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Neural network modelling of NO_3^- time series from small headwater catchments

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Abstract A variety of different processes is known that determine water and solute fluxes in headwater catchments. Water resources management of these systems, however, relies in most cases on empirical experience with respect to its overall response. A promising method to bridge the gap between comprehensive scientific investigations and the need to manage the systems on the basis of limited data sets seems to be the application of artificial neural networks (ANN). Here, time series of NO_3^- concentrations in the runoff of two forested headwater catchments in south Germany are investigated. Furthermore, the application of nonlinear methods presented here reveals a rather intricate behaviour also on the temporal scale, and considerable differences between the two catchments. This demonstrates the validity of ANN as universal descriptive tools.

INTRODUCTION

Long lasting non-point emissions affect the quality of freshwater systems and shallow groundwater. Often, headwater catchments in mountainous regions are especially sensitive and reveal severe effects on ecosystem function, species diversity, and quality of these water resources. One expectation is a slow shift in water quality in the long run; however, short-term exceedance of certain threshold values is much more relevant for the survival of biota and sustained drinking water supply.

Furthermore, short-term dynamics of time series can give valuable hints on relevant processes and driving variables at the scale of observation. Due to the expected complex interplay of a variety of processes, however, this kind of information provided by the system may not be easy to interpret.

The application of process-oriented models in a bottom-up approach as a means to overcome these difficulties suffers, e.g. from problems of parameter identification (Beven, 1996) and the non-uniqueness of model results (Janssen & Heuberger, 1995; Konikow & Bredehoeft, 1992). Thus, in spite of a sound physical basis for many of these models, model application in practice often results in a mere fitting exercise.

On the other hand, the effective dimensionality of hydrochemical data sets often seems to be rather small (Christophersen & Hooper, 1992; Evans *et al.*, 1996). Thus the motivation is given to apply data-oriented models to identify the driving variables and to visualize the interdependencies revealed.

SIMULATION WITH ARTIFICIAL NEURAL NETWORKS

ANN are now increasingly used to analyse comprehensive, multidimensional data sets. With regard to theory and potential of neural networks the reader is referred to, e.g. Rumelhart & McClelland (1986) and Hecht-Nielsen (1990). Here the feedforward multilayer perceptron type has been used. The number of hidden layers was set to one. The logistic function has been used as activity function. The learning algorithm is the resilient propagation (Riedmiller & Braun, 1992), combined with a stochastic approach: To overcome the problem of getting stuck in a local minimum of the error hyperplane, the weight matrix is altered randomly within a given range when the network fails to decrease the model error. As is usual, the data set has been split into training, validation and testing subsets. The objective function for selecting the best network has been the maximum of the sum of model efficiency for the training and the validation data set. Here model efficiency (R_{eff}) is defined according to Janssen & Heuberger (1995) as $R_{eff} = 1 - \sigma^2_{x\bar{x}} / \sigma^2_{xx}$ where $\sigma^2_{x\bar{x}}$ = unbiased mean squared error of the simulation and σ^2_{xx} = variance of the data set. The simulator used is the Stuttgart Neural Network Simulator (SNNS) (Zell *et al.*, 1995) with a slight modification by the first author.

CHARACTERIZATION WITH NONLINEAR METHODS

Application of pertinent and recently developed methods of time series analysis (e.g. Grassberger *et al.*, 1991) has led to successful identification of the detailed temporal structure of hydrological data sets (Porporato & Ridolfi, 1997). Nonlinear prediction methods led to precise and reliable forecasts of catchment behaviour, especially important for management purposes such as flood estimates (Rinaldo *et al.*, 1995).

As our ANN investigation focuses on the detection of general temporal dynamics, it seems natural to characterize the latter in detail independently. Among a plethora of methods available, here we will present just two: the cumulative periodogram (Hipel & McLeod, 1994) and data compressibility, calculated as Lempel-Ziv complexity (Lempel & Ziv, 1976). They will be accomplished by other techniques in an accompanying poster presentation (Lange *et al.*, 1997).

DATA SET

In this article, time series of NO_3^- concentration in the runoff of two forested headwater catchments in south Germany are investigated. This ion is known to exhibit strong spatial heterogeneity on the subcatchment scale (Lischeid *et al.*, 1997). The Lehstenbach catchment is located in the Fichtelgebirge at 11°53'E, 50°8'N. The catchment size is 4.2 km^2, the altitude is 694–877 m a.s.l. The bedrock consists of deeply weathered variscian granite, on which dystric cambisols developed. More than 90% of the stand consists of Norway spruce (*Picea abies* (L.) Karst.) (Lischeid *et al.*, 1997).

A substantial part of the data set has been published by Bayerisches Landesamt für Wasserwirtschaft (1994) or kindly provided by Bittersohl & Moritz (personal communication). For the simulation runs, about 300 runoff water samples of a 10-year monitoring programme were available.

The Steinkreuz catchment is the second main investigation site of BITÖK. It belongs to the Steigerwald region and is located at 10°28'E, 49°52'N. The area size is 0.55 km^2, altitude is 405–460 m a.s.l. On interlayered Triassic clayey and sandstone layers eutric cambisols developed. The mixed deciduous stand is predominated by European beech (*Fagus sylvatica* L.) and Sessile oak (*Quercus petraea* L). Here, the runoff water concentration data set comprises about 200 analyses, covering a 2.5-year period.

RESULTS

Here only some striking features can be shown. Technical details will be described elsewhere (Lischeid, 1998; Lange *et al.*, 1997).

Figure 1 summarizes the most important results of the neural network simulation. Every training was repeated 10 times, differing only in the initialization of the weight matrix. Mean and standard deviation of the performance of different ANN, depending on network topology (number of nodes in the input, hidden and output layer) for the Lehstenbach and Steinkreuz catchments are shown for the training, validation and test data set separately. Input variables were daily mean values of air temperature and runoff, and additionally the averages of the preceding 30-day period for air temperature and runoff, respectively. Figure 2 shows measured and simulated time series for both catchments, modelled with the network that showed best performance for the training, validation and test data set. For both catchments, air temperature and discharge were used as input variables. Taking into

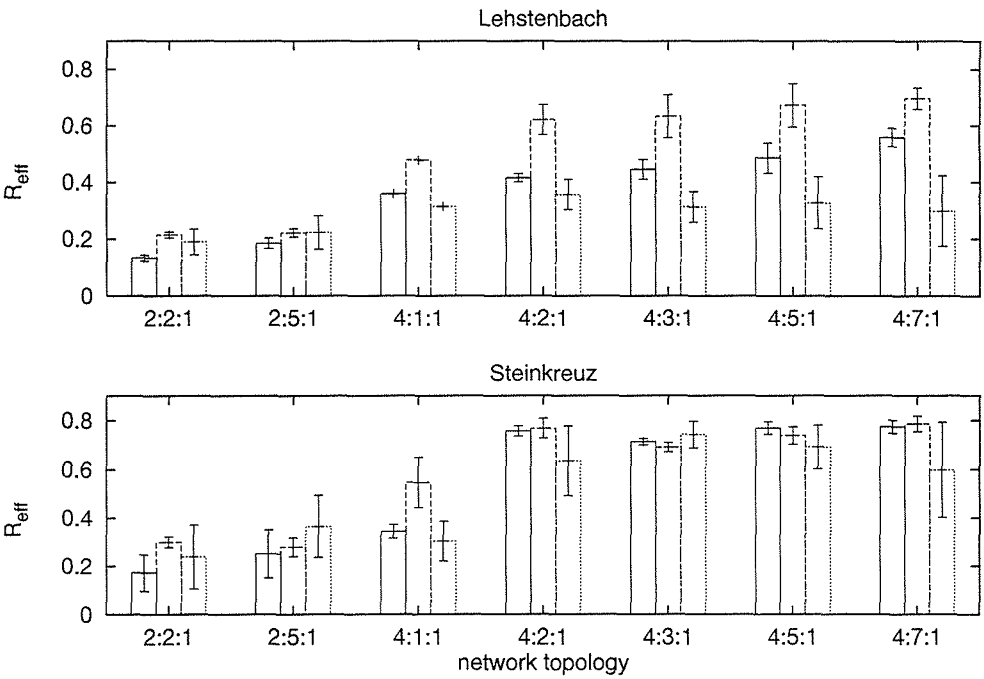

Fig. 1 Performance of different ANN, depending on network topology. See text for details.

Table 1 Lempel-Ziv complexity (algorithmic compressibility) of investigated data sets. Precipitation is included for comparison.

Site	Runoff	Temperature	NO_3^-	Precipitation
Lehstenbach	0.87	0.66	0.92	0.88
Steinkreuz	0.51	0.59	0.59	0.28

account short-term history (moving averages of the precedent period) increases performance of the networks significantly (Fig. 1). Performance of the models did not depend on the length of this period within the 3–90 days range for both catchments. Results are shown for a 30-day period.

Although the number of data points for the Lehstenbach catchment is about four-thirds that of the Steinkreuz catchment, performance of the network is not as good. On the other hand, the differing time span of the two data sets has to be considered (10 years *vs* 2.5 years).

The overall information content is quantified via the Lempel-Ziv complexity (LZC) (Table 1). A completely random sequence would have a LZC value of unity in the normalization chosen. One would expect that a very simple input signal (LZC near zero) could not reproduce signals with high LZCs, unless the model combining them imprints structure not contained in the data. According to this expectation, one would conclude from Table 1 that it seems plausible to reconstruct NO_3^- from runoff and air temperature in the case of the Steinkreuz catchment, although this seems to be a tedious task, whereas the Lehstenbach nitrate data contain components not present in both input signals.

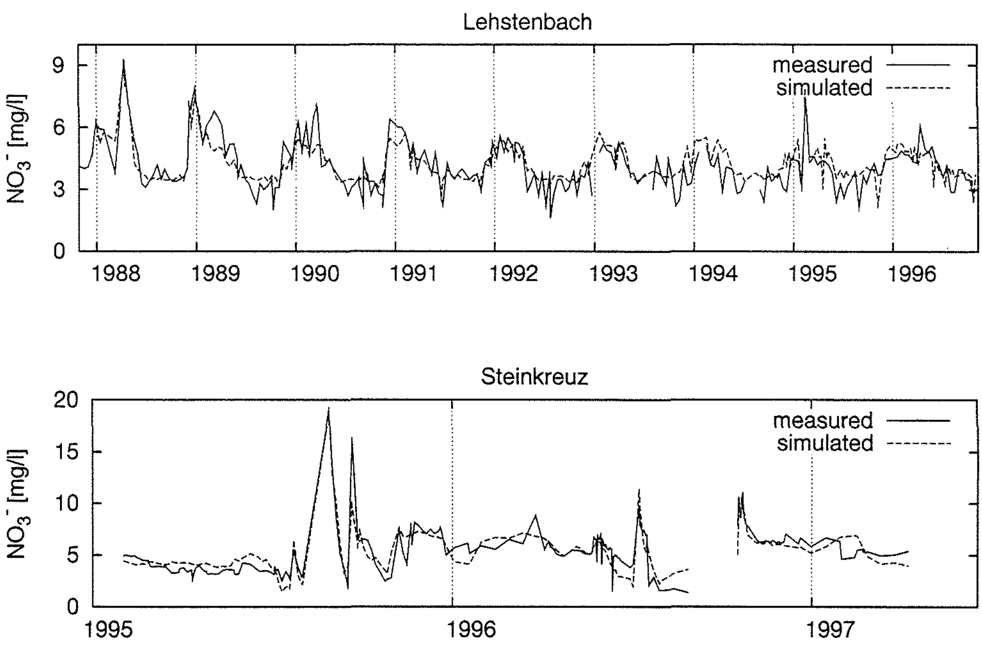

Fig. 2 Time series of measured and simulated NO_3^- concentration in the Lehstenbach (4:7:1 network) and Steinkreuz (4:5:1 network) catchment runoff.

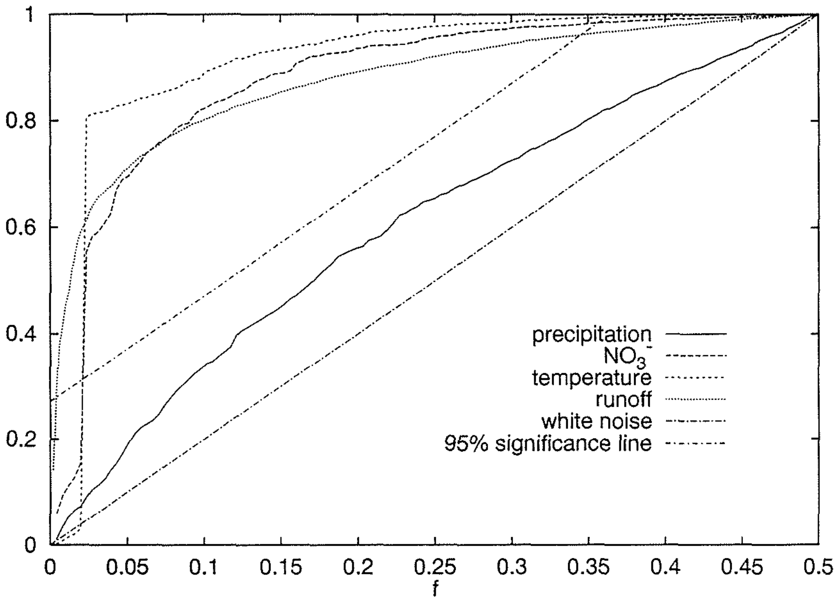

Fig. 3 Cumulative periodograms for the Lehstenbach data. Included is the theoretical white-noise line and the 95% significance line for the given data set length (periodograms which stay within the two straight lines for more than 95% of the values are compatible with white noise).

However, this conclusion is not supported when considering cumulative periodograms (Figs 3 and 4). For the Lehstenbach catchment, the frequency structure of NO_3^- is quite similar to that of air temperature at low frequencies, e.g. shares the pronounced seasonality visible as steep increase, and interpolates between runoff and temperature for higher frequencies. It is suggestive to construct the NO_3^- periodogram via frequency-dependent "linear combination" of temperature and runoff and to transform back to receive the original sequence (only in a metaphorical sense of course, as the phase information has been lost through the transformation). On the other hand, the Steinkreuz NO_3^- behaves markedly different: here, runoff and temperature are completely controlled by low-frequency components (the temperature exhibits a diurnal component as well), whereas nitrate shows a continuous and complicated spectrum over the whole range, possibly indicating intermittent behaviour (Wang, 1990).

DISCUSSION

Understanding short-term dynamics of solute concentrations in catchment runoff is crucial for a scientific description of the system as well as for water resources management. It could be shown that in fact time series of NO_3^- in catchment runoff can be mapped by a rather simple empirical model, based on air temperature and discharge. The fact that rather different dynamic behaviour could be reconstructed from the input may indicate that the number of active degrees of freedom in the system is in fact very low—a necessary precondition for reliable forecasts.

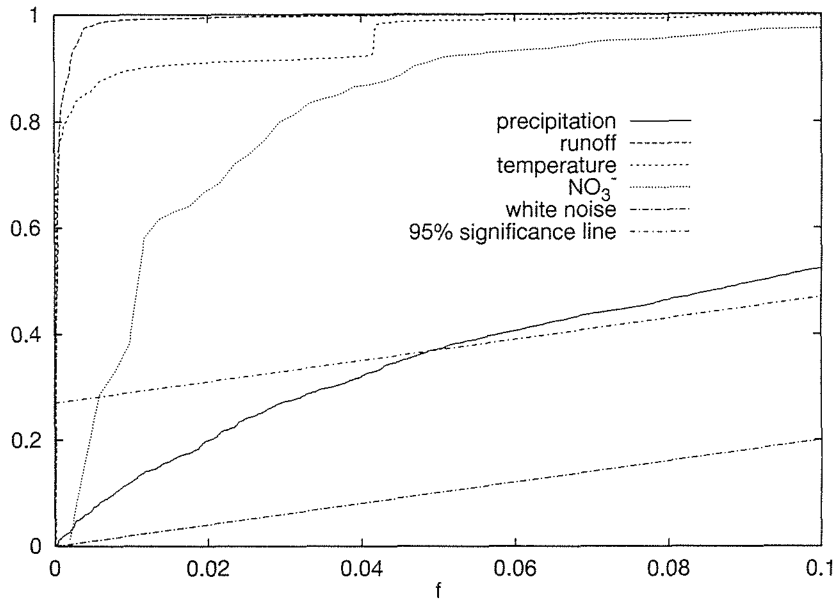

Fig. 4 Cumulative periodograms for the Steinkreuz data. Notice that in this case, also the precipitation shows non-random behaviour.

It is remarkable that for the Steinkreuz catchment especially the model results fit the measured peak concentration values fairly well (Fig. 2). On the basis of the nonlinear methods presented here, this remains unexplained. However, the success implies that ANN are able to cope with very different sorts of dynamic behaviour. This flexibility is accompanied by the unavoidable disadvantage that no hint is given towards the origin of the very clear difference in nitrate dynamics for the two catchments.

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