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A competitive neural network approach for meteorological situation clustering

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Abstract

A complete competitive scheme is proposed in this work in order to perform a classification analysis of meteorological data in the 'Campo de Gibraltar' region (in the South of Spain) from 1999 to 2002. The main objectives of the study presented here have been the characterization of the meteorological conditions in the area, using a competitive neural network based on Kohonen learning rule. Standard Principal Component Analysis (PCA) and VARIMAX rotation have allowed interpreting the physical meaning of the classes obtained from the competitive scheme. Quantitative (using three quality indices) and qualitative (from the analysis of the data projection) criteria based on Fisher Discriminant Analysis were introduced to verify the results of the clustering. A randomized procedure is developed to assure the best performance of the models and to select the best model in the experiments. The different experiments developed extracted five classes, which were related to typical meteorological conditions in the area.

Keywords: Artificial intelligence; Cluster analysis; Automated meteorological classification; Artificial neural network; Multivariate techniques

1. Introduction

It is extremely important to consider the effect of meteorological conditions on atmospheric pollution, since they clearly influence dispersion capability of the atmosphere. Severe pollution episodes in the urban environment are not usually attributed to sudden increases in the emission of pollutants, but to certain meteorological conditions which diminish the ability of the atmosphere to disperse pollutants (Ziomas et al., 1995; Cheng and Lam, 2000). The study of meteorological conditions could be done by analyzing meteorological variables individually. However, this analysis suffers from at least one shortcoming because air pollution is known to respond to the complete meteorological data which comprises an air mass, rather than to certain selected meteorological variables (Kalkstein, 1991).

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In the last years the use of cluster analysis to better elucidate the dependency of air quality on meteorology has proliferated. It has been used successfully in numerous studies which relate air quality and meteorological situations. Thus, Eder et al. (1994) and Zelenka (1997) used clustering results to develop "unique" or "separate" regression models for ozone and acid aerosols, respectively. In the work of Ludwig et al. (1995) cluster analysis is used to categorize meteorological data and determine the combination of conditions associated to daily ozone maxima.

Davis et al. (1998) used similar techniques to those used by Eder et al. (1994), where principal component analysis (PCA) and *k*-means clustering procedure were used with the objective of determining synoptic meteorological scenarios. Similar approaches have been used in Berman et al. (1995), Lam and Cheng (1998), and Triantafyllou (2001). More recently, Kim Oanh et al. (2005) have also developed an automated scheme to classify the synoptic meteorological conditions governing over Northern Thailand. Because a quantitative approach utilizes a variety of meteorological variables for the classification of synoptic patterns, it involves intensive statistical data treatment, normally accomplished in the literature by a combination of the PCA and clustering techniques.

In Avila and Alarcón (1999) a clustering analysis of meteorological variables was applied as a classification tool, while PCA was performed to help interpret the groupings. The meteorological classification was compared to an independent grouping based on PCA.

Up to date, no meteorological classification approach has been applied to the assessment of the relationships between climate and air pollution in the 'Campo de Gibraltar' region (in the south of Spain). The main objectives of this work were firstly to analyse the capability of a competitive network (Kohonen, 1987) with unsupervised learning to find different classes from the meteorological data available, and secondly, a quantitative analysis (through four quality indices (QI) based on Fisher Discrimination Analysis) and a qualitative analysis (with the aid of the visualization capabilities of the Fisher projection) of the data clustered. PCA (Jollife, 1986) with a VARIMAX rotation (Kaiser, 1958) has been applied to make class interpretation easier, while Fisher transformation (Fisher, 1976) has been used to verify and control the quality of the procedure. These networks require no priori assumptions about the model in terms of mathematical relationships or data distribution. Our interest is to classify meteorological situations for the later purpose of determining whether the meteorological situations can be used for air pollution forecasting and for developing future control or warning strategies. In general, the modelling of "separate" models (one for each cluster) will give better performance results, rather than the modelling of a unique model for the whole data (Zelenka, 1997). This approach will allow formulating better effective mitigation strategies and better predictions to help or warn elderly and sick people.

The paper is organized in several sections. Section 2 presents the study area and the data collected. In Section 3 the basic concepts of clustering and Kohonen competitive learning approach are briefly described as well as how PCA and Fisher analyses are used to identify, visualize and compare the clustering results. Section 4 reports the results obtained. Finally, the conclusions and future researches are shown in Section 5.

2. The study area and the data

The 'Campo de Gibraltar' is the southern-most region of the Iberian Peninsula. It is 584 km^2, and is surrounded by western mountains (a Natural Park called 'Los Alcornocales') that rise up to 700 m, and the Rock of Gibraltar in the South–East, with a maximum altitude of 420 m. Its climate is Mediterranean and winds are predominantly easterly and westerly. About 300,000 inhabitants live in the different towns spread in the region (Algeciras, 120,000; La Linea, 65,000). It is a very complex scenario, where many stationary sources are present (Fig. 1): an oil-refinery and some petrochemical factories close to it, a coal-fired and several fuel-oil power plants, a large steel factory and a paper factory.

The port of Algeciras, one of the most important ship-trading ports in Europe, and the airport of Gibraltar are other possible sources of particulate and gaseous air pollution in the area. Due to the economic development of the region, many construction activities, which are important particle emission sources, have been carried out lately. In addition, the region is one of the paths that African air masses from Sahara and Sahel deserts take, increasing significantly particulate air concentration in different areas of Spain and Europe (Rodriguez

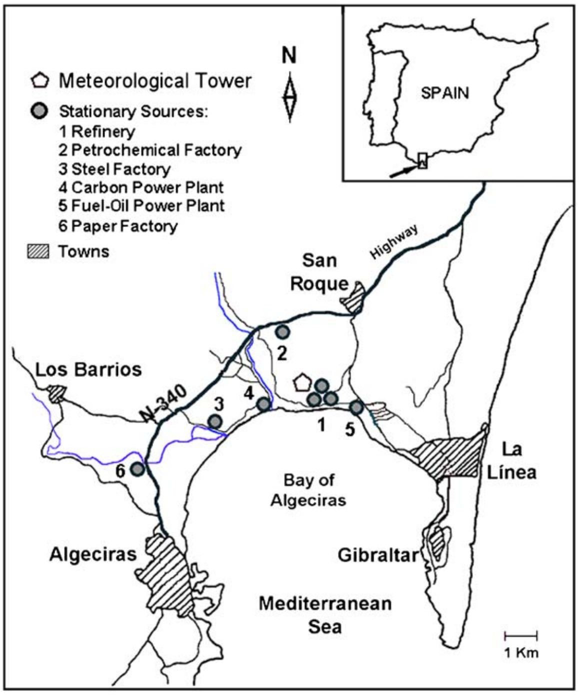

Fig. 1. Location of the towns, large factories and the monitoring stations.

et al., 2001, 2002). Thus, many (particulate) air pollution episodes have been detected by the different monitoring stations that the Environmental Agency of the Andalusian Regional Government has in the region. Therefore, and considering the new European Directives for atmospheric emissions (2001/80/EC, 1999/32/EC), more research is needed in this area. In summary, this is a heavily industrialized area where, up to date, very few air pollution studies have been made.

The study was initiated in November 1999 and continued until December 2002. The meteorological data were obtained from the meteorological tower located at the refinery (point 1 on the map of Fig. 1). The meteorological variables employed include daily average net radiation (RAD), precipitation (PRC), surface temperature (TMP), wind speed (WSP), sea level pressure (SLP), relative humidity (RHM), absolute humidity (AHM), mixing height (MXH), and the absolute frequencies of the different wind sectors (N, NNE, NE, ENE, etc.). In this study, no imputation missing data methods were used to avoid the introduction of artificial data in the clustering procedure.

The meteorological characterization was determined by the statistical analysis applied to the different parameters measured in the tower (surface wind speed and wind direction, temperature, atmospheric pressure, etc.), and other indirectly estimated variables (absolute humidity, mixing height, ventilation factor, etc.). The mixing height was estimated from surface data, using the method of Batchvarova and Gryning (1990) for the growth of the daytime mixed layer and the Benkley and Schulman method for the nocturnal mixing height estimation (Lena and Desiato, 1999). The surface roughness length was set to 1 m (typical urban value), while the temperature gradient above the mixing layer was assumed to be $0.05\,\mathrm{K\,m^{-1}}$ for MXH values less than 100 m, and $0.005\,\mathrm{K\,m^{-1}}$ above 100 m. The equation for the growth of the daytime mixing layer was solved numerically by Finite Differences Method (FDM) (González, 2003).

3. Methodology

3.1. Competitive neural approach

Typically, a Kohonen neural network (or self-organizing map—SOM) has two layers of nodes, the input layer and the Kohonen or output layer. The input layer is fully connected to a 1-D or 2-D (or another different topology) output grid. During the training process, input data (the 20 meteorological variables) are introduced in the network through the processing elements (nodes or neurons) in the input layer. Associated with the output nodes in the Kohonen layer there is a weight vector of values. The neurons of competitive networks learn to recognize groups of similar input vectors. The weights of the winning neuron are adjusted with the Kohonen learning rule (Kohonen, 1987). The weight vector (w) is changed for a given neuron if the output is not equal to zero (the winning neuron), according to: $\mathrm{d}w = \alpha(x - w)$, where x is the neuron's input, and α the learning rate. Thus, the neuron whose weight vector is closer to the input vector is updated to be even closer. The result is that the winning neuron is more likely to win the competition the next time a similar vector is presented, and less likely to win when a very different input vector is presented. The training stage stops when any of the following conditions are met: the maximum number of epochs (an epoch is a presentation of all input patterns) is reached, the performance has been minimized to the goal, or a maximum amount of time has been exceeded. One of the limitations of competitive networks is that some neurons may not always get allocated, that is, some neuron weight vectors may start out far from any input vectors and never win the competition, no matter how long the training is continued. Tendency terms or biases (b) are used to give the neurons that rarely win the competition an advantage over the neurons that often win. The learning algorithm calculates the bias change for a given neuron by first updating each neuron's conscience (c), i.e. the running average of its output (o): $c = (1-\alpha)c + \alpha o$. The conscience is then used to compute a bias change for the neuron that is the greatest for smaller conscience values: $\mathrm{d}b = \exp(1-\log(c)) - b$. For each epoch, each training vector is presented once in a different random order to the network. Weight and bias values are updated accordingly after each individual presentation.

The Kohonen networks have the ability to extract the statistical properties of the data set, and are also able to model any statistical distribution which may lack a closed-form analytical expression (Fu, 1994). That is the reason why these kinds of network have been used in the present study. However, in order to get good results, the network should be trained with statistically representative or meaningful data of the total input. In this application, the data statistics are not well understood and, therefore, the whole data set is required for good modelling. Due to the inherent process randomness and because these methods depend on initial centres, the order of the presentation and the geometric properties of the data (Jain et al., 1999), a relatively high number of experiments (30 were proposed in this study) has to be done and their results checked. Also, different experiments have been done to determine different numbers of classes, by changing the number of iterations and checking the appropriate performance of each solution (Masters, 1993). A unidimensional competitive Kohonen network (or SOM 1-D with k output units) can be seen as a stochastic form of classical k-means clustering technique (Tou and Gonzalez, 1974), and its performance is very similar to this algorithm (Fu, 1994; Jain et al., 1999). Both techniques try to minimize the sum of squared distances from each example to its cluster centre. These clustering methods are just algorithms: even though they aim to optimize a criterion, finding the global optimum is not guaranteed (Ripley, 1996). In the reviewed literature, k-means is normally applied after a hierarchical clustering method, such as average linkage, to find the number of clusters to be searched. With a competitive network this first stage could be implemented by using a large number of classes (greater than the plausible number of clusters) and analysing the dead neurons. This was the first experiment developed (results in Table 2). Then, a second stage experiment was designed with a refinement of the algorithm which uses a conscience term to avoid the death of neurons in the searching process of the most frequent number of clusters. Our aim is to interpret this second stage competitive experiment with the aid of PCA-VARIMAX transformation, and to control its quality using quantitative and qualitative properties of Fisher transformation.

3.2. Principal component analysis (PCA) and Fisher discriminant analysis

PCA is a well-known multivariate statistical method which allows finding new directions (components) that explain most of input data variability and which are linear combinations of input variables. A transformation matrix is constructed from the eigenvectors of the input correlation matrix and they are ordered according to their corresponding eigenvalues (Thurston and Spengler, 1985). More details on the mathematical background of PCA can be found in Jollife (1986). Many applications of PCA on synoptic meteorological approaches can be found in Avila and Alarcón (1999), Davis et al. (1998), Lam and Cheng (1998), Cheng and Lam (2000), Borchi and Marenco (2002), Kim Oanh et al. (2004), and Colette et al. (2005). Here, VARIMAX criterion has been used (Johnson and Wichern, 1998). The number of significant factors to be considered is diagnosed from the eigenvalues by discarding any direction corresponding to eigenvalues lower than unity (Kaiser, 1958; Colette et al., 2005). An attempt to interpret the physical meaning of the resulting competitive clustering is made by using the projection of the patterns (of each cluster) onto the VARIMAX axes.

Fisher discriminant method achieves an optimal linear dimensionality reduction for classification problems in a supervised way (Bishop, 1995; Duda and Hart, 1973). Fisher criterion is derived by requiring maximum class separation in the output space, and looks for a linear combination of the variables which maximizes the ratio of its between-group variance to its within-group variance (Bishop, 1995). Therefore, the method calculates the between-group covariance matrix (B) and the within-group covariance matrix (W). Then, the Fisher transformation matrix can be found, as in PCA algorithm, from the eigenvectors associated to the highest eigenvalues of the matrix ratio $B \cdot W^{-1}$ (Ripley, 1996). Three QI, based on Fisher method, are proposed here to compare the results obtained from the experiment quantitatively. The QI are computed as follows: QI1: trace(B)/trace(W), QI2: norm(diag(B)/diag(W)), and QI3: norm(eigenvalues(B/W)). Additionally, the sum of standard mean squared errors (MSE) for each class is also used (QI4). Quality index four is the usual criterion which k-means clustering methods attempt to minimize. These QI are introduced in order to have some quantitative measurements of the clustering method applied at hand. However, as we mentioned above, clustering methods are just algorithms that are not guaranteed to converge into a global optimum. The first three QI are measurements of the between-group and within-group ratio (Tou and Gonzalez, 1974; Fukunaga, 1990; Bishop, 1995; Ripley, 1996), that is, three alternative formulae to measure the discriminant capability of each model. 2-D projections (through Fisher transformation) of the clusters have been used as a qualitative measurement. Generally, these first two axes contain most of the variance in the experiments. The interest of this representation has been shown in Section 4—Results and discussion. The best model is selected using a Majority Voting Scheme (MVS) (Ng and Singh, 1998), and the model selected have the votes of the majority of the indices.

4. Results and discussion

The results of applying rotated PCA-VARIMAX to the meteorological data of the period 1999–2002 are shown in Table 1. Only those components associated with eigenvalues greater than unity were extracted. With the rotated PCA-VARIMAX transformation method seven different meteorological conditions could be extracted: component labelled as MET1 is strongly loaded on TMP, RAD and AHM, and is associated with the thermal low, especially observed during warm periods. It is also characterized by high MXH values and wet conditions derived from evaporation processes. It can be interpreted as the influence of convective turbulence in the area. MET2 shows the contrast between the drier conditions linked to north-western winds and the wetter conditions associated with other

Table 1
PCA-VARIMAX eigenvectors. Only absolute values greater than 0.40 are shown in the table

	MET 1	MET 2	MET 3	MET 4	MET 5	MET 6	MET 7	h^2
TMP	0.93							0.900
RAD	0.82							0.831
AHM	0.75	*0.41*						0.779
NW		−0.78						0.715
NNW		−0.81						0.735
RHM	*−0.40*	0.61						0.674
W			−0.75					0.717
WNW			−0.79					0.789
ESE			0.58					0.566
E			0.59	*0.45*				0.781
WSP				0.92				0.892
MXH	*0.45*			0.80				0.888
SE				*−0.49*				0.556
SSE					0.80			0.705
NNE					0.77			0.647
SSW						0.71		0.553
SLP	*−0.46*					−0.64		0.660
PRC						0.69		0.598
NE							0.76	0.721
ENE							0.74	0.702
% var.	17.4	30.4	43.0	51.9	59.9	66.8	72.0	

Communalities are shown in the last column, while the last row shows the cumulative percentage of variance explained by the components.

prevailing winds. MET3 shows the contrast between the most prevailing winds in the area: westerly winds (W, WNW) and easterly winds (E, ESE). MET4 reflects the influence of high winds and good dispersion conditions, that is, mechanical turbulence. This component is positively correlated with easterly winds (E), while the negative moderate correlation with southeast winds appears to indicate the presence of coastal sea breezes during low wind speed conditions. MET5 shows the presence of winds from SSE and NNE sectors, usually associated with transitional situations and low wind speeds. MET6 is positively correlated with PRC and SSW winds and negatively correlated with SLP. It seems to represent rain conditions associated with cyclonic winds from the SSW sector. Finally, MET7 seems to reflect the persistence of northeast winds in the area.

Table 2
Relative frequencies of the different number of classes

Number of classes	1	2	3	4	5	6	7
Relative frequency	0	0	0.0187	0.1375	0.3883	0.3080	0.1320

Table 3
Comparison results between *k*-means clustering and Kohonen competitive network in the search of five clusters

Quality indices	Kohonen competitive network		*k*-means	
	Mean value	Std value	Mean value	Std value
QI1	6.31	0.42	6.05	0.22
QI2	15.80	1.44	15.44	1.41
QI3	1.18E+05	3.22E+05	1.21E+05	2.83E+05
QI4	66634	1834.8	67735	261.11

PCA suggests the existence of seven meteorological conditions through the analysis of the eigenvectors associated to the eigenvalues greater than unity. Although these directions can be physically interpreted and represent the seven most relevant directions in terms of variance explained, they are not likely to represent seven clusters in the data. In fact, PCA is not a discriminant transformation, and though the new space is better oriented, clusters do not have to be extracted more easily. Anyway, and as a starting point, the Kohonen network was trained to look for seven clusters. Table 2 shows that five is the most frequent final number of clusters. The Kohonen network had the ability to discover the final number of clusters in an unsupervised way. This outcome achieved by Kohonen networks is very interesting and useful.

The competitive network performance was compared with *k*-means clustering procedure in a

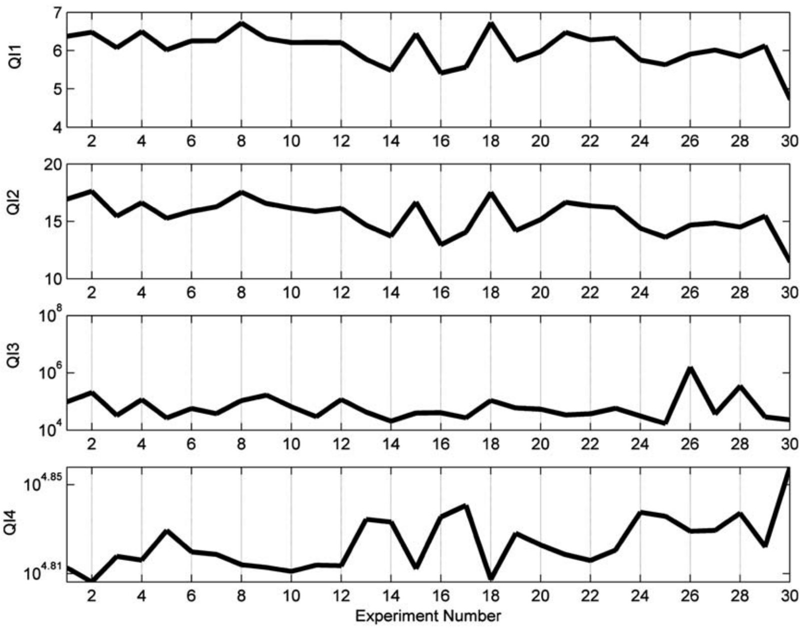

Fig. 2. Quality indices computed for the competitive final experiment.

30-times experiment searching for five clusters. Table 3 shows the mean and standard deviation values of the 30 repetitions. Although differences are not very important, it can be noticed that Kohonen network obtained better results in QI 1, 2 and 4 (better performance is achieved when QI1-3 are higher, and QI4 are smaller).

In the final experiment with a SOM 1-D with five output neurons (one for each cluster), different numbers of epochs were considered for the competitive network (100, 500, and 5000). However, more than 100 epochs led to very slightly changes in the network weights. This final experiment with five classes (and 100 epochs) was repeated 30 times. Thus, the results could be compared and the uncertainty from the randomness in the weight initialization and from the order of pattern presentation was eliminated. The combination (made by MVS) of the results from the quantitative QI (see Fig. 2) allows selecting the second experiment as the best one. For this experiment, the patterns of the five classes found by the competitive network were projected onto PCA-VARIMAX new axes (called MET1-7), as shown in Fig. 3. Projections on the rotated VARIMAX principal components lead to a plausible physical interpretation of the five classes. Actually, the different classes obtained by the Kohonen network seem to be a combination of

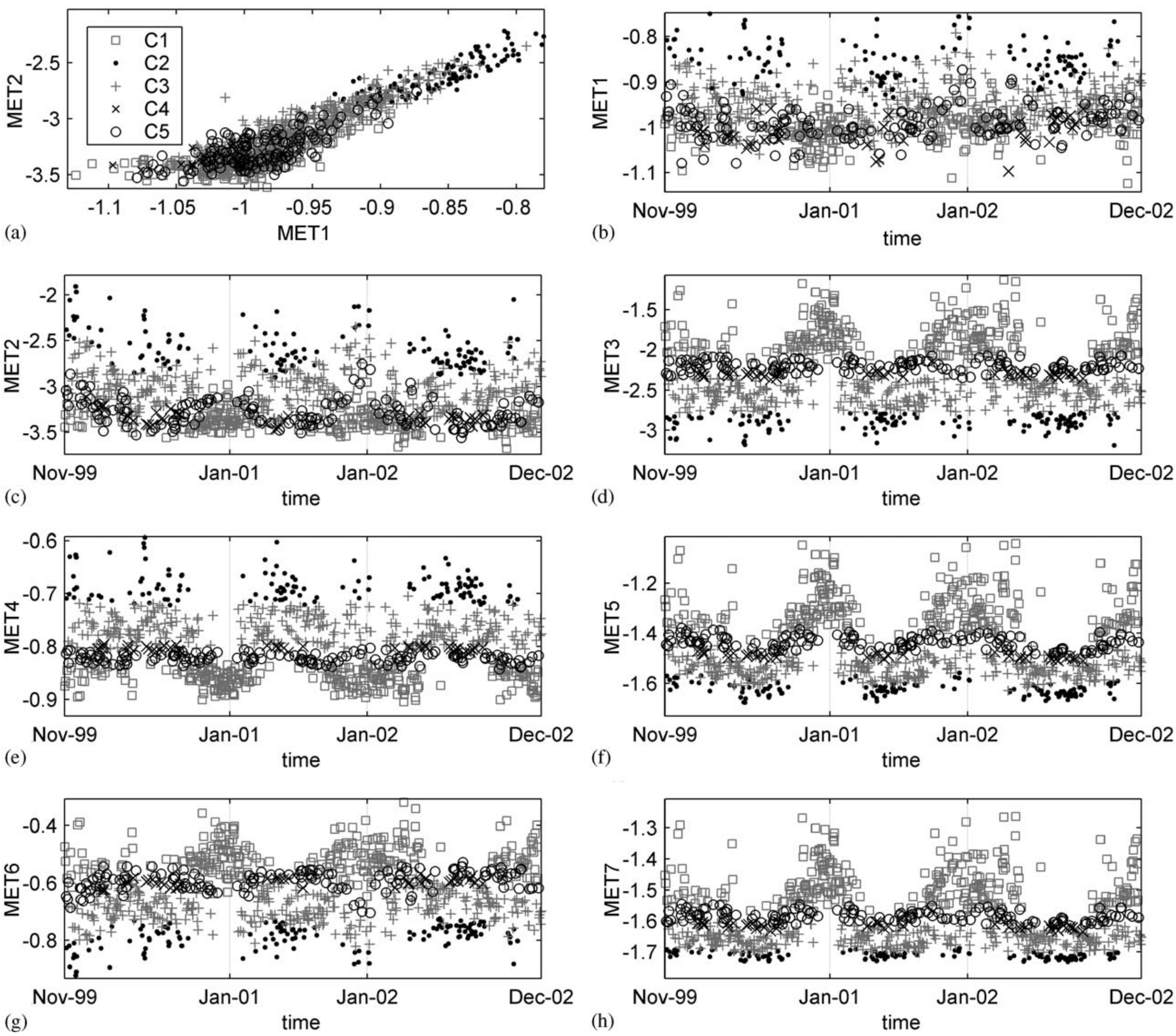

Fig. 3. Projection onto PCA-VARIMAX axes. (a) Data clustering projected onto the first two principal axes (MET1 and MET2); (b) projection onto MET1; (c) MET2; (d) MET3; (e) MET4; (f) MET5; (g) MET6; (h) MET7.

the meteorological situations formerly labelled as MET1-7. The description of classes C1–C5 is as follows: C1 has a clear seasonal behaviour, specially focussed on winter and autumn months. From its projections on the different principal components, it seems that this class reflects opposite conditions to that of persistent easterly winds, showing situations of non-easterly dry winds, small wind speed and mixing heights. Rainy days are also part of this class. C2 is specially focussed on warm months, including thermal low situations, persistent easterly winds and those from sectors W and WNW. C3 is similar to C2, but with higher sea level pressure and lower net radiation values. C4 seems to be a subclass of C5 but focussed on the warm months. C5 is strongly influenced by relative humidity what could explain its seasonal behaviour with increases in winter time. It has also the highest values on variable NNW (daily frequency of the appearance of winds from this sector). From the analysis of these projections it seems that there are slightly differences between the meteorological situations labelled as MET3, MET5 and MET7. This is another interesting result extracted from the use of the methodology proposed here. Seasonal behaviour of the series seems to really affect the clustering process, and different classes have been established during each year's season. Furthermore, their projections on the principal component axes seem to repeat from year to year, which is a plausible result. However, longer series should be considered to infer climatological situations.

Fig. 4 shows how different data clustering can be qualitatively controlled through the visualization of 2-D Fisher projection of the database (the first two Fisher dimensions explained at least 99% of variance). Anyway, like all unsupervised methods, the clustering techniques must be judged by their results. There is no guarantee to find the global optimum. A successful clustering produces groups which can be interpreted by domain experts (Ripley, 1996). In Fig. 4, $u1$ and $u2$ are the new basis (linear combination of the original basis xi), and the database is projected using the Fisher transformation matrix. Fig. 4a shows the projection of the selected clustering (experiment number 2). In Fig. 4b it can be seen that, although QI1 and QI2 are practically identical to those in Fig. 4a, the

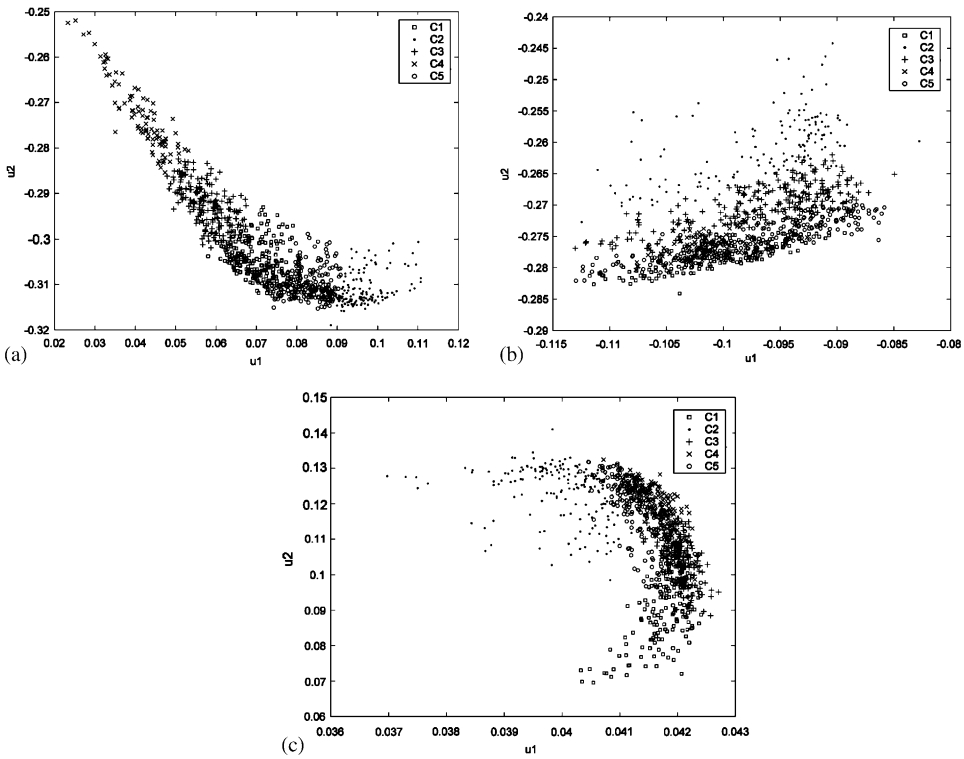

Fig. 4. Metereological clustering projected onto Fisher axes. (a) The best clustering (experiment number 2), (QI1, QI2, QI3, QI4) = {6.48, 17.615, 2.07E+05, 64024}. (b) Experiment number 8 (QI1, QI2, QI3, QI4) = {6.71, 17.54, 1.07E+05, 64992}. (c) Experiment number 28 (QI1, QI2, QI3, QI4) = {5.84, 14.50, 3.46E+05, 68745}.

smaller value of QI3 makes the clustering worse. Fig. 4c illustrates that if QI1 and QI2 are high, the value of QI3 seems to be irrelevant, and the clustering will be bad.

5. Conclusions

The following concluding remarks can be made from the results discussed above:

- Using this approach, a Kohonen SOM 1-D seems to be a plausible alternative to a classical two-stage hierarchical-partitioning clustering technique.
- Five different meteorological classes (C1–C5) have been found using a competitive neural network and identified by using the projection onto the rotated-PCA with VARIMAX criterion.
- The model with the best classification results can be selected using the quantitative QI based on Fisher method.
- The Fisher visualization of the clustering allows checking the clustering in a qualitative way.

The results obtained here can be used in future works to design a separate system of air pollution prediction for each meteorological class, which will improve the results of a unique global system for all the patterns from the database. Our future research includes modelling of the relationship between air pollutants concentrations and meteorological variables within each cluster using backpropagation feedforward neural networks or radial basis function neural networks as regression models. Additionally, SOM networks with different output *n*-dimensional topologies (rectangular, hexagonal, toroidal, etc.) should be researched in order to test the applicability of the method and its topological preserving characteristic in the domain of meteorological clustering.

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