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Estimating soil solution electrical conductivity from time domain reflectometry measurements using neural networks

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Abstract

Time domain reflectometry (TDR) is a widely used method for measuring the dielectric constant (K_a) and bulk electrical conductivity (σ_a) in soils. The TDR measured σ_a and K_a can be used to calculate the soil solution electrical conductivity, σ_w. The σ_w, in turn, can be related to the concentration of an ionic tracer. Several models of the σ_w–σ_a–K_a relationship can be found in the literature. Most of these models require extensive calibration experiments in order to obtaining best-fit parameters. In this paper, we attempt to model the σ_w–σ_a–K_a relationship using neural networks (NN). We used TDR measured K_a and σ_a along with five different soil physical parameters (sand, silt, clay, and organic matter content and bulk density) measured in nine different soil types using three different σ_w levels in each soil type. In total, 2953 K_a and σ_a measurements were obtained. The NN estimated σ_w was found to have a root mean square error (RMSE) of 0.05–0.13 dS m^{-1} for the nine different soil types whereas the RMSE of two traditional σ_w–σ_a–K_a models was 0.12–0.87 dS m^{-1}. Furthermore, the traditional models exhibited larger errors for low σ_a and K_a, whereas the NN estimated σ_w did not show any trend in the errors. A sensitivity analysis showed that the NN model was more sensitive to small changes in σ_a compared to K_a. Of the five soil physical parameters, the silt and clay content affected the σ_w–σ_a–K_a relationship the most. The results presented shows that using NN, the σ_w–σ_a–K_a relationship can be predicted using soil physical parameters without need for elaborate soil specific calibration experiments.

Keywords: Neural networks; Time domain reflectometry; Electrical conductivity

1. Introduction

Time domain reflectometry has become an important tool for measurement of soil water content (θ) and bulk electrical conductivity (σ_a). The TDR instrument sends a high frequency electromagnetic signal along a probe buried in the soil. The signal is reflected at the end of the probe and the travel time of the signal can be measured from the resulting waveform. The travel time can be related to K_a, which in turn can be related to θ. Additionally, the attenuation of the reflected signal can be related to σ_a.

The σ_a of the soil is depending both on the electrical conductivity of the pore water (σ_w) and θ. Thus, the σ_w can only be predicted if θ is constant, or if the relationship between σ_w, σ_a, and θ (or K_a) is determined. The σ_w can be related to the concentration of an ionic tracer. Several different models of the σ_w–σ_a–K_a relationship have been developed

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(Rhoades et al., 1976; Mualem and Friedman, 1991; Persson, 1997). These models, however, have several drawbacks. For example, the $\sigma_w-\sigma_a-K_a$ relationship is highly dependent on soil type, requiring detailed soil specific calibration experiments. The model calibration process is among the most problematic impediments to routine application of TDR for σ_w measurements (Mullin et al., 1999). Thus, a model capable of σ_w estimations in multiple soil types is highly desirable. However, no such study has been presented so far and, therefore, forms the basis for the present investigation, where a neural network (NN) is used.

The NN is conceived to mimic the functioning of the human brain by acquiring knowledge through a learning process and finding optimum weights for the different connections between the individual nerve cells. Mathematically, a NN can be treated as a universal function approximator. The ability to 'train' and 'learn' the output from a given input makes NN capable of describing large scale complex problems. During the last decade, NN has been applied, with success, to various hydrological processes, such as rainfall-runoff modeling (Hsu et al., 1995), rainfall forecasting (French et al., 1992), water quality modeling (Maier and Dandy, 1996), streamflow modelling (Cannon and Whitfield, 2002), reservoir operation, river basin classification, etc. (Govindaraju, 2000). In soil science, NNs have been used to predict water retention characteristics from other, more easily measured, soil variables like particle size distribution and bulk density (Pachepsky et al., 1996; Schaap and Bouten, 1996; Koekkoek and Booltink, 1999). The NN is, thus, a useful tool for achieving accurate data without cumbersome calibration. Recently, Persson et al. (2001) used NN to calibrate TDR measurements. They showed that a NN gave better prediction of the $\sigma_w-\sigma_a-K_a$ relationship than other commonly used models. However, they used only a single soil type (sand) and, thus, effects of different soil textures were not investigated. With the encouraging results obtained using NNs for water retention characteristics estimations using soil physical parameters in mind, it seems possible that the same procedure could be used to predict the $\sigma_w-\sigma_a-K_a$ relationship. Similar work has also been previously presented by Persson et al. (2002) for the $K_a-\theta$ relationship.

The purpose of the present study is to investigate the use of NN to understand (or derive) the $\sigma_w-\sigma_a-K_a$ relationship from physical parameters of the soil. The performance of NNs is compared to the ones achieved using common calibration models. An attempt is also made to study the influence of different soil physical parameters on the behaviour of NN.

2. Materials and methods

2.1. Soil sampling

Soils from six different locations were used in this study. Four of these locations are situated in southern Sweden. At three sites, both the topsoil (0–0.1 m depth) and the subsoil (0.4–0.5 m depth) were collected, at the fourth site only the topsoil was collected. Two samples were also collected in the catchment of M'Richet el Anze, located 110 km southwest of Tunis, Tunisia. These samples were collected from the topsoil at the hollow and at the slope of the catchment. Thus, totally nine different soil samples were used. A description of some selected soil properties is found in Table 1.

2.2. Laboratory experiments

The soil samples were oven dried and passed through a 2 mm sieve. Then, the soil was packed into Plexiglas soil columns, 0.076 m in diameter and 0.1 m long (Soil Measurement System, Tucson, AZ), to the bulk densities encountered in the field. One three-rod TDR probe with a length of 0.08 m and a wire spacing of 0.03 m (model 6111, Soilmoisture Equipment Corp., Santa Barbara, CA) was inserted in the cent of the column. TDR measurements were carried out using a Tektronix 1502C cable tester with an RS232 interface connected to a laptop computer. Estimates of K_a and σ_a were calculated from the TDR trace using the WinTDR99 software (developed by the Soil Physics Group at Utah State University).

First, each sample was saturated by upward infiltration. Distilled water with KBr added to increase the σ_w to 0.30 dS m^{-1} was used. When studying the $\sigma_w-\sigma_a-K_a$ relationship it is important that the σ_w is known and constant in the soil sample. Thus it was necessary to leach the soil with water of constant σ_w.

Table 1
Soil properties

Location	Sand (g kg^{-1})	Silt (g kg^{-1})	Clay (g kg^{-1})	Organic matter (g kg^{-1})	Bulk density (g cm^{-3})
Revinge					
Topsoil	828	160	12	45	1.30
Subsoil	818	151	31	17	1.60
Löddeköpinge					
Topsoil	800	165	35	43	1.56
Subsoil	788	183	29	34	1.58
Odarslöv					
Topsoil	680	272	48	58	1.48
Värpinge					
Topsoil	571	342	87	33	1.65
Subsoil	405	446	149	20	1.48
M'Richet el Anze					
Hollow	120	240	640	26	1.27
Slope	80	430	490	36	1.44

The upward infiltration was continued until the σ_w of the effluent and the TDR measured σ_a reached a constant value. Approximately five pore volumes of water was added since this proved to be more than sufficient for the soils used in this study. The flow rate was 0.008 m h^{-1} during daytime and 0.002 m h^{-1} during the night. Then, suction was applied at the bottom of the column to drain water. The drainage experiments were always started after a >15 h period of low flow. This was due to that during low flow the difference in σ_w between mobile and immobile water is likely to be small. Suction was increased stepwise from 0 to 70 kPa (system limit) with an increment of 10 kPa. The TDR measurements were taken automatically every half minute at the beginning of the experiment, the measurement frequency was then decreased gradually to once every 30–60 min as θ decreased slower when the drainage experiment progressed. The drainage experiment was continued 24–48 h, at this time there was no change in the TDR measured K_a and σ_a. The σ_w of the extracted water was measured several times during the experiment.

The leaching/drainage experiment was repeated twice using water with σ_w of about 1.2 and 3.0 dS m^{-1}. These σ_w levels should cover the range of interest in most non-saline agricultural soils. First, the samples were leached using upward infiltration. Again, about five pore volumes proved to be sufficient for reaching a constant σ_a. Then, suction was applied according to above. Thus, for all soil samples the K_a–σ_a relationship for three different σ_w were determined. In total, 2953 data points were collected. All experiments were carried out at a constant temperature of 20 °C and the data were, thus, not temperature corrected.

2.3. Models of the σ_w–σ_a–θ relationship

There are several different σ_w–σ_a–K_a or σ_w–σ_a–θ models presented in the literature. A comparison of the performance of some existing models can be found in Persson (1997), Wraith and Das (1998) and Persson et al. (2001). In the present study, we compared two commonly used models for comparison with the NN performance. The first model used was the one presented by Rhoades et al. (1976)

$$\alpha_a = \sigma_w(a\theta^2 + b\theta) + \sigma_s \quad (1)$$

where a and b are soil specific parameters and σ_s is the surface conductivity of the soil matrix. The parameter σ_s is difficult to measure directly, thus it is often used as a fitting parameter. The θ was calculated from the TDR measured K_a using a soil specific calibration equation which previously have been determined in each of the nine soil types (data not shown). The second model used for comparison of the σ_w

estimation was the one presented by Mualem and Friedman (1991),

$$\sigma_a = \sigma_w \theta^\beta / \theta_s + \sigma_s \quad (2)$$

where θ_s is the water content at saturation and β is a calibration coefficient. Mualem and Friedman (1991) found that $\beta = 2.5$ fits most soils. The θ_s was set equal to the porosity, which was estimated using the bulk density and an assumed particle density of 2.65 g cm^{-3}

2.4. Neural networks

The NN is a non-linear model that makes use of a parallel programming structure capable of representing arbitrarily complex non-linear processes that relate the inputs and outputs of any system (Hsu et al., 1995). It provides better solutions than traditional statistical methods when applied to poorly defined and poorly understood complex systems that involve pattern recognition (Poff et al., 1996). Although NN do not provide a model that is readily physically explainable, it is a viable technique to develop input–output simulations and forecast models for situations when the objective is an accurate forecast (Uvo et al., 2000).

The NN are structured, similarly to the biological neural network, by interconnected layers composed of neurons. An artificial neuron is the unit of the architecture of the NN. It basically consists of a transfer function and two scalar number, a weight and a bias. It receives a scalar input that is multiplied by the weight and added to the bias. The transfer function is applied to this result. The scalar number that is a result from the application of the transfer function will be the input to the neurons in the next layer. Every neuron in one layer is connected to each neuron of the neighbour layers. In a feedforward NN, each neuron receives input from the neurons of the previous layers and feeds the neuron of the next layer with inputs.

To develop and train a NN involve (a) choosing a training set that contains input–output pairs; (b) defining a suitable network (number of layers and number of neurons in each layer); (c) training the network to relate the inputs to the corresponding outputs by estimating the NN weights; and (d) testing the identified NN. If compared to a conceptual model, (b) is equivalent to the development of the model and (c) is the estimation of the parameters of the designed model.

The process of training the NN consists of a self organizing learning process through a procedure that minimizes the error between the NN output and the target values. The objective of the training is to find the weights of each neuron that will result in the minimum error.

General properties of NN, as well as their applications within hydrology, water resources, and soil science have been thoroughly covered in a number of publications (Smith, 1993; Bishop, 1995; Maier and Dandy, 2000; Cannon and Whitfield, 2002; Pachepsky et al., 1996). For background information, the reader is referred to this literature; here only specific properties of the NN employed are given.

In the present study, we chose to use a two-layer (one hidden and one output layer) feedforward NN trained by a backpropagation algorithm using the Levenberg–Marquardt optimisation (Hagan and Menhaj, 1994). Backpropagation can be explained as the adjustment of NN weights and biases by backpropagating the differences between the NN output and actual target. Prior to NN application, the original input and target time series were standardized to ensure that every input receives equal attention during the training (Maier and Dandy, 2000). Typically the data available for NN calibration is split in two parts, one for training and one for test (or validation). For our data set, 20% of the data points were randomly selected as the test data set. This division is made in order to use early stopping, a common and practical method to avoid over-fitting but ensure proper generalization (Bishop, 1995). Early stopping means that the NN is trained with the training set and its performance for the test set is checked after each epoch (parameter adjustment based on one sequence through all values). When a consistent increase in the performance for the test set is observed, training is stopped and the NN considered trained. After that the quality of the NN ability to estimating σ_w is checked using the test data set as input. The test set is an independent part of the data set that is not, at any moment, used during the training process. All NN simulations were run using the neural network toolbox of UNIX Matlab^R (version 6.1, The Mathworks Inc., Natick, MA) software.

To every neuron in the hidden layer, was allocated a log-sigmoid transfer function defined as

$$ov = \frac{1}{1 + e^{-iv}} \quad (3)$$

where iv is the input value to the neuron and ov the output value from the neuron. To the output layer, a pure linear transfer function was allocated.

Determination of the number of neurons and how to divide these into separate layers are delicate issues. Large (or complex) NNs require a lot of data to generalize well and are computationally intensive; small (or simple) NNs may not be able to reproduce intricate I/O relationships (Bishop, 1995). As mentioned before, we chose to use a NN with one hidden layer and one output layer with a single neuron. The number of inputs to the NN was seven, i.e. the two measured parameters K_a and σ_a along with five soil physical parameters describing the soil type (Table 1); bulk density, sand, silt, clay, and organic matter content. To determine the optimal number of neurons in the hidden layer we used the principle of constructive algorithms, which essentially is start testing the number of neurons from a minimal and add neurons until performance ceases to increase (Kwok and Yeung, 1997). Each NN was trained 20 times and the average output (here after referred to as output) was compared to the targets. The root mean square error (RMSE) and the coefficient of determination (r^2) between target and output resulting from the trained NN with different number of hidden neurons were compared and the design associated to the smaller RMSE was accepted as the most suitable NN design for our problem. We increased the number of hidden neurons from one to 18. The minimum RMSE combined with maximum r^2 was found using a NN with 10 hidden neurons. Thus, 10 hidden neurons were used in the following simulations.

A sensitive test was performed to the chosen NN so that a better understanding of the influence of each input on the output could be examined. The trained NN was fed by the seven input series multiplied by 1.1 one at a time and the RMSE was analysed for each of the runs. A large increase in the RMSE represented a higher sensitivity of the NN to that input. Based on the results from the sensitivity analysis, two NN with a reduced number of input parameters were constructed. In one NN, we omitted the sand content and in the other sand content, organic matter content, and bulk density were omitted. Again, all NNs were trained 20 times and the average output was compared to the test data.

3. Results and discussion

3.1. The TDR measured σ_w–σ_a–K_a relationship in different soil types

In most leaching/drainage experiments, the σ_w of the inflowing water was slightly different to the effluent above the soil surface after the TDR measured σ_a reached a constant level. However, the effluent and the extracted water had similar σ_w. Therefore, it was assumed that the σ_w was constant within the samples and equal to the effluent and extracted water. Thus, this value was used in the analysis. In Fig. 1, all 2953 measured K_a and σ_a values are presented.

In Table 2, the RMSE and r^2 values of Rhoades et al. (1976) and Mualem and Friedman (1991) models are presented along with the best-fit parameters. Both models (Eqs. (1) and (2)) gave RMSE of about 0.2 dS m^{-1} for most soil types. In the M'Richet el Anze hollow soil, however, both models gave much higher RMSE. The encountered magnitude of the errors in the σ_w estimation is similar to the ones presented in the literature (Persson, 1997; Persson et al., 2001). Both models performed equally well in all cases except in the Revinge subsoil, where Eq. (2) gave significantly higher RMSE. The σ_s was

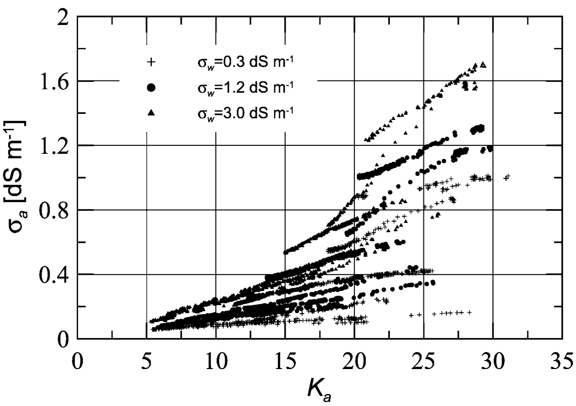

Fig. 1. All TDR measured K_a and σ_a in the nine soil types for three different σ_w.

Table 2
The NN performance compared to the Rhoades et al. (1976) and Mualem and Friedman (1991) models

Soil type	Rhoades et al. (1976)			Mualem and Friedman (1991)			NN	
	Best-fit parameters	r^2	RMSE (dS m^{-1})	Best-fit parameters	r^2	RMSE (dS m^{-1})	r^2	RMSE (dS m^{-1})
Revinge								
Topsoil	$a = 1.43$, $b = 0.18$, $\sigma_s = 0.07$ dS m^{-1}	0.987	0.125	$\beta = 1.83$, $\sigma_s = 0.07$ dS m^{-1}	0.939	0.303	0.996	0.074
Subsoil	$a = 0.73$, $b = 0.14$, $\sigma_s = 0.06$ dS m^{-1}	0.961	0.211	$\beta = 2.31$, $\sigma_s = 0.06$ dS m^{-1}	0.771	0.543	0.984	0.126
Löddeköpinge								
Topsoil	$a = 3.74$, $b = 0.02$, $\sigma_s = 0.06$ dS m^{-1}	0.979	0.155	$\beta = 1.75$, $\sigma_s = 0.06$ dS m^{-1}	0.971	0.184	0.989	0.116
Subsoil	$a = 2.94$, $b = 0.29$, $\sigma_s = 0.06$ dS m^{-1}	0.984	0.193	$\beta = 1.60$, $\sigma_s = 0.06$ dS m^{-1}	0.977	0.186	0.988	0.127
Odarslöv								
Topsoil	$a = 1.73$, $b = 0.26$, $\sigma_s = 0.13$ dS m^{-1}	0.946	0.248	$\beta = 2.73$, $\sigma_s = 0.12$ dS m^{-1}	0.960	0.218	0.994	0.082
Värpinge								
Topsoil	$a = 4.07$, $b = 0.38$, $\sigma_s = 0.23$ dS m^{-1}	0.971	0.154	$\beta = 2.05$, $\sigma_s = 0.20$ dS m^{-1}	0.962	0.146	0.996	0.055
Subsoil	$a = 2.47$, $b = 0.20$, $\sigma_s = 0.32$ dS m^{-1}	0.970	0.183	$\beta = 1.69$, $\sigma_s = 0.31$ dS m^{-1}	0.977	0.153	0.996	0.053
M'Richet el Anze								
Hollow	$a = 3.79$, $b = 1.09$, $\sigma_s = 0.62$ dS m^{-1}	0.712	0.873	$\beta = 2.28$, $\sigma_s = 0.48$ dS m^{-1}	0.615	0.587	0.972	0.117
Slope	$a = 2.64$, $b = 0.62$, $\sigma_s = 0.85$ dS m^{-1}	0.985	0.123	$\beta = 2.66$ $\sigma_s = 0.83$ dS m^{-1}	0.982	0.136	0.995	0.069

similar for both models. As expected, σ_s increased as the clay content increased. The relationship between clay content and σ_s found in our data was similar to that obtained by Rhoades et al. (1989). The β was in the range 1.6–2.7 as suggested by Mualem and Friedman (1991).

3.2. NN performance

The RMSE decreased as the number of neurons in the hidden layer increased up to 10, after this the RMSE was more or less constant. The results are shown in Fig. 2, where the average RMSE of the standardized data is plotted against the number of hidden neurons. Consequently, 10 hidden neurons were chosen in the following NN runs.

In all soil types, the NN σ_w estimation showed very low RMSE, which were between 0.05 and 0.13 dS m^{-1} (Table 2). It should be noted here that the RMSE and r^2 values for the NN and Eqs. (1) and (2) showed here are from the test data only. The RMSE of the NN estimation were significantly lower than the RMSE of the traditional models. Even the M'Richet el Anze hollow soil had similar RMSE as the other soil types, the traditional models showed much larger RMSE for this soil type. Thus, the NN seems to work equally well in all soil types whereas the traditional models seems to work better in certain soils.

An interesting feature of the NN σ_w estimation was that it did not show any trend in the residual when plotted against σ_a or K_a. The traditional σ_w–σ_a–K_a models (Eqs. (1) and (2)) typically give larger errors

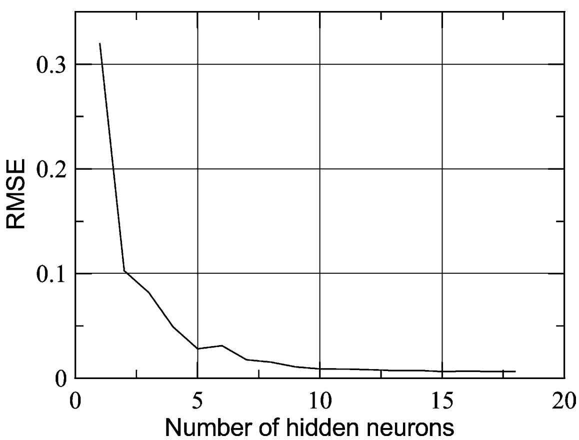

Fig. 2. The average root mean square error (RMSE) of 20 neural network runs plotted against the number of neurons in the hidden layer. Note that the RMSE is calculated using the standardized data.

Table 3
The results of the sensitivity analysis

Change in inputs	r^2	RMSE (dS m^{-1})
No change	0.991	0.097
Sand content × 1.1	0.955	0.234
Silt content × 1.1	0.932	0.289
Clay content × 1.1	0.935	0.285
Organic content × 1.1	0.968	0.191
Bulk density × 1.1	0.950	0.221
K_a × 1.1	0.947	0.254
σ_a × 1.1	0.825	0.580
No sand content	0.989	0.098
No sand content, organic matter content or bulk density	0.984	0.131

for low K_a and low σ_a. Rhoades et al. (1976) model even give negative σ_w in some soil types at low K_a when using $\sigma_w = 0.3$ dS m^{-1}. This clearly shows that the traditional $\sigma_w-\sigma_a-K_a$ models can give excellent results for some parts of the $\sigma_w-\sigma_a-K_a$ relationship, but lack flexibility to cover their entire range. The NN, on the other hand, performs equally well in all soil types at all K_a and σ_a.

The results for the sensitivity analysis are presented in Table 3, where the average r^2 and RMSE for all 20 NN runs using the data from all soil types are shown. Clearly, the NN model is most sensitive to changes in σ_a when compared to changes in K_a. Thus, when estimating σ_w from TDR measurements the accuracy of the σ_a measurements are more important than the accuracy of the K_a (or θ) measurements. Of the soil physical parameters the silt and clay contents were the most important to the NN model. This was not surprising since fine textured soils have a high specific surface area, which contributes to the series coupled surface conductivity (Rhoades et al., 1976; Rhoades et al., 1989). The sand content also showed to be fairly important, however, we believe that the main reason for this is that it is highly correlated to the clay content for our particular data set. The bulk density and organic matter content were the parameters that least affected the NN model. This was also expected since these parameters did not change much between the different soil types. However, the organic matter content is probably important to the $\sigma_w-\sigma_a-K_a$ relationship in soils with high organic matter content as it should contribute to the series coupled surface conductivity.

In Table 3, the results from the NNs with reduced number of inputs are also presented. When the sand content was omitted there was hardly any change in the r^2 and RMSE. This was expected since the sand, silt, and clay content always sum up to 100%. Thus, including only two of these parameters is sufficient. The other reduced NN only used silt and clay content, K_a, and σ_a as inputs. These parameters were chosen since these were the most important for the $\sigma_w-\sigma_a-K_a$ relationship. The results show that these parameters are sufficient for getting a reasonable result for the soil types used in this study. This NN is, of cause, less effective, but it is more widely applicable since bulk density and organic matter content does not need to be known.

Evidently, the five soil physical parameters were enough to describe the different $\sigma_w-\sigma_a-K_a$ relationships in our nine soil types. However, we believe that if more soil types were included, more physical parameters would be necessary. Parameters that are likely to significantly affect the $\sigma_w-\sigma_a-K_a$ relationship are soil pH and cation exchange capacity.

4. Conclusion

We investigated the $\sigma_w-\sigma_a-K_a$ relationship for three different levels of σ_w in nine different soil types. The soils included loamy sand, sandy loam, loam, silty clay, and clay soils. Two commonly used models (Rhoades et al., 1976; Mualem and Friedman 1991) were used to describe the $\sigma_w-\sigma_a-K_a$ relationship and compared to results from a NN model. Both these models gave reasonable σ_w estimation with a RMSE of about 0.2 dS m^{-1} for most soil types. However, an extensive calibration data set is needed for determining the calibration parameters of these $\sigma_w-\sigma_a-K_a$ relationships. By using NN, no a priori model of the $\sigma_w-\sigma_a-K_a$ relationship was needed, instead five soil physical parameters were used as inputs along with the measured K_a and σ_a to get the σ_w estimations in the different soils. The RMSE of the NN predicted σ_w were 0.05–0.13 dS m^{-1} for the nine different soil types whereas the RMSE of two traditional $\sigma_w-\sigma_a-K_a$ models were 0.12–0.87 dS m^{-1}. Furthermore, the traditional models exhibited larger errors for low σ_a and K_a and Rhoades et al. (1976) model even gave negative σ_w in some cases. The σ_w estimated by NN did not show any such trend in the errors. A sensitivity analysis showed that the NN model were more sensitive to small changes in σ_a compared to K_a. Of the five soil physical parameters, the silt and clay content affected the $\sigma_w - \sigma_a - K_a$ relationship the most. The NN predictions were least sensitive to changes in organic matter content. The results presented shows that using NN, the $\sigma_w - \sigma_a - K_a$ relationship could be estimated using soil physical parameters without need for elaborate soil specific calibration experiments. The Matlab NN code is available from the first author upon request.

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