

Polluted aquifer inverse problem solution using artificial neural networks

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Abstract: The problem of identifying an unknown pollution source in polluted aquifers, based on known contaminant concentrations measurement in the studied areas, is part of the broader group of issues, called inverse problems. This paper investigates the feasibility of using Artificial Neural Networks (ANNs) for solving the inverse problem of locating in time and space the source of a contamination event in a homogeneous and isotropic two dimensional domain. ANNs are trained in order to implement an input-output relationship which associates the position. Once the output of the system is known, the input is reconstructed by inverting the trained ANNs. The approach is applied for studying a theoretical test case where the inverse problem is solved on the basis of measurements of contaminant concentrations in monitoring wells located in the studied area. Groundwater pollution sources are characterized by varying spatial location and duration of activity. To identify these unknown pollution sources, concentration measurements data of monitoring wells

are used. If concentration observations are missing over a length of time after an unknown source has become active, it is more difficult to correctly identify the unknown pollution source. In this work, a missing data scenario has been taken into consideration. In particular, a case where only one measurement has been made after the pollutant source interrupted its activity has been considered.

Introduction

Groundwater represents an important resource for the production of drinking water. However, groundwater is exposed to man-made pollution. When groundwater is polluted, the restoration of quality and removal of pollutants is a very slow, hence, lengthy, and, sometimes, a practically impossible task. As a consequence a management aimed at protecting the groundwater quality and at safeguarding the groundwater resources has a vital importance for life support systems.

Groundwater contamination, in some cases, may result from pollutions whose origin is found at times and places different than where the contaminations have been actually noticed. Such situations require the development of techniques that allow the identification of these unknown pollution sources. The determination of the initial conditions of pollution is of considerable interest in the framework of the implementation of the European Union Directive 2004/35/EC: this directive concerns environmental liability with regard to the prevention and compensation of environmental damages, based on the affirmation of the principle of *polluter-payer*.

The problem of determining the unknown model parameters is usually identified as “inverse problem”. Solving the inverse problem is the main goal of modelling groundwater flow and contaminant transport. With respect to the resolution of the inverse problem, in this work we propose the use of an innovative ANNs based methodology for solving the inverse problem of locating in time and space the source of a contamination process in a homogeneous and isotropic two dimensional domain. The identification and remediation of polluted aquifers represents nowadays an important challenge in groundwater resource management. In order to efficiently manage the groundwater quality, it is fundamental to know pollution source characteristics such as location, magnitude and duration of the activity. Inaccuracies/inadequacies in determining the pollution sources may lead to inefficient or unsuccessful management/remediation efforts. Information regarding the pollution sources is also necessary and useful for addressing the judicial issues of responsibility and compensation for environmental damage.

In the case presented in this paper, the inverse problem is solved on the basis of measurements of contaminant concentrations in monitoring wells located in the studied theoretical area. During the last decade, there has been seen a significant activity in ANNs applied to various hydrogeological problems such as groundwater modelling, modelling of hydrogeological parameters, modelling of various kinds of aquifers contamination, water quality modelling. Several studies have been dedicated to the development of different models

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for solving the inverse problem, however works using the ANNs approach are less popular. Among these latest, one can highlight Rizzo and Dougherty (1994), Zio (1997), Gümrah et al. (1999), Mahar & Datta (2000), Fanni et al. (2002), Rajanayaka et al (2002), Sciuntu (2004), Singh and Datta (2006), Zhiqiang et al. (2006), Bashi-Azghadi et al. (2010), Foddis et al (2012).

In this work, in order to identify the spatial location (X,Y) and the duration of the activity (T) for a theoretical unknown pollution source, a new approach is applied. Several ANNs are trained to solve the direct problem, presenting as input the spatial location (X,Y) and the duration of the activity (T) for an unknown pollution source and as desired output, the measures of contaminant concentrations acquired in the monitoring wells at the current time t . After the training phase, the trained ANN is inverted in order to solve the inverse problem. Starting from the contaminant concentration in the monitoring wells, the unknown contaminant source characteristics are found. Thanks to a drastic reduction of the input/output data the computational time is strongly decreased. Moreover the implemented method is useful not only to identify the location and duration activity of unknown pollution sources, but also to bound the study area defining the best location of the monitoring wells in the domain and to optimize the investigation costs.

Materials and methods

In the first step, several ANNs are trained to solve the direct problem. In this part of the procedure, the networks are trained, by means of a set of examples, to associate the contaminant concentration in monitoring wells to the position and duration of pollution sources activity. The input patterns are the features describing spatial position and activity duration of the pollution sources. The output patterns are contaminant concentration observation data at given monitoring wells. After the training, the ANN generalization capability can be exploited to estimate the contaminant concentration in monitoring wells corresponding to a new pollution source.

In the second step, the trained ANN is inverted in order to solve the inverse problem. On the basis of values of known contaminant concentrations in monitoring wells, the pollution sources position and the activity duration can be identified.

In the following paragraph the methodology is deeply described.

ANN pattern construction: flux and transport model of the theoretical aquifer

ANNs are trained by using a set of patterns created by means of the flux and transport contaminant modelling software TRACES (Transport of Radio Active Elements in the Subsurface [Hoteit et al.(2004)]). As documented by Hoteit et al.(2004), TRACES performs the simulation of flow and reactive transport in saturated porous media. It is based on mixed and discontinuous finite element methods for solving hydrodynamic state and mass transfer problems. The patterns describe, for a theoretical hydrogeological basin, both spatial location and duration of activity of the contamination source and the set of contaminant concentrations measurements in the monitoring wells.

The theoretical hydrogeological basin and its principal features have been defined as reported in Table 1.

In order to solve the partial differential equations by means of the numerical model, a regular quadrangular two-dimensional mesh is superimposed in the whole domain for a total of 50 cells in the 2D directions (see Figure 1). Each cell is large 20×20 m².

ANNs patterns are constructed through a suitable number of hy-

Tab. 1: *theoretical aquifer features.*

Theoretical aquifer type: confined and isotropic aquifer system composed by one horizontal layer characterized by only one stratigraphic unit with a constant thickness. It is delimited by no-flow boundaries on the North and South sides.	
Domain dimension	1000*1000m ²
Hydraulic head on the west boundary	9 m
Hydraulic head on the east boundary	8 m
Horizontal hydraulic conductivity [k_o]	0.0001 m/s
Effective porosity	10%

drogeological scenarios that take under consideration the restrictive hypothesis of groundwater contaminated by a single generic conservative pollutant injected in a single point (pollutant source). Overall, 40 constant punctual pollution sources with a constant contaminant concentration of $100 \mu\text{g}/\text{m}^3$ were uniformly distributed in the aquifer domain (see Figure 1). It is also assumed the presence of a pumping well with a constant pumping rate ($0.0012 \text{ m}^3/\text{s}$) and the pumping start from the beginning of the simulation. No variation of the initial parameters of the model during the simulation time and no recharge rate are applied to the aquifer. The initial contaminant concentration, in the domain, is assumed equal to zero. Training patterns are constructed by simulating the 40 different pollution sources for 3 timing of activity source duration (10, 20 and 30 years), resulting in $40 \times 3 = 120$ samples maps of contaminant distributions. The samples obtained from the simulation model are the matrix of contaminant concentration for 50 monitoring cells distributed in order to cover the entire basin area of the domain (Figure 1).

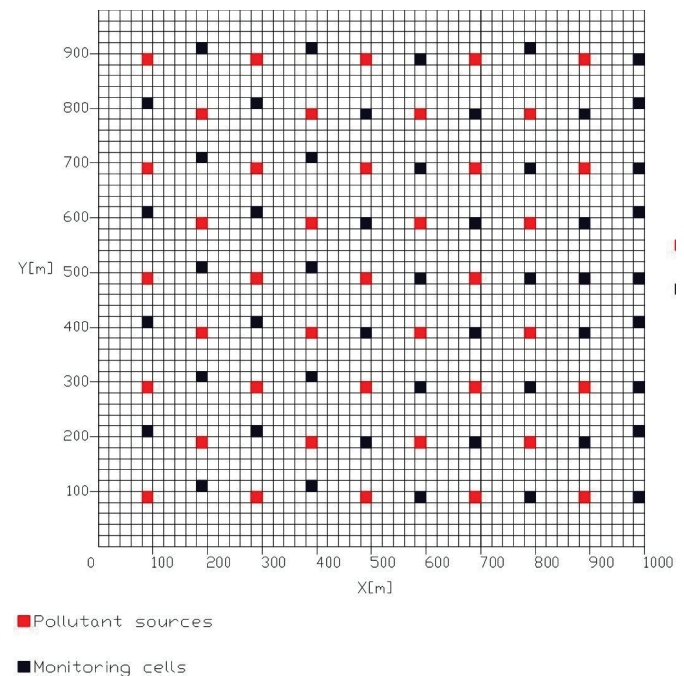


Fig. 1: *distribution of the pollutant sources and the monitoring cells in the domain*

Through TRACES, the trend of the piezometric head and contaminant concentrations in the domain in stationary state is developed (Figure 2)

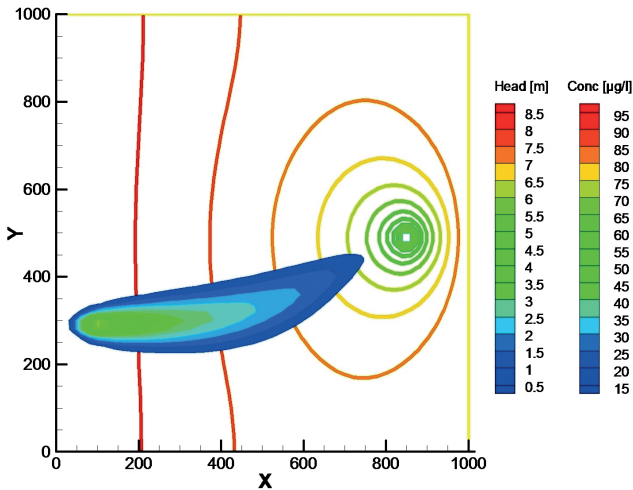


Fig. 2: hydraulic head and contaminant concentration distribution for a generic pollutant source after 10 years activity at the top of the aquifer domain.

The huge amount of data carried out by each time step of simulation is not suitable to be inputted in an ANN. Therefore, feature extraction techniques have been implemented to reduce data dimensionality. Several feature extraction procedures have been compared in order to choose the best one, in this affecting size and structure of ANNs.

Multi Layer Perceptron (MLP) network model

An ANN consists of a number of interconnected processing elements (Perceptrons) called neurons, which are logically arranged in two or more layers and interact with each other through weighted connections. In particular, the Multi Layer Perceptrons (MLPs) fall within the class of methods for function approximation by means of combination of elementary functions (Taylor, Fourier series, etc.). In general, MLPs could have whichever number of layers, but it has been demonstrated that an MLP with only one intermediate layer (hidden layer) is a universal approximator (Cybenko, 1989). For this reason throughout the paper, the MLP are considered having only one hidden layer without further specification. MLPs have the two-fold advantage of using transcendent functions and determining the parameters by means of examples. This second property makes possible to develop a model of the system without an analytical formalization but simply on the basis of a suitable set of input/output pairs of example patterns. The features of the developed ANN depend on the nature of the problems analysed and there are no theoretical guidelines for determining the best way out. The model is specific to the system under study and it cannot be built a priori. The training of the ANN consists in applying a learning rule that modifies the weights of the connections on the basis of the difference between the calculated and the desired output of the network. The aim of the training is to make the ANN able to generalize the acquired information, i.e. to give the correct output even for examples not included in the training set. This aspect is crucial for the application described in this work, because the assumption is to reconstruct the input by inverting the trained ANN. In practice, the aim of training is abstracting the input-output relationship which generated the examples of the training set and implementing it into the ANN. After that, the

ANN is inverted to solve the inverse problem by fixing the output and reconstructing the corresponding input of the ANN.

Input data reduction

The ANN input data are the positions (X,Y) and the activity duration (T) of the pollution sources for the 120 hydrological scenarios. These correspond to 40 sources for 3 timing considered. The three input parameter (X,Y,T) are pre-processed by normalizing so that they fall in the interval [-1,+1]. The algorithm is presented in Equation 1.

$$p_n = \frac{2 \cdot (p - p_{\min})}{(p_{\max} - p_{\min})} - 1 \quad (1)$$

where: p_n is the normalized input value, p is the input, p_{\max} and p_{\min} are maximum and minimum values respectively. The pre-processed input patterns matrix has size 3×120 .

Output data reduction

Thanks to TRACES a total of 120 matrices of concentrations at the monitoring cells have been generated, corresponding to as many scenarios. Each component $a_{i,j}$ of the matrix corresponding to a specific scenario represents the concentration value at the well j and the time i . In the studied case, the total absence of complete breakthrough curves of concentration time series at all the time steps is hypothesized. So, for each one of the 50 monitoring cells, only one observation is taken into consideration, in particular the concentration of the final time t is taken. Therefore, each scenario is described by a 50 values vector, corresponding to the 50 monitoring cells. These cells correspond to as many hypothetical monitoring wells. However, these vectors are too large to be subsequently processed through the ANN, requiring too many examples and a large network with a lot of hidden neurons. In this way, the ANN becomes too big and it may lose its specific feature consisting in the calculation speed. Moreover, the number of 50 hypothetical wells is too large for a small domain such that taken into account. For these reasons, a procedure has to be adopted to select the most suitable monitoring cells, in order to reduce both the size of ANN and the cost of measurements in applying the method to a real case. Several data pre-processing methods can be used to this purpose. The scheme in Figure 3 represents the procedure applied in this work.

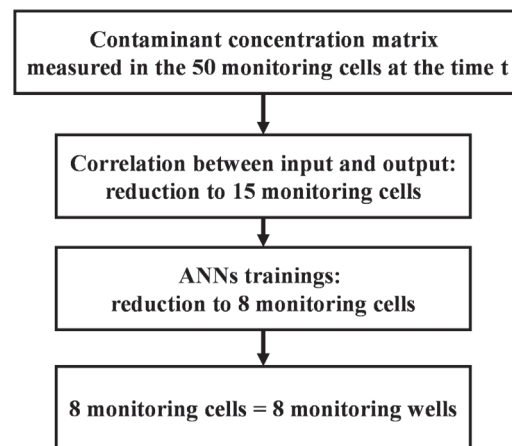


Fig. 3: sketch of the monitoring wells selection procedure.

First the 120 vectors are joined to make a unique matrix of output patterns. The dimension of this matrix is 50×120 .

Then the correlation of each one of the 50 monitoring cells with each input is evaluated, obtaining three distinct classifications of the 50 monitoring cells. Only the five cells more correlated with each input are kept into consideration. Based on this initial reduction, at most 15 monitoring cells are kept (Figure 4), the number being lower when the same monitoring cells is within the first five in more than one classification. So the output patterns matrix size becomes 15×120 .

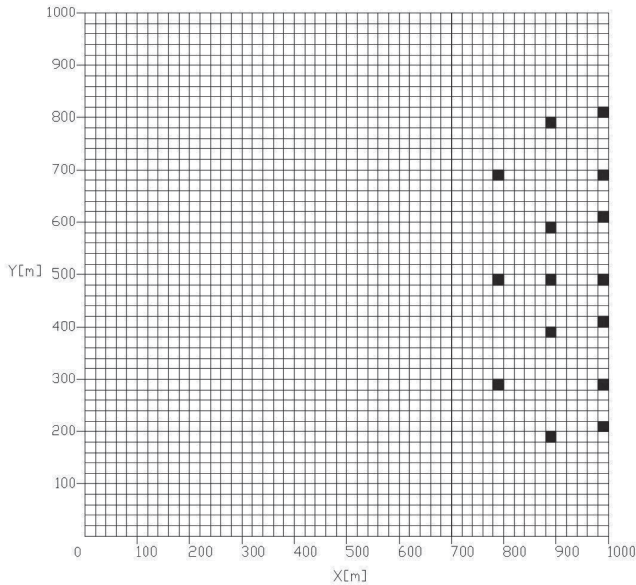


Fig. 4: distribution of the 15 monitoring cells selected on the basis of correlation with inputs..

The number of hypothetical monitoring wells is still too large. In order to further reduce this number, an iterative procedure based on the application of an ANN was developed. ANNs are over-trained with the training set made up of all the patterns, and then the correlation between the inputs and the calculated outputs are evaluated. The monitoring cell corresponding to the lowest correlation is removed together with the associated output neuron. After this, the reduced ANN is trained. The iterative procedure ends when the minimum value of correlation is below a prefixed threshold.

For each training, the number of the hidden neurons is determined by means of a trial and error procedure by performing several trainings and assuming a growing number of hidden neurons. For each training phase, the output layer becomes smaller, and consequently the hidden layer decreases too. For a reason which will be clarified below, the number of hidden neurons must be less or equal to the number of output neurons. At the end of the iterative procedure, the number of monitoring wells has been reduced to 8 (Figure 5).

As a consequence, the dimensions of the output pattern matrix are 8×120 , the rows corresponding to the monitoring wells and the columns to the scenarios. As for the input matrix, the output matrix has been normalized in the interval $[-1, +1]$

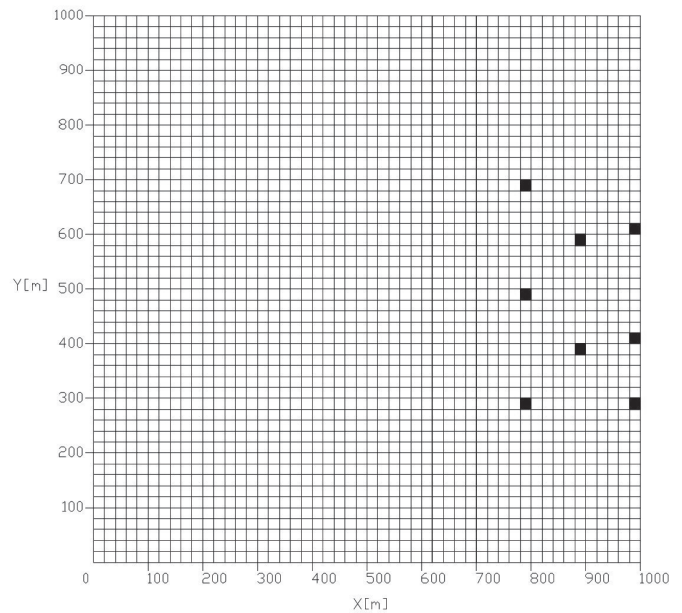


Fig. 5: distribution of the 8 monitoring cells selected on the basis of the ANNs trainings..

ANN Training

The 3 inputs-8 hidden-8 outputs structured MLP is initially trained by means of the Levenberg-Marquardt (LM) algorithm to solve the direct problem, namely associating the contaminants concentration in monitoring wells to the time-space coordinates of the pollutant source. The trained MLP is subsequently inverted to solve the inverse problem, namely deriving the time-space coordinates of the unknown pollutant source starting from the measurement of contaminants concentration in monitoring wells.

The training procedure consists in modifying iteratively the connection weights of the ANN, in order to minimize the mean squared error (error function) of the output with respect to the desired one. In particular, LM algorithm performs an approximated second-order minimization of the error function. In an iteration the error function with respect to the whole training set is calculated and a consequent small modification of connections weights is applied. The operations performed during a single iteration is called epoch.

The training of the ANN is a critical part of the proposed process. A special attention has to be paid to guarantee the generalization capability of the trained MLP, namely the capability to solve, with the desired rate of approximation, the direct problem for cases out of the training set. To this end it is important both to have a meaningful training set and to avoid overfitting. The first requirement can represent a difficulty when the available examples are limited or, as in this case, generating a consistent number of patterns is too costly. In such cases, a solution can be represented by the Leave one Out Cross Validation (LOO) technique, which offers a way to mitigate also the overfitting, which in general is avoided by adopting the cross-validation method. This consists in calculating, during the training phase, the error made by the MLP on a validation set, which is distinct from the training set. When such error gets to rise the training is stopped.

In the LOO, the examples patterns are divided in p sets, where p is the number of examples. Each set is divided in two subsets: one composed by $p-1$ examples is used as training set and the remaining

example is used as validation set. Therefore in this work, the training set is made of 119 examples. One by one, each example is used as validation set, so that an overall number of 120 trainings have been performed. This preliminary study is performed to establish an optimal number of training epochs. In this work, a number of 100 epochs has been deduced by this analysis. This number of epochs has been then used as a standard for all trainings in this work.

In the studied case, the LOO procedure is not used to train the network that will be used in a particular case, but only to estimate the generalization capability of the 120 trained networks. If one wish to consider a new source not included in the 120 patterns, all the patterns will be used for the training set and the new case will be used for the test set. The developed methodology allows us to reach the reasonable presumption that the error for the new case will not be greater than the errors experienced in the 120 networks already trained.

Inverse problem solution

Given an MLP trained as described above, the inversion procedure has to be applied to characterize the unknown pollution source.

The MLP (Figure 6) realizes a relationship between input and output patterns described by the following algebraic equations system:

$$\begin{cases} \text{Input layer} & \underline{W}_1 \cdot \underline{x} + \underline{b}_1 = \underline{y} \\ \text{Hidden layer} & \underline{h} = \sigma(\underline{y}) \\ \text{Output layer} & \underline{W}_2 \cdot \underline{h} + \underline{b}_2 = \underline{u} \end{cases} \quad (2)$$

Where: \underline{x} is the input of the network, \underline{W}_1 is the weights matrix of the input layer, \underline{b}_1 is the bias vector of the input layer, \underline{y} is the input of the hidden layer, \underline{h} is the output of the hidden layer, $\sigma(\cdot)$ is the hidden neurons logistic activation function, \underline{u} is the output of the network, \underline{W}_2 is the weights matrix of the output layer, \underline{b}_2 is the bias vector of the output layer.

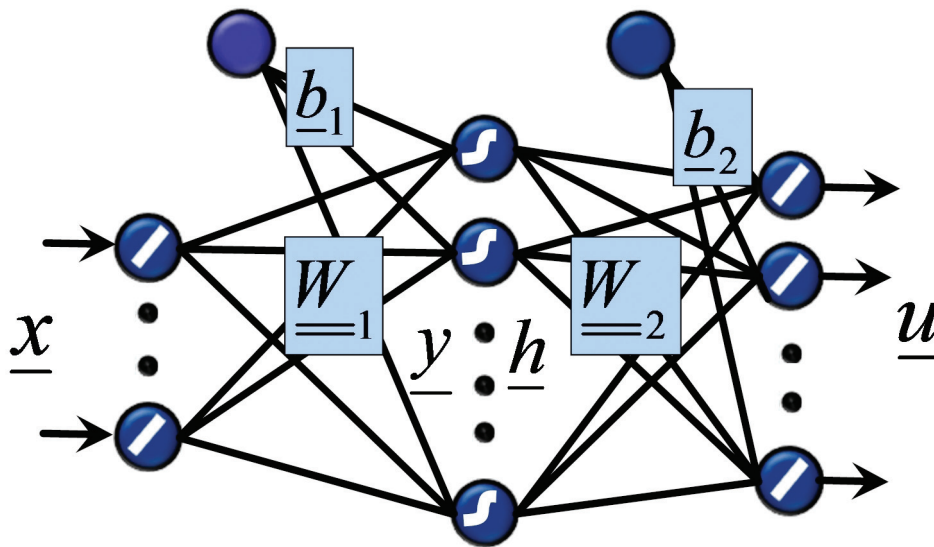


Fig. 6: Structure of the MLP.

On the basis of the known output of the system, which derives from a set of measurements in the monitoring wells at a certain time, the corresponding input can be calculated exploiting the method described in (Carcangiu et al, 2007; Fanni et al, 2003).

During the inversion process, as explained below, the difference between the calculated input and the desired input is considered. On the basis of the third equation described in the equation system, starting from the output \underline{u} , the vector \underline{h} can be determined. Provided that the matrix \underline{W}_2 is full rank, and taking into account that in the present case such matrix is squared, the solution corresponding to the minimum sum squared error is equal to:

$$\underline{h} = \underline{W}_2^{-1} \cdot (\underline{u} - \underline{b}_2) \quad (3)$$

More in general, the matrix \underline{W}_2 is rectangular, so it cannot be directly inverted. In order to guarantee the uniqueness of the solution, the rows (number of output neurons) must be more than the columns (number of hidden neurons). In this case, the equations system results overdetermined and the uniqueness is ensured by assuming the solution which corresponds to the minimum mean squared error. Such solution can be found by solving the following modified equations system, whose coefficients matrix is squared.

$$\underline{W}_2^T \underline{W}_2 \underline{h} = \underline{W}_2^T (\underline{u} - \underline{b}_2) \quad (4)$$

Even in this case, the uniqueness is conditional on the fact that the matrix \underline{W}_2 is full rank.

The second equation in (2) states a biunivocal relation between \underline{y} and \underline{h} , therefore the vector \underline{y} is:

$$\underline{y} = \sigma^{-1}(\underline{h}) \quad (5)$$

Finally, provided that the matrix $\underline{\underline{W}}_1$ is full rank, the input pattern \underline{x} can be calculated as:

$$\underline{x} = \left(\underline{\underline{W}}_1^T \cdot \underline{\underline{W}}_1 \right)^{-1} \cdot \underline{\underline{W}}_1^T (\underline{y} - \underline{b}_1) \tag{6}$$

where the mark T represents the transposition operator. The desired source position and duration of activity have been obtained by backward applying the pre-processing of the vector \underline{x} obtained by inverting the ANN.

Results and discussion

The described procedure has been applied to the problem described in section 1.1. The results show very good performances in locating the pollutant source, obtaining correct results in the 67% of the cases for the X coordinate and in the 59% of the cases for the Y coordinate. In the most of the cases the identification error is less than one cell size (20×20 m²). On the other hand, the maximum error is less than the size of two cells. Figure 7 shows the hydrogeological domain with spatial coordinates X and Y corresponding to the 40 pollution sources positions. The black circles represent the correct source positions while the blue, red and green circles are the positions calculated by means of the MLP inversion. The Figure 7 corresponds to the 40 pollution sources, with 10, 20 and 30 years activity time respectively.

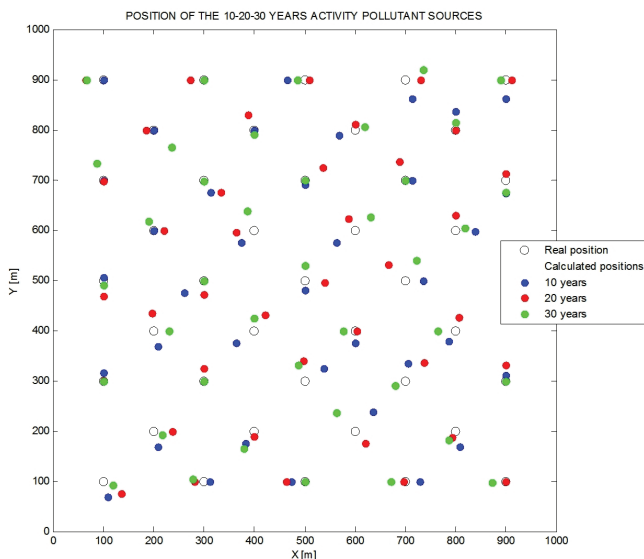


Fig. 7: real and calculated position of the 10, 20 and 30 years activity pollutant sources

Table 2 illustrates the percentages of success in identifying the unknown pollution sources. The localization of the source is considered 100% correct if the error is less than the side of the cell (20 m). The prediction of the activity duration is considered 100% if the error is less than one year.

Tab. 2: performance of the inversion of the MLP.

Patterns results examples	%
X,Y,T 100% correct	14
T 100% correct / X,Y error < 20m	40
T 100% correct / X,Y error > 20m	17
T error < 6 years / X,Y error < 20m	23
T error < 6 years / X,Y error > 20m	6

The method proves to be suitable in predicting the position of the source, whereas less satisfying results have been obtained concerning activity duration prediction, with 76% of correct answers. Concerning 10 and 30 years as the duration of the sources activity of, the activity duration resulted to be wrong in only one case. Conversely, for the 20 years sources duration activity, the resulting wrong cases are 26 out of a total of 40. Anyway, the maximum error committed in time estimation is 5,26 years. In Table 3 the average and maximum errors for the three source parameters are reported.

Tab. 3: results related to the identification of the pollution sources features.

	X [m]	Y [m]	Time [years]
Em – mean error	14.19	14.33	0.70
EM – maximum error	39.17	39.82	5.26

In most cases the MLP is able to correctly detect the duration of the pollution activity. This is probably due to the different dynamics of the pollutant processes depending on the distance of the source from the boundaries and from the pumping well.

Figure 8 shows the performance concerning duration activity prediction. As one can see, for the sources duration activity of 10 and 30 years, only one case is wrong. For the 20 years sources duration activity, the wrong cases have been higher than the correct cases with 26 wrong cases out of a total of 40 cases. Nevertheless the resulting mean error is equal to 2.66 years. The minimum and maximum errors were respectively of 6 months and 5 years and 3 months. Various trials performed to improve these results have shown that these results are strongly influenced by the instability of the MLP training.

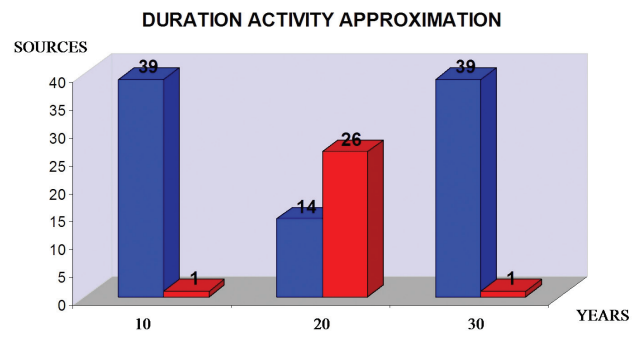


Fig. 8: duration activity approximation of the ANNs.

Figure 9 shows the position of the sources where the prediction of duration activity is wrong. The positions are uniformly distributed throughout the domain and in general the position of the source is precise. Such result could suggest an interpretation of the anomalous performance in the case of 20 years activity duration. It seems that the procedure is able to locate the source, but probably the plume exhibits an irregular behaviour in the intermediate time, which is not the case in both the beginning, when the pollutant is strongly concentrated, and in the long time, when the plume reached a regime distribution. In order to improve the performance of the system a greater number of examples should be generated of the midterm cases, but this is not the aim of the present work, which instead was to put in evidence the characteristics of the system which can affect the performance.

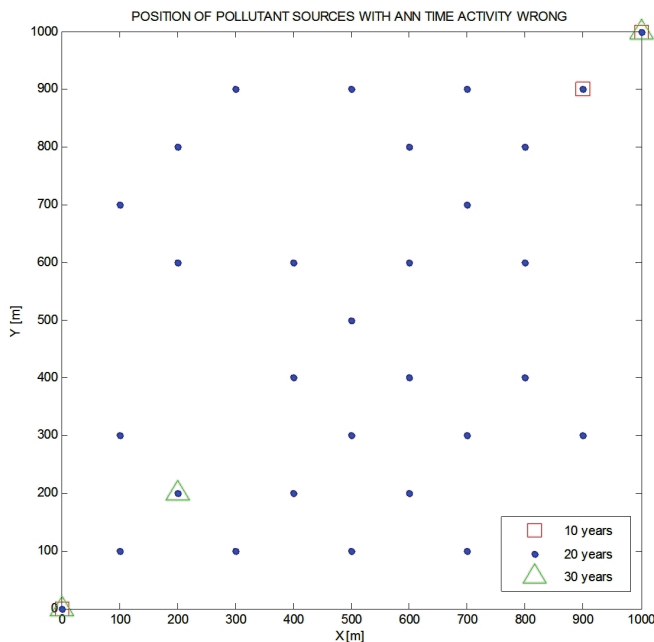


Fig. 9: position of pollutant sources with ANN activity wrong.

Conclusion

The presented inverse problem solution method allows estimating time-space coordinates of unknown contaminant sources. Various source scenarios have been constructed in order to generate the examples used for training MLPs. These scenarios have been performed by varying the pollutant source position and the duration of the source activity in the domain. The inverse problem has been solved using measurements of contaminant concentration acquired in the monitoring wells at a certain time t . In the presented case the method may be useful not only to identify the location and activity of unknown pollution sources, but also to delimitate the study area and optimize the investigation costs by determining the best monitoring wells location. The proposed methodology has been developed for a simple theoretical case, however the method may be applied to real cases characterized by a high uncertainty in the aquifer formation because of its heterogeneity, single plume or multiple plumes, plumes overlapping, continuous or instantaneous sources and lack of information on the pollutant source behaviour. Therefore, further research to improve the method and extend its application is still needed.

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