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An automated decision support system for aided assessment of variogram models

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ABSTRACT

In the present paper, an extensive cross-validation procedure, based on the analysis of numerical indices and graphical tools, is described and discussed. The procedure has been implemented in a software application designed to support practitioners in the variogram model assessment. It provides an extensive report, which summarizes a large post-processing stage and suggests how to interpret the performed analysis to rate the model to be validated. Besides classical accuracy indices, two new integrated tools based on the variogram of residuals are introduced, which take the spatial nature of the dataset into account. Finally, inspecting the summary report, the user can decide whether the considered model is satisfactory for his/her goals or it needs to be improved. Finally, a case study is presented related to the variogram assessment of groundwater level measured in a porous shallow aquifer of the Apulia Region (South-Italy).

Software availability

Name of the software: SRF-XValid
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E-mail: emanuele.barca@ba.irsa.cnr.it
First available: 2014
Program Language: Surfer VBA
Note: SRF-XValid is not on sale but it can be requested from the authors for research purposes

1. Introduction

Applied Earth and environmental sciences often deal with regionalized data with the aim of studying the behaviour of one or more spatially distributed properties.

Geostatistics provides a number of techniques based on Random Functions theory (Journel and Huijbrechts, 1978), which are generally applied to estimate the value of a spatially measured variable at an unsampled location within a given study area. The main issue concerning any geostatistical approach is the assessment of spatial dependencies, through parametric classes of covariance and variogram functions, which basically describe the dependence of a process along the space where it is defined.

Since a poorly assessed *variogram model* (VM) can strongly affect the final results of any geostatistical study, much time and effort are devoted to the VM assessment and validation. In general, a VM is considered *good* if it shows a strong consistence with the observational data. The fulfilment of such a property is assessed by means of a family of procedures that goes under the name of *cross-validation* (Clark, 1986; Davis, 1987). Roughly, the *cross-validation* consists in estimating $z^*(x_i)$ values in any location x_i where observed values $z(x_i)$ are available. The underlying approach is the well-known *leave-one-out* method (Isaaks and Srivastava, 1989; Cressie, 1993), which consists in iteratively removing $z(x_i)$ from the dataset and estimating it on the basis of the VM and the remaining observed data. The deviations between estimated and observed values at any x_i are statistically analysed in order to make some inference about the *goodness* of the VM through the analysis of accuracy indices (Jolly et al., 2005; Theodossiou and Latinopoulos, 2006; Spöck, 2012) and the expert judgement of the geostatistician. During the last decades, the scientific literature has proposed a great number of such indices to support geostatisticians in validating the VMs (Willmott and Matsuura, 2005).

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Nevertheless, the scientific debate is still open; divergent opinions arise about the effectiveness of such indices and many works claim the greater relevance of some of them compared to others on the basis of good theoretical arguments (Willmott et al., 2009; Chai and Draxler, 2014; Zhang and Wang, 2010). Last, but not the least, geostatistical beginners, often ignoring the real meaning of available indices, choose just a few of them or, worse, prefer to fit VMs by using automatic procedures, neglecting any expert-based judgement. The reason underlying these divergent opinions is the intrinsic complexity of the VM validation. In our opinion, all of the proposed indices explain the deviation of the model from observed data from different perspectives. Consequently, for a cross-validation being really effective, it should analyse an extensive number of different indices, each representative of as many features of the model behaviour as possible. Coherently with this standpoint, this paper outlines a procedure that involves a wide range of independent indices and is consequently called *extensive cross-validation*.

Finally, a useful and friendly software application, SRF-XValid, implementing the above mentioned procedure and capable of performing such extensive cross-validation is presented. The software has been developed in VBA for Surfer (Golden Software Inc.) and integrates the existing Surfer cross-validation facilities, introducing several further important extensions. The software is flexible enough to allow the user to check very sophisticated models, such as anisotropic and multi-component ones. In conclusion, as a representative case study, SRF-XValid is applied to a groundwater-level dataset surveyed in the shallow, porous aquifer of Tavoliere di Puglia located in the northern part of the Apulia Region, Italy.

2. Material and methods

2.1. The issue of environmental models assessment in the geostatistical scope

The present paragraph focuses on the calibration and sensitivity analysis of environmental models in the context of the Gaussian processes framework (Geostatistics). In the geostatistical scope, the primary goal of the modeller is the assessment of the variogram model. Given a physical spatial variable (rainfall depth, piezometric level, air temperature, etc.), such model describes the average dissimilarity between observation couples at different spatial locations. In practice, given a lag-distance h and a generic location x_0, the variogram model is a continuous function providing the average variance between x_0 and all the locations x_i falling within the annulus of centre x_0, major radius = h + lag-tolerance and minor radius = h-lag-tolerance over the geographic observational domain (see Fig. 1).

Due to the aforementioned definition, the variogram model can be classified as a *lazy learner*, since it doesn't provide directly the predictions of the studied variable at un-sampled locations and needs a companion method (called kriging) for solving the set of algebraic equations to respond to specific queries. From the mathematical standpoint, the variogram is basically a function selected from a limited set of permissible functions (see Table 1) with specific properties known in advance. These properties, such as the monotonicity, the conditionally negative-definiteness, the geographic domain etc., pose different issues for its assessment with respect other kind of models. In general terms, the assessment of the variogram follows the steps described in Oreskes et al. (1994): the first assessment stage is the model *calibration*, followed by a second stage called *validation* or *sensitivity analysis*. The calibration is made up of two steps in a similar way to the regression analysis: i) the selection of a specific permissible model and ii) the estimation of the optimal set of the model parameters according some objective functions (generally, error-based). The step (i) is operationally carried out by means of the visual inspection of the experimental variogram, an empirical estimation of the variogram model, whose shape aids the variographer in the selection of the most suited model. The step (ii) can be carried out by a trial-and-error strategy or automated by means of several estimation algorithms: the weighted least square, the generalized least square, the restricted maximum likelihood etc. (Zhang et al., 1995; Genton, 1998; Lark and Cullis, 2004). More in details, differently from the classical approach (Oreskes et al., 1994), the calibration stage involves the whole observational dataset; the goal is of exploiting all the information available to improve the calibration stage performance. Concerning the validation (or sensitivity) stage, it should be highlighted that, due to the aforementioned variogram properties, many of the main sensitivity methodologies are of little use in this scope. In fact, the three main parameters of the variogram (see Fig. 4), namely the *nugget*, the *length* and the *scale*, embed the major information needed for an effective sensitivity analysis. In particular, the length accounts for the model slope, the nugget for the model bias (the y-axis positive intercept) and the scale for the maximum variance of the couples located at the maximum lag-distance (Chilès and Delfiner, 1999).

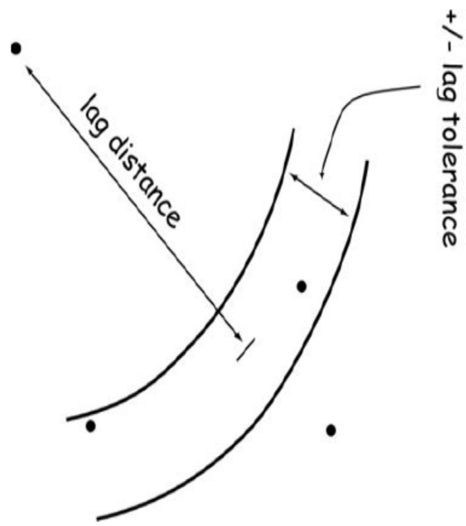

Fig. 1. Detail of the annulus containing the couples falling within the class lag ± tolerance.

As final remark, it should be highlighted that the variogram itself has become recently a master tool to carry out the sensitivity analysis on very complex models showing its capability in capturing the variance of the variable of interest, which, as it has been demonstrated (Razavi and Gupta, 2016a; 2016b), is directly and intrinsically tied to the most used sensitivity methods, such as the variance-based, the local derivative and the distributional approaches (Shahsavani and Grimvall, 2011; Gan et al., 2014; Pianosi and Wagener, 2015). Therefore, the sensitivity analysis is therefore performed by tuning the mentioned parameters and analysing the produced *response surfaces* in terms of kriging predictions and kriging standard deviations maps. The tuning is carried out with the *one-factor-at-time* strategy (Pianosi et al., 2016; Sarrazin et al., 2016); since, in general, the length is preferred for the parameters adjustment and only if the length tuning resulted ineffective it is followed by the nugget tuning. In Fig. 2 is sketched the effect on the variogram shape of the parameters adjustment.

Concerning the validation (or sensitivity) stage, following Pianosi et al. (2015), Pianosi et al. (2016), it can be defined an operational workflow to set up a robust decision support system for