Knowledge extraction from artificial neural networks: Case study on reference evapotranspiration in southeastern of rolling pampas of Argentina

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Abstract. Evapotranspiration is an important component of hydrologic balance and represent essential information for irrigation scheduling and water resources planning. The study aimed: a) to evaluate the performance of artificial neural networks (ANNs) with combinations of meteorological inputs for estimating reference evapotranspiration and b) to discuss the knowledge learned by the networks during the training process. Daily evapotranspiration values computed following the Penman-Monteith equation ($ET0_{PM}$), were used as target outputs for the implementation of the ANNs. Data of global radiation (Rg), net radiation (Rn) and extraterrestrial radiation (RTA) were alternated in combinations with air temperature (Ta), vapor pressure deficit (DPV) and wind (u) as inputs to networks. The ANNs with best performance for each combination of inputs were retained in order to evaluate the performance based on multi-criteria analysis. According to the results, it can be concluded that it is possible to estimate accurately daily $ET0_{PM}$ values. A decomposition method based on Garson's algorithm was applied to quantify the relative importance for each input variable. It was examined how model selection in ANNs can be guided by complementary procedures. The application of these methods in evaluation of ANNs models is discussed, paying attention especially on detection of the better predicting variables and analysis of errors.

Key words: Radiation, Deficit Pressure Vapor, Synaptic Weight, Decomposition Method

1 Introduction

Artificial Neural Networks (ANNs) are mathematical models similar to biological neurons, with computational capacity to solve problems of approximation, prediction and optimization [1]. [2]. The application of neural networks in environmental problems is relatively newer than in other research areas, but is becoming popular because of their ability of capturing nonlinear relationships between the variables, and hence, providing key advantages over traditional statistical techniques.

Specifically, the applications in water resources modeling is increasing. Estimation of reference evapotranspiration (ET0), the basic step toward the calculation of crop water requirements, is a case. Several models were developed to predict ET0 from meteorological elements and the most recommended model is Penman-Monteith (PM) procedure presented in [3]. Sometimes, the use of the standard method is restricted by the lack of input variables and, therefore, empirical methods become essential.

Despite the reference in literature about adequate performance of ANNs to approximate reference evapotranspiration under different climate conditions [4], [5], [6],[7], [8], [9], [10], [11], [12], few studies [8], [9], [10], [11], [12] carried out the estimation with a number of variables more reduced than the request for the Penman Monteith-FAO56 method [3].

Because of need of alternative methods for dealing with missing data, some models based on regression have already been evaluated for climate local conditions [13] [14]. Regardless of an acceptable approximation to estimate mean values on 10-days period, a better approximation for daily scale is required. In this sense, the capacity of ANNs to solve approximation problems could be a feasible alternative.

A major drawback often associated with ANNs is to be deficient in understanding the knowledge learnt by the trained network. Since the assimilated knowledge from data during training is represented by the network topology, the activation functions and the synaptic weights, a number of methods have been proposed to extract knowledge based on analysis of synaptic weights or sensitivity analysis [15] [16].

The objectives were: a) to evaluate the performance of models based on artificial neural networks (ANNs) to approximate daily values of reference evapotranspiration ($ET0_{PM}$) with a limited number of input variables and b) to quantify the relative contribution of inputs to model based on connection weight analysis.

2 Material and methods

2.1 Study area, meteorological data and estimation of daily reference evapotranspiration

The southeastern region of rolling pampas is characterized with a climate of the *Cfb* humid subhumid type, according Köppen classification. The present study is focused at Balcarce, Buenos Aires Province, Argentine (37° 45' S, 58º 18´ W, 130 m altitude).

Meteorological data were obtained from a conventional weather station localized at Experimental Station of Instituto de Tecnologia Agropecuaria INTA Balcarce. The site includes observations of daily maximum and minimum air temperatures, relative humidity, wind speed, and daily sunshine duration. Measurements were made at a height of 2 m above the soil surface.

The reference evapotranspiration values, that are target outputs for the artificial neural networks (ANNs), were computed on the daily basis of Penman-Monteith method ($ET0_{PM}$) for the period 1971-2000, following the recommendations in [3]:

$$ET0_{PM} = \frac{0{,}408\,\delta\,(Rn - G) + \gamma \frac{900}{Ta + 273} u\,(DPV)}{\delta + \gamma\,(1 + 0{,}34\,u)} \quad \textbf{(1)}$$

where the $ET0_{PM}$ is reference crop ET calculated using the PenmanMonteith-FAO56 method (mm d^{-1}), Rn is the daily net radiation (MJ $m^{-2}d^{-1}$), G is the daily soil heat flux (MJ $m^{-2}d^{-1}$), Ta is the mean daily air temperature at a height of 2 m (°C), u is the daily mean wind speed at a height of 2 m (m s^{-1}), es is the saturation vapor pressure (kPa), ea is the actual vapor pressure (kPa), δ is the slope of the saturation vapor pressure versus the air temperature curve (kPa°C^{-1}), and γ is the psychrometric constant (kPa°C^{-1}). In this study, the daily values of Δ, Rn, es and ea were calculated using the equations (for albedo, α=0.23 for green vegetation surface) given by Allen et al. (1998). The soil heat flux (G) was assumed to be zero over the calculation for time step of 24 h [3]. The measured RH, Tmax and Tmin values were used to calculate ea and es.

At Balcarce, the daily reference evapotranspiration ($ET0_{PM}$) shows a seasonal pattern with maximum occurring in January (4.9 mm d^{-1}) and minimum in July (0.8 mm d^{-1}). Relative contribution of radiation term is dominant with values about 70% from October to March [18].

The series on study was finished at 2000 due the increasing missing data in more actual series for some of driving variables to give $ET0_{PM.}$ At present and as routine procedure, multiple regression models are used to complete the missing data, at the local weather station.

2.2 Development of ANNs

A schematic representation of neuron model is given in the Fig. 1.

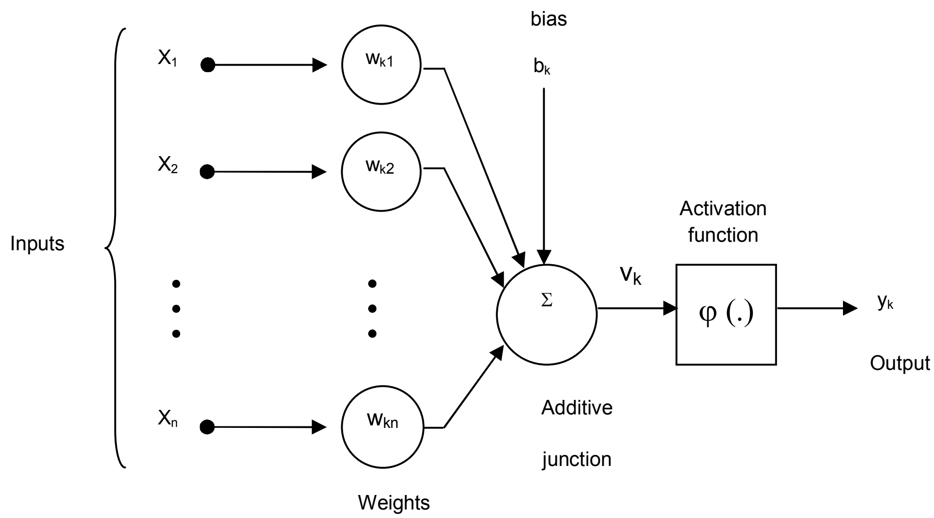

Figure 1. Model of artificial neuron adapted from [1].

Mathematically, the artificial neuron can be described by the equation:

$$y_k = \varphi\left(\sum_{i=1}^{n} x_i \mathrm{w}_{\mathrm{ki}}\right) + \mathrm{b_k} \qquad \textbf{(1)}$$

Where yk is the output neuron; φ is the activation function; X1, X2, ..., Xn are the input signals; and wij are the synaptic weight of k neuron and b_k is the bias. The characteristics of a neural network are: structure or architecture, training algorithm and activation functions. The development of a model based in neural network consists in the definition of these characteristics.

In order to specify a network structure, the relevant input variables and the appropriate number of hidden units respect to samples have chosen. It has been shown that only one hidden layer is required to approximate any continuous function [17]. Models with one hidden layer and one output were utilized in this study; therefore the size of each network was defined by the number of input and nodes in the hidden layer. The maximal number of neurons was defined as related to the number of training samples.

The solar radiation (Rg), net radiation (Rn) and radiation on top of the atmosphere or extraterrestrial radiation (RTA) were combined in the input layer with mean air temperature (Ta), deficit of pressure vapor (DPV) and wind velocity (u). The criteria of mandatory input of some variable linked to available energy to evaporate (Rn, RG or RTA), in all ANNs, was due to the predominant contribution of radiation term in reference evapotranspiration, when estimated by Penman-Monteith model [18].

The daily global radiation (Rg) values were obtained from relative sunshine hours, according a model adjusted for local conditions [19]. The relative sunshine was obtained as the quotient between actual sunshine hours and theoretical sunshine for each day of the year in the location. The radiation on top of the atmosphere (RTA) or extraterrestrial radiation, which only needs latitude data and day of the year, was also combined with maximum daily temperature (Tmax) and minimum daily temperature (Tmin), similar as inputs in Hargreaves method [20].

Activations functions for the hidden units are needed to introduce non-linear components. In this study, two types of transformed of sigmoid activation functions (i.e. logistic and hyperbolic tangent) were applied in the hidden layer and linear ones in the output layer. The sigmoid response, in general, allows a network to map a nonlinear process. A linear function was used in output.

Training of a ANN with the above topology was achieved by adjusting the weights of the neurons through an iterative algorithm that minimizes the error between the predicted outputs and the actual data. The training was carried out under conjugated algorithm of errors propagation using the daily values of $ET0_{PM}$ as target output in the ANNS.

Lack of generalization can be caused by overfitting. A very common technique to avoid this defect is an early stopping criterion that ends training before convergence. So each ANNs architecture was trained under automatic early stopping criterion associated to cross validation method. For this reason, the data set was split into training, validation and test groups to apply cross-validation [21]. Training, testing, and validation sets were representative of the same population. In order to evaluate the hypotheses of equality of frequencies distributions between values of training set with test and validation ones, respectively the non parametrical Kolmogorov-Smirnov test was applied ($p < 0,05$) .

The selection of ANNs architectures was based on the application of a selected algorithm integrated on the IPS (Intelligent Problem Solver) of the Neural Network module of Statistica Software [22]. The inputs and the outputs of data sets were automatically normalized to improve the performance of ANN models. Conjugate of retropropagation of errors algorithm, a second-order non linear optimization technique, was used in training process. The maximal number of neurons was fixed related to the number of examples training. The model with the lowest cross validation error was chosen and then, the ANN with best performance for each combination was retained and evaluated.

The description of ANNs was carried out following: a) the variables used as input, b) the sequence n-m-x, where n is the number of inputs, m is the number of neuron at hidden layer and x is the number of outputs; c) the activation function; d) number of free parameters.

2. 3 Evaluation of ANN models

The evaluation of ANNs performance to estimate daily values of reference evapotranspiration was based on comparison of their performance estimates from FAO-56 (ETo_{PM}). Multi-criteria analysis were used on the basis of root mean of squared error (RMSE), mean absolute error (MAE), mean bias error (MBE) and regression coefficients (a, b, R^2) between estimates from ANNs and measured values. The Student test was used to statistically evaluate the value of either the intercept (H0: a=0) or slope of the straight line (H0: b=1) at the 5% probability level. To assess the capacity of generalization of the ANNs, descriptions of performance are given over both validation and test sets.

2.4 Extraction of knowledge from ANN models

Once the ANNs were trained on a specific network topology, then the modeling of attributes process using ANN involved the extracting knowledge from each network. The embedded knowledge is in the form of connection weights. Garson's method [34] was performed from adjusted synaptic weights of each ANNs. The contribution of each input neuron to the output (c_{ijo}) was computed via each hidden neuron as the product of the input-hidden connection (w_{ij}) and the hidden-output connection (w_{jo}):

$$\mathrm{c_{ijo}} = w_{ij} \times w_{jo} \quad (2)$$

The relative contribution of each input *k* to hidden neuron *j* can be expressed as:

$$r_{ijo} = \frac{|\mathrm{c_{ijo}}|}{\sum_{K=1}^{m} |\mathrm{c_{kjo}}|} \quad (3)$$

The total contribution of input *i* is:

$$S_i = \sum_{J=1}^{n} r_{ijo} \quad \textbf{(4)}$$

Finally, the relative contribution of each input is:

$$RI \quad = S_i / \sum_{k=1}^{m} Sk \quad \textbf{(5)}$$

3 Results and discussion

Frequencies distribution of $ET0_{PM}$ values from training set did not differ from respective test and validation sets. Therefore, the requirement of series to be part of to same population was attended. This fact is relevant because cross-validation was applied during training process, and this method is sensitive to the way that available data are divided [21].

The descriptions of structure and function of the ANNs trained to estimate daily values of $ET0_{PM}$ are summarized in Table 1. A more reduced number of free parameters were needed to approximate the process if radiation (RN, RTA or RG) was combined with some driving variable of the aerodynamic component of evapotranspiration (DPV or u), whereas than the input of another variable of radiation component (Tar) resulted in ANNs with more parameters, except for RG.

Table 1. Description of artificial neural networks (ANNs) trained to estimate daily values of reference evapotranspiration ($ET0_{PM}$) at Balcarce.

ANN	Inputs	Estructure	Activation in hidden layer	Number of free parameters
1	Rn Tar	MLP 2-7-1	Logistic	29
2	Rn DPV	MLP 2-3-1	Hyperbolic Tangent	13
3	Rn Tar DPV	MLP 3-6-1	Hyperbolic Tangent	31
4	Rn u	MLP 2-3-1	Hyperbolic Tangent	13
5	Rn Tar u	MLP 3-4-1	Hyperbolic Tangent	21
6	Rg Tar	MLP 2-3-1	Hyperbolic Tangent	13
7	Rg DPV	MLP 2-3-1	Logistic	13
8	Rg Tar DPV	MLP 3-8-1	Hyperbolic Tangent	41
9	Rg u	MLP 2-3-1	Logistic	13
10	Rg Tar u	MLP 3-6-1	Logistic	31
11	RTA Tar	MLP 2-7-1	Logistic	29
12	RTA DPV	MLP 2-4-1	Logitic	17
13	RTA Tar DPV	MLP 3-3-1	Logistic	16
14	RTA u	MLP 2-5-1	Logistic	21
15	RTA Tar u	MLP 3-3-1	Hyperbolic Tangent	16
16	RTA Tmax Tmin	MLP 3-10-1	Logistic	51

The 2 input models that combined Tar and radiation exhibited a bigger number of nodes in hidden layer than those with DPV or u, inside of each group, except for Rg. This can be explained due multicollineal variables require more sized structure in the network due the presence of mutual information.

From regression analysis and errors of estimation between outputs of the ANNs and $ET0_{PM}$ values was possible to distinguish some combinations of variables with better performance. The analyses were carried out on both data sets (validation and test). In Table 2 are reported the results on validation set. In general, the input of DPV improved the performance, whichever the radiation used. The MAE values ranged from 0.2 to 0.6 mm d^{-1} were equivalent to 9 and 22% of observed mean values of validation series. Furthermore, the ANNs with DPV did not imply structures with high number in hidden layer. The combination of RTA with Tmax and Tmin did not improve the performance respect model with DPV.

The RTA was not input in the six best ANNs of the group when ranked in function of minor RSME. The difference in RSME between the best ranked ANN with RTA (ANN12) was about 19% and 49% and RTA in comparison to their analogue models with Rg (ANN8) and Rn (ANN3), respectively. The last ANN ranked in function of minor RSME (ANN14) increased 62% the RSME respect their analogue combination with Rn (ANN4).

The RSME increased 20% when RTA was combined with Tar instead Tmax and Tmin (ANN11 vs ANN16). A better explanation from this combination can be associated with the humidity description from difference in maximum and minimum temperatures. Following [20] The a and b parameters obtained by regression analyses between the target output and estimates from ANNs did not differ significantly from 0 and 1, respectively, being possible to infer that ET estimated from ANNs did not differ from reference evapotranspiration ($ET0_{PM}$), except for the ANNs

Table 2. Errors of estimation of the ANNs trained to approximate daily reference evapotranspiration (ET_{0PM}) for the validation set (pairs of data=2121)

ANN	Model MLP	a mm d^{-1}	b	R^2	RSME mm d^{-1}	MAE mm d^{-1}	MBE mm d^{-1}
1	$ET0_{PM}$ (Rn Tar)	-0.0402	0.9333	0.93	0.4790	0.3848	0.2205
2	$ET0_{PM}$ (Rn DPV)	0.0168	0.9734	0.96	0.3155	0.2231	0.0506
3	E $T0_{PM}$ (Rn Tar DPV)	-0.0115	0.9782	0.96	0.3045	0.2164	0.0669
4	$ET0_{PM}$ (Rn u)	-0.0302	0.9750	0.91	0.4825	0.3620	0.0939
5	$ET0_{PM}$ (Rn Tar u)	0.0115	0.9549	0.93	0.4303	0.3205	0.1051
6	$ET0_{PM}$ (Rg Tar)	-0.0318	0.9425	0.93	0.4571	0.3600	0.1849
7	$ET0_{PM}$ (Rg DPV)	0.0230	0.9863	0.93	0.4280	0.3292	0.0111
8	$ET0_{PM}$ (Rg Tar DPV)	0.0052	0.9757	0.94	0.3819	0.2866	0.0564
9	$ET0_{PM}$ (Rg u)	-0.0033	1.0031	0.88	0.5413	0.4138	-0.0043
10	$ET0_{PM}$ (Rg Tar u)	0.0002	0.9717	0.94	0.3923	0.2960	0.0719
11	$ET0_{PM}$ (RTA Tar)	-0.0403	0.9239	0.83	0.7191	0.5287	0.2479
12	$ET0_{PM}$ (RTA DPV)	-0.0657	0.9955	0.92	0.4596	0.3311	0.0772
13	$ET0_{PM}$ (RTA Tar DPV)	-0.0854	1.0088	0.92	0.4544	0.3312	0.0629
14	$ET0_{PM}$ (RTA u)	-0.0351	0.9506	0.76	0.7826	0.5540	0.1657
15	$ET0_{PM}$ (RTA Tar u)	0.0132	0.9408	0.82	0.6858	0.4977	0.1421
16	$ET0_{PM}$ (RTA Tmax Tmin)	0.0061	0.9303	0.87	0.5983	0.4505	0.1794

RMSE: root mean square error; MAE: mean absolute error; MBE: mean bias error.

In Table 3 the results on test set to are reported. The accuracy of the model on the test data gives a realistic estimate of the performance of the model on completely unseen data and in order to confirm the actual predictive power of the network. The same ANNs ranking according RSME values was maintained for test evaluation. The losses on generalization (RSME of test set – RSME of validation test) varied between 0 and 6.4%. The ANN 9 was the model that showed more decline in predictive power.

In general, the input of DPV improved the performance, whichever the radiation used. The MAE values ranged from 0.2 to 0.6 mm d^{-1} were equivalent to 9 and 22% of observed mean values of validation series. Furthermore, the ANNs with DPV did not imply structures with high number in hidden layer. The combination of RTA with Tmax and Tmin did not improve the performance respect model with DPV.

The RTA was not input in the six best ANNs of the group when ranked in function of minor RSME. The difference in RSME between the best ranked ANN with RTA (ANN12) was about 19% and 49% and RTA in comparison to their analogues with Rg (ANN8) and Rn (ANN3), respectively. The last ANN ranked in function of minor RSME (ANN14) increased 62% the RSME respect their analogue combination with Rn (ANN4).

The RSME increased 20% when RTA was combined with Tar instead Tmax and Tmin (ANN11 vs ANN16). A better explanation from this combination can be associated with humidity description from difference in maximum and minimum temperatures. Following [20], the temperature difference is linearly related to relative humidity. The a and b parameters obtained by regression analyses between the target output and estimates from ANNs did not differ significantly from 0 and 1, respectively, being possible to infer that ET estimated from ANNs did not differ from reference evapotranspiration ($ET0_{PM}$), except for two ANNs.

Table 3. Errors of estimation of the ANNs trained to approximate daily reference evapotranspiration (ET_{0PM}) for the test set (pairs of data=2159)

ANN	Model MLP	RSME mm d^{-1}	MAE mm d^{-1}	MBE mm d^{-1}
1	$ET0_{PM}$ (Rn Tar)	0.4798	0.3814	-0.1323
2	$ET0_{PM}$ (Rn DPV)	0.4798	0.3814	-0.1323
3	E $T0_{PM}$ (Rn Tar DPV)	0.3075	0.2318	-0.0539
4	$ET0_{PM}$ (Rn u)	0.2973	0.2237	-0.0697
5	$ET0_{PM}$ (Rn Tar u)	0.5243	0.3999	-0.0146
6	$ET0_{PM}$ (Rg Tar)	0.4396	0.3404	-0.0509
7	$ET0_{PM}$ (Rg DPV)	0.4728	0.3728	-0.1042
8	$ET0_{PM}$ (Rg Tar DPV)	0.4325	0.3388	-0.0229
9	$ET0_{PM}$ (Rg u)	0.3872	0.2962	-0.0520
10	$ET0_{PM}$ (Rg Tar u)	0.6057	0.4635	0.0709
11	$ET0_{PM}$ (RTA Tar)	0.4197	0.3192	-0.0237
12	$ET0_{PM}$ (RTA DPV)	0.7136	0.5205	-0.1725
13	$ET0_{PM}$ (RTA Tar DPV)	0.4653	0.3377	-0.1050
14	$ET0_{PM}$ (RTA u)	0.4634	0.3390	-0.0925
15	$ET0_{PM}$ (RTA Tar u)	0.7939	0.5858	-0.0971
16	$ET0_{PM}$ (RTA Tmax Tmin)	0.6917	0.5086	-0.0974

RMSE: root mean square error; MAE: mean absolute error; MBE: mean bias error.

Despite the importance of radiation component in reference evapotranspiration values from Penman Monteith method [18], the contribution of Rn was not predominant in the models tested with reduced number of variables (ANN1 to ANN5). The relative contribution of aerodynamic components (DPV and u) was similar when Rn was regarded in input (ANN2 and ANN4), but did not for models with Rg (ANN 7 vs ANN9) or RTA (ANN12 vs ANN14).

When Tar was input with DPV or u, the RI values of Rn decreased (ANN3 and ANN5). In general, the contribution relative of Rg tended to increase in each model (ANN6 to ANN10) respect the same combination with Rn and other variables (ANN1 to ANN5). It was conspicuous the contribution the one variable to model in ANN12 (RTA) and ANN15 (u). The Ri of RTA was minor when air temperature was input as maximum and minimum daily values than the average value (ANN16 vs ANN11).

Table 4. Relative contribution of inputs (RI) to neural network to approximate daily reference evapotranspiration ($ET0_{PM}$).

						RI			
ANN	Inputs	Rn	Rg	RTA	Ta	Tmax	Tmin	DPV	U
1	Rn Ta	0.36			0.64				
2	Rn DPV	0.41						0.59	
3	Rn Ta DPV	0.16			0.47			0.37	
4	Rn u	0.45							0.55
5	Rn Ta u	0.21			0.41				0.38
6	Rg Ta		0.39		0.61				
7	Rg DPV		0.46					0.54	
8	Rg Ta DPV		0.41		0.20			0.39	
9	Rg u		0.61						0.39
10	Rg Ta u		0.42		0.38				0.20
11	RTA Ta			0.55	0.45				
12	RTA DPV			0.80				0.20	
13	RTA Ta DPV								
14	RTA u			0.33					0.67
15	RTA Ta u			0.11	0.06				0.83
16	RTA Tmax Tmin			0.24		0.48	0.28		

4 Conclusions

A description of the knowledge that was learned by the ANNs during their training was obtained by applying a simple knowledge extraction method. An advantage of this method is that additional information about the model performance is obtained, including the relative contribution of inputs via analysis of connection weights in the ANNs.

In addition, techniques of knowledge extraction could be carried out in further studies in order to determine the types of problems where artificial neural networks would yield better results than other methods. The results reported here also contribute to coping with problems of scarce or missing data and thus can be used to guide priorities for data acquisition.

An application example is analyzed to illustrate the use of the model and demonstrate its capabilities of effectively analyzing and predicting the reference evapotranspiration.

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