APPLIED ISSUES

Water quality assessment using diatom assemblages and advanced modelling techniques

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SUMMARY

1. Two types of artificial neural networks procedures were used to define and predict diatom assemblage structures in Luxembourg streams using environmental data.

2. Self-organising maps (SOM) were used to classify samples according to their diatom composition, and multilayer perceptron with a backpropagation learning algorithm (BPN) was used to predict these assemblages using environmental characteristics of each sample as input and spatial coordinates (X and Y) of the cell centres of the SOM map identified as diatom assemblages as output. Classical methods (correspondence analysis and clustering analysis) were then used to identify the relations between diatom assemblages and the SOM cell number. A canonical correspondence analysis was also used to define the relationship between these assemblages and the environmental conditions.

3. The diatom-SOM training set resulted in 12 representative assemblages (12 clusters) having different species compositions. Comparison of observed and estimated sample positions on the SOM map were used to evaluate the performance of the BPN (correlation coefficients were 0.93 for X and 0.94 for Y). Mean square errors of 12 cells varied from 0.47 to 1.77 and the proportion of well predicted samples ranged from 37.5 to 92.9%. This study showed the high predictability of diatom assemblages using physical and chemical parameters for a small number of river types within a restricted geographical area.

Keywords: backpropagation algorithm, benthic diatoms, Kohonen self-organising map, stream ecology

Introduction

The distribution and abundance of the species that constitute biological communities are influenced by competition (Schoener, 1989; Eklöv, 1997) as well as the availability of environmental resources that are fundamental for growth and reproduction (Di Castri & Younes, 1990; Chapin *et al*., 1997). These two concepts, namely species–species and species–environment relationships, illustrate the non-linear and complex relationships that often govern a community and the difficulties that ecologists confront when trying to interpret these kinds of data. Limitations of many modelling methods result in data being reduced to relatively simple metrics, such as species richness, which often leads to a loss of valuable information and ecological reality. Two problems arise, however, when working with complex data sets, first the necessity to use methods that take into account non-linear responses, and secondly the need to include community information that can be used to predict ecosystem quality.

The usefulness of efficient mathematical tools in community ecology is apparent (Giske, Huse & Fiksen, 1998), and ecologists have used mathematical approaches such as linear regression (e.g. Ricker, 1975), multiple linear regression (e.g. Oberdorff,

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Hugueny & Guegan, 1997), canonical correspondence analysis (e.g. ter Braak, 1986), principal component analysis (e.g. Grossman, Nickerson & Freeman, 1991) and multiple dimensional scaling (e.g. Legendre & Legendre, 2000). However, one of the drawbacks of these methods is that they do not take sufficient account of data complexity and non-linearity (Blayo & Demartines, 1991). Artificial neural networks (ANNs) are techniques that have been shown to work well with complex and non-linear datasets (Lek *et al.*, 1995; Scardi, 1996; Recknagel *et al.*, 1997). ANN methods are based on transmission of information through connections similar to those that occur in the animal nervous system. Different kinds of ANN exist, usually classified as supervised or unsupervised learning (Lek & Guegan, 2000). The most common types of ANN used in ecology are supervised multilayer perceptron neural networks with a backpropagation learning algorithm (BPN) (e.g. Brosse *et al.*, 1999; Maier & Dandy, 2000) and unsupervised self-organising maps (SOM) (e.g. Brosse, Giraudel & Lek, 2001; Michaelides, Pattichis & Kleovoulou, 2001). SOM is usually used for ordination and classification (e.g. Chon *et al.*, 1996; Lek, Guiresse & Giraudel, 1999), whereas BPN is commonly used to develop predictive models (e.g. Clair & Ehrman, 1998; Laberge, Cluis & Mercier, 2000). The aim of this study is to present an ecological modelling method combining SOM and BPN. The SOM–BPN combination has been tried in medical imaging (e.g. Reddick *et al.*, 1997; Glass *et al.*, 2000) and in electrical engineering (e.g. Srinivasan *et al.*, 1998) and has given satisfactory results for prediction. The present study, carried out in the framework of the European project PAEQANN (Predicting Aquatic Ecosystem Quality using Artificial Neural Networks, http://aquaeco.ups-tlse.fr/), used a database of benthic diatom inventories and environmental variables of headwater streams in Luxembourg.

Methods

Database

As part of the PAEQANN project, epilithic samples were collected from streams (stream orders one to three according to Strahler, 1963 and Leopold, Wolman & Miller, 1964) in spring and autumn from 1994 until 1997. The data, consisting of 289 samples of benthic diatoms and environmental variables, were collected according to French and European standard sampling methods (Kelly *et al.*, 1998; AFNOR, 2000). In brief, benthic diatoms were collected in riffle areas from stones, which are not moved under normal hydrological conditions, by scraping the upper surface of the stones with a toothbrush. Samples were directly fixed in 4% formaldehyde solution (Prygiel & Coste, 2000). Diatom valves, cleaned with concentrated hydrogen peroxide (H_2O_2 40%) to eliminate organic matter and hydrochloric acid in each sample to dissolve calcium carbonates were mounted in Naphrax®. Up to 400 valves were counted and identified in each sample (Iserentant *et al.*, 1999). An agglomerative hierarchical clustering analysis (Ward's method for linkage and Euclidean distances) of diatom inventories showed no correlation between sampling season (spring or autumn) and diatom assemblages, hence the data were pooled.

The habitats where diatom samples were collected were characterised using nineteen topographical, physical and chemical variables: width, slope, distance from source, water temperature, dissolved oxygen, conductivity, total phosphorus, pH, NO_3^-, NO_2^-, NH_4^+, PO_4^{3-}, Na^+, Cl^-, K^+, SO_4^{2-}, biological oxygen demand $(BOD)_5$, total hardness and carbonate hardness. Some chemical variables were measured directly at the sampling site (e.g. pH, conductivity) whilst others were analysed in the laboratory following standard procedures (e.g. NO_3^-, NO_2^-, NH_4^+, PO_4^{3-}). Topographical parameters (width, slope and distance from source) were measured on 1/20 000 maps.

A total of 411 diatom taxa were recorded from the 289 samples. Because of the dominance of rare species (e.g. 50% of the taxa occurred no more than three times in 289 samples) and to facilitate the work of managers, the species data-matrix was reduced (see below).

ANN models

Two ANN algorithms were used to model the structure of the diatom assemblages: (i) SOM, an unsupervised neural network, was used to ordinate diatom assemblages in a two dimensional grid and (ii) BPN, a supervised neural network, was used to predict the assemblages classified by SOM.

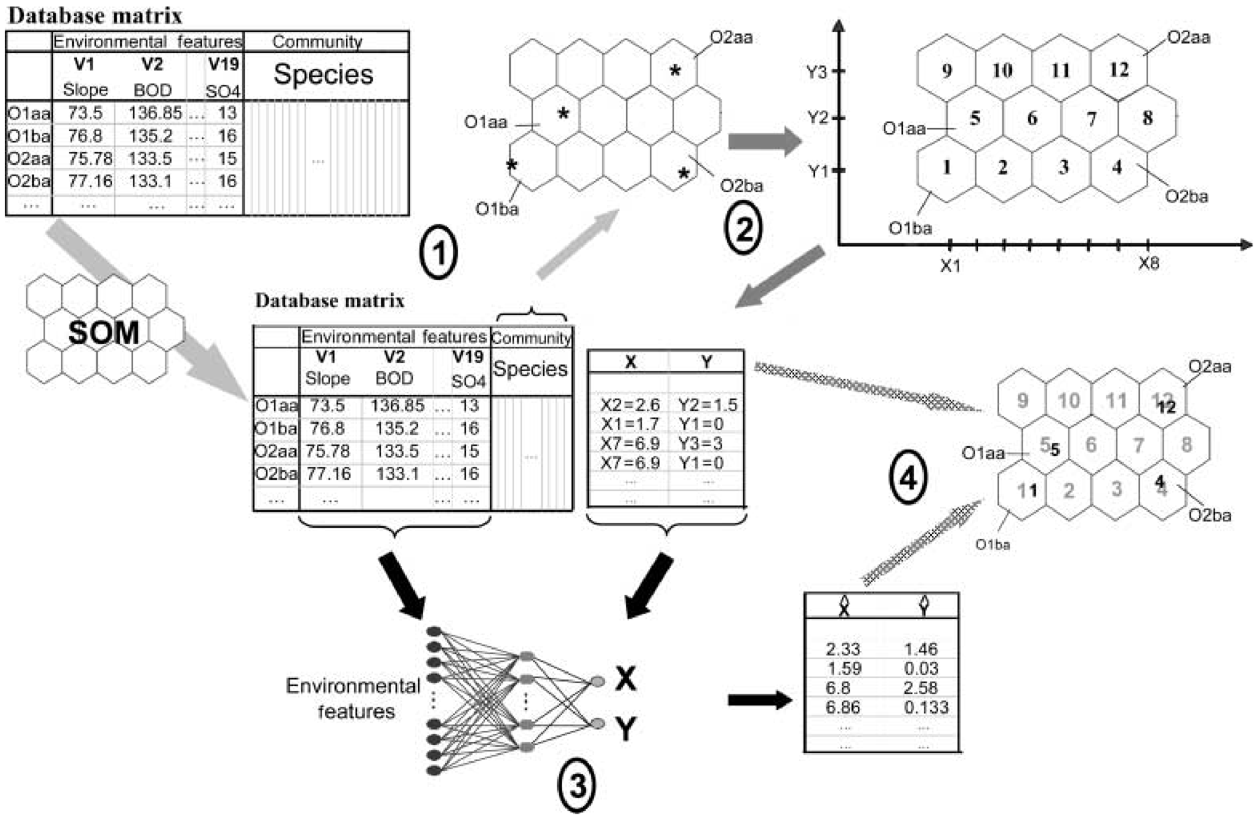
In brief, SOM, also referred to as a Kohonen neural network, approximates the probability density function of the input variables and performs a non-linear projection of the multivariate data into a two-dimensional space (Kohonen, 1982, 2001). SOM consists of two layers of neurones (i.e. computational units) connected by weights (connection intensities): the input layer is connected to a vector of the input dataset and the output layer forms a map consisting of a rectangular grid laid out in several neurones (cells). During the learning process the weights are modified to minimise the distances between weight and input vectors. This results in classifying the input data according to their similarities and preserving the connection intensities.

Backpropagation learning algorithm is one of the most popular ANN algorithms (Rumelhart, Hinton & Williams, 1986; Lek & Guegan, 2000) as it has the ability to learn patterns when given training data, and to generalise results from the training dataset. BPN is composed of three layers (input, hidden and output layers) of interconnected processing elements (neurones) and each neurone is connected with neurones of the previous layer by weighted links and activated by the sigmoid transfer function $f(x) = 1/(1 + e^{-x})$, where x is input data. During training the network is designed to compare expected and calculated values, and to modify connection weights to reduce the mean square error (MSE).

A detailed description of both algorithms and their applications in ecology are given in Chen & Ware (1999) and Lek & Guegan (2000).

Modelling processes

For the prediction of the diatom assemblages in this study, SOM was used to give groups of diatom assemblages and BPN was used to predict these assemblages. A complete modelling sequence is constructed following four steps (Fig. 1):



	Environmental features				Community
	V1 Slope	V2 BOD		V19 SO4	Species
O1aa	73.5	136.85	...	13	
O1ba	76.8	135.2	...	16	
O2aa	75.78	133.5	...	15	...
O2ba	77.16	133.1	...	16	
...	...	...	...	...	

X	Y
X2=2.6	Y2=1.5
X1=1.7	Y1=0
X7=6.9	Y3=3
X7=6.9	Y1=0
...	...
...	...

$\hat{X}$	$\hat{Y}$
2.33	1.46
1.59	0.03
6.8	2.58
6.86	0.133
...	...
...	...

Fig. 1 Schematic diagram showing the modelling process in four steps: (1) The SOM algorithm is used on the species data matrix to reduce the dimensionality and classify the samples according to similarities in the species composition; (2) Each sample (characterised by a diatom composition) is represented by spatial coordinates (X and Y) associated to their environmental features; (3) The BPN algorithm used the environmental features of the samples as input and the coordinates of each sample as output; (4) The predicted values ($\hat{X}$, $\hat{Y}$) for each sample are plotted on a 12-celled SOM map to test the predictability of the BPN. The number of the cell where it was observed is noted.

(1) First, data dimensions were reduced by eliminating taxa showing low density and/or low occurrence by SOM. SOM reduced the diatom assemblage matrix (density and taxon occurrence) to a number of assemblages using the connection intensity values that represent the abundance of each taxon in the assemblages. Data reduction, using the connection intensities of the SOM, allowed species with connection intensities <10% to be discarded. In the final data matrix, 71 taxa were selected from 411 total taxa for the ANN models. SOM were then trained again with densities of 71 taxa to classify different groups of assemblages based on their species similarities. In SOM classification, the number of output neurones (i.e. the map size) is important: if the map size is too small, differences among assemblages might not be adequately described, conversely, if the map size is too big the differences among assemblages become trivial (Wilppu, 1997). Thus, we trained the network with different map sizes, and chose the optimum map size based on the minimum values for quantisation and topographic errors, which are used to evaluate the map quality (Park et al. 2003). In this study, a 12-celled map was used, (i.e. a rectangular map of 4 × 3 cells), with each of the 12 cells considered as representing a different diatom assemblage.

(2) A SOM map is represented by a two-dimensional lattice, where each point of the grid can be defined by X and Y coordinates. Each sample is then characterised by the X and Y coordinates of the centre of the cell where it has been placed, and by the original data using the environmental variables. A new matrix is therefore constructed with, for each sample, its environmental features and the coordinates of the centre of the cell in which it is observed. BPN was used to predict the coordinates of the samples in the SOM with the environmental variables. Two output neurones were used to predict the X and Y coordinates of the cell centres of the SOM map. A Jacknife leave-one-out validation procedure (Efron, 1983; Efron & Tibshirani, 1995), where each sample is tested using a model trained by all the other observations, was used to test the predictive quality of the model. Nineteen environmental variables were used as input variables in input neurones to predict the coordinates of the SOM cells (X and Y, i.e. two output neurones). Thirteen neurones were used in the hidden layer of the artificial network and the network converged after 500 iterations according to the best compromise between bias and variance (Geman, Bienenstock & Doursat, 1992; Kohavi, 1995).

(3) The estimated X, Y coordinate values of each sample were plotted on the same SOM map and a sample was estimated as being well predicted if it was plotted in the cell area where it had been observed (i.e. included in the expected samples).

The simulating program in the Matlab environment that was used for this work is available from the first author request.

For each cell, two indices were used to assess the quality of the model:

(1) The total mean square error ($\mathrm{MSE_t}$) was calculated by considering the sum of the abscissa MSE ($\mathrm{MSE_{abs}}$) and ordinate MSE ($\mathrm{MSE_{ord}}$):

$$\mathrm{MSE_t} = \mathrm{MSE_{abs}} + \mathrm{MSE_{ord}} = \frac{\sum_{i=1}^{N}\left(X_{\mathrm{obs}_i} - X_{\mathrm{pred}_i}\right)^2 + \left(Y_{\mathrm{obs}_i} - Y_{\mathrm{pred}_i}\right)^2}{N} \tag{1}$$

where N is the number of samples in a cell, X_{obs} is the observed abscissa, X_{pred} is the predicted abscissa, Y_{obs} is the observed ordinate and Y_{pred} is the predicted ordinate.

(2) The percentage of well predicted samples (P_{wp}), which is defined as the ratio of samples predicted inside the specific cell and the total number of samples classified in the cell, varied from 0 (all samples were predicted outside the cell) to 100 (all samples were predicted inside the cell) was calculated as:

$$P_{\mathrm{wp}}(\%) = \frac{n}{N} \times 100 \tag{2}$$

where n is the number of samples predicted to lie inside a cell and N is the total number of samples in a cell. A cell is considered as well predicted if P_{wp} is high and $\mathrm{MSE_t}$ is low (i.e. the samples are inside and near the centre of the cell).

As SOM placed samples into different cells according to their similarities of taxa composition, all samples in a cell have similar taxa assemblages. To identify the relations between assemblages and the cell number the taxa were analysed by their connection intensities. This was performed using the density probabilities of each taxon in SOM cells using correspondence analysis (CA) (Hill, 1973) and divisive hierarchical clustering analysis (DHC) (Kaufman & Rousseeuw, 1990). Canonical correspondence analysis

(CCA) (ter Braak, 1986) was used to define the relationship between diatom assemblages and environmental conditions using the 16 physical and chemical variables and the 19 relevant diatom taxa (Table 2) of the groups defined by the CA and DHC.

Results

Diatom assemblages were classified according to the gradient of species composition on the SOM map, with each cell corresponding to a specific diatom assemblage (Fig. 2). The number of samples in each cell ranged from eight (in cell six) to 39 (in cell nine) (Table 1).

Using a Jacknife leave-one-out validation procedure of the BPN, the correlation coefficients between observed and predicted values of *X* and *Y* spatial coordinates were 0.93 and 0.94, respectively. Most samples were well located, although some misallocations were noted in cells three, six, seven and 10 (Fig. 3). The highest MSE and the smallest proportion of well predicted samples were obtained for these four cells and relatively small numbers of samples were found in cells six, seven and 10 (Table 1). The coexistence of diatom taxa at one sampling site is controlled by the environmental descriptors. In this study, cells one, two, five and nine on the left side of the SOM map are characterised by samples with higher conductivity, carbonate hardness and pH than cells four, eight and 12 on the right side of the map. The influence of geology is also evident, as samples to the left were from sandstone areas, whilst samples to

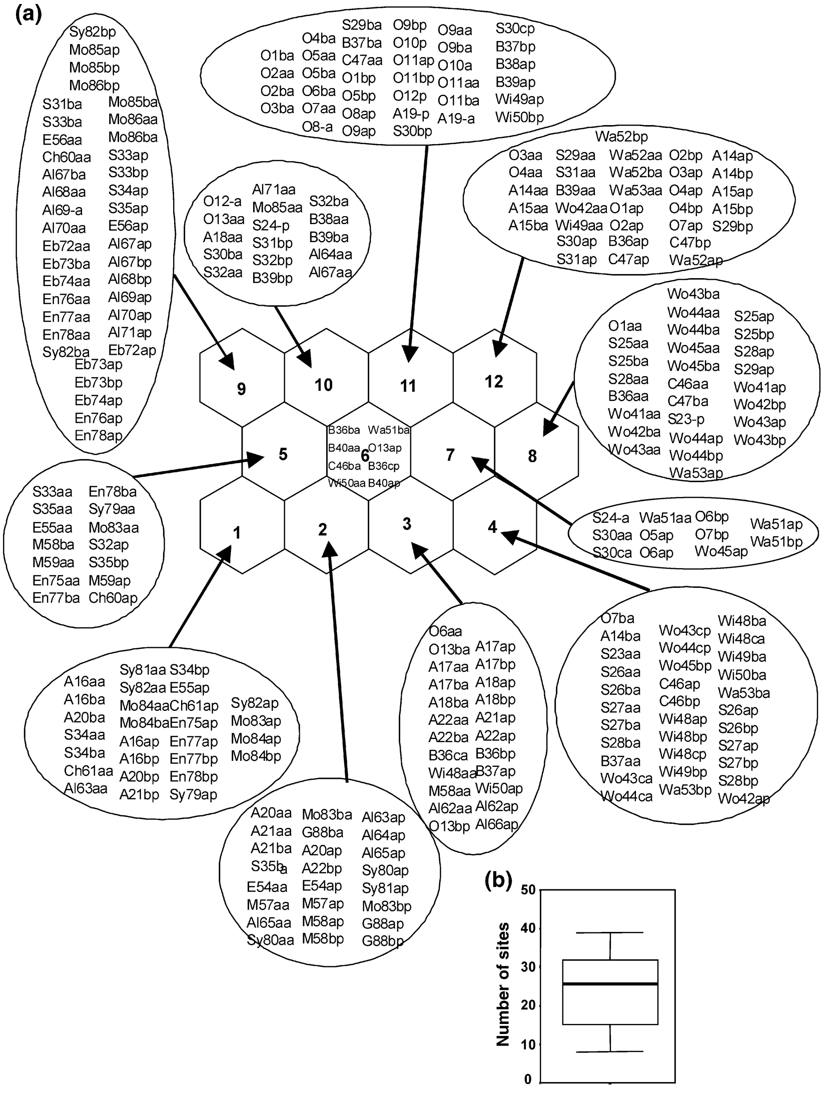


Fig. 2 (a) A SOM map of species abundance of 289 samples of diatom assemblages from the Luxembourg streams plotted according to similarities in species composition. The name of each sample is represented by an abbreviation ending with two letters, where the first letter denotes sampling area and the second letter shows if the sample was collected during spring (p) or autumn (a). The number of samples in each cell varied from eight to 39 (see also Table 1). (b) A box plot of the distribution of the samples in the cells of the SOM map. The tails of the box represent the maximum and the minimum values of the number of samples per cell, and the horizontal line in the box represents the average value.

Table 1 Summary table giving the number of samples (N) plotted in each cell of the SOM, the total mean square errors ($\mathrm{MSE_t}$), the number of well predicted samples (n) in each cell (cf. page 211) and the percentage of well predicted samples [P_{wp} (%)]

No. of cells	N	$\mathrm{MSE_t}$	n	P_{wp} (%)
1	27	0.6988	20	74.1
2	24	0.7316	17	70.8
3	23	1.0607	14	60.9
4	32	0.7802	24	75.0
5	14	0.485	13	92.9
6	8	1.7672	3	37.5
7	11	0.8974	5	45.4
8	27	0.6378	21	77.8
9	39	0.4669	36	92.3
10	16	1.7259	8	50.0
11	36	0.8641	26	72.2
12	32	0.7311	23	71.9

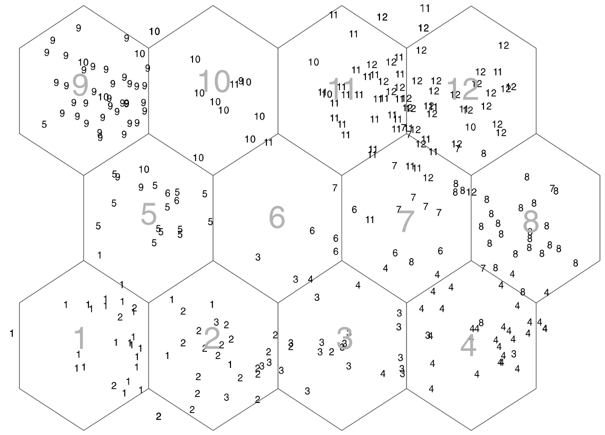


Fig. 3 Predicted results of a leave-one-out validation procedure of the BPN model. The samples are plotted with their predicted coordinates. The samples predicted within the corresponding area were considered as well predicted. Each sample is plotted using the number of the cell where it was observed. The observed coordinates are represented in the centre of each cell, and the predicted coordinates are at their precise position on the map.

the right were dominated by schist. Cells in the bottom of the SOM map (one, two, three and four) show higher values of $\mathrm{PO_4^{3-}}$, $\mathrm{NO_2^-}$ and $\mathrm{BOD_5}$ than cells nine, 10, 11 and 12, in the upper areas. This finding indicates that samples in the bottom of the SOM map are affected by anthropogenic disturbances such as organic pollution or eutrophication.

Both CA and DHC analyses showed three main diatom groups and several subgroups (Fig. 4). The three main groups were also defined by k-means clustering analysis. Three main groups of assemblages were also revealed in the SOM map (as shown in Table 2). The first group was composed of cells four, seven, eight, 11 and 12, the second of cells three, six and 10 and the third of cells one, two, five and nine (Fig. 4c).

While the samples allocated to a given cell have similar diatom assemblages, those in neighbouring cells are less similar, and dissimilarity increases with distance between cells. Species that have a probability of presence of over 0.8 are given in Table 2. The diatom compositions of each cell were clearly related to their ecology, and in agreement with the observations of van Dam, Mertens & Sinkeldam (1994). For example, alkaliphilic taxa such as *Amphora pediculus* (Kützing) Grunow, *Cocconeis placentula* var. *lineata* (Ehrenberg) Van Heurck, *Rhoicosphenia abbreviata* (C.A. Agardh) Lange-Bertalot and*Mayamaea atomus* var. *permitis* (Hustedt) Lange-Bertalot and alkalibion taxa such as *Gomphonema olivaceum* (Hornemann) Brébisson are located in the left part of the SOM map (cells one, five and nine). Neutrophilic taxa, such as *Achnanthidium minutissimum* (Kützing) Czarnecki, *G. olivaceum* var. *minutissimum* (Hustedt) Lange-Bertalot, *Navicula gregaria* Donkin, *Fistulifera saprophila* Lange-Bertalot & Bonik, *Nitzschia palea* (Kützing) W.M. Smith and*Gomphonema parvulum* Kützing are found on the right side (cells four, eight and 12) (Table 2 and Fig. 4). The diatom assemblages also show a pollution-gradient from the top to the bottom of the SOM map. For instance, *F. saprophila, M. atomus* var. *permitis, Eolimna minima* Grunow, and*N. gregaria* Donkin are α-mesosaprobic to polysaprobic and eutrophic species and are mainly found in cells one, two, three and four, whilst *A. minutissimum*, a common β-mesosaprobic diatom, is found in high abundance (over 47%) in several other cells (nine, 10, 11 and 12). Hence, the cells at the bottom of the map correspond to sites with high pollution, whilst the cells at the top correspond to minimally disturbed or unpolluted rivers.

Canonical correspondance analysis (CCA) showed the relationship between diatom assemblages and environmental conditions, revealing clear ecological and physical-chemical gradients (Fig. 5). Ecological, physical and chemical gradients were clearly defined and indicated the water quality. According to van Dam *et al.* (1994) the species in group one, *Fragilaria capucina* Desmazières ssp. *rumpens* (Kützing) Lange-

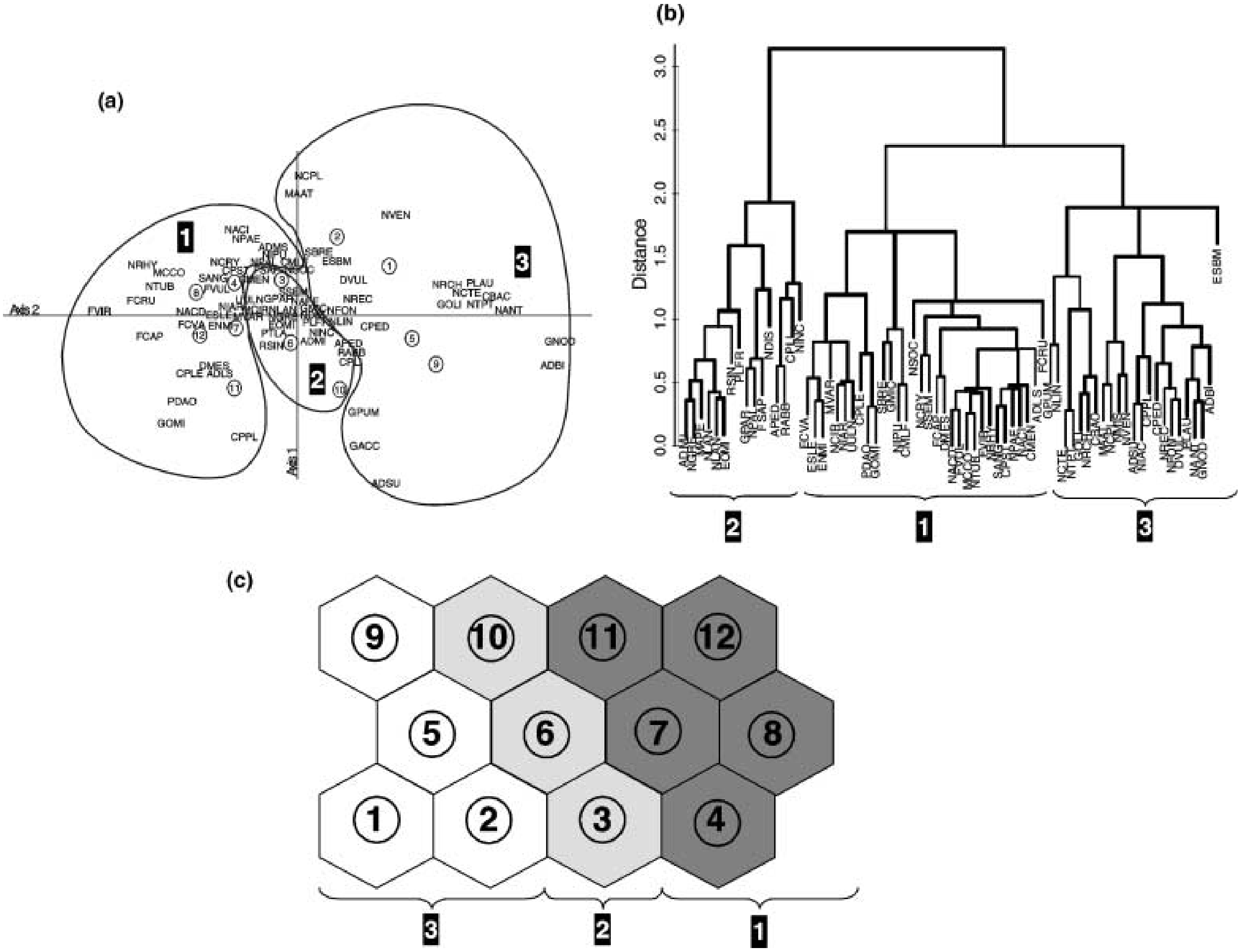


Fig. 4 (a) Correspondence analysis (CA) of the 12 SOM cells (numbers one to 12) and the diatom species probability in these cells (their abbreviations are listed in Appendix). Axes 1 and 2 account for 65.7% of the variation and the three main diatom groups are shown; (b) Divisive hierarchical clustering (DHC) analysis showing groups of affinity. The three groups were defined using *k*-means clustering analysis (10 iterations); (c) The three groups determined by CA and DHC analyses represented on the SOM map. Each group is represented by a different shade: dark grey for group 1, light grey for group 2 and white for group 3.

Bertalot, *G. olivaceum* var. *minutissimum* and *Psammothidium daonense* (Lange-Bertalot) Lange-Bertalot are considered as neutrophilous, whilst those in group three are mostly alkaliphilic taxa such as *Caloneis bacillum* (Grunow) Cleve, *Navicula cryptotenella* Lange-Bertalot and *Navicula tripunctata* (O.F. Müller) Bory and also alkalibion taxa such as *G. olivaceum*. These taxa were correlated with gradients of carbonate hardness, pH, conductivity and total hardness, which are the most important structuring parameters in the CCA. The secondary gradient of the CCA was an organic pollution gradient represented by BOD_5, NO_2^- and PO_4^{3-}. The taxa in the upper left part of the CCA are α-meso-polysaprobic species such as *E. minima*, *Eolimna subminuscula* Manguin and*F. saprophila*, and polysaprobic taxa like *N. palea*. Sites plotted in the lower part of the CCA represent mainly undisturbed conditions in Luxembourg's streams.

Discussion

Assessing the ecological integrity of running water often requires the development of integrated methods that consider the complex inter-relationships between community assemblage and environmental factors. Many existing methods use the species composition of the communities, reduced to species richness (e.g. Belkessam, Oberdorff & Hugueny, 1997; Guegan, Lek

Table 2 Relevant diatom taxa in each SOM cell (i.e. of each diatom assemblage). Taxa are considered as relevant if the probability of their presence in a cell is >0.8. Underlined text shows representative taxa of group 1, italics shows representative taxa of group 2, bold lettering shows representative taxa of group 3. These three groups correspond to the groups revealed by cluster analysis (Fig. 4)

Cell 1	Cell 2	Cell 3	Cell 4	Cell 5	Cell 6	Cell 7	Cell 8	Cell 9	Cell 10	Cell 11	Cell 12
NGRE	NGRE	ADMI	NGRE	ADMI	ADMI	ADMI	NGRE	ADMI	ADMI	ADMI	ADMI
NLAN	APED	NGRE	NLAN	APED	NGRE	MAPE	EOMI	APED	APED	NGRE	NGRE
MAPE	ADMI	MAPE	MAPE	RABB	NLAN	EOMI	GPAR	GPUM	EOMI	PTLA	PTLA
APED	MAPE	FSAP	EOMI	CPLI	PTLA	FSAP	ADMI	**NTPT**	PLFR	RSIN	NLAN
NTPT	PLFR	NLAN	FSAP	**NTPT**	MAPE	NGRE	NLAN	**NCTE**	RABB	GOMI	FCVA
ADMI	PTLA	NPAL	NPAL	NGRE	RSIN	PTLA	FSAP	CPLI	MAPE	CPLE	
NDIS	EOMI	EOMI	GPAR	EOMI	APED	RSIN	FCVA	**GOLI**	RSIN	APED	
NCTE	GPAR	GPAR	ADMI	NDIS	EOMI	GPAR	MAPE	NDIS	NLAN	NLAN	
EOMI	NPAL	ESBM	PTLA	**NCTE**	GPAR	NLAN	FCRU	NGRE	*CPLI*	MAPE	
RABB	**NCTE**	RSIN	FCVA		*CPLI*	PDAO	PTLA	RABB	*NINC*	PDAO	
SBRE	ESBM	PLFR	FCRU		*NINC*		NPAL			PLFR	
CBAC		*NINC*	RSIN				RSIN				
			ENMI				NDIS				
			ESBM								
			MVAR								

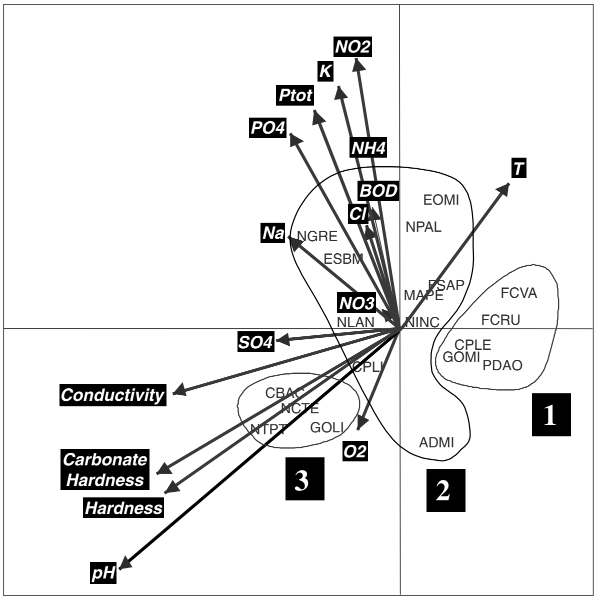


Fig. 5 Canonical correspondence analysis (CCA) biplot of 19 diatom taxa, which are relevant (Table 2) in the three groups defined by the CA and DHC (Fig. 4 and Table 2), and 16 selected physical and chemical environmental variables. The three main diatom groups are shown.

& Oberdorff, 1998; Mastrorillo *et al.*, 1998), or bioassesment indices such as 'River Invertebrate Prediction and Classification System' (RIVPACS) (Armitage *et al.*, 1983; Wright, Furse & Armitage, 1993) or the 'Index of Biotic Integrity' (IBI) (Karr, 1981; Oberdorff & Hughes, 1992).

The European Water Framework Directive (European Parliament, 2000, directive 2000/60/EC, http://europea.eu.int/comm/environment/water) considers benthic diatoms as one of the key groups of organisms for assessing the ecological quality of rivers. Several studies have related diatom assemblage composition to environmental factors. For example, diatom assemblages have been shown to be strongly related to pH (e.g. Eloranta, 1990; van Dam, 1997), and using this information a number of prediction models have been developed (e.g. Renberg & Hellberg, 1982; ter Braak & van Dam, 1989; Birks, Juggins & Line, 1990; ter Braak & Juggins, 1993; Racca *et al.*, 2001). Similarly, relationships between diatoms and salinity have also been studied (Ziemann, 1971; Juggins, 1992). However, one of the weaknesses of these approaches is that they consider environmental parameters independently, although some studies have used several environmental variables (e.g. Lange-Bertalot, 1979; Denys, 1991a,b; van Dam *et al.*, 1994).

Attempts to describe a complex assemblage structure using a single attribute, such as species richness, diversity or equitability, have been criticised, as valuable information may be lost (Begon, Harper & Townsend, 1996). The use of simple metrics is mainly because of the paucity of methods that can handle large databases (Giske *et al.*, 1998). This problem is, however, becoming less prevalent with the use of CCA, weighted averaging (WA) regression, weighted averaging partial least square (WA-PLS) regression and ANNs. The advantage of ANNs is that these techniques are tolerant to noisy data (Hepner *et al.*, 1990), they are able to handle outliers (Lippman, 1987) and they are efficient for predicting non-linear data and for explaining complex relationships between the variables (Rumelhart *et al.*, 1986). In brief, they are well-adapted tools for analysing large and complex data matrices.

In the present study, the association of two ANN methods, SOM and BPN, gave satisfactory results for the prediction of diatom assemblages. These results are in agreement with those obtained in other fields of research, where the two ANN methods have been used together in imagery (Reddick *et al.*, 1997; Glass *et al.*, 2000) and engineering and computing technology (Srinivasan *et al.*, 1998). The map obtained by the SOM procedure distributed the diatom samples into 12 cells, with each SOM cell representing a specific diatom assemblage according to the environmental conditions of sampling sites assigned in each cell. Both CA and DHC supported this conjecture, showing the existence of three main diatom assemblages. These three assemblages were also revealed in the SOM map, when the probability of each species in each cell was studied.

Backpropagation learning algorithm was used to predict the diatom assemblages in streams from their spatial coordinates on the SOM map. Cells three, six, seven and 10 had the highest MSE and the lowest proportion of well-predicted samples. One obvious reason for the poor prediction power is that BPN performs poorly when that number of samples per cell is low (Hagan, Demuth & Beale, 1995). In the Luxembourg area, only a few intermediate situations can be found (sites with intermediate conductivities, carbonate hardness and pH), as the country is divided in two very different geological regions: schistose substrates in the north and sandstone or limestone in the south. These two geological regions result in strongly different water chemistry characteristics of headwater streams. For instance, only eight of the total 289 samples were placed in cell six. The learning step was stopped just before over-learning of the network to allow the model to maintain its ability to generalise (i.e. if the learning step is too long, the model becomes specialised and is not able to generalise on new data). However, the BPN predicted all the other diatom assemblages relatively well, placing the samples in the cells of the map where they were also classified by the SOM method. The correlation coefficients obtained for the spatial coordinates were also high (>0.9) indicating the model's quality of prediction.

The use of advanced modelling techniques for predicting the structure and the diversity of key aquatic communities such as diatoms is the principal research subject of the European research project PAEQANN (N° EVK1-CT1999-00026, http://aquaeco.ups-tlse.fr/). This project is under the directive of the European Community (European Parliament, 2000, directive 2000/60/EC). One of major aims of the European Water Framework Directive is to evaluate the deviation of an ecosystem from the highest ecological quality expected in the absence of human-induced stress. The European Community has recently proposed that diatoms be used to assess river quality. This study shows the accuracy of ANN methods to predict diatom assemblages in a defined geographical area for a small number of river types. The use of predictive modelling could be an important step in defining the reference conditions for diatom assemblages in European rivers and streams.

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Appendix 1: List of the 71 diatom taxa used in the model

Taxa names	Abbreviations
Achnanthidium biasolettianum (Grunow) Round & Bukhtiyarova	ADBI
Achnanthidium subatomus (Hustedt) Lange-Bertalot	ADSU
Planothidium lanceolatum (Brébisson) Round & Bukhtiyarova	PTLA
Planothidium frequentissimum (Lange-Bertalot) Round & Bukhtiyarova	PLFR
Psammothidium lauenburgianum (Hustedt) Bukhtiyarova & Round	PLAU
Achnanthidium minutissimum (Kützing) Czarnecki	ADMI
Amphora pediculus (Kützing) Grunow	APED
Caloneis bacillum (Grunow) Cleve	CBAC
Cocconeis pediculus Ehrenberg	CPED
Cocconeis placentula Ehrenberg var. *euglypta* (Ehrenberg) Grunow	CPLE
Cocconeis placentula var. *lineata* (Ehrenberg) Van Heurck	CPLI
Cocconeis placentula var. *pseudolineata* Geitler	CPPL
Cyclotella meneghiniana Kützing	CMEN
Cyclotella pseudostelligera Hustedt	CPST
Encyonema minutum (Hilse) D.G. Mann	ENMI
Encyonema silesiacum (Bleisch) D.G. Mann	ESLE
Diatoma mesodon (Ehrenberg) Kützing	DMES
Diatoma vulgaris Bory	DVUL
Eolimna minima Grunow	EOMI
Eolimna subminuscula Manguin	ESBM
Fistulifera saprophila Lange-Bertalot & Bonik	FSAP
Fragilaria capucina Desmazières var. *capucina*	FCAP
Fragilaria capucina Desmazières ssp. *rumpens* (Kützing) Lange-Bertalot	FCRU
Fragilaria capucina Desmazières var. *vaucheriae* (Kützing) Lange-Bertalot	FCVA
Ulnaria ulna (Nitzsch) Compère	UULN
Fragilaria virescens Ralfs	FVIR
Frustulia vulgaris (Thwaites) De Toni	FVUL
Gomphonema micropus Kützing	GMIC
Gomphonema olivaceum (Hornemann) Brébisson	GOLI
Gomphonema olivaceum (Hornemann) Brébisson *var. minutissimum* (Hustedt) Lange-Bertalot	GOMI
Gomphonema parvulum Kützing	GPAR
Gomphonema pumilum (Grunow) Reichardt & Lange-Bertalot	GPUM
Gyrosigma nodiferum (Grunow) Reimer	GNOD
Melosira varians C.A. Agardh	MVAR
Meridion circulare (Greville) C.A. Agardh var. *circulare*	MCIR
Meridion circulare (Greville) C.A. Agardh var. *constrictum* (Ralfs) Van Heurck	MCCO
Mayamaea atomus (Kützing) Lange-Bertalot	MAAT
Mayamaea atomus var. *permitis* (Hustedt) Lange-Bertalot	MAPE
Nitzschia acicularis (Kützing) W.M. Smith	NACI
Nitzschia acidoclinata Lange-Bertalot	NACD
Nitzschia capitellata Hustedt	NCPL

Appendix 1: (Continued)

Taxa names	Abbreviations
Navicula cryptocephala Kützing	NCRY
Navicula cryptotenella Lange-Bertalot	NCTE
Navicula gregaria Donkin	NGRE
Geissleria acceptata (Hustedt) Lange-Bertalot & Metzeltin	GACC
Navicula antonii Lange-Bertalot	NANT
Adlafia minuscula (Grunow) Lange-Bertalot	ADMS
Craticula molestiformis (Hustedt) Lange-Bertalot	CMLF
Navicula reichardtiana Lange-Bertalot	NRCH
Navicula rhynchocephala Kützing	NRHY
Navicula tripunctata (O.F. Müller) Bory	NTPT
Navicula veneta Kützing	NVEN
Nitzschia archibaldii Lange-Bertalot	NIAR
Nitzschia dissipata (Kützing) Grunow	NDIS
Nitzschia fonticola Grunow	NFON
Nitzschia inconspicua Grunow	NINC
Navicula lanceolata (Agardh) Ehrenberg	NLAN
Nitzschia linearis (Agardh) W.M. Smith	NLIN
Nitzschia palea (Kützing) W.M. Smith	NPAL
Nitzschia paleacea (Grunow) Grunow	NPAE
Nitzschia pusilla (Kützing) Grunow	NIPU
Nitzschia recta Hantzsch	NREC
Nitzschia sociabilis Hustedt	NSOC
Adlafia suchlandtii (Hustedt) Moser, Lange-Bertalot & Metzeltin	ADLS
Nitzschia tubicola Grunow	NTUB
Psammothidium daonense (Lange-Bertalot) Lange-Bertalot	PDAO
Rhoicosphenia abbreviata (C.A. Agardh) Lange-Bertalot	RABB
Reimeria sinuata (Gregory) Kociolek & Stoermer	RSIN
Sellaphora seminulum (Grunow) D.G. Mann	SSEM
Surirella angusta Kützing	SANG
Surirella brebissonii Krammer & Lange-Bertalot	SBRE