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Optimal Spatiotemporal Prediction of Karstwater Levels

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ABSTRACT
In many fields of applied statistics samples from several locations in an investigation area are taken repeatedly over time. Especially in environmental monitoring the chemical and physical conditions in water, air and soil are measured using fixed and possibly mobile monitoring stations. The monitoring studies are aimed to model the phenomenon of interest (e.g., ground-level ozone, rain fall acidity or groundwater levels in karststone) and to predict the phenomenon at unsampled locations as well as into the future. For this purposes the spatiotemporal dynamic linear model is proposed, which builds up the framework for recursive best linear predictions. On one hand the spatiotemporal recursive best linear predictor is strongly connected with the predictors arising from the Kalman filter. On the other hand, this spatiotemporal predictor includes the method of linear Bayesian kriging as a special case. Thus the proposed method for spatiotemporal prediction is related to frequently used geostatistical and time series analysis methods. The spatiotemporal modeling and prediction approach will be applied to hydrogeological data of yearly averaged karstwater levels from 50 wells monitoring a Triassic karstwater reservoir in a mining region of Hungary from 1970 to 1990.

KEY WORDS: Environmental Monitoring, Geostatistics, Hydrogeology, Kalman Filtering, Karstwater Levels, Kriging, Linear Bayes Prediction, Recursive Prediction, Time Series Analysis.

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The Transdanubian Mountains in Hungary are an karstic area. Bauxite and coal mines are established in this area long ago. In the fifties mining was intensified thus it was needed to lower the karstwater levels in the surrounding of the mines. By this the groundwater drops locally for about more than 100 meters. When the ecological consequences became apparent, e.g. forest decline and dried out springs, an environmental monitoring program was set up and started in the year 1970.

Karstwater is the groundwater in water conducting karststone layers. The karstwater level is mainly affected by infiltration of rain, evaporation and the outlet at springs. But in more detail, e.g. the evaporation depends on temperature, wind and the plants on the surface. Further, the outlet at springs depends on the karstwater level itself through the hydrologic pressure. Because of the complexity of all these effects and their interrelations deterministic models are inappropriate to predict the karstwater level in space and time. Therefore a spatiotemporal stochastic model will be used hereafter to monitor and predict the anthropogeneous effect by water extraction on the natural karstwater level.

In the last decade many spatiotemporal prediction methods were discussed, see e.g. Oehlert (1993), Handcock and Wallis (1994), Haas (1995), Huang and Cressie (1996). However standard procedures were not established yet. The aim of this work is to illustrate a method for optimal spatiotemporal on-line prediction within the concept of spatiotemporal dynamic linear models proposed by Berke (1998b,c). For this reason, yearly averaged karstwater levels from 50 monitoring wells from the period of 1970 to 1990 will be spatiotemporally analyzed. The data show up a temporal downwards trend as well as a clear spatial trend. Further the spatial structure, i.e. the variogram, is temporally dependent.

The outline of this work is as follows. Section 2 starts with a description of the data and the monitoring network. In section 3 several spatial statistics will be calculated, i.e. the variogram and trend parameters. The temporal behavior of this
spatial statistics is examined as well. Spatiotemporal dynamic linear modeling of the data and predictive inferences are the topic of section 4. The paper ends with a discussion of the results and further research directions.

2. DESCRIPTION OF THE KARSTWATER LEVEL DATA

Monitoring of the karstwater levels in the Transdanubian Mountains dates back to the early fifties (cf. Márkus et al., 1999a,b). But in 1970 a more extensive monitoring network was set up. The observations from the monitoring wells are taken irregularly during the year. Thus it is reasonable to analyze yearly averages of the karstwater level data. To do so is not trivial because the geological structure of the region contains several types of faults and sediments which affect the hydrogeological pattern, i.e., the permeability. So it is clear that there are several karstwater reservoirs that are almost independent of each other. For this reason data from 50 monitoring wells are chosen. This part of the monitoring network covers the subregion of the Transdanubian Mountains called the Bakony Mountains and the Balaton Highlands. The region of interest is placed to the north of the Lake Balaton. It is assumed that these 50 wells monitor the same Triassic karstwater reservoir.

In figure 1 a map shows the relative positions of the monitoring wells in this region of size $60 \times 60$ km. The data set contains the karstwater levels in meters above sea level and the spatial coordinates of the wells (north and east coordinates in km). The elevation data was incomplete and not used.

The main water extraction site to lower the karstwater level is to the east of well number 18 and to the north of well number 49. In other words, the water was pumped out of the center of the south-western part of the monitoring region. There exist several other drinking water pumps in this region but their overall effect is negligible compared to that of the main water extraction site.

A first step in spatiotemporal data analysis is to plot the data series, if a fixed monitoring network was used to sample the data. Figure 2 shows the 50 time series
in one plot together. These time series are called hydrographs by hydrogeologists.

All hydrographs show a downwards trend in time. However the temporal variability of the hydrographs show different pattern. In fact, some hydrographs are crossing, others are in parallel. These are effects that may depend on the distance and direction of the well to the water pumping station. Also the sediments permeability and many other sources have influence on the behavior of the hydrographs. Furthermore figure 1 shows the presence of 39 missing values. 10 of these occur in 1970 due to an extension of the monitoring network in 1971.

After the visual inspection of the time series it is useful to calculate yearly summary statistics over all spatial observations. These indicate that (a) the maximum karstwater level in this region varies from 298 m in 1970 down to 293 m in 1990, (b) the median falls more than 25 m from 194 m almost continuously down to 168 m in 1990, and (c) the minimum drops for more than 45 m from 108 m down to 61 m.
3. YEARLY SPATIAL STATISTICS

To explore the spatial issues of the monitoring data yearly triple scatter plots have been inspected at first. From these it can be deduced that the data imply a spatial trend that could be represented by second order polynomials in the north and east coordinates, i.e. a hill like trend model. Surprisingly (with respect to the crossings in the multiple time series plot of figure 1) the yearly spatial trend structure is stable over the whole monitoring period from 1970 to 1990.

These findings are formalized in the following way. The phenomenon under study is a spatiotemporal process $Z$. The sample data are an infill realization from this process. But due to missing values and the redesign of the network in 1971 the data are modeled as if they were a sequence of spatial processes:

$$Z = \left\{ \{Z_t(s) : s \in D \} \right\}_{t \in T},$$
where $\mathcal{D} \subset \mathbb{R}^2$ denotes the monitoring area, $s = (x, y) \in \mathbb{R}^2$ is any spatial location within this area, and $t \in \mathcal{T} \subset \mathbb{N}$ is the time index, i.e. the years. Inferences about the spatiotemporal process follow from yearly spatial linear modeling of the sample data. Further, the spatial processes are composed by two additive components: the trend $\mu_t(s)$ and the residual components $\delta_t(s)$, in particular these components are time dependent. The trend component is of the form

$$
\mu_t(s) = x_t(s)'\beta_i \quad s \in \mathcal{D}, \ t \in \mathcal{T}.
$$

In this notation $x_t(s)'\beta_i$ denotes the polynomials to model the spatial trend. For example, a first order polynomial at site $s = (u, v) \in \mathcal{D}$ is of the form

$$
\mu_t(s) = 1\beta_{i,0} + u\beta_{i,1} + v\beta_{i,2}, \quad s = (u, v) \in \mathcal{D}.
$$

The assumption that a second order polynomial could be used to model the spatial trend is tested by investigation of some experimental semivariograms. Firstly the experimental semivariograms are based on the raw data and the ordinary least squares estimation (OLSE) residuals from first and second order polynomial trend surfaces, respectively. This indicated that second order polynomials are much better. The first order polynomials result in estimates for the sill parameter that are two times larger than that of the second order trend surface. However the north coordinate is for both models in none of the years significant. The yearly semivariograms of the raw data exhibit no sill and disagree with the ergodic hypothesis. Finally, the following trend surface polynomial was fitted to the data year by year

$$
\mu_t(s) = \beta_{i,0} + u\beta_{i,1} + u^2\beta_{i,2} + uv\beta_{i,3} + v^2\beta_{i,4}, \quad s = (u, v) \in \mathcal{D}, \ t \in \mathcal{T}.
$$

Since the data are spatially correlated it is preferable to use the method of generalized least squares estimation (GLSE) over OLSE to fit the trend surfaces. However this presumes the knowledge of the second order moments that are of interest now. Iterative methods could be used for this purpose, e.g. iterative GLSE or maximum likelihood methods. But then one should be aware that the iterative procedures may result in biased estimates. In fact that turned out to be the case here.
Thus the experimental semivariogram based on the OLSE trend surface residuals is compared to that based on GLSE residuals after the first iteration. In figure 3 the experimental semivariograms for the years 1970 and 1990 are compared. At least for the first and critical 6 or 7 distance classes the experimental semivariograms agree to each other and to the fitted spherical structure models. For larger distances the fit is not perfect. However following a rule of thumb, the structure model should be fitted to the first half of the experimental semivariogram. Therefore OLSE is used to generate trend surface residuals from which the experimental semivariogram is calculated. And then iterated GLSE is used to estimate the polynomial trend surface parameters $\beta_i$.

Furthermore, from figure 3 follows that, with respect to the linear increase of the experimental semivariograms from 0 on, the use of the spherical model (cf. Cressie, 1993, p. 61) without nugget effect is adequate. Therefore the spherical model was fitted to the classical method of moments estimator (cf. Cressie, 1993, p. 69) of the experimental semivariogram based on the OLSE trend residuals using the first 11 of 20 distance classes. Here the weighted least squares estimation method of Cressie (1993, p. 98) was used. The results of this year by year fitting process to the 21 spatial processes of the years 1970 to 1990 is displayed in figure 4. Since the residuals are based on a scaled coordinate system (explained below) the range parameter is rescaled here, i.e. multiplied by the scaling factor. The sill is not affected by this scaling. The range seems to vary more or less on the same level, see figure 4a. Suspicious is one possible outlier for the year 1970. This may be regarded as an effect of the 10 missings in this year. On the other hand, the sill parameter estimates exhibit a clear upwards trend, see figure 4b.

This is interpreted as follows. The range parameter (cf. Cressie, 1993, p. 131) defines the zone of influence of the spatial process. In hydrogeological context this is regarded as the distance that the water flows within a certain time. This means that the water is moving about 11 km in one year. This parameter is stationary in time since the permeability of the ground, i.e. the geological formations and sediments
Figure 3a. Experimental semivariograms for year 1970 from OLSE trend residuals (○) and GLSE trend residuals (●) together with the estimated spherical models (—).

Figure 3b. Experimental semivariograms for year 1990 from OLSE trend residuals (○) and GLSE trend residuals (●) together with the estimated spherical models (—).