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Multivariate Geostatistical Approach to Space-Time Data Analysis

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A large number of hydrological phenomena may be regarded as realizations of space-time random functions. Most available hydrological data sets exhibit time-rich/space-poor characteristics, as well as, some form of temporal periodicity and spatial non-stationarity. To better understand the space-time structure of such hydrological variables, the observed values at each measurement site are considered as separate, but correlated time series. Moreover, it is assumed that the time series are realizations of a mixture of random functions, each associated with a different temporal scale, represented by a particular basic variogram. To preserve the observed temporal periodicities, the experimental direct and cross variograms are modelled as linear combinations of a number of hole function variograms. In a further step, the principal component analysis is used to determine groupings of measurement stations at different temporal scales. The proposed procedure is then applied to monthly piezometric data in a basin south of Paris, France. The temporal scales are determined to be the 12-month seasonal and the 12-year climatic cycles. At each temporal scale different spatial groupings are observed which are attributed to the contrast between the nearly steady state climatic variations versus the almost transient seasonal fluctuations.

1. INTRODUCTION

A great number of variables in hydrology can be viewed as spatiotemporal processes. Monthly precipitation readings or daily piezometric measurements may be considered as space-time functions presenting continuous complex fluctuations. Geostatistics offers a variety of methods to model such processes as realizations of random functions. These procedures, however, have been primarily applied to spatial data. Most published works in geostatistical hydrology also show a tendency to de-emphasize the role of the time dimension in order to comply with spatial models. Temporal integration of variables or steady-state assumptions are common approaches to accomplish this spatial conversion. For instance, one may consider annual rainfall depths in space as a regionalized variable. Steady-state piezometric surface is another example of a complex spatial function. Applying such space-oriented approaches to spatiotemporal processes, however, may lead to the loss of valuable information in the time dimension.

One obvious solution to this problem is to consider the spatiotemporal phenomenon as a realization of a random function in $n + 1$ dimensions (i.e., n dimensions in the physical space plus one time dimension.) This approach demands the extension of the existing spatial techniques into the space-time domain. Despite the straightforward appearance of this extension, there are a number of theoretical and practical problems that should be addressed prior to any successful application of geostatistical methods to space-time data. These problems include qualitative differences between spatial and temporal processes, imbalance between quantities of temporal and spatial information, and the presence of temporal periodicity and spatial non-stationarity.

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There are some major differences between temporal and spatial phenomena. For example, the one dimensional temporal data is ordered, while the usually 2 or 3 dimensional spatial variables do not exhibit such order, as past, present, and future. Moreover, a spatiotemporal phenomenon contains temporal and spatial scales which are fundamentally different, and cannot be compared to each other in a physical sense. To resolve this difference an operational solution is to split the space-time correlation either into a product [*Rodriguez-Iturbe and Mejia*, 1974], or a sum [*Bilonick*, 1987; *Rouhani and Hall*, 1989] of space and time components.

A further problem is caused by the typical arrangements of hydrological data sets. These sets are usually composed of few scattered clusters of observation points, each with a long time series. Such configurations are often dictated by the economy of sampling that yields information which is rich in time, but poor in space. As a consequence, the accuracies of the estimated temporal and spatial structures are quite different.

Another important issue is about the fact that many space-time data exhibit some form of temporal periodicity and spatial non-stationarity. One usually observes a variety of temporal periodicities, such as: periodic seasonal cycles, pseudo-periodic climatic cycles, as well as, non-periodic long-term trends. The periodic component can be approached in two different ways serving different purposes. The first approach regards the periodic component as a part of the trend, where estimation is conducted subject to periodic unbiasedness conditions, such as in trigonometric kriging. This method appears to be more efficient for filtering periodic components [see *Seguret*, 1989]. The second approach, on the other hand, considers the series as stationary, where the periodic component is included in the correlogram or the variogram (see, for example *Chatfield* [1984, p. 112]). This latter method, which is suitable for data analysis based on nested variograms or spectral analysis, has been adopted in this paper to better understand the spatiotemporal structure of a hydrological data set.

The temporal periodicities are often superimposed by strong spatial drifts. This spatial non-stationarity is not always limited to the mean. In certain instances, even when local stationarity of mean can be justified, the spatial variograms still show wide variations. For example, the portion of an aquifer with a closer hydraulic contact with surface waters exhibits a wider range of fluctuations, when compared to the more confined zones. In some cases, these spatial non-stationarities may be ignored, in others, however, they raise serious doubts about the homogeneity assumption.

In response to these problems, we decided to take a different approach, in which the time series at each measurement point are considered as separate, but correlated one-dimensional regionalized variables. In other words, we focus our attention on the dimension which is richer in information. We believe that our proposed approach is more suited to deal with the apparent spatial non-stationarities and temporal periodicities in our data sets. These can be treated more efficiently, if measurements at each site are considered as realizations of a separate random function. This collection, composed of a finite number of one-dimensional random functions, can be considered as a family of correlated random functions. The only drawback is the increase in the number of direct and cross variograms or covariances, which need to be modelled and estimated. If m observation points are considered, the number of involved structures amounts to $m(m + 1)/2$. However, in many studies, the number of measurement points are limited and so the proposed multivariate approach can be applied quite easily. Given the inherent imbalance in hydrological space-time data, this approach appears to be a rational alternative.

Solow and Gorelick [1986] propose a similar approach to deal with streamflow data, where measurements from each gage are considered as separate but correlated time series. Their approach is based on simple co-kriging (i.e., linear co-interpolation without any constraint on weights) of streamflow residuals which are detrended prior to the estimation. Covariance values are determined experimentally and no model is fitted. Such an approach demands the additional verification of positive definiteness of the covariance matrices that are calculated on a sample set with missing values. The proposed approach by *Solow and Gorelick* [1986] is only applicable to regularly spaced measurements in time. The above authors apply their procedure to the co-kriging of streamflow residuals at missing time intervals which are then added to the historical averages to determine missing streamflow values. In the present work, we make our geostatistical model more general by requiring a weaker stationarity hypothesis in the time dimension, and by making it applicable to measurements taken at irregular time intervals. Furthermore, modelling direct and cross variograms at different time scales adds more insight about the data, which will be discussed later. In an additional step we propose to use the principal component analysis to determine groupings of measurement stations at different temporal scales.

The proposed approach allows temporal estimation, such as estimation of missing data, hindcasting, and forecasting, which is appropriate for cases of few gages with long time series. This approach, in its present form, does not allow spatial estimation at an ungaged site. There is, however, another way that our multivariate approach can be applied to spatiotemporal data that permits spatial estimation. This is accomplished by viewing measurements in space at each time interval as realizations of a separate but correlated random function. Spatial interpolation and extrapolation can then be conducted by calculating direct and cross variograms in space and using time realizations $t \pm \tau$, $\tau = 1, \cdots, T$, as auxiliary correlated variables. In the following sections, we focus on the former approach, where the spatiotemporal data is viewed as a multivariate time series process.

2. Multivariate Approach

Description of multivariate geostatistical estimation processes can be found in the works of such authors, as *Matheron* [1971], *Journel and Huijbregts* [1978], and *Myers* [1982]. *Wackernagel* [1988] proposes a multivariate technique to interpret spatial information, based on a combination of variography, principal component analysis, and co-kriging. In the present work, we consider a spatiotemporal data set, $\{z_i(t_\alpha);\ i = 1, \cdots, N;\ \alpha = 1, \cdots, T\}$, measured at N locations at T time intervals, as samples of a set of N regionalized variables. These variables in turn can be viewed as a realization of a set of one-dimensional random functions $\{Z_i(t);\ i = 1, \cdots, N\}$. In this paper, we deal with a set of monthly piezometric heads measured at N wells over a period of up to T months. So we consider the piezometric data at each well to be a realization of a temporal random function, which is correlated to random functions associated with the other wells.

We then postulate the so-called "intrinsic" hypothesis that the increments, $Z_i(t_\alpha) - Z_i(t_\alpha + \tau)$, τ time intervals apart, are second order stationary,

$$E[Z_i(t) - Z_i(t + \tau)] = 0$$
$$E[\{Z_i(t) - Z_i(t + \tau)\}\{Z_j(t) - Z_j(t + \tau)\}] = 2\gamma_{ij}(\tau) \tag{1}$$

where $\gamma_{ij}(\tau)$ is defined as the cross variogram. In the particular case where variables themselves, Z_i and Z_j, can be assumed second-order stationary and uncorrelated for large time lags,

$$\gamma_{ij}(\tau) \rightarrow \sigma_{ij} \qquad \text{for } \tau \rightarrow \infty \tag{2}$$

where σ_{ij} is the covariance of Z_i and Z_j.

The experimental value of this variogram can be calculated directly as,

$$\gamma_{ij}(\tau_k) = (1/2T_k) \sum_{\alpha=1}^{T_k} \{(z_i(t_\alpha) - z_i(t_\alpha + \tau')\} \cdot \{z_j(t_\alpha) - z_j(t_\alpha + \tau')\} \tag{3}$$

where τ' is the time lag belonging to a class of lags τ_k, and T_k is the number of increment pairs in such a class.

3. Linear Model of Coregionalization

Using the technique of nested variogram modelling [*Journel and Huijbregts*, 1978], the experimental direct and cross variograms of the observed spatiotemporal data are modelled as sums of variograms at different temporal scales.

$\gamma_{ij}^u(\tau)$, which in turn, can be defined in terms of elementary variogram functions, $g_u(\tau)$,

$$\gamma_{ij}(\tau) = \sum_{u=1}^{S} \gamma_{ij}^u(\tau) = \sum_{u=1}^{s} b_{ij}^u g_u(\tau) \tag{4}$$

The elementary variogram functions, $g_u(\tau)$, have to be conditionally negative definite, and the matrices of coefficient b_{ij}^u, for fixed u, must be positive semi-definite. This multivariate model considers the phenomenon of interest to be generated by a sum of several random processes, each related to a specific temporal scale, as defined by its corresponding $g_u(\tau)$. The coefficients b_{ij}^u are determined semi-automatically by the computer program LINMOD, developed by *Wackernagel* [1989]. Recently, a more powerful least squares fitting procedure has been proposed by *Goulard* [1989].

To preserve the periodic behavior of our data in time, we have used the so-called "hole function" variograms as our basic models, defined as

$$g_u(\tau) = 1 - \exp(-\tau/r_u) \cos(2\pi\tau/l_u) \tag{5}$$

where r_u represents the range or the extent of oscillation of the hole function, $g_u(\tau)$, while l_u is the period of the cyclic variogram. A hole function variogram is a valid model for one-dimensional processes for positive values of r_u, l_u, and τ. In R^2, it is valid for $l_u \geq 2\pi r_u$, while in R^3 it is valid for $l_u \geq 2(3)^{1/2}\pi r_u$ [*Yaglom*, 1986]. The above basic variograms can represent cyclic trends in the piezometric data, including the 12-month seasonal trend and the longer climatic cycle.

Experimentally these basic processes can only be distinguished if their variograms have an impact on the shape of experimental curves. If this is the case, it would be possible to decompose the variogram into several temporal variograms, that leads to an analysis of the relationship between variables at different temporal scales. These relationships are described by the $N \times N$ matrices $\mathbf{B}_u$ of coefficients b_{ij}^u denoted as coregionalization matrices. The characteristics which are exhibited by each $\mathbf{B}_u$ matrix may be quite different from the one that is implied by the classical variance-covariance matrix, $\mathbf{V}$. In fact, under the same assumptions as for relation (2), $\mathbf{V}$ is related to the $\mathbf{B}_u$, as follows

$$\mathbf{V} = \sum_{u=1}^{S} B_u \tag{6}$$

which suggests that $\mathbf{V}$ is apparently a mixture of correlation structures at different spatial scales.

Each coregionalization matrix can be viewed as the variance-covariance matrix of a particular temporal scale. So a principal component analysis in R-mode can be performed by decomposing them, such that

$$\mathbf{B}_u\mathbf{Q}_u = \mathbf{D}_u\mathbf{Q}_u \tag{7}$$

with

$$\mathbf{Q}_u^T\mathbf{Q}_u = \mathbf{I} \tag{8}$$

where, $\mathbf{Q}_u$ is an orthonormal matrix of eigenvectors, $\mathbf{D}_u$ is a diagonal matrix of eigenvalues, $\mathbf{I}$ is the identity matrix, and superscript T implies a transposed matrix. The eigenvalues maximize the variance represented by the trace of $\mathbf{B}_u$ and the eigenvectors can be chosen to span an orthonormal system of axes called principal axes [see *Courant and Hilbert*, 1968]. The principal axes associated with most important eigenvalues explain the essential features of a coregionalization matrix.

The coordinates of the variables on a pair of principal axes lie inside a unit circle centered at the origin because the orthonormal matrix $\mathbf{Q}_u$ satisfies the equation of the unit hypersphere [*Volle*, 1985, p. 116]. The relative positions of variables on the above unit circle allow us to sort them in different groups. So for each time scale, associated with a $g_u(\tau)$, we can determine different groupings, which may reveal varying spatial characteristics of our temporal variables.

The above implies that the original set of correlated random functions $\{Z_i(t); i = 1, \cdots, N\}$ are decomposed into a set of uncorrelated random functions $\{Y_p^u(t); u = 1, \cdots, S; p = 1, \cdots, N\}$, each defined as the regionalized factor of pth principal component at uth temporal scale, such that

$$Z_i(t) = \sum_{u=1}^{S} \sum_{p=1}^{N} a_{up}^i Y_p^u(t) \tag{9}$$

which defines the linear model of coregionalization in a space-time context. The transformation coefficients, a_{up}^i, are contained in matrices $\mathbf{A}_u$ and obtained by setting,

$$\mathbf{A}_u = \mathbf{Q}_u(\mathbf{D}_u)^{1/2} \tag{10}$$

This paper primarily focuses on the principal component analysis at different temporal scales. It should be noted, however, that varying forms of mapping can be performed based on co-kriging of measured values. For instance, given our piezometric data, we can estimate the following:

1. The piezometric head at ith observation well at an arbitrary time interval, $Z_i(t_0)$, which allows hindcasting as well as forecasting;

2. The temporal component $Z_i^u(t_0)$ that represents the behavior of the piezometric head at the ith observation well of the uth temporal cyclic trend at an arbitrary time interval, which may be used for filtering and forecasting purposes; and

3. The regionalized factor $Y_p^u(t_0)$ of the pth principal component at the uth temporal scale, where for $p = 1$, it reflects the essential regional features of piezometric surface at uth cyclic trend.

In all above estimations the desired value is calculated as a linear sum of observed data, such as

$$\sum_{j=1}^{N} \sum_{\alpha=1}^{T} \lambda_\alpha^j z_j(t_\alpha) \tag{11}$$

where, λ_α^j is the estimation weight of the observed value at the jth location at the αth time interval.

The co-kriging of Z_i at an arbitrary time interval t_0 is a form of forecasting or hindcasting that can be used for estimation of missing values. This estimate is yielded by solving the following linear system

$$\sum_{k=1}^{N} \sum_{\beta=1}^{T} \lambda_{\beta}^{k} \gamma_{jk}(t_{\alpha}, t_{\beta}) - \mu_j = \gamma_{ji}(t_{\alpha}, t_0)$$
$$\sum_{\beta=1}^{T} \lambda_{\beta}^{j} = \delta_{ji} \tag{12}$$

for

$$j = 1, \cdots, N \qquad \alpha = 1, \cdots, T$$

where, $\gamma_{jk}(t_{\alpha}, t_{\beta})$ is the cross variogram between $Z_j(t_{\alpha})$ and $Z_k(t_{\beta})$, δ_{ji} is a Kronecker delta, and μ_j is the jth Lagrange multiplier.

The uth temporal component at the ith location at an arbitrary time interval t_0, $Z_i^u(t_0)$ can also be estimated by a similar co-kriging system. The local mean of each temporal component of the groundwater data may be arbitrarily set to zero, which then reflects the general trend of piezometric head variations at a specific temporal scale, such as seasonal or climatic cycles.

The co-kriging system for estimation of $Z_i^u(t_0)$ is

$$\sum_{k=1}^{N} \sum_{\beta=1}^{T} \lambda_{\beta}^{k} \gamma_{jk}(t_{\alpha}, t_{\beta}) - \mu_j = b_{ji}^{u} g_u(t_{\alpha}, t_0)$$
$$\sum_{\beta=1}^{T} \lambda_{\beta}^{j} = 0 \tag{13}$$

for

$$j = 1, \cdots, N \qquad \alpha = 1, \cdots, T$$

where, b_{ji}^{u} are coefficients as defined in Equation (4) and $g_u(t_{\alpha}, t_0)$ is the uth elementary variogram between time intervals t_{α} and t_0.

The regionalized factor $Y_p^u(t_0)$ representing the pth principal component at the uth temporal scale can also be estimated. In our example, the first principal component at any scale represents a regional index for variations of piezometric surface at different cycles. The co-kriging system

$$\sum_{k=1}^{N} \sum_{\beta=1}^{T} \lambda_{\beta}^{k} \gamma_{jk}(t_{\alpha}, t_{\beta}) - \mu_j = a_{up}^{i} g_u(t_{\alpha}, t_0)$$
$$\sum_{\beta=1}^{T} \lambda_{\beta}^{j} = 0 \tag{14}$$

for

$$j = 1, \cdots, N \qquad \alpha = 1, \cdots, T$$

where, a_{up}^{i} are transformation coefficients as defined in Equation (9), and $g_u(t_{\alpha}, t_0)$ is the uth elementary variogram between time intervals t_{α} and t_0. For more information readers are referred to *Wackernagel* [1988, 1989], and *Wackernagel et al.* [1988] for the application of the above multivariate procedure to spatial data. An alternative viewpoint, as mentioned in the introduction, is the one implied by trigonometric kriging that considers periodicity as a part of the trend [*Seguret*, 1989].

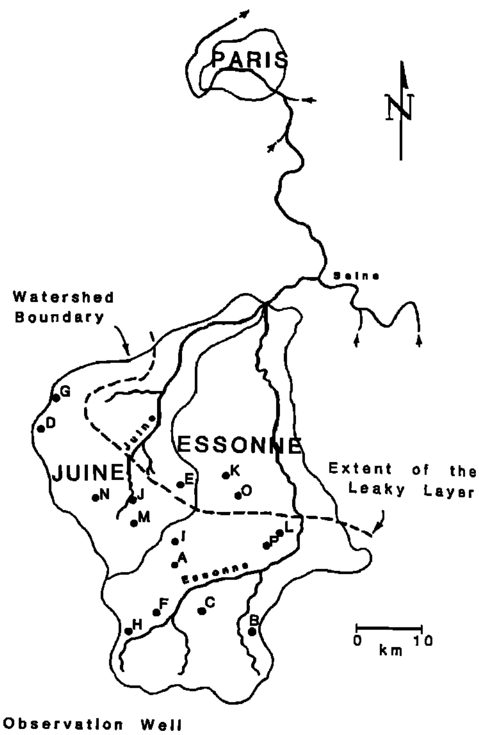

Fig. 1. Juine and Essonne Basins, located to the south of Paris, France. (Observation wells are identified by letters A to P.)

4. CASE STUDY

Our data set is composed of monthly piezometric readings from January 1967 to December 1982 at 16 observation wells in the Essonne and the Juine watersheds located in the Seine River basin in France, as shown in Figure 1. This region is underlain by two aquifers, which according to the geological time of their formations are termed as the Oligocene and the Eocene layers. The upper unconfined Oligocene layer is separated from the semi-confined lower Eocene aquifer by a leaky layer which covers the northern part of the region as shown in Figure 1. In the southern section of the basins there are no well defined boundaries between these two layers. All the observation wells used in this work represent piezomet-

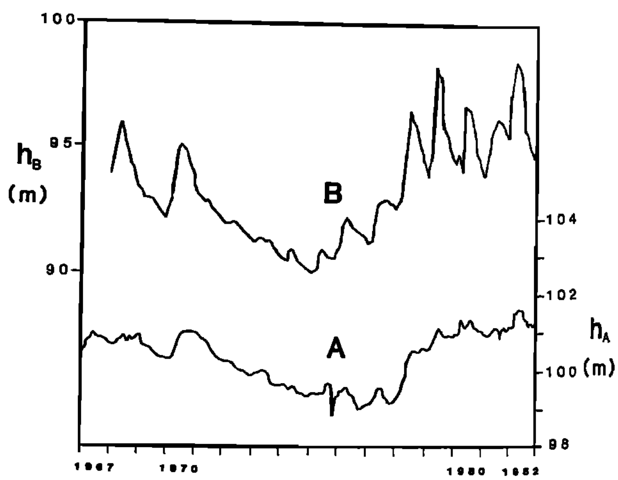

Fig. 2. Monthly piezometric heads at Wells A and B, denoted by h_A and h_B, respectively.

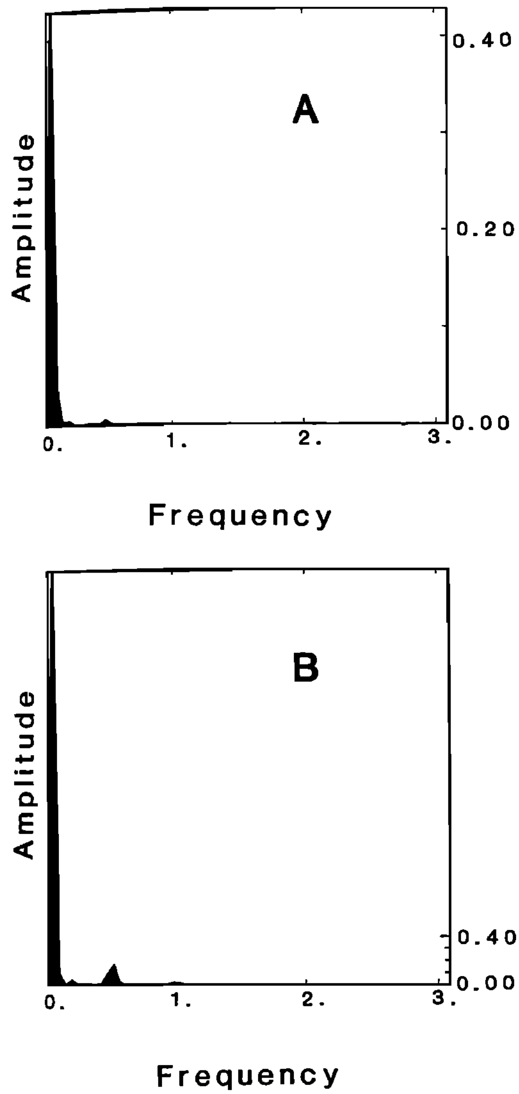

Fig. 3. Periodograms of monthly piezometric heads at Wells A and B. (Frequencies are given in 2π/months.)

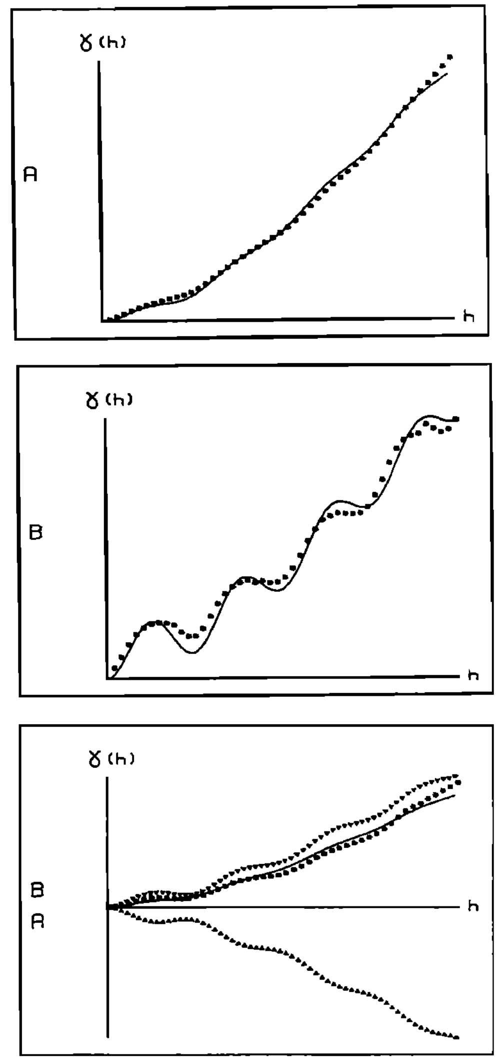

Fig. 4. Experimental and fitted variograms for Wells A and B as well as their cross variogram. (The dotted lines around the cross variogram represent its actual limits, defined by cases of perfect positive and negative correlations.)

ric heads in the Oligocene layer. For more information about the geology and hydrology of this region readers are referred to the report prepared by Centre d'Informatique Géologique of Ecole Nationale Supérieure des Mines de Paris for *Service Géologique Ile-de-France* [1984].

The analysis of our raw data indicated that piezometric heads in every well exhibit two cyclic trends. To illustrates these features, readings from well A and B are shown in Figure 2. As can be seen both show the impacts of the 12-year climatic cycle and the 12-month seasonal trend. The Fourier analysis of the available information, despite being based on limited data, clearly indicates the relative dominance of these two cycles in the resulting periodograms, as shown in Figure 3. Although these periodograms should be viewed with caution, more detailed climatological study of the region [*Service Géologique Ile-de-France*, 1984] confirms the existence of the above 12-year and 12-month cycles based on the analysis of long precipitation records. Therefore, it seems logical to view piezometric data at each well as the sum of two cyclic random processes, each with a hole function variogram as defined by Equation (5). The first hole function variogram represents the seasonal variations, while the second one describes the observed climatic cycles.

Further study of our data, however, reveals that the relative impacts of these cycles may vary from well to well. For instance, Figure 2 clearly illustrates that Well B has a much stronger seasonal component than Well A. Such clear point-to-point variations cast doubt on the assumption of spatial stationarity. In fact, it is more realistic to view measurements from each well as a realization of a separate temporal variable, which in turn, is correlated with random variables of other wells. This method not only accommodates for the observed non-stationarities, but also preserves the physical relationship that exists between these piezometric readings through the cross-correlation structures. Furthermore, the general emphasis of this multivariate procedure is on the time dimension described by the time scales of $g_u(\tau)$, while the spatial variations are included in coregionalization matrices. Such an approach is more consistent with the available time-rich/space-poor data sets.

At the next stage the 136 experimental direct and cross variograms were plotted and automatically fitted using two hole function basic variograms with different ranges and periodicities. The first basic variogram represents the seasonal cycle with a period of 12 months and a range of 120 months, while the second one depicts the climatic trend with a period of 144 months and a range of 1440 months. The least squares fits yield the corresponding coregionalization coefficients, b_{ij}^{u} as defined in Equation (4). Generally, the fits are quite satisfactory. Figure 4 shows three sample variograms out of a total of 136. The illustrated structures are the direct variograms at A and B and their cross variogram as well as their fitted variograms. The dashed intervals on the cross variogram show the cases of perfect positive and negative correlations. Observed and fitted cross variograms should not go beyond these limits.

Having determined the coefficients b_{ij}^{u}, we can perform principal component analysis on the resulting two coregionalization matrices and the original variance-covariance matrix. The results are demonstrated on unit circles (Figure 5) showing the coefficients of each well in the first and the second principal axes of each matrix. As can be seen the first two axes describe a large percentage of fluctuations of each matrix: 96.7% for variance-covariance matrix, 98.8% for 12-year climatic coregionalization matrix, and 98.5% for seasonal coregionalization matrix. The patterns for the variance-covariance and the climatic matrices are very similar, which does not distinguish between wells based on their first principal axes. On the other hand, the seasonal matrix, shows drastically different patterns that permit us to sort the wells into two groups. Wells B, C, F, and to some extent A all have relatively strong seasonal components, while all the rest have minor or negligible seasonal variations. Figure 1 reveals that these four wells are located in the southeastern corner of the Essonne basin. These results persuaded us to conduct further study of the hydrogeology of this area. Early studies have identified this area as a zone of low to moderate permeability with transmissivities ranging from 5×10^{-3} to 5×10^{-2} m^2/s. So we were expecting the readings from these wells show more moderate seasonal components relative to wells, such as E, L, O, and P, whose transmissivities are as high as 3×10^{-1} m^2/s. However, latter studies revealed that this zone has the lowest porosity in the Essonne and the Juine basins. While the porosity in these basins varies between 2 to 13%, the porosity in the southeastern zone is as low as 0.1%. So it seems the distinguishing factor is the porosity. This leads us to view each cycle dominated by a different flow regime.

The seasonal cycle due to its short period could be regarded as a nearly transient flow condition. Considering the importance of storativity in the transient flow conditions, we see more pronounced monthly oscillations in the southeastern corner that can be distinguished from the rest of the region. This seasonal cycle appears to strengthen as one move from A to B in a southeasterly direction, as indicated in Figure 5. The climatic cycle, on the other hand, is relatively slow and represents an almost steady state condition. At such a condition the flow is determined by the transmissivity, while the impact of the storativity is minimized. So due to mild variations of transmissivity in this region, all wells exhibit similar characteristics at the climatic scale. These observations clearly confirm the results of our multivariate analysis.

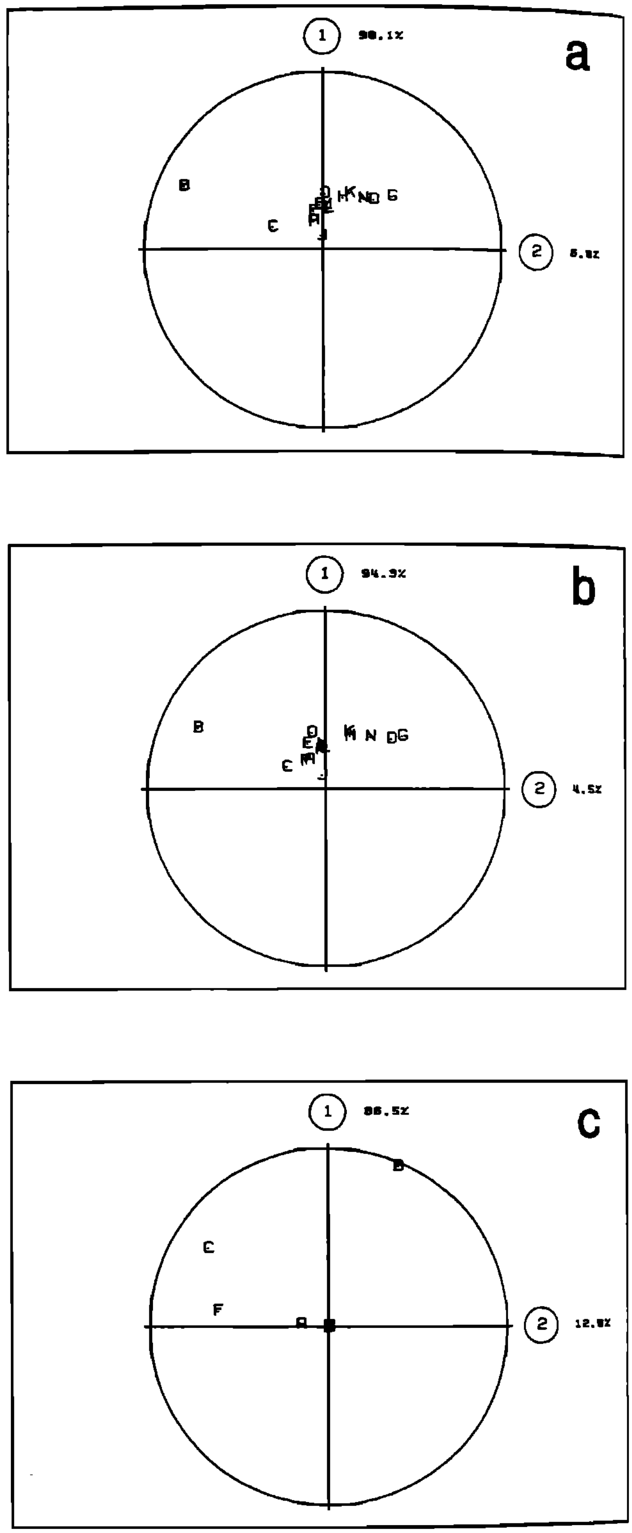

Fig. 5. Principal component results shown on unit circles of the first two axes for (*a*) the classical variance-covariance matrix; (*b*) the climatic coregionalization matrix; and (*c*) the seasonal coregionalization matrix. (Each well is identified by its corresponding letter.)

5. Conclusion

The multivariate geostatistical approach enables us to study space-poor/time-rich geohydrological data sets by paying due attention to the temporal dimension. Viewing each time series as a realization of a correlated random function, composed of a sum of multi-scale random processes, permit us to analyze the data without masking the important temporal periodicities and spatial non-stationarities. As noted earlier, this approach can easily be used to estimate the missing data or to forecast piezometric heads at each observation well. Similarly, the temporal components at each observation site as well as regional index at each temporal scale can be estimated and used for filtering purposes. Current studies, such as *Switzer* [1989] on weighting of fitted stationary covariances with observed non-stationary spatial covariances, or *Seguret* [1989] on trigonometric kriging will complement our proposed approach and makes it an efficient procedure for space-time estimation.

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