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The Multivariate (Co)Variogram as a Spatial Weighting Function in Classification Methods[1]

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The multivariate variogram and the multivariate covariogram are used as spatial weighting functions for forming spatially homogeneous groups automatically. The groups are created after either deflating similarities between distant samples with the multivariate covariogram or by inflating dissimilarities between distant samples with the multivariate variogram. These approaches can be seen as generalization of the Oliver and Webster proposal. Two data sets show the efficiency of the two weighting functions when compared to the classical approach which does not take spatial information into account. In one case study, the weighting of similarities by the multivariate covariogram showed more interpretable results than the weighting of dissimilarities by the multivariate variogram.

KEY WORDS: multivariate (co)variogram, (dis)similarity, metric, cluster analysis.

INTRODUCTION

Several authors have recognized the importance of taking spatial information into account in cluster analysis for geographically referenced samples. Oliver and Webster (1989) reviewed the most important work that had been carried out on this subject and proposed an original solution to the problem of forming spatially homogeneous groups. Their solution was to weight the dissimilarities between samples by means of the variogram:

$$d_{ij}^{*} = d_{ij} \frac{\gamma\,(\mathbf{h})}{(C + C_o)} \tag{1}$$

where $\gamma\,(\mathbf{h})$ = variogram model fitted to the experimental variogram $\gamma^{*}(\mathbf{h})$, $(C + C_o)$ = variogram's sill (note that since $C + C_o$ is a constant, it has no

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influence on the resulting classification), d_{ij} = original dissimilarity between samples i and j, d^*_{ij} = modified dissimilarity between samples i and j, and

$$2\gamma^*(\mathbf{h}) = \frac{1}{N_h} \sum_{(i,j) \in D_h} (z(\mathbf{x_i}) - z(\mathbf{x_j}))^2 \tag{2}$$

where $z(\mathbf{x_i})$ = sample's value at location $\mathbf{x_i}$, $\mathbf{h}$ = geographical displacement vector, D_h = collection of sample pairs for which $\|\mathbf{x_i} - \mathbf{x_j}\| \in [\|\mathbf{h} \pm \Delta\mathbf{h}\|]$, and N_h = cardinality of D_h.

For all monotonic increasing variograms, the closer the samples are spatially, the more the dissimilarities decline. With bounded models with finite range, a, there is no modification for samples spaced at a geographic distance equal to or greater than the range. One result of this is to downweight the large dissimilarities that occur between close neighbors. The main difficulty of this approach lies in the choice of a variogram model, which is a univariate spatial function, to represent spatial structure of the dissimilarities (which are generally a multivariate measure). To take into account the multivariate character of dissimilarities, Oliver and Webster (1989) proposed using the variogram of the first principal component of the PCA, or to use a variogram that is a compromise between the variograms of the first few principal components.

We propose either to use the multivariate covariogram as a weighting function to decrease (relatively) similarities of distant samples or to use the multivariate variogram as a weighting function to increase (relatively) dissimilarities between distant samples. In addition, we propose calculating the multivariate (co)variogram in the same metric used to calculate the (dis)similarities in order to obtain a multivariate function which describe the spatial variation of (dis)similarities. Examples using the various approaches are presented for comparison.

The method presented in this paper is also an alternative to the clustering methods that impose a strict spatial contiguity constraint, as proposed by many authors (among others, Ray and Berry, 1966; Lebart, 1978; Monestiez, 1978; Lefkovitch, 1980; Legendre and Legendre, 1984; Legendre, 1987). The difference between these and our method is briefly discussed below.

MULTIVARIATE VARIOGRAM

Mackas (1984), Young (1987), and Harff and Davis (1990) have already proposed the use of multivariate variograms in different ways. Mackas (1984) computed a multivariate variogram, based upon chord metric, to describe multivariate spatial structure of a planktonic community. Harff and Davis (1990) suggest a multivariate variogram, based upon the Mahalanobis metric, to krige a vector of regionalized variables. This makes it possible to obtain a regular grid where p variables are estimated at each node without having to resort to a cokriging system. These authors then proceed with a Bayesian-type classification of the nodes on the grid, and define geographically compact groups.

Bourgault and Marcotte (1991) formalized the multivariate variogram as it applies to stationary random functions, demonstrating the relation that exists between the multivariate variogram and the multivariate autocovariance function. This is precisely the same as the relation encountered in univariate geostatistics. For a regionalized vector of p stationary variables and for every metric **M**, the multivariate covariogram and the multivariate variogram are defined as follow:

$$\underline{\text{multivariate covariogram}}$$

$$K(\mathbf{h}) = E[(\mathbf{Z}(\mathbf{x}) - \boldsymbol{\mu})\, \mathbf{M}(\mathbf{Z}(\mathbf{x} + \mathbf{h}) - \boldsymbol{\mu})^t] \tag{3}$$

$$\underline{\text{multivariate variogram}}$$

$$2G(\mathbf{h}) = E[(\mathbf{Z}(\mathbf{x}) - \mathbf{Z}(\mathbf{x} + \mathbf{h}))\, \mathbf{M}(\mathbf{Z}(\mathbf{x}) - \mathbf{Z}(\mathbf{x} + \mathbf{h}))^t] \tag{4}$$

where $\mathbf{Z}(\mathbf{x})$ = row vector of p second-order stationary random functions, $\boldsymbol{\mu} = E[\mathbf{Z}(\mathbf{x})]$, and $\mathbf{M}$ = a $p \times p$ positive-definite symmetric matrix used as metric in the calculation of (dis)similarities. (Examples of such metrics are: the identity matrix (Euclidean), the inverse of the variance-covariance matrix (Mahalanobis), a diagonal matrix with the inverse of the standard deviations, the chi-square metric, etc. . . . The interested reader is referred to Sneath and Sokal (1973) for more details about metrics). Assuming second-order stationarity, the multivariate autocovariance function is related to the multivariate variogram by:

$$K(\mathbf{h}) = G(\infty) - G(\mathbf{h}) \tag{5}$$

where $G(\infty)$ = sill of the multivariate variogram. From Eq. (4), $G(\mathbf{0}) = 0$, thus $K(\mathbf{0}) = G(\infty)$.

Journel (1988) recognized the traditional univariate variogram (2) as a distance squared measure, and its counterpart, the univariate covariogram, as a proximity (or similarity) measure. Thus, the multivariate variogram (Eq. 4) represents the mathematical expectation of a multivariate dissimilarity squared measure, and the multivariate autocovariance function (Eqs. 3 and 5) represents the mathematical expectation of a multivariate similarity measure.

As in the Mackas (1984), the multivariate variogram is estimated by averaging multivariate dissimilarities (squared) in a similar way to the traditional variogram (Eq. 2):

$$2G^*(\mathbf{h}) = \frac{1}{N_h} \sum_{(i,j)\in D_h} d_{ij}^2 \tag{6}$$

where d_{ij} = dissimilarity between samples i and j calculated with a given metric, and N_h and D_h are as defined previously.

We propose to modify the similarity measure between individuals (computed from the multivariate vectors of observations), based on the Oliver and Webster (1989) proposal, by means of the multivariate autocovariance function:

$$S_{ij}^{*2} = S_{ij}^{2}\, K(\mathbf{h}) \tag{7}$$

Alternatively, one may modify the dissimilarities between individuals with the multivariate variogram function:

$$d_{ij}^{*2} = d_{ij}^{2}\, G(\mathbf{h}) \tag{8}$$

Note that this latter approach is slightly more general since it allows for multivariate variograms without sills. The spatial modifier defined by Eq. (7) is stronger in the sense that it favors formation of groups which are more spatially homogeneous. With a stationary model when samples are separated by a distance exceeding the range, a null similarity is computed from Eq. (7), whereas dissimilarities are simply multiplied by a constant in Eq. (8). Both methods perform correctly when a pure nugget effect is modeled. Spatial modifier (Eq. 7) will compute null similarities, and either leave unchanged the initial random partition formed by non-hierarchical (N-H) clustering algorithm or will not do any grouping with the hierarchical algorithm. This is coherent with the meaning of the nugget effect: that the size of the spatial structures are smaller than the sampling mesh. Therefore, we cannot observe any groups within the data set. On the other hand, spatial modifier (Eq. 8) will modify all dissimilarities by a constant, the clustering will be identical to the one performed on original dissimilarities in the absence of any spatial information.

The new (dis)similarity matrix can serve as a starting point for any hierarchical or non-hierarchical (N-H) clustering algorithm. We used a N-H clustering algorithm where the sample-group (dis)similarity is computed as the arithmetic average of the (dis)similarities between the sample and all the samples of the group considered. The N-H algorithm used is the following:

Step 0: An initial random partition with k groups (provided by the user) is performed.

Step 1: For each sample, the modified (with Eqs. 7 or 8) (dis)similarity is calculated with all the other samples; the average (dis)similarity is computed for each of the k groups. The sample is assigned to the group with the smallest average dissimilarity or greatest average similarity.

Step 2: If no samples changed assignation in step 1, then the algorithm is stopped. Otherwise we go to step 1 for the next iteration. The algorithm can also be stopped after a fixed number of iterations or when the average sample-group (dis)similarity does not improve sufficiently.

(In the two cases studied below, the algorithm was stopped after no change in group membership was obtained over a full iteration).

EXAMPLE 1: LAKEVIEW MOUNTAINS

The data selected to illustrate the various approaches were taken from the study by Morton et al. (1969) of the batholite in the Lakeview Mountains region of California. These data result from the analysis of 147 rock samples for Na, Mg, Al, Si, K, Ca, and Fe. The samples were spread over a square grid (650 m × 650 m). Morton et al. (1969) observed that the geochemical variations revealed an aureole structure, which consists of a mafic core bordered with felsite. David and Dagbert (1974) also obtained an aureole pattern for the first factor of a correspondence analysis performed on these data (Fig. 1). This factor sets Fe, Mg, and Ca opposite to Si and K: the center of the batholite is rich in Fe, Mg, and Ca, while the periphery is rich in Si and K.

For clustering, the variables were standardized, and the similarities were calculated using:

$$S_{ij}^2 = D_{\max}^2 - D_{ij}^2 \tag{9}$$

where D_{ij}^2 = Mahalanobis distance between samples i and j,

$$D_{ij}^2 = (\mathbf{z}(\mathbf{x}_i) - \mathbf{z}(\mathbf{z}_j))\, \mathbf{C}^{-1}\, (\mathbf{z}(\mathbf{x}_i) - \mathbf{z}(\mathbf{x}_j))' \tag{10}$$

$D_{\max}^2 = \max\,(D_{ij}^2)$ with $\mathbf{z}(\mathbf{x}_i)$ = row vector of p variables observed at location $\mathbf{x}_i$, and $\mathbf{C}^{-1}$ = inverse of the experimental variance-covariance matrix.

To facilitate the comparison between different clustering approaches, we fixed the partitioning to have six groups. Figure 2 shows the map obtained by a N-H clustering of the original dissimilarities, which reveals dispersed, non-contiguous groups. This map also indicates that there is a tendency to form a fairly homogeneous central group (#5). The arrangement of the groups suggests the presence of a concentric spatial structure, but the picture is far from clear.

The multivariate spatial structure of the data is described by the omnidirectional experimental multivariate variogram shown as the plotted points in Fig. 3. This multivariate variogram is calculated according to Eq. (6) with $\mathbf{M} = \mathbf{C}^{-1}$ (the Mahalanobis metric; $\mathbf{C}$ is the variance-covariance matrix). It is modeled as an isotropic spherical variogram with a range of nine units (1 unit = 650 m), a sill of 2.4 and a nugget effect of 5.0. This multivariate variogram was used to modify the Mahalanobis distances between samples using Eq. (8), whereas the multivariate covariogram was used to modify (using Eq. 7) the similarities (calculated with Eq. 9).

Figure 4 shows the maps obtained by N-H clustering on the modified dissimilarities (4a) and the modified similarities (4b). We find that there are six

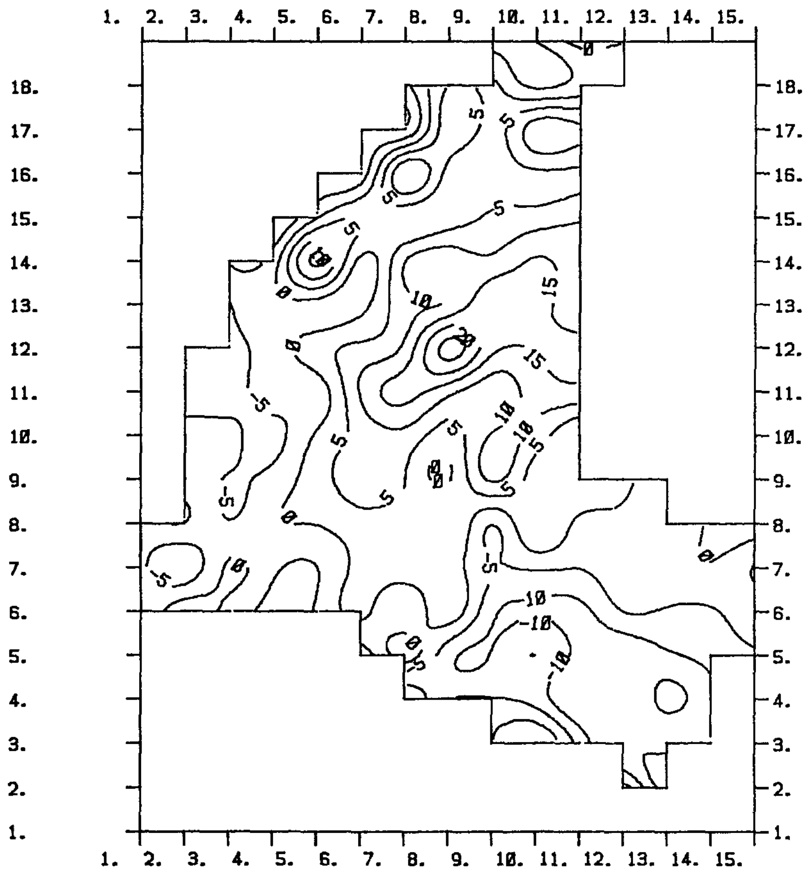


Fig. 1. Isarithmic map of the first factor of a correspondence analysis of the Lakeview Mountains data obtained by kriging (grid is 650 m × 650 m).

compact groups, five of which are located toward the edges around a central group. The results for both maps are practically identical, but the central group obtained with the modified similarities is slightly smaller than the one obtained with the modified dissimilarities. The dendrogram in Fig. 5, constructed from a matrix of Mahalanobis distances between the vectors of averages representing the groups, indicates that the groups toward the periphery are more similar to each other than they are to the central group. These maps are a good representation of the known aureole structure.

EXAMPLE 2: SCHEFFERVILLE

For this example, 448 samples of lake-floor sediment were taken from an area about 50 km north of Schefferville, Québec. The samples were collected by the Ministère de l'Energie et des Ressources du Québec (Beaumier, 1987),

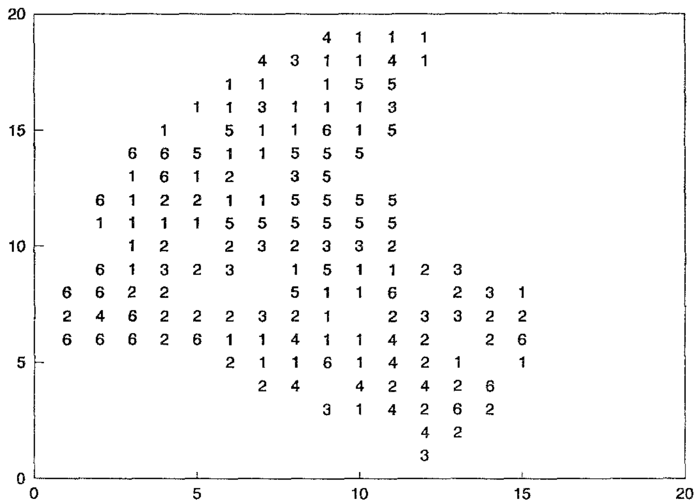


Fig. 2. Map of groups obtained by N-H clustering on original dissimilarities for the Lakeview Mountains data (coordinates are in grid units).

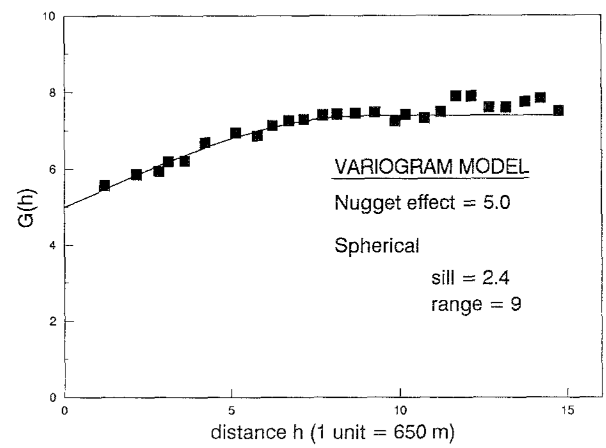
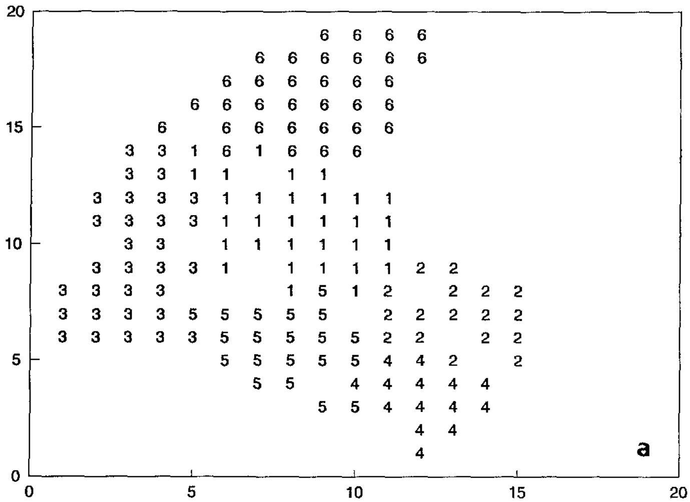


Fig. 3. Experimental multivariate variogram, calculated using Mahalanobis metric, on the Lakeview Mountains data (1 unit on the abscissa = 650 m).

and analyzed for 38 elements. Only Al, Fe, K, and Mg were used in this analysis, since they represent the most important lithological variation. Figure 6 shows the general geology of the studied area. The main feature of the geological pattern is a stratification oriented at N32°W; five geological formations may be identified. The formation at the extreme west of the map consists es-



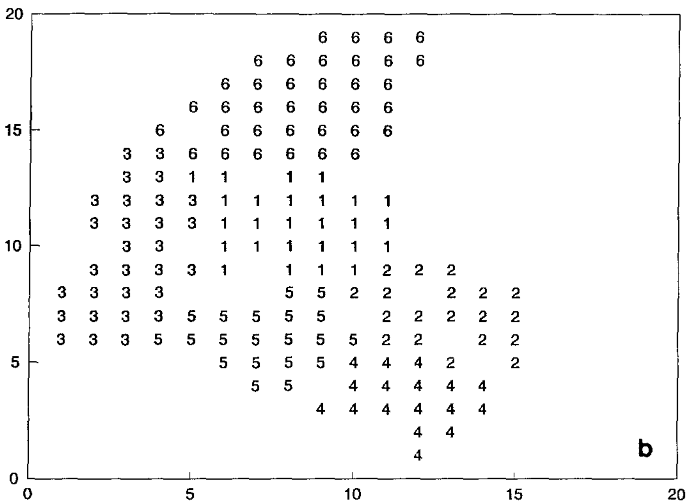


Fig. 4. Maps of groups obtained by N-H clustering on dissimilarities modified by (a) the multivariate variogram, and (b) on similarities modified by the associated multivariate covariogram (coordinates are in grid units).

sentially of igneous mafic rock (basalt and gabbro). The formation to the east of the map is also composed of igneous mafic rock, and contains a band of ultramafic rock (periodotite). The central formation is composed of igneous mafic rock, too, but it has been covered by considerable glacial deposits along the length of the stratigraphy. The igneous mafic rock formations are separated

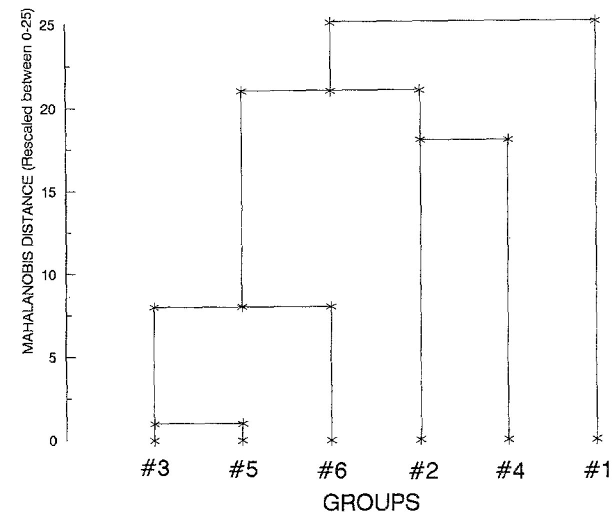


Fig. 5. Dendrogram, based on Mahalanobis distances, for centroids of the groups shown in Fig. 4b (the Mahalanobis distances were rescaled between 0–25).

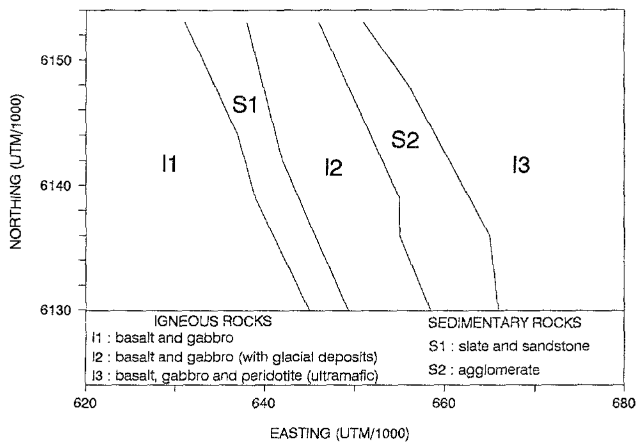


Fig. 6. General geology of the Schefferville area (coordinates are in kilometers).

by sedimentary formations (sandstone, greywacke, conglomerate) (Dimroth, 1978).

We have used standardized logarithms of the elements Al, Fe, K, and Mg to calculate the dissimilarities. The original similarities were calculated using:

$$S_{ij}^2 = d_{\max}^2 - d_{ij}^2 \quad (11)$$

where d_{ij} = distance (in the variable space) between samples i and j with the identity metric, and $d_{\max} = \max(d_{ij})$. The partitioning was fixed at five groups, which corresponds to the number of geological formations (Fig. 6).

Figure 7 shows the map of the groups obtained by N-H clustering without modifying the dissimilarities. These groups are dispersed and intermingled. The map is a poor representation of the geology described in Fig. 6.

Figure 8 shows the experimental multivariate variograms calculated for two orthogonal directions, using the identity metric. A spherical variogram model with geometric anisotropy is adopted. Largest range (15000 m) and shortest range (9000 m) respectively occur along (N32W) and across (N58E) the stratigraphy.

Figure 9 shows the map obtained by modifying the dissimilarities using the multivariate variogram anisotropic model. Groups 1, 3, and 4 are spatially more homogeneous than they were before; however, the link with the known geology remains uncertain.

Figure 10 shows the map obtained by modifying the similarities using the multivariate covariogram anisotropic model. This time, the groups are kept well apart from one another, and they reflect the anisotropy of the geological pattern very well. This is the map that compares best with the geological map. The boundary between the two formations to the west of the map is well defined by the classification (5-3, Fig. 10); the other boundaries, however, do not correspond exactly to those of the geological map. The formation to the east of the map is divided into two groups (1 and 4), which is probably caused by the

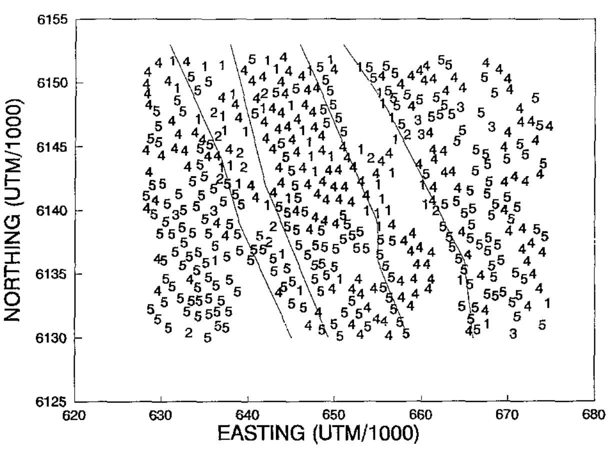


Fig. 7. Map of groups obtained by N-H clustering from the original dissimilarities of the Schefferville area (coordinates are in kilometers).

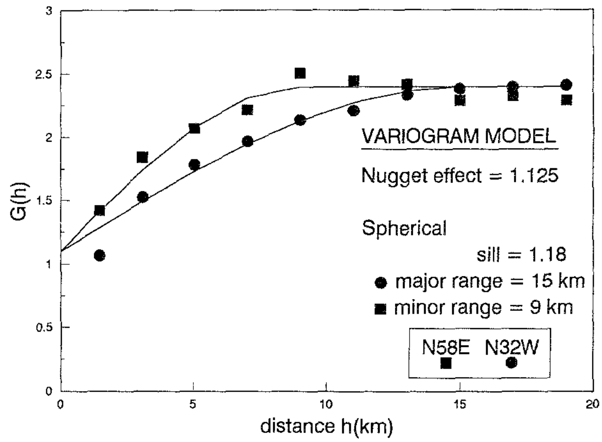


Fig. 8. Experimental anisotropic multivariate variogram, calculated using the Euclidean metric, on the Schefferville data.

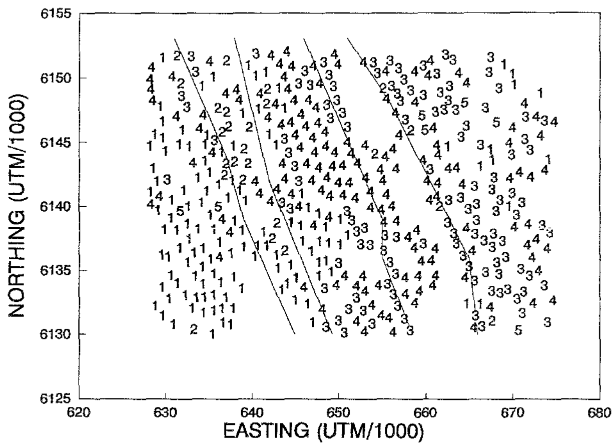


Fig. 9. Map of the groups obtained by N-H clustering on the dissimilarities modified using the anisotropic multivariate variogram of the Schefferville area (coordinates are in kilometers).

influence of the band of ultramafic rock contained in that formation. The ultramafic rocks are associated with group 1. The group 1 samples in the southern part of the sedimentary formation in the easternmost section of the map come from a lake that is fed by a river that cuts through the ultramafic band. The central formation contains groups 2 and 3. The lakes in this formation have

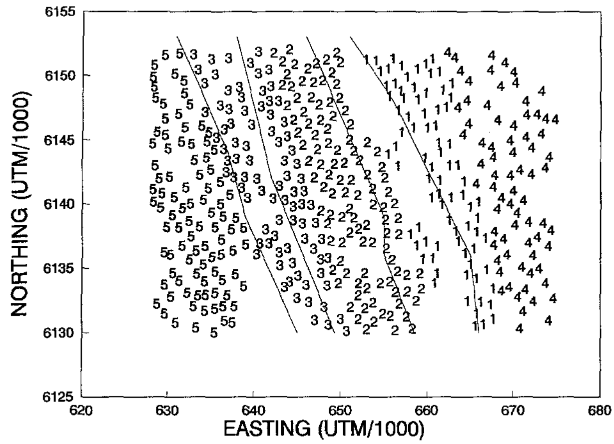


Fig. 10. Map of the groups obtained by N-H clustering on the similarities modified using the anisotropic multivariate covariogram of the Schefferville area (coordinates are in kilometers).

probably received sediments from many different sources, such as igneous mafic rocks and glacial deposits, which makes it difficult to classify them spatially.

In the absence of a perfect geological image, the map of the groups modified by the multivariate covariogram is the one which leads to the best geological analysis. In knowing that there are two major geological families in this region, igneous mafic rocks and sedimentary rocks, a second N-H clustering with only two groups was performed.

Figure 11a shows the map obtained after the dissimilarities had been weighted by the multivariate variogram, and Fig. 11b shows the map obtained after the similarities had been modified by the multivariate covariogram. A comparison of these two maps reveals, once again, that the groups obtained from the weighted similarities are more spatially homogeneous. In Fig. 11a, group 1 combines more readily with the igneous rock, and group 2 with the sedimentary rock and with the zone of glacial deposits. The groups in the map of Fig. 11b delimit very well the boundaries between the igneous mafic rocks and the sedimentary formations to the east and to the west of the map. The igneous formation at the center of the map does not appear, but is combined with the two sedimentary formations (group 1), possibly because of the influence of the glacial deposits. It should be noted here that the weighting of similarities by the multivariate does not preclude that samples which are very far apart geographically be joined together (group 2), even if the distance between these samples is greater than the range (the western part of group 2 is located more than three times the range from its eastern part). This is possible because the

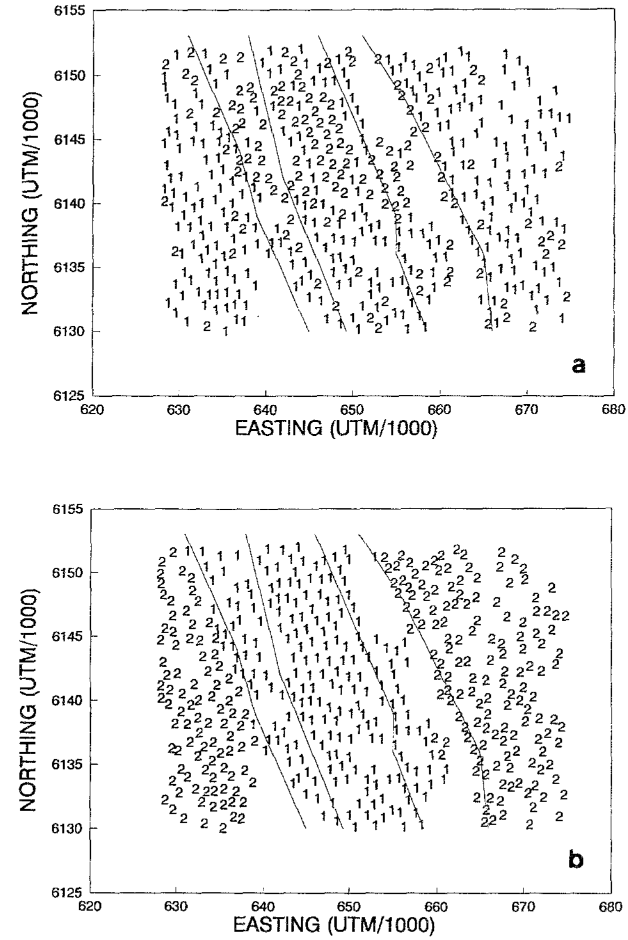


Fig. 11. Maps of the groups obtained by N-H clustering, for two partitions only: (a) on dissimilarities modified using the anisotropic multivariate variogram, and (b) on similarities modified using the anisotropic multivariate covariogram of the Schefferville area (coordinates are in kilometers).

average similarity remains large over all the samples of these two geological formations, in spite of the large number of null similarities for the pairs of samples formed between these two formations. Weighting dissimilarities by the multivariate variogram can also lead to similar results although this was not observed here.

DISCUSSION AND CONCLUSIONS

This work was triggered by a suggestion of Legendre (1987) to weight the dissimilarity matrix values by a linear function of the geographic distances among points before clustering. The proposal of Oliver and Webster (1989) is a more sophisticated way of reaching the goal. The present study describes another improvement of the same method, that integrates the multivariate nature of the data most often used for clustering.

The multivariate variogram is a function of the spatial structure that has all the attributes sought by Oliver and Webster (1989). It is a function of the data, describing their regionalization while taking into account the spatial correlations among the variables, in accordance with the metric used. It is no longer necessary to perform a principal components analysis to find a compromise variogram, and the weighting conforms to the metric selected for calculating the (dis)similarities.

The spatial constraint induced by the multivariate variogram is not always sufficient to produce a clear picture of the groups under study. In our case studies, the weighting of the similarities by the multivariate covariogram yields better results (more spatially contiguous and better related to the known geology) than those obtained by spatial weighting of dissimilarities with the multivariate variogram.

There may be some concern that the spatial weighting introduced by the multivariate covariogram is so strong that it could impose spatially homogeneous groups even when this is inappropriate, since its chief effect is to downweight the similarities that occur between distant samples. This would be easy to detect, however, by varying the initial partitioning (N-H method) for a fixed number of groups; with non-spatially-organized data, one would expect significant differences between the groups obtained for each initial partitioning. Also, for such data, the nugget component of the multivariate variogram should be large.

In the case studies presented, we obtained better results, i.e., more in agreement with known geology, with spatial modifier Eq. (7). It may be that in other contexts, or with different metrics or different clustering algorithms, spatial modifier Eq. (8) would prove more useful. The choice of one or the other may rest, in the end, on our perception of how much spatial homogeneity the groups should exhibit. If the groups are expected to be spatially very homogeneous or compacts, then Eq. (7) is more appropriate. If the groups are expected to be intermingled to a certain degree, then Eq. (8) is preferable.

Compared to the clustering methods that impose a strict constraint of spatial contiguity and necessarily lead to the formation of geographically unique groups of observation points, our method of weighting similarities or dissimilarities possesses two advantages: first, it is computationally simpler, since the inclusion of the geographic information can be done as a pre-treatment, prior to the clustering itself, which can then be obtained from standard, unmodified clustering programs; second, it may produce disconnected groups of similar objects, as was the case in Fig. 11b (this grouping was obtained three times out of ten, starting with different initial random partitions).

When only the intrinsic hypothesis can be used (i.e., the multivariate covariogram does not exist), the spatial weighting of dissimilarities could be done with the multivariate variogram with Eq. (8). Pseudo-covariance models such as: constant-$G(\mathbf{h})$ are to be avoided since the classification results will depend on the choice of the arbitrary constant. When the intrinsic hypothesis is not fulfilled (i.e., the multivariate variogram does not exist), one may define a multivariate generalized covariogram in the same way as the multivariate variogram. However, it could be preferable to eliminate the effects of the physical causes responsible for the trends before doing any classification.

One of the referees pointed out that a good strategy to determine the number of groups could be to use a two-stage procedure. First use an N-H clustering with spatial modifier Eq. (7) or (8) and a large number of groups to obtain spatially contiguous groups. Second, perform a second classification or a multivariate analysis of the mean vectors of these groups without spatial weighting to cluster groups that are similar in the variable space but geographically distant.

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