matrix of the usual LSC solution. Evidently, the prediction accuracy of the CV-matching solution will always be worse than the prediction accuracy of the original LSC solution, regardless of the form of the filtering matrix **R**. This is not surprising since LSC provides the best (in the MSE sense) unbiased linear predictor from the available measurements, which cannot be further improved by additional linear operations.

Our goal is to determine an optimal filtering matrix that satisfies the CV-matching constraint in (12), while minimizing the loss of the prediction accuracy in the recovered signal, in the sense that

$$trace\,(\mathbf{C_{e'}} - \mathbf{C_e}) = trace\,(\delta\mathbf{C_{e'}}) = \text{minimum} \tag{17}$$

where $\delta\mathbf{C_{e'}} = (\mathbf{I} - \mathbf{R})\,\mathbf{C_{\hat{u}}}\,(\mathbf{I} - \mathbf{R})^{\mathrm{T}}$ represents the part of the error CV matrix of the CV-matching predictor that depends on the choice of the filtering matrix.

The determination of the filtering matrix that satisfies the CV-matching constraint (12) and also minimizes the loss in the MSE prediction accuracy of $\mathbf{\hat{u}}'$ according to (17), is analytically described in Kotsakis (2007). Here we only present the final result without going into any technical details regarding its mathematical proof.

The optimal filtering matrix is

$$\mathbf{R} = \mathbf{C_u^{1/2}}(\mathbf{C_u^{1/2}}\mathbf{C_{\hat{u}}}\mathbf{C_u^{1/2}})^{-1/2}\mathbf{C_u^{1/2}} \tag{18}$$

or equivalently

$$\mathbf{R} = \mathbf{C_{\hat{u}}^{-1/2}}(\mathbf{C_{\hat{u}}^{1/2}}\mathbf{C_u}\mathbf{C_{\hat{u}}^{1/2}})^{-1/2}\mathbf{C_{\hat{u}}^{1/2}} \tag{19}$$

Note that the above result was originally derived in Eldar (2001) under a completely different context than the one discussed in this paper, focusing on applications like matched-filter detection, quantum signal processing and signal whitening.

4. Numerical example

A numerical example is presented in this section to demonstrate the performance of the transformed CV-matching solution $\mathbf{\hat{u}}'$ in comparison with the classic LSC solution $\mathbf{\hat{u}}$. This particular test refers to a standard noise filtering problem for a set of simulated gravity anomaly data. The image shown in Fig. 1(a) is the actual realization of a free-air gravity anomaly field that has been simulated within an 50×50 km^2 area with a uniform sampling resolution 2 km, according to the following model of spatial CV function

$$C_u(P,Q) = \frac{C_o}{1 + (r_{PQ}\,/\,a)^2} \tag{20}$$

where C_o = 220 mgal^2, r_{PQ} is the planar distance between points P and Q, and the parameter a is selected such that the correlation length of the gravity anomaly signal is equal to 7 km.

The noisy data grid is shown in Fig. 1(b) with the underlying noise level set to

±15 mgal. The additive random errors have been simulated as uncorrelated random variables, thus enforcing a white noise background for the gridded data. In Fig. 1(d) we see the filtered signal as obtained from the classic LSC algorithm (i.e. Wiener filtering), whereas in Fig. 1(c) is shown the result obtained from the optimal CV-matching transformation that was described in the previous section.

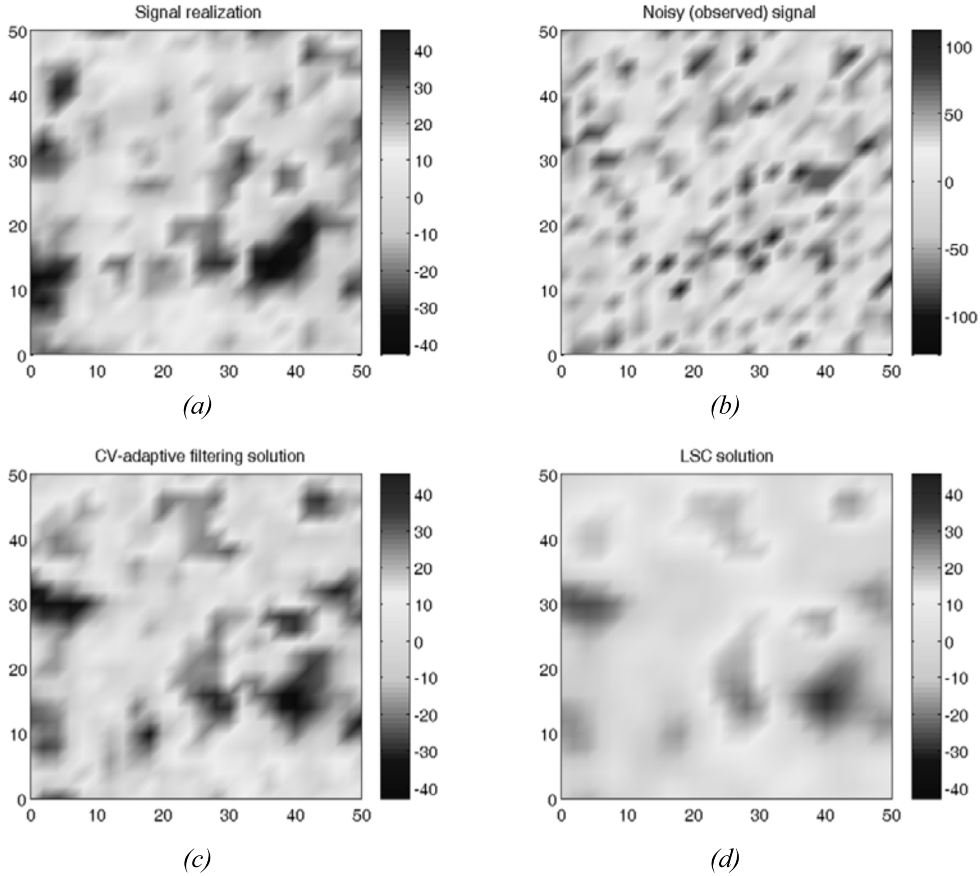

Figure 1. *Plots of: (a) the true (simulated) gravity anomaly signal, (b) the noisy observed signal, (c) the CV-matching transformed signal, and (d) the LSC-filtered signal*

Although the LSC method provides the most accurate (in the MSE sense) filtered signal, the result obtained from the transformed CV-matching solution clearly looks more similar to the original field that is depicted in Fig. 1(a). The emulation of the spatial variability of the primary SRF by the CV-matching solution $\hat{\mathbf{u}}'$, in contrast to the smoothed representation obtained by the LSC predictor $\hat{\mathbf{u}}$, can also be seen in the histograms plotted in Fig. 2, as well as in the signal statistics listed in the following table.

Table 1. *Statistics of the true (simulated) signal, the LSC-filtered signal and the CV-matching transformed signal (all values in mgal)*

	Max	Min	Mean	σ
True signal	45.33	–42.88	–0.04	14.96
LSC solution	27.42	–29.10	0.74	10.29
CV-matching solution	41.47	–42.48	0.73	14.64

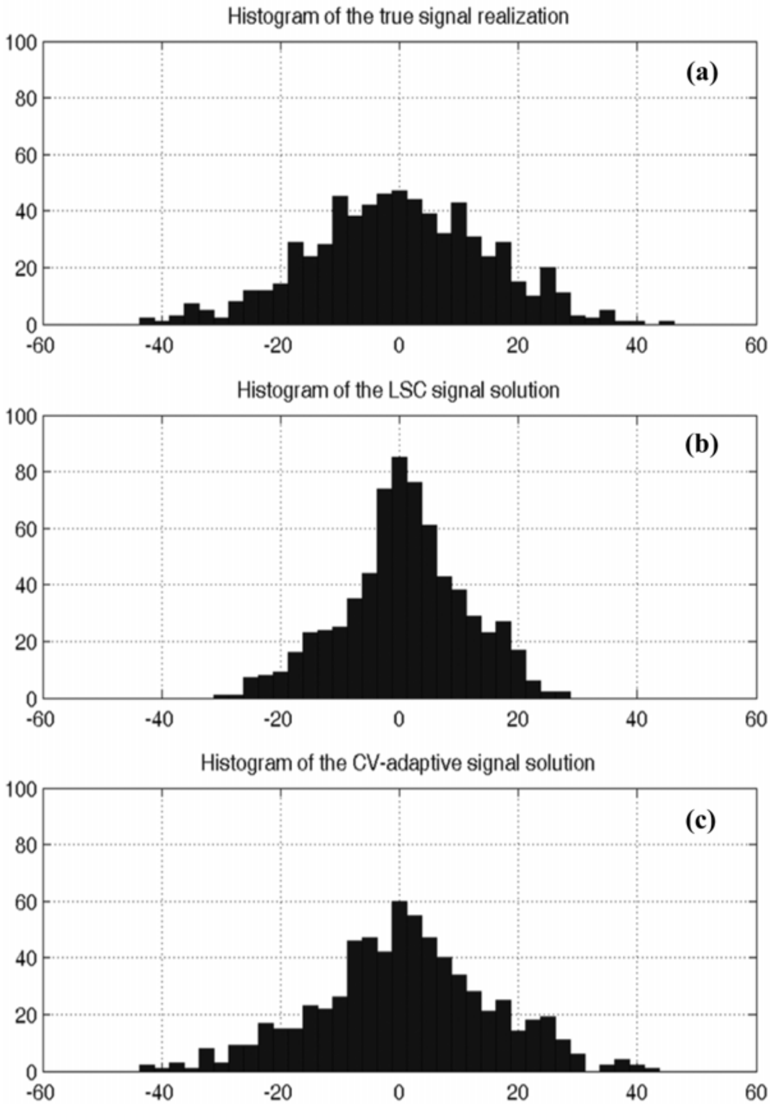

Figure 2. *Histograms of: (a) the true (simulated) gravity anomaly signal, (b) the LSC-filtered signal, and (c) the CV-matching transformed signal*

5. Conclusions

Due to its inherent smoothing effect, the LSC solution does not reproduce the spatial correlation structure of the primary SRF that needs to be recovered from its observed functionals. The technique presented in this paper overcomes this problem by transforming the original LSC solution through a CV-matching operator under a “minimum prediction accuracy loss” optimal criterion. In contrast to stochastic simulation schemes which provide multiple equiprobable signal realizations according to some CV model of spatial variability (e.g. Christakos 1992), the methodology presented in this paper gives a unique field estimate that is statistically consistent with an a-priori model of its spatial covariance function. The uniqueness is imposed through an optimal criterion that minimizes the loss in local prediction accuracy (in MSE sense) which occurs when we transform the LSC solution to fit the spatial correlation of the primary SRF over all prediction points.

Note that similar predictors have also appeared in the geostatistical literature by constraining the unbiased solutions obtained by various forms of kriging through a covariance-adaptive condition, thus yielding SRF predictors that match not only the first moment but also the second moment of the unknown SRF (Cressie 1993, Aldworth and Cressie 2003).

Evidently, the rationale of the proposed technique relies on the knowledge of the *true* covariance function of the underlying SRF, an assumption which is also inbuilt in the theoretical development of the LSC method itself (Moritz 1980). In practice, an *empirical* signal covariance function is often first estimated from a noisy data record and then used in the implementation of the LSC procedure for the (sub-optimal) recovery of the primary SRF at a number of prediction points. It is thus reasonable to question whether it would be meaningful to let the spatial variability of the LSC solution to be adapted to an empirical covariance function by following the CV-matching approach presented in this paper. A more reasonable methodology in this case would be to incorporate a variance component estimation approach, in the sense that the final predicted field adapts to an “improved” model of spatial variability (i.e. with respect to the one imposed by the empirical CV function). In contrast to the standard CV-matching constraint introduced in (10), we may impose the alternative CV-tuning constraint

$$\mathbf{C}_{\hat{\mathbf{u}}'} = \sigma^2 \, \mathbf{Q}_{\mathbf{u}} \qquad (21)$$

where the CV matrix $\mathbf{Q}_{\mathbf{u}}$ is formed through the empirically determined signal CV function, and σ^2 is an unknown variance factor which controls the consistency between the empirical and the true CV function for the underlying unknown signal. Tackling the above problem along with the study of one-step CV-matching linear predictors, instead of the two-step constructive approach that was presented herein, may be an interesting subject for future investigation.

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