Journal of Geochemical Exploration 136 (2014) 14–23

Contents lists available at ScienceDirect

Journal of Geochemical Exploration

journal homepage: www.elsevier.com/locate/jgeoexp

Application of an inverse neural network model for the identification of optimal amendment to reduce copper toxicity in phytoremediated contaminated soils

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ARTICLE INFO

Article history:
Received 22 January 2013
Accepted 15 September 2013
Available online 23 September 2013

Keywords:
Soil contamination
Copper
Amendment optimization
Artificial neural networks (ANN)
Inverse modeling

ABSTRACT

Artificial neural network ANN prediction approaches applied to the modeling of soil behavior are often solved in the forward direction, by measuring the response of the soil (outputs) to a given set of soil inputs. Conversely, one may be interested in the assessment of a given set of soil inputs that leads to given (target) soil outputs. This is the inverse of the former problem. In this study, we develop and test an inverse artificial neural network model for the prediction of the optimal soil treatment to reduce copper (Cu) toxicity assessed by a given target concentration of Cu in dwarf bean leaves (BL) from selected soil inputs. In this study the inputs are the soil pH, electrical conductivity (EC), dissolved organic carbon (DOC) and a given target toxicity value of Cu, whereas the output is the best treatment to reduce the given toxicity level. It is shown that the proposed method can successfully identify the best soil treatment from the soil properties (inputs). Two important challenges for optimal treatment prediction using neural networks are the non-uniqueness of the solution of the inverse problem and the inaccuracies in the measurement of the soil properties (inputs). It is shown that the neural network prediction model proposed can overcome both these challenges. It is also shown that the proposed inverse neural network method can potentially be applied with a high level of success to the phytoremediation of contaminated soils. Before large-scale application, further validation is needed by performing several experiments and investigations including additional factors and their combinations to capture the complex soil behavior.

1. Introduction

Soils contaminated with trace elements have serious consequences for terrestrial ecosystems, agricultural production and human health (Adriano, 2001). Trace element contamination is considered as a negative effect of industrial activities which must be monitored, assessed and managed (Alloway, 1995). For instance several authors have reported that soil contamination is accompanied by a loss of biodiversity, land cover and finally a lack of nutrients and water (Freitas et al., 2004; Mench and Baize, 2004; Zvereva and Kozlov, 2007). The exposure of plants to contaminants causes the same consequences as environmental stress and results in a lower biomass and lower vegetation (Zvereva and Kozlov, 2004). According to the international organization for standardization, the bioavailability of soil contaminants is defined as the fraction of available contaminant in the soil acquired by a target-organism through physiological processes (Harmsen, 2007). Consequently, the characterization and prediction of metal phytoavailability in soils is a crucial step for assessing the efficiency of soil remediation strategies such as the addition of soil amendments including organic matter (compost, farm manure and biosolids), lime or other alkaline materials (Bolan et al., 2003; Brown et al., 2003; Lombi et al., 2003; Ma et al., 2006; McBride, 1994; Oste et al., 2001; Puschenreiter et al., 2005) which have the capacity to adsorb complex or (co)precipitate trace elements in the soil.

Various treatments can be suggested or tested experimentally with a view to reducing the toxicity of a specific contaminated soil to plants by observing the growth or death of the plants. It is therefore of immense practical importance to be able to determine the optimal soil treatment with an amendment to a specific soil in order to reduce the soil toxicity which can be controlled and measured by metal concentrations in vegetation. It is usual to try to predict the effectiveness of these treatments, e.g. by how much the metal concentration will be reduced in plant leaves. One can specify a maximum allowable limit value (target) of metal concentration in a specific soil and seek to identify the corresponding optimal treatment to reduce the toxicity below the specified target. Examples of the areas where such predictive capability is of great value are the monitoring and management of industrial sites. Thus it is necessary to develop rapid and accurate prediction tools to control and analyze contamination sites and to manage soil use. This requires an extensive data bank of soil input–output data. However, measuring these parameters is time-consuming, difficult and expensive.

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http://dx.doi.org/10.1016/j.gexplo.2013.09.002

In such cases, there is no clear standard rule for the selection of the optimal soil treatment and one needs to determine the response of the soil. This is the so called inverse problem identification which must be solved to answer the following question: what are the controlled inputs (e.g. amendments) that have resulted in this given output (metal concentrations in the plant leaves). Recently, several applications based on inverse neural network models referred as (ANNi) were developed by several authors to optimize the performance of polygeneration system parameters (Hernández et al., 2013) to control the strategy for absorption chillers (Labus et al., 2012), to optimize the operating conditions for compressor performance (Cortés et al., 2009), to optimize the operating conditions for heat and mass transfer in foodstuffs drying (Hernández, 2009), to predict the chemical oxygen demand removal during the degradation of alazine and gesaprim commercial herbicides (El hamzaoui et al., 2011) and to optimize solar-assisted adsorption refrigeration system (Laidi and Hanini, 2013).

The solution of the inverse problem has several practical applications in soil analysis, but has not been extensively studied so far, presumably due to the difficulties associated with the resolution of the nonlinear inverse problem. Over the last few years ANNs have been widely used in the field of soil science for the prediction of soil hydraulic properties (Minasny et al., 2004; Schaap et al., 1998), the generation of digital soil maps (Behrens et al., 2005; McBratney et al., 2003) and the modeling of the behavior of trace metals (Anagu et al., 2009; Buszewski and Kowalkowski, 2006; Gandhimathi and Meenambal, 2012). In this case, the ANN is trained to find these relations using an iterative calibration process. The ANN approach is beneficial compared to traditional regression methods if the input–output relationship is complex or unknown (Hambli, 2009; Hambli et al., 2006; Sarmadian and Taghizadeh Mehrjardi, 2008; Schaap and Leij, 1998). Moreover, ANN can be used as an inverse modeling approach. ANN modeling has been previously applied for solving inverse problems in other engineering fields (Hambli et al., 2006; Jenkins, 1997; Rafiq et al., 2001), but has not been previously used in conjunction with soil analysis. Inverse ANNs have several advantages compared to other inverse identification techniques. First, ANNs are very general. It is proven that ANNs can accurately represent any sufficiently smooth nonlinear mapping (Jenkins, 1997; Rafiq et al., 2001). Second, the accuracy of the solution is independent of the number of inputs (Jenkins, 1997; Rafiq et al., 2001). This is an important point, because accurate prediction of the optimal soil treatment may require a large number of soil inputs. Third, ANNs are particularly useful in cases where solving the forward problem model is time-consuming (Hambli et al., 2006).

In this study, we have developed and tested an inverse artificial neural network (ANN) model for the prediction of optimal soil treatment to reduce toxicity assessed by a given target concentration of Cu in dwarf bean leaves (BL) from a given set of soil properties (inputs).

In order to prepare the training data for the inverse ANN, 16 (4×4) soil samples were collected from different soil profiles from a Cu sulfate and Chromated Copper Arsenate (CCA) contaminated site located in south-western France. The measured soil variables were soil pH, soil electrical conductivity (EC), dissolved organic carbon (DOC) and the concentration of Cu in BL grown in the laboratory on these contaminated soils treated with inorganic and organic amendments, with 4 replications for each measurement (4×4 measurements). The inverse ANN model was then developed and trained to predict the best soil treatment. The inputs were the soil pH, EC, DOC, and a given target toxicity value of Cu, whereas the output is the best treatment to reduce the given toxicity level.

In previous studies (Cortés et al., 2009; El hamzaoui et al., 2011; Hernández, 2009; Hernández et al., 2013; Labus et al., 2012; Laidi and Hanini, 2013), the authors generated the resulting corresponding mathematical equations obtained from the trained direct ANNs representing the investigated processes behaviors and used optimization algorithms based on these equations to assess the optimal input parameters. In general, optimization involves finding the minimum or/and maximum of these n objective functions subjected to some constraints. For example in El Hamzaoui et al. (2011) study, the authors proposed an innovative methodology to calculate the optimum operating conditions. In a first step, the explicit mathematical equation was obtained by the ANN after training (ANN weights) as an objective function using Matlab code. In a second step, the Nelder–Mead simplex method was applied to calculate the optimal (unknown) reaction time to obtain a chemical oxygen demand. Current inverse ANN differs from these previous works by two features: (i) The aim here was to predict an output as a non-numerical data (amendment type) where prediction of a minimum or a maximum response do not apply. And (ii) during the training phase, the amendment type was considered as an input which refers to a given amendment to reduce copper toxicity in phytoremediated contaminated soils (Fig. 2). Therefore, the current inverse prediction does not require the generation of the complicated ANN mathematical equations obtained from the trained direct ANNs. Two important aspects in the estimation of the optimal soil treatment from the measured soil inputs is the non-uniqueness of the solution of the inverse problem and the inaccuracies that may exist in the measurement of the soil inputs. The non-uniqueness of inverse solutions is a challenge for any inverse problem algorithm, because several solutions exist for the same inverse problem. The convergence of the solution may therefore be compromised. The second challenge is the inaccuracy that may exist in the actual measurements of soil inputs. The inverse ANN algorithm should be robust enough to be able to provide reasonable predictions of optimal soil treatment even when the soil input measurements are not perfectly accurate. Both challenges are addressed for the proposed inverse ANN algorithm. Results show that the inverse ANN model leads to a rapid and accurate prediction of the optimal soil treatment.

2. Material and methods

From a practical point of view, the following three steps are required for the development of the inverse ANN model:

(i) Performing suitable experiments to measure the effects of selected soil inputs (properties, inorganic and organic amendments) on the soil toxicity assessed by concentration of Cu in dwarf BL.
(ii) Forward training the neural network based on the results of step (i) (mapping inputs to outputs).
(iii) Inverse ANN prediction (prediction of the inputs given a target set of outputs).

The present section of the paper is divided into three sub-sections. The first sub-section presents the soil experiments. The second sub-section describes the inverse ANN approach and the third sub-section deals with the inverse ANN prediction considering the non-unique solutions of the inverse problem.

2.1. Soil sampling and preparation

16 soil samples (four replicates) were collected from 16 plots (1×3 m) from the BIOGECO phytostabilization platform installed on a former wood preservation site located in south-western France, Gironde County (44°43′N; 0°30′W), This site has been contaminated with high concentrations of Cu. The history of the site and its characteristics are detailed in (Bes et al., 2010; Mench and Bes, 2009). Long-term aided phytostabilization experiments are established at the site. The plant communities cultivated in the zone of the field trial were *Agrostis capillaris*, *Elytrigia repens*, *Rumex acetosella*, *Portulaca oleracea*, *Hypericum perforatum*, *Hypochaeris radicata*, *Euphorbia chamaesyce*, *Echium vulgare*, *Agrostis stolonifera*, *Lotus corniculatus*, *Cerastium glomeratum*, and *Populus nigra* (Bes et al., 2010). Four different amendments were applied on the site and carefully mixed in the topsoil (0–0.30 m) with a stainless steel spade with four replicates: untreated soil (UNT), 0.2% of dolomite limestone (DL), 5% of compost