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Artificial neural networks as a tool in ecological modelling, an introduction

Sovan Lek ^{a,*}, J.F. Guégan ^b

^a CNRS, UMR 5576, CESAC-Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse cedex, France

^b Centre d'Etude sur le Polymorphisme des Micro-organismes, Centre I.R.D. de Montpellier, U.M.R. C.N.R.S.- I.R.D. 9926, 911 avenue du Val de Montferrand, Parc Agropolis, F-34032 Montpellier cedex 1, France

Abstract

Artificial neural networks (ANNs) are non-linear mapping structures based on the function of the human brain. They have been shown to be universal and highly flexible function approximators for any data. These make powerful tools for models, especially when the underlying data relationships are unknown. In this reason, the international workshop on the applications of ANNs to ecological modelling was organized in Toulouse, France (December 1998). During this meeting, we discussed different methods, and their reliability to deal with ecological data. The special issue of this ecological modelling journal begins with the state-of-the-art with emphasis on the development of structural dynamic models presented by S.E. Jorgensen (DK). Then, to illustrate the ecological applications of ANNs, examples are drawn from several fields, e.g. terrestrial and aquatic ecosystems, remote sensing and evolutionary ecology. In this paper, we present some of the most important papers of the first workshop about ANNs in ecological modelling. We briefly introduce here two algorithms frequently used; (i) one supervised network, the backpropagation algorithm; and (ii) one unsupervised network, the Kohonen self-organizing mapping algorithm. The future development of ANNs is discussed in the present work. Several examples of modelling of ANNs in various areas of ecology are presented in this special issue. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Ecological modelling has grown rapidly in the last three decades. To build his models, an ecologist disposes a lot of methods, ranging from numerical, mathematical, and statistical methods to techniques originating from artificial intelligence

(Ackley et al., 1985), like expert systems (Bradshaw et al., 1991; Recknagel et al., 1994), genetic algorithms (d'Angelo et al., 1995; Golikov et al., 1995) and artificial neural networks, i.e. ANN (Colasanti, 1991; Edwards and Morse, 1995).

ANNs were developed initially to model biological functions. They are intelligent, thinking machines, working in the same way as the animal brain. They learn from experience in a way that no conventional computer can and they can rapidly solve hard computational problems. With

* Corresponding author. Tel.: +33-561-558687; fax: +33-561-556096.

E-mail address: lek@cict.fr (S. Lek)

the spread of computers, these models were simulated and later research was also directed at exploring the possibilities of using and improving them for performing specific tasks.

In the last decade, research into ANNs has shown explosive growth. They are often applied in physics research like speech recognition (Rahim et al., 1993; Chu and Bose, 1998) and image recognition (Dekruger and Hunt, 1994; Cosatto and Graf, 1995; Kung and Taur, 1995) and in chemical research (Kvasnicka, 1990; Wythoff et al., 1990; Smits et al., 1992). In biology, most applications of ANNs have been in medicine and molecular biology (Lerner et al., 1994; Albiol et al., 1995; Faraggi and Simon, 1995; Lo et al., 1995). Nevertheless, a few applications of this method were reported in ecological and environmental sciences at the beginning of the 90's. For instance, Colasanti (1991) found similarities between ANNs and ecosystems and recommended the utilization of this tool in ecological modelling. In a review of computer-aided research in biodiversity, Edwards and Morse (1995) underlined that ANNs have an important potential. Relevant examples are found in very different fields in applied ecology, such as modelling the greenhouse effect (Seginer et al., 1994), predicting various parameters in brown trout management (Baran et al., 1996; Lek et al., 1996a,b), modelling spatial dynamics of fish (Giske et al., 1998), predicting phytoplankton production (Scardi, 1996; Recknagel et al., 1997), predicting fish diversity (Guégan et al., 1998), predicting production/biomass (P/B) ratio of animal populations (Brey et al., 1996), predicting farmer risk preferences (Kastens and Featherstone, 1996), etc. Most of these works showed that ANNs performed better than more classical modelling methods.

2. Scope of this particular issue

The pressures to understand and manage the natural environment are far greater now than could ever have been conceived even 50 years ago, with the loss of biodiversity on an unprecedented scale, fragmentation of landscapes, and

addition of pollutants with the potential of altering climates and poisoning environments on a global scale. In addition, many ecological systems present complex spatial and temporal patterns and behaviours.

Recent achievements in computer science provide unrivaled power for the advancement of ecology research. This power is not merely computational: parallel computers, having hierarchical organization as their architectural principle, also provide metaphors for understanding complex systems. In this sense, in sciences of ecological complexity, they might play a role like equilibrium-based metaphors had in the development of dynamic systems ecology (Villa, 1992).

ANNs have recently become the focus of much attention, largely because of their wide range of applicability and the ease with which they can treat complicated problems. ANNs can identify and learn correlated patterns between input data sets and corresponding target values. After training, ANNs can be used to predict the output of new independent input data. ANNs imitate the learning process of the animal brain and can process problems involving very non-linear and complex data even if the data are imprecise and noisy. Thus they are ideally suited for the modelling of ecological data which are known to be very complex and often non-linear.

For this reason, we organized the first workshop on the applications of ANNs in ecological modelling in Toulouse in December of 1998. This special volume gathers some of the papers presented.

3. What is an artificial neural network

An ANN is a 'black box' approach which has great capacity in predictive modelling, i.e. all the characters describing the unknown situation must be presented to the trained ANN, and the identification (prediction) is then given.

Research into ANNs has led to the development of various types of neural networks, suitable to solve different kinds of problems: auto-associative memory, generalization, opti-

mization, data reduction, control and prediction tasks in various scenarios, architectures etc. Chronologically, we can cite the Perceptron (Rosenblatt, 1958), ADALINE, i.e. Adaptive linear element (Widrow and Hoff, 1960), Hopfield network (Hopfield, 1982), Kohonen network (Kohonen, 1982, 1984), Boltzmann machine (Ackley et al., 1985), multi-layer feed-forward neural networks learned by backpropagation algorithm (Rumelhart et al., 1986). The descriptions of these methods can be found in various books such as Freeman and Skapura (1992), Gallant (1993), Smith (1994), Ripley (1994), Bishop (1995), etc. The choice of the type of network depends on the nature of the problem to be solved. At present, two popular ANNs are (i) multi-layer feed-forward neural networks trained by backpropagation algorithm, i.e. backpropagation network (BPN), and (ii) Kohonen self-organizing mapping, i.e. Kohonen network (SOM). The BPN is most often used, but other networks has also gained popularity.

3.1. Multi-layer feed-forward neural network

The BPN, also called multi-layer feed-forward neural network or multi-layer perceptron, is very popular and is used more than other neural net-

work types for a wide variety of tasks. The BPN is based on the supervised procedure, i.e. the network constructs a model based on examples of data with known outputs. It has to build the model up solely from the examples presented, which are together assumed to implicitly contain the information necessary to establish the relation. A connection between problem and solution may be quite general, e.g. the simulation of species richness (where the problem is defined by the characteristics of the environment and the solution by the value of species richness) or the abundance of animals expressed by the quality of habitat. A BPN is a powerful system, often capable of modelling complex relationships between variables. It allows prediction of an output object for a given input object.

The architecture of the BPN is a layered feed-forward neural network, in which the non-linear elements (neurons) are arranged in successive layers, and the information flows unidirectionally, from input layer to output layer, through the hidden layer(s) (Fig. 1). As can be seen in Fig. 1, nodes from one layer are connected (using interconnections or links) to all nodes in the adjacent layer(s), but no lateral connections within any layer, nor feed-back connections are possible. This is in contrast with recurrent net-

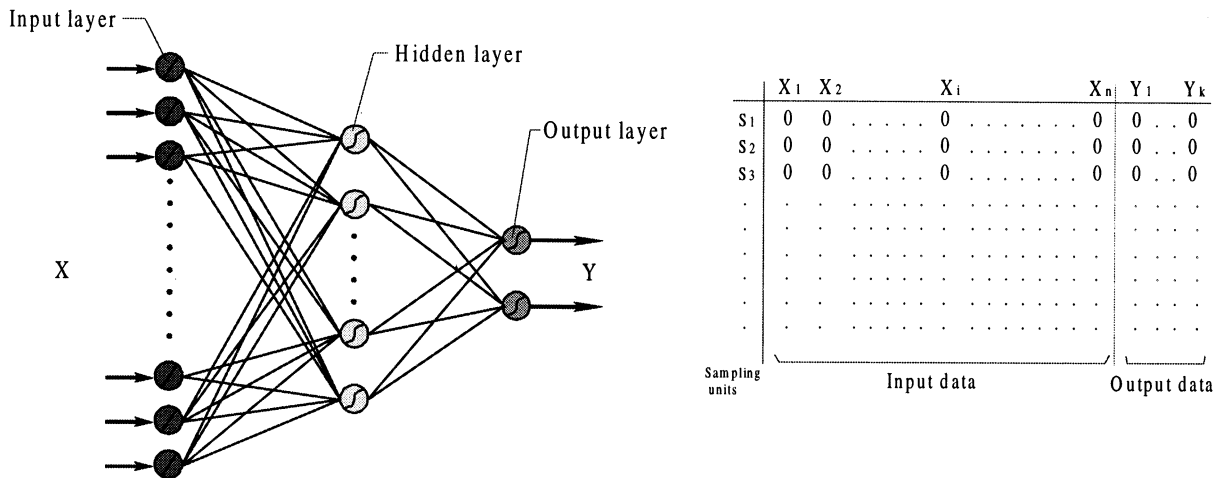


Fig. 1. Schematic illustration of a three-layered feed-forward neural network, with one input layer, one hidden layer and one output layer. The right-hand side of the figure shows the data set to be used in backpropagation network models. X_1, \dots, X_n are the input variables, Y_1, \dots, Y_k are the output variables, S_1, S_2, S_3, \dots are the observation data.

works where feed-back connections are also permitted. The number of input and output units depends on the representations of the input and the output objects, respectively. The hidden layer(s) is (are) an important parameters in the network. BPNs with an arbitrary number of hidden units have been shown to be universal approximators (Cybenko, 1989; Hornick et al., 1989) for continuous maps and can therefore be used to implement any function defined in these terms.

The BPN is one of the easiest networks to understand. Its learning and update procedure is based on a relatively simple concept: if the network gives the wrong answer, then the weights are corrected so the error is lessened so future responses of the network are more likely to be correct. The conceptual basis of the backpropagation algorithm was first presented in by Webos (1974), then independently reinvented by Parker (1982), and presented to a wide readership by Rumelhart et al. (1986).

In a training phase, a set of input/target pattern pairs is used for training and presented to the network many times. After the training is stopped, the performance of the network is tested. The BPN learning algorithm involves a forward-propagating step followed by a backward-propagating step. A training set must have enough examples of data to be representative for the overall problem. However, the training phase can be time consuming depending on the network structure (number of input and output variables, number of hidden layers and number of nodes in the hidden layer), the number of examples in the training set, the number of iterations (see Box 1).

Typically, for a BPN to be applied, both a training and a test set of data are required. Both training and test sets contain input/output pattern pairs taken from real data. The first is used to train the network, and the second to assess the performance of the network after training. In the testing phase, the input patterns are fed into the network and the desired output patterns are compared with those given by the neural network. The agreement or disagreement of these two sets gives an indication of the performance of the neural network model.

Box 1. A brief algorithm of backpropagation in neural networks

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- (1) Initialize the number of hidden nodes
 - (2) Initialize the maximum number of iterations and the learning rate (η). Set all weights and thresholds to small random numbers. Thresholds are weights with corresponding inputs always equal to 1.
 - (3) For each training vector (input $X_p = (x_1, x_2, \dots, x_n)$, output Y) repeat steps 4–7.
 - (4) Present the input vector to the input nodes and the output to the output node;
 - (5) Calculate the input to the hidden nodes: $a_j^h = \sum_{i=1}^n W_{ij}^h x_i$. Calculate the output from the hidden nodes: $x_j^h = f(a_j^h) = \frac{1}{1 + e^{-a_j^h}}$.

Calculate the inputs to the output nodes: $a_k = \sum_{j=1}^L W_{jk} x_j^h$ and the corresponding outputs: $\hat{Y}_k = f(a_k) = \frac{1}{1 + e^{-a_k}}$.

Notice that $k = 1$ and $\hat{Y}_k = \hat{Y}$, L is the number of hidden nodes.

- (6) Calculate the error term for the output node: $\delta_k = (Y - \hat{Y})f'(a_k)$ and for the hidden nodes: $\delta_j^h = f'(a_j^h)\sum_k \delta_k W_{jk}$
- (7) Update weights on the output layer: $W_{jk}(t+1) = W_{jk}(t) + \eta \delta_k x_j^h$ and on the hidden layer: $W_{ij}(t+1) = W_{ij}(t) + \eta \delta_j^h x_i$

As long as the network errors are larger than a predefined threshold or the number of iterations is smaller than the maximum number of iterations envisaged, repeat steps 4–7.

Another decision that has to be taken is the subdivision of the data set into different sub-sets which are used for training and testing the BPN. The best solution is to have separate data bases, and to use the first set for training and testing the model, and the second independent set for validation of the model (Mastrorillo et al., 1998). This situation is rarely observed in ecology studies, and partitioning the data set may be applied for testing the validity of the model. We present here two partitioning procedures:

1. if enough examples of data sets are available, the data may be divided randomly into two parts: the training and test sets. The proportion may be 1:1, 2:1, 3:1, etc. for these two sets. However, the training set still has to be large enough to be representative of the problem and the test set has to be large enough to allow correct validation of the network. This procedure of partitioning the data is called k -fold cross-validation, sometimes named the hold-out procedure (Utans and Moody, 1991; Geman et al., 1992; Efron and Tibshirani, 1995; Kohavi, 1995; Kohavi and Wolpert, 1996; Friedman, 1997).
2. if there are not enough examples available to permit the data set to be split into representative training and test sets, other strategies may be used, like cross-validation. In this case, the data set is divided into n parts usually small, i.e. containing few examples of data. The BPN may now be trained with $n-1$ parts, and tested with the remaining part. The same network structure may be repeated to use every part once in a test set in once of the n procedures. The result of these tests together allow the performance of the model to be determined. Sometimes, in extreme cases, the test set can have only one example, and this is called the leave-one-out or sometime Jackknife procedure (Efron, 1983; Kohavi, 1995). The procedure is often used in ecology when either the available database is small or each observation is unique information and different to the others.

3.2. Kohonen self-organizing mapping (SOM)

Kohonen SOM falls into the category of unsupervised learning methodology, in which the relevant multivariate algorithms seek clusters in the data (Everitt, 1993). Conventionally, at least in ecology, reduction of multivariate data is normally carried out using principal components analysis or hierarchical clustering analysis (Jongman et al., 1995). Unsupervised learning allows the investigator to group objects together on the basis of their perceived closeness in n dimen-

sional hyperspace (where n is the number of variables or observations made on each object).

Formally, a Kohonen network consists of two types of units: an input layer and an output layer (Fig. 2). The array of input units operates simply as a flow-through layer for the input vectors and has no further significance. In the output layer, SOM often consist of a two-dimensional network of neurons arranged in a square (or other geometrical form) grid or lattice. Each neuron is connected to its n nearest neighbours on the grid. The neurons store a set of weights (weight vector) each of which corresponds to one of the inputs in the data. The SOM algorithm can be characterized by several steps (see Box 2).

Box 2. A brief algorithm of self-organizing mapping neural networks
Let a data set of observations with n -dimensional vectors:

Initialise the time parameter t : $t = 0$.

- (1) Initialise weights W_{ij} of each neuron j in the Kohonen map to random values (for example, random observations).
 - (2) Present a training sample $x(t) = [x_1(t), \dots, x_n(t)]$ randomly selected from the observations.
 - (3) Compute the distances d_i between x and all mapping array neurons j according to: $d_j(t) = \sum_{i=1}^n [x_i(t) - W_{ij}(t)]^2$ where $x_i(t)$ is the i^{th} component of the N dimensional input vector and $W_{ij}(t)$ is the connection strength between input neuron i and map array neuron j at time t expressed as a Euclidean distance.
 - (4) Choose the mapping array neuron j^* with minimal distance d_{j^*} : $d_{j^*}(t) = \min[d_j(t)]$.
 - (5) Update all weights, restricted to the actual topological neighbourhood $NE_{j^*}(t)$: $W_{ij}(t+1) = W_{ij}(t) + \eta(t)(x_i(t) - W_{ij}(t))$ for $j \in NE_{j^*}(t)$ and $1 \leq i \leq n$. Here $NE_{j^*}(t)$ is a decreasing function of time, as is the gain parameter $\eta(t)$.
 - (6) Increase the time parameter t
 - (7) If $t < t_{\text{max}}$ return to step 2
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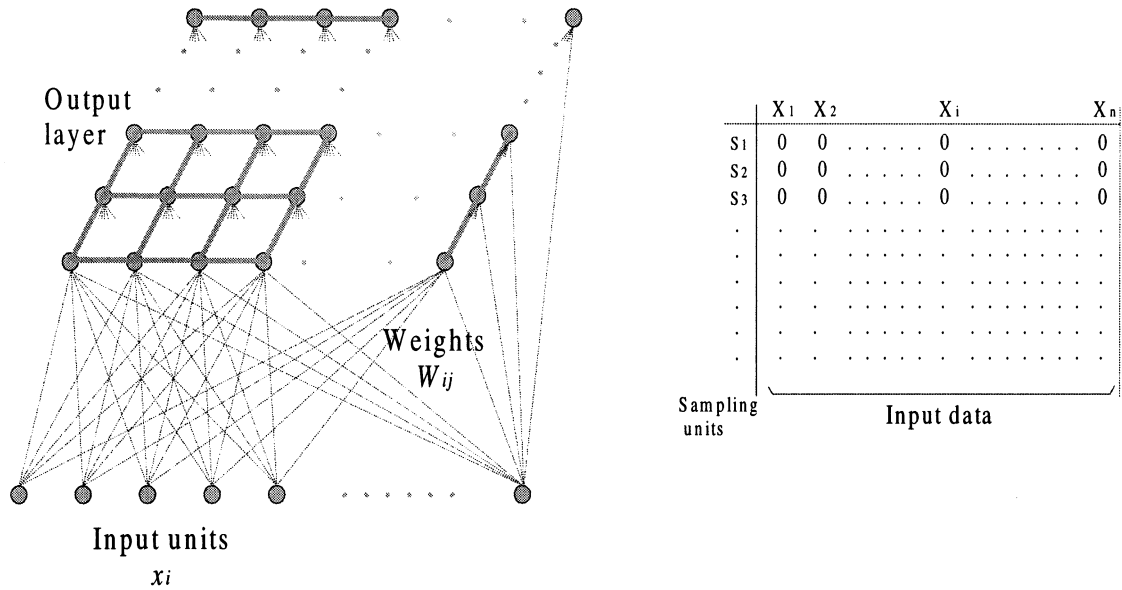


Fig. 2. A two-dimensional Kohonen self-organizing feature map network. The right-hand side shows the data set to be used in Kohonen self-organizing mapping models. X_1, \dots, X_n are the input variables, S_1, S_2, S_3, \dots are the observation data.

Since the introduction of the Kohonen neural network (Kohonen, 1982, 1984), several training strategies have been proposed (see e.g. Lippmann, 1987; Hecht-Nielsen, 1990; Freeman and Skapura, 1992) which deal with different aspects of the use of the Kohonen network. In this section, we will restrict the study to the original algorithm proposed by Kohonen (1984).

4. Overview of the presented papers

During the three days of the workshop on ANN applications in ecology, 45 oral communications and posters were presented. They were thoroughly discussed by 100 or so participants coming from 24 countries. The session started with the general review 'state-of-the-art of ecological modelling with emphasis on development of structural dynamic models' (Jørgensen, see paper in the next chapter). Then applications of ANNs in several fields of ecology were presented: primary production in freshwater and marine ecosystems (seven papers), remote sens-

ing data (six papers), population and community ecology and ecosystems (six papers), global change and ecosystem sensitivity (six papers), fishery research in freshwater and marine ecosystems (four papers), evolutionary ecology and epidemiology (three papers), population genetics (two papers) and seven remaining papers which rather concerned the methodological aspects, i.e. improvement of ANN models in ecological modelling. Some of these papers have been selected for publication in this special issue. The aim of this special issue, as well as of this first workshop, was both to contribute to an improvement of methodology in ecological modelling and to stimulate the integration of ANNs in ecological studies.

Most of the papers propose the use of a backpropagation algorithm in ANN models. Certain papers suggest improvement by including the Bayesian (see Vila et al.' paper) or radial base functions (see Morlini's paper). Only a few papers used unsupervised learning to model remote sensing data, microsatellite data, or marine ecology data (see Foody's paper).

5. Future developments of ANNs in ecological modelling

In 1992, during the first international conference on mathematical modelling in limnology (Innsbruck, Austria), Jørgensen (1995) presented a review on ecological modelling in limnology. He noted the rapid growth of ecological modelling and proposed a chronological development in four generations of models. The first models covered the oxygen balance in streams and the prey-predator relationships (the Lotka-Volterra model) in the early 1920s. The second phase of modelling (in the 1950s and 1960s) was particularly concerned with population dynamics. The third generation started from the 70's with more complicated models and rapidly became tools in environment management, e.g. eutrophication models. In the fourth generation, more recent models are becoming increasingly able to take the complexity, adaptability and flexibility of ecosystems into account.

As the modelling techniques available in the fourth generation of ecological models, researchers have a lot of methods ranging from numerical, mathematical and statistical methods to techniques based on artificial intelligence, particularly ANNs. During the last 2 decades of the current century, the growing development of computer-aided analysis, easily accessible to all researchers has facilitated the applications of ANNs in ecological modelling.

To use ANN programmes, ecologists can obtain freeware or shareware using different web sites in the World. Users interested could find these programmes by filling in 'neural network' as a keyword in the search procedure of the web explorer. Thus, they can obtain many computer ANN programmes functioning with all operating systems (Windows, Apple, Unix stations, etc.). Moreover, increasingly specialized ANN packages are proposed at acceptable prices for personal computers and most professional statistical software now proposes ANN procedures included (e.g. SAS, Splus, Matlab, etc.).

The development of computers and ANN software must allow ecologists to apply ANN methods more easily to resolve the complexity of

relationships between variables in ecological data. A lot of reports, and especially the papers presented in this first workshop on the applications of ANNs in ecology, demonstrate the importance of these methods in ecological modelling. The second workshop on this subject is programmed for November 2000 in Adelaide University (Australia), and is being organized by F. Recknagel (Email: frecknag@waite.adelaide.edu.au) and S. Lek (Email: lek@cict.fr). You are cordially invited to participate in this meeting.

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