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Artificial Neural Networks to predict decreasing saturated hydraulic conductivity in soils irrigated with saline-sodic water.

Younes Daw Ezlit[a], Ahmed Ibrahim Ekhmaj[a] and Mukhtar Mahmud Elaalem[a]

[a] Department of Soil and Water Science, Faculty of Agriculture, University of Tripoli, Libya

Abstract

Multilayer Artificial Neural Networks (ANNs) with the backpropagation algorithm were used to estimate the decrease in relative saturated conductivity due to an increase in sodicity and salinity. Data from the literature on the relative saturated hydraulic conductivity measured using water having levels of sodicity and salinity in different types of semiarid soils were used. The clay content of these soils is predominantly montmorillonite. The input data consisted of clay percentage, cation exchange capacity, electrolyte concentration, and estimated soil exchangeable sodium percentage at equilibrium stage with the solution applied. The data was divided into three groups randomly to meet the three phases required for developing the ANNs model (i. e. training, evaluation, and testing).The activation function selected was the TANSIG layer in the middle, while the exit function was the PURELIN layer. The comparisons between the experimental and predicted data on relative saturated hydraulic conductivity during training and testing phases showed good agreement. This was evident from the statistical indicators used for the evaluation process. For the training phase, the values of mean absolute error (MAE), root mean square error (RMSE), the correlation coefficient (r) and the determination coefficient (R^2) were 0.08, 0.13, 0.91, and 0.83, respectively. The performance of the ANNs model was evaluated against a part of the data selected randomly form the whole set of data collected (i. e. data not used during the model testing phase). The resultant values for MAE and RMSE, r and R^2 were 0.12, 0.16, 0.82 and 0.68, respectively. It should be noted that many factors were not considered, such as soil pH, type of clay, and organic matter, due to the limitations of the data available. Using these factors as input in ANNs might improve model predictions. However, the results suggested that the ANNs model performs well in soils with very low levels of organic matter.

1. Introduction

The shortage of fresh water for irrigation has led to overuse of water with high levels of salinity and sodicity. Salinity is the increase of concentration of soluble salts in the water solution, while sodicity is the relative concentration of sodium (Na^+) compared with divalent cations, mainly calcium (Ca^{2+}) and magnesium (Mg^{2+}) in water or soil solution (Ezlit et al. 2010). Using water with high levels of salinity and sodicity may initiate soil structure stability problems in irrigated areas. The increase of salinity in the root zone limits the growth and development of crops and reduces yield. Rising sodicity induces structural instability in soils containing a significant clay percentage. Degradation of soil structure results in negative changes in soil hydraulic properties, reduces aeration and soil logging, and adversely affects nutrient balance in the root zone. Sodicity is also common in soils irrigated with water containing considerable bicarbonate concentrations. This is because bicarbonate anions raise soil pH and can result in precipitation of divalent cations and an increase in the relative sodium concentration (Ezlit et al. 2011).

Sodicity is usually evaluated in terms of the sodium adsorption ratio (SAR) in irrigation water. The exchangeable sodium percentage (ESP) was employed to determine the level of sodicity in soils. ESP is closely related to SAR and in the literature it is used interchangeably to express the level of sodicity. In addition, the magnitudes of defflocculation are expressed in terms of decreases in saturated hydraulic conductivity (K_{sat}), and occasionally in the change in infiltration rates (Simunek and Suarez 1997). Coupling the percentage of the hydraulic conductivity reduction to the real measured values of ESP of the soil or SAR of the applied water allows quantification of the sodicity effect. This approach has been intensively applied since first introduced by Quirk and Schofield (1955). They measured the decrease in K_{sat} as a result of water sodicity and salinity using soil columns equilibrated with Mixed-Salt solutions at given SAR values and different electrolyte concentrations.

Quirk and Schofield (1955) introduced two indicators to evaluate the degree of adverse sodicity effect in relation to the total salinity concentration and the SAR of the water applied. These indicators are the threshold electrolyte concentration (TEC) and turbidity concentration (TC). TEC was defined as the salt concentration at which the soil permeability starts decreasing to a certain sodicity level. The value of TEC is very important in setting an irrigation management program using highly saline sodic water. TC was defined as the salt concentration at which clay fractions appear in the percolate. TC indicates that the soil structure is highly affected and should not be reached in practice. It should be noted that some level of K_{sat} reduction occurs due to pore clogging as a natural process of water movement conveying fine particles. Fine particles may plug some of the fine effective pores. In addition, soil slaking occurs the first time water is added. For a given soil, Quirk and Schofield (1955) proposed a critical decrease in K_{sat} of 10 to 15% of the optimal Ksat value. However, McNeal et al. (1966) recommended using a 25% reduction as critical of TEC for some American soils tested using backed columns. In addition, Cook et al. (2006) adopted a 20% reduction in Ksat as a critical value to determine TEC; this was later adopted by Ezlit (2009). Ezlit (2009) used an improved experimental design based on the Quirk and Schofield (1955) method to produce the TEC for a number of Australian soils (i.e. semiarid soils). The results showed

that the TEC varies from one soil to another. Bennett and Raine (2012) used the same technique to demonstrate the need for producing a TEC curve for a single soil to better manage irrigation using highly saline sodic water.

Various researchers have developed general soil stability guidelines based on the TEC concept for different soils in relation to the total salinity concentration and SAR of the water applied (e.g. Quirk and Schofield 1955, Rengasamy et al. 1984, and Ayers and Westcot 1985). These guidelines are useful for general demonstration of the effect of sodicity. However, these guidelines were derived for specific soils, and may not be suitable for other soil types (Ezlit 2009). The variation in the TEC for different soils is significant due to many interrelated and dynamic factors (Rengasamy et al. 1984). The variation in TEC is mainly caused by the differences in the clay mineral types and content, as well as soil texture (McNeal and Coleman 1966, Frenkel et al. 1978). Setting good irrigation management using saline sodic water requires identification of the level of soil structural stability under applications of saline sodic water.

Modeling soil structure instability due to sodicity was first introduced by McNeal (1968). The McNeal (1968) method is based on a semi-empirical model that relates the montmorillonite swelling approach from Norrish (1954) (i.e. swelling factor) to the change in relative reduction in saturated hydraulic conductivity as relative RK_{sat}. In addition, Lagerwerff et al. (1969) proposed a different semi-empirical model that relates RK_{sat} calculated using the Kozeny-Carmen equation (Carman 1937, 1948) to clay swelling calculated based on the diffuse double layer theory. Furthermore, Yaron and Thomas (1968) provided a simple empirical equation to predict RK_{sat} from the average ESP of the soil. Jayawardane (1979) proposed the equivalent salt solutions method to predict RK_{sat} due to rising sodicity. Jayawardane (1979) defined the equivalent salt solutions as solutions with combinations of sodium adsorption ratio (SAR) and solute concentration (Co) that produce the same extent of clay swelling in a given soil. In addition, Ezlit (2009) and Ezlit et al. (2013) provided a modification of the McNeal model with guidelines to predict the model parameters.

Research on these models showed more or less appropriateness (e.g. Russo and Bresler 1977, and Mustafa and Hamid 1977). Nevertheless, in all aforementioned models, obtaining the model parameters for a specific soil is required. The process of parameter determination is complicated, time consuming, and tedious experiments are needed.

The situation of the unsaturated conditions is more complex. Different models have also been proposed to quantify the decrease in unsaturated hydraulic conductivity to be applied under field conditions. Examples of those approaches are Simunek et al. (1996) and Russo and Bresler (1977). Simunek et al. (1996) used a reduction function based on the McNeal (1968) model and a soil pH effect function. The Simunek (1996) approach assumes that the effect of sodicity in soils under saturated conditions is similar to that in unsaturated conditions.

Despite considerable studies, there is no generic approach to predicting the TEC for different soils based on readily available soil data. However, this model can be developed by utilizing the new techniques in computer technology. The best available technique is artificial neural networks (ANNs).

ANNs are able to accurately approximate complicated non-linear input/output relationships. The ANNs methodology has been used in applications where the characteristics of the processes are difficult to describe using simple physical equations. There are a number of studies (e.g. Elizondo et al. 1994, Schultz and Wieland 1997, Ekhmaj et al. 2007) in which some environmental phenomena are described by mathematical models based on an ANNs approach. For solute transport problems, ANNs applications have been used successfully to predict the transport parameters and solute distribution in groundwater (Morshed and Kaluarachchi 1998, Almasri and Kaluarachchi 2005). Nevertheless, no study has been conducted to use the input– output mapping of ANNs to predict the effect of sodicity seen in the decrease in saturated hydraulic conductivity associated with applications of saline-sodic water. The current study aims to develop an ANNs model to simulate the decrease in saturated hydraulic conductivity associated with applications of saline-sodic water using RK_{sat} data obtained from laboratory experiments.

2. Material and Methods

2.1 Data collection

TEC experiments for 10 semi-arid soil groups from different sources were used in this study. The soils selected have very low organic matter levels and represent semi-arid soils from the US and Australia. Table 1 provides a summary of the main soil input data used to develop the ANNs model. In all data sourced, the experimental design used is similar to that adopted by Quirk and Schofield (1955), where different NaCl-CaCl$_2$ solutions having different SAR and solute concentrations (C_0) were applied to soil columns. The RK_{sat} values were calculated by dividing the measured K_{sat} using a NaCl-CaCl$_2$ solution by the K_{sat} measured for normal water (low SAR and higher C_0). The measured RK_{sat} in solution having a value of SAR and C_0 for a given soil were treated as an individual case.

Individual cases of RK_{sat} data (the values ranged from 0.1 to 1) corresponding to Electrolyte concentration (C_0) (ranged from 2.5 to 640 mmol$_c$/Litre), exchangeable sodium percentage (ESP) (ranged from zero to 100%), cation exchange capacity (CEC) (between 94.45 and 433.2 mmol$_c$/Kg$_{soil}$), clay content (%) (from 5.7 to 53.4) were organized in Excel spreadsheets as cases. The data collected represents the quality of the water applied and the soil properties.

The ESP values were estimated from the measured sodium adsorption ratio (SAR) for applied water using the USSL Staff (1954) SAR-ESP relationship. Both solute concentration (C_0) and ESP as a function of SAR determine the degree of the sodicity effect on the soil's stability due to the water applied. The CEC is one of the main soil properties. CEC is a relative function of the type of clay and organic matter. Since the data selected represents soils having less than 1% organic matter, most of the CEC values come from clay content. Thus, CEC is expected to improve the predictions generated by the model. Clay content reflects the percentage of soil that can affect the conductivity if entirely dispersed. However, not all clay types can result in soil deflocculation, the effect of clay can be better refined by using the percentage of dispersed clay such as montmorillonite. However, not all the data available in the literature has such values, though the data selected for this study is generally from soils predominant in montmorillonite clay which makes total clay percentage a useful variable for the model.

2.2 Standardization of the data:

The data collected were processed to meet the requirement of the ANN model. Data were arranged as numbered cases (i = 1, 2,..., n), and transformed according to the following expression as suggested by Vamsidhar et al. (2010):

$$v = \frac{v - min_A}{max_A - min_A} (new\_max_A - new\_min_A) + new\_min_A$$

(1)

Where: min_A and max_A are the minimum and maximum values of an attribute such as C_0, ESP, clay %, CEC and RK_{sat}. Min-max normalization maps a value, v, of the A attribute to v' in the range [new $min_{A'}$; new max_A]. In this study, all data values fall between 0 and 1, which is required by the model's algorithm. New min_A was set at 0.0 and new $maxA$ equal to 1.0.

Table 1: Main properties of the soils used to develop the ANNs Model

Soil No.	Soil name (As reported)	Clay %	CEC (mmolc/kg)	Number of cases (RKsat, ESP, C0, clay %, CEC)	Source
1	Alluvial	36.9	433.2	30	Jayawardane (1977)
2	Red Brown	40.6	245.7	12	
3	Imperial soils group a	5.7	94.6	20	McNeal (1968), Mc-Neal et al. (1968)
4	Imperial soils group b	16.2	153.8	20	
5	Imperial soils group c	48.5	336	20	
6	Gray Vertisols	53.4	258.4	25	Ezlit (2009)
7	Sodosols	12.9	99	24	
8	Brown Vertisols	47.1	270	24	
9	Soil 9	37	252.2	33	Leigh (2010)
10	Soil 8	38	275.4	30	

The data were divided into three groups. Group A were used for the model training and comprises 50% of the data collected (119 cases). Group B was employed for the internal process of the ANNs model. Group C was used for the internal model validations and comprises 25% of the data collected (59 cases). The testing phase used the third group which comprises 25% of the data set (60).

2.3   ANNs Model

Matlab program (Version 7.0) of Neural Networks Toolbox (Graphical User Interface) was used to develop the ANN model for this study. The activation function selected was the "TANSIG" layer in the middle, while the exit function was the layer. The model used is demonstrated in figure 1.
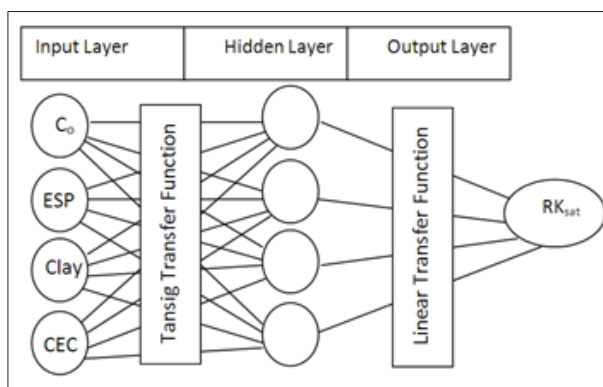

Figure 1. The architecture of (4 – 4 – 1) backpropagation neural networks used in this study

2.3   Performance Evaluation Criteria

In order to evaluate the developed neural network model, a number of statistical parameters were used. These indicators are the correlation coefficient between experimental and estimated RK_{sat} (r), determination coefficient (R^2), mean absolute error (MAE) and root mean square error ($RMSE$).

$$MAE = \frac{\left(\sum_{i=1}^{i=n}|O_i - P_i|\right)}{n} \quad (2)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{i=n}(O_i - P_i)^2} \quad (3)$$

$$r = \frac{\sum_{i=1}^{i=n}(O_i - \overline{O})(P_i - \overline{P})}{(n-1)S_0 S_p} \quad (4)$$

Where O_i and P_i are the estimated and experimental values of RK_{sat}, S_o is the sample standard deviation of the observed data, S_p is the sample standard deviation of the predicted data and n is number of pairs of observations. All data were processed and loaded into the neural modeling application Matlab program (Version 7.0) Neural Networks Toolbox (Graphical User Interface).

3.   Results and Discussion

3.1 Development of the ANN model

Despite the many models proposed to quantify the decrease of saturated hydraulic conductivity, none can be used without determining the model parameters for a given soil. The perfect relationship with limited factors is not available in the literature. That is because of the complexity of the sodicity effect within the soil. Therefore, there are no standard rules to building the networks structure; the optimum networks was identified using a trial and error process. The best results were obtained using a multilayer networks including the backpropagation algorithm. The input layer consists of 4 neurons for CEC, C_0, ESP, and clay content. The output layer has only one neuron to provide the predicted RK_{sat}. The hidden layer was started with a small number of neurons and increased progressively until the optimum structure was reached. Too few neurons could lead to underfitting and difficulties in mapping
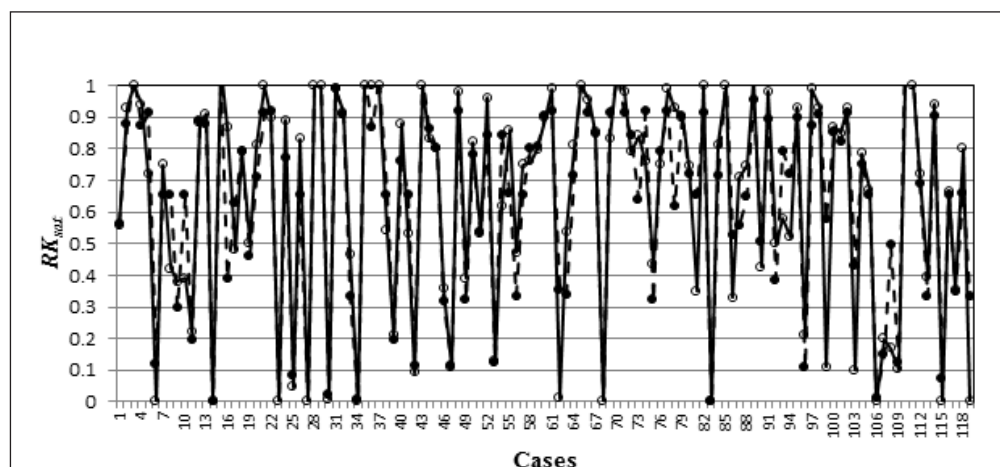

Figure 2. Plots of experimental (solid line with filled circles) versus estimated values (dashed with unfilled circles) of RK_{sat} for the training phase.

the process, while having too many neurons leads to overfitting and increased training time. The optimum model structure was accomplished through trial and error to determine the number of hidden layers and the number of neurons in each layer. It was found that the optimum networks structure to simulate the decrease in RK_{sat} for the networks of four neurons in the input layer needs one hidden layer with 4 neurons to provide one neuron in the output layer. Therefore, the optimum structure was 4-4-1 as illustrated in Figure 1.
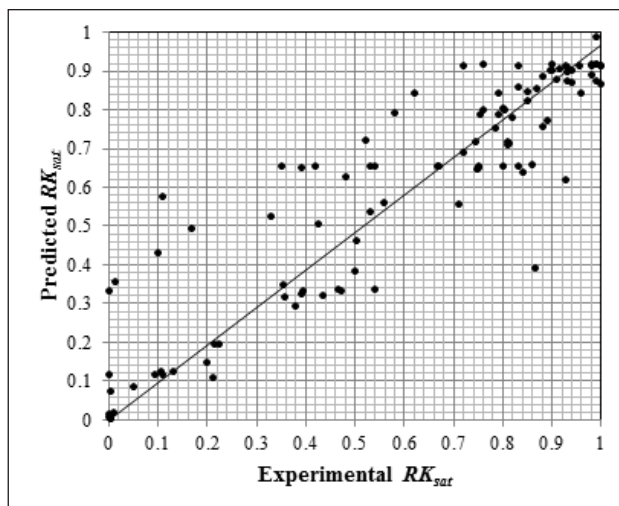

Figure 3. The correlation between the predicted and the experimental RKsat during the training phase.

The ANNs model predictions compared with the real data selected during the training phase are illustrated in Figure 2. It can be noted that the predicted values of RK_{sat} are in good agreement with the experimental values. The good performance of the model is evident from the values of MEA and *RMSE* which are 0.08 and 0.13, respectively. The correlation between the predicted and the experimental RK_{sat} data during the training phase is shown in Figure 3. The correlation coefficient obtained was 0.91, and the R^2 is about 0.83. From 119 values of RK_{sat} plotted, few points fall away from the regression line. This shows that the model was able to estimate RK_{sat} values in most cases during the training phase. However, there are some points where the model tends to overestimate RK_{sat} compared with the experimental data. This may be due to the random errors which are inherent to the experiments. However, the statistic indices confirm that the model of RK_{sat} was appropriate during the training phase.

The plots of experimental versus estimated values of RK_{sat} for the data selected in the testing phase are illustrated in Figure 4. Generally, the performance of the ANN model was good. The model was able to describe the change in RK_{sat}, as is evident from the values of RMSE and MAE in the testing phase, 0.16 and 0.12, respectively. The performance of the model may also be considered acceptable based on the value of the correlation coefficient, which is 0.82. The value of R^2 was 0.68. For the testing phase, statistical indices indicate that the model was to some extent able to predict the decrease due to sodicity. In addition, the parameters chosen to describe soil characteristics were significant in the model (Figure 5). However, the model tends to overestimate RK_{sat} compared with the experimental data. That is probably due to differences associated with random errors which are inherent to the experiments. The data sourced from the literature obtained under different conditions and standards regarding soil columns and solute preparations, which may lead to errors. The amount and the timing of water application were also different for the different experiments, which may result in uncertainty regarding the final RK_{sat}. Such variations are expected in view of the absence of a standard methodology to obtain the TEC curves for a given soil. The variation can also be attributed to the differences in the ratio of dominant clay type (i.e. montmorillonite) in the clay percentage. For example, montmorillonite clay has less thickness and dispersion occurs due to the nature of clay swelling. A slight difference in the montmorillonite ratio could affect RK_{sat}, however, other clay types may be less sensitive to the increase in sodicity levels in ambient solutions, and may also have no role in the dispersion process. The change in soil pH is one of the factors that may cause variation and induce unexpected results as it may alter CEC and significantly change ESP. However, the magnitude of this change is complicated and may differ with the chemical complex and the orientation of the clay particles. Thus, there is a need to set a standard method to estimate RK_{sat} for different soils, which may improve the predictions generated by the model.
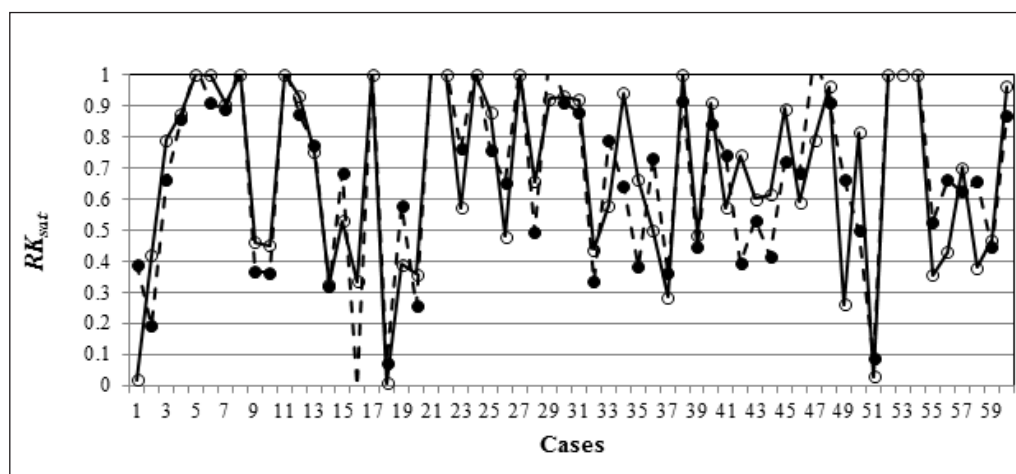

Figure 4. Plots of experimental (solid line with filled circles) versus estimated values (dashed with unfilled circles) of RK_{sat} for the testing phase.
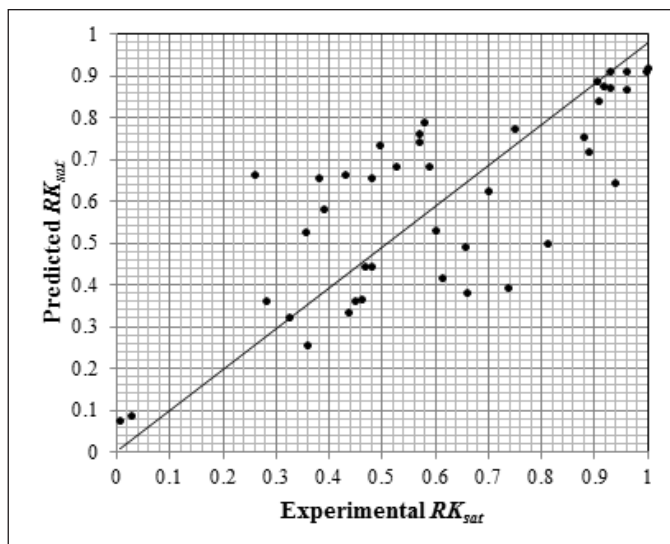
Figure 5. The correlation between the predicted and experimental RK$_{sat}$ during the testing phase

4. Conclusions and Recommendations

Despite the complexity of soil sodicity mechanisms, which hinders the task of generating a generic model to describe the change in conductivity, the ANNs model developed herein describes the decrease in saturated hydraulic conductivity with appropriate accuracy. The performance of ANNs can be attributed to their structural and functional characteristics, such as nonlinear model capability. For the purpose of soil management under irrigation using sodic and saline water, the ANNs model developed here provided enhanced information on the soil's structural instability compared with traditional indictors. However, many factors were not considered in this study, such as soil pH, type of clay and organic matter. This is because of the limitation in the available data. Therefore, there is a need to further examine this model taking other factors into consideration. However, the results suggest that the ANN model performs well in soils with low percentage of organic matter (< %1). In addition, the model can be coupled with chemical, water and solute movement to enhance the modeling process. It is recommended that the research continue in this area toward enhancement and improvement the ANNs model for improved results.

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