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ORIGINAL ARTICLES

A comparison of methods for assessing the relative importance of input variables in artificial neural networks

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ABSTRACT

Artificial neural networks are considering powerful statistical modeling technique in the agricultural sciences; however, they provide little information about the contributions of the independent variables in the prediction process. The goal of relative importance analysis is to partition explained variance among multiple predictors to better understand the role played by each predictor. In the present study, a modification to Connection Weights Algorithm and a novel algorithm are proposed to assess the relative importance of independent variables in multilayer perceptron neural network and a comparison in the field of crop production with the Connection Weights Algorithm, Dominance Analysis, Garson's Algorithm, Partial Derivatives, and Multiple Linear Regression is presented. The performance of the two proposed algorithms is studied for empirical data. The Most Squares method (the second proposed algorithm) is found to be a better method in comparison to the above mentioned methods and seem to perform much better than the other methods, and agree with the results of multiple linear regressions in terms of the partial R^2 and consequently, it seem to be more reliable.

Key words: Artificial neural networks, relative importance, statistical modeling.

Introduction

The relationships between variables in agriculture are almost very complicated. One of the most appropriate methods to illustrate these relationships is Artificial Neural Networks (ANNs). A number of authors have shown the interest of using ANNs instead of linear statistical models (Özesmi and Özesmi, 1999). The main application of ANNs is the development of predictive models to predict future values of a particular dependent variable from a given set of independent variables. The contribution of the input variables in predicting the output is difficult to be explained within the network. Consequently, input variables are entered into the network and an output value is generated without understanding the inter-relationships between the variables, and therefore, providing no explanation by the network (Ripley, 1996). The study of contributions of input variables for ANNs models has been attempted only by few authors. For example (Duh, *et al.*, 1998) have presented a methodology to understand how an input is correlated to the predicted output by the ANNs. They have tested this methodology on three datasets and have shown that the results correspond well to the partial least squares method interpretation for linear models. (Olden and Jackson, 2002) have reviewed a number of methods (Neural Interpretation Diagram, Garson's algorithm and sensitivity analysis) and demonstrated utility of these methods for interpreting neural network connection weights. (Olden *et al.*, 2004) have provided a comparison of different methodologies for assessing variable contributions in artificial neural networks using simulated data exhibiting defined numeric relationships between a response variable and a set of predictor variables. They proposed an approach called connection weights method to outperform other methods in quantifying importance of variables. They have shown that the connection weight method is the least biased among others. This method has also been used in comparison to other available methods in assigning the relative contribution of input variables in prediction of the output by (Watts and Worner, 2008).

Materials and Methods

An experiment was set up during the summer seasons of 2012 and 2013, Soil Salinity Laboratory, Alexandria, Egypt to investigate the effect of irrigation with saline water (0.5, 2.75, 5.5 dS/m) on yield and yield components of maize as well as the relative importance of yield components. Well water was used as a source of saline water. Grains of maize cultivar (Gemmeiza 12) were obtained from Crops Research Institute, Agricultural Research Center, Egypt. The soil and irrigation water were analyzed according to **(**Chapman and Pratt, 1978) before sowing and had the following characteristics:

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Table 1: Physical and chemical analyses of soil before sowing.

Sand %	Silt %	Clay %	Soil texture	E.C. dS/m	pH	S.P. %	SAR
74.0	10.4	15.6	Sandy loam	1.82	7.53	43.33	1.49

Table 2: Chemical analyses of irrigation water.

Treatments	PH	E.C.	Cations, meq/ L.				Anions, meq/L.		
		dS/m	Ca^{2+}	Mg^{2+}	K^+	Na^+	HCO_3^-	Cl^-	SO_4^{2-}
Tap water	7.6	0.62	2.2	1.73	0.18	2.75	3.55	2.11	1.2
Well water	7.8	5.44	1.8	2.4	3.9	48.0	2.9	32.0	13.9

The experimental design was Randomized Complete Block Design (RCBD) with four replicates; the experimental unit was a cemented plot with a dimension of 150 cm in long and 75 cm in wide with an area of 1.125 m^2. Every cemented plot contains four rows, the grain were sown in the first of May and before sowing the plots were prepared by adding calcium superphosphate 15.5% P_2O_5 at a rate of 100 kg/feddan (Hectare = 2.38 feddan) and potassium sulphate 48% K_2O_4 at a rate of 50 kg/feddan, the nitrogen fertilizer rates were added at the rate of 125 kg N/feddan as ammonium sulphate 20.5% N at three doses, the first at sowing, the second at the first irrigation, and the third at the second irrigation.

At the end of the experiment the following characters were measured:

Number of rows/ear, number of grains/row, 100 kernels weight (g), and grain yield (g/plot).

The data were subjected to the analysis of standardized and stepwise multiple linear regression according to (Snedecor and Cochran, 1982) and dominance analysis using SAS computer software (SAS Institute Inc., 2003).

A program was proposed by the author, based on Microsoft Access 2007 and containing modules written in visual basic computer language, was used to perform the comparison among the different relative importance methods, figure 2.

Neural network training and architecture:

A three layer feed forward neural network was trained using back propagation algorithm. The three layered feed forward network contains one input layer, one hidden layer and one output layer. The input layer contains 3 neurons corresponding to 3 independent variables, number of rows/ear (X1), number of grains/row (X2), and 100 kernels weight (g) (X3) whereas the output layer contains one neuron corresponding to one dependent variable, grain yield (g/plot) (GY). The sigmoid activation function was used at both the hidden layer and the output layer. The structure of the multilayer perceptron neural network used in this study and its connections between layers is shown in Figure 1.

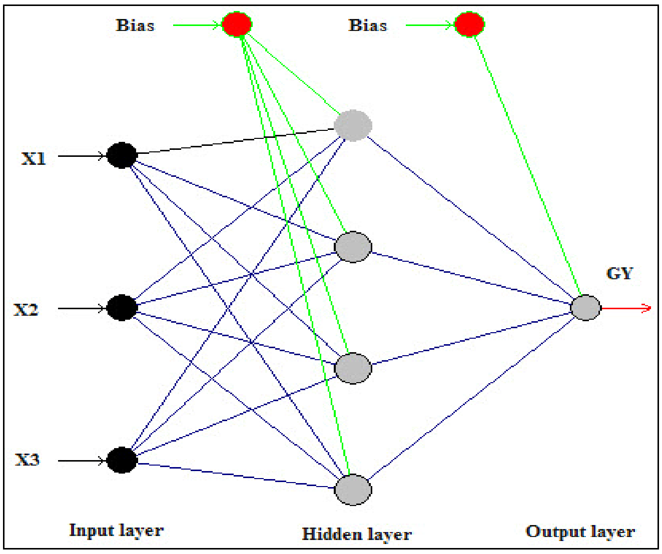

Fig. 1: Structure of the multilayer perceptron neural network used in this study.

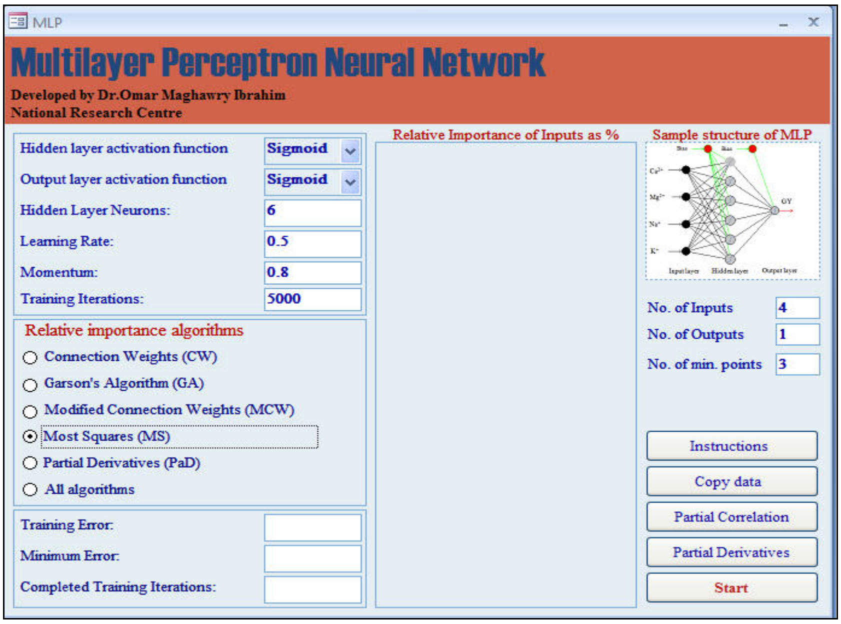

Fig. 2: Interface of the proposed program used to perform the comparison among the studied methods.

Results and Discussion

Effect of water salinity on yield and yield components of maize:

Data presented in Table (3) show that irrigation with saline water adversely and significantly influenced number of grains/row, 100 kernels weight (g), and grain yield of maize plants (g/plot) as compared with control plants. However, number of rows/ear was not significantly affected by water salinity. The reduction in grain yield of maize plants was 32.13% and 61.31% when the plants were irrigated with 2.5 and 5.5 dS/m, respectively. These results are in agreement with (Khodary, 2004).

Table 3: Effect of water salinity on number of rows/ear, number of grains/row, 100 kernels weight (g), and grain yield (g/plot) of maize plants, (combined analysis of the two seasons).

Salinity	Number of Rows/ear	Number of grains/row	100 kernels weight(g)	Grain yield(g/plot)
Control	11.50 a	30.25 a	23.68 a	407.02 a
2.5 dS/m	11.50 a	19.25 b	20.40 a	262.03 b
5.5 dS/m	12.00 a	15.75 b	17.25 b	170.50 c

Relative importance of independent variables methods:

The relative importance of predictor or input variables is the contribution of each of the variables for predicting the dependent variable. The proposed methods are defined after a brief description of the connection weights algorithm in order to quantify the relative importance of independent variables in predicting the output variable for neural network.

1- Connection weights algorithm (CW):

The connection weights algorithm **(**Olden and Jackson, 2002) calculates the sum of products, Table (5) of final weights of the connections from input neurons to hidden neurons, Table (4) with the connections from hidden neurons to output neuron, Table (4) for all input neurons. The relative importance of a given input variable can be defined as:

$$RI_x = \sum_{y=1}^{m} w_{xy} w_{yz}$$

Where RI_x is the relative importance of input neuron x, $\sum_{y=1}^{m} w_{xy} w_{yz}$ is sum of product of final weights of the connection from input neuron to hidden neurons with the connection from hidden neurons to output neuron, y is the total number of hidden neurons, and z is output neurons. This approach is based on estimates of network final weights obtained by training the network. It is observed that these estimates of final weights may vary with the change in the initial weights used for starting the training process.

Table 4: Final connection weights.

Input-hidden				
	Hidden1	Hidden2	Hidden3	Hidden4
X1	-0.8604	1.0651	-0.1392	1.0666
X2	-6.6167	1.5145	-5.3051	1.3358
X3	-1.7338	1.4107	-1.4207	0.7845
Hidden-output				
	Hidden1	Hidden2	Hidden3	Hidden4
GY	-5.2075	2.0158	-4.4617	1.5858

Table 5: Connection weights products, relative importance and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Sum	Relative importance	Rank
X1	4.4805	2.1469	0.6212	1.6914	8.94	9.75%	3
X2	34.4562	3.0529	23.6698	2.1184	63.30	69.03%	1
X3	9.0286	2.8436	6.3388	1.2442	19.46	21.22%	2
Sum	47.97	8.04	30.63	5.05	91.69	100%	

2- The first proposed algorithm (MCW):

This method is referred to as Modified Connection Weights. In this proposed algorithm, the connection weights of the artificial neural network model is obtained after training the network, after the calculation of sum of product of final weights of the connections from input neurons to hidden neurons with the connections from hidden neurons to output neuron for all input neurons, a correction term (partial correlation) is multiplied by this sum and the absolute value is taken, this is called the corrected sum, Table (6), then to calculate the relative importance of each input, the corrected sum of each input is divided by the total corrected sum as illustrated in the following equation.

$$RI_x = \frac{\left|\sum_{y=1}^{m} w_{xy} w_{yz} \times r_{ij.k}\right|}{\sum_{x=1}^{n} \sum_{y=1}^{m} w_{xy} w_{yz}}$$

where RI_x is the relative importance of neuron *x*, $\sum_{y=1}^{m} w_{xy} w_{yz}$ is sum of product of raw weights of the connection from input neuron to hidden neurons with the connection from hidden neurons to output neuron, $r_{ij.k}$ is partial correlation of input *i* with output *j* after input *k*, $\sum_{x=1}^{n} \sum_{y=1}^{m} w_{xy} w_{yz}$ is the total corrected sum of all inputs.

The correction term is the partial correlation; the partial correlation is the correlation that remains between two variables after removing the correlation that is due to their mutual association with the other variables. The correlation between the dependent variable and an independent variable when the linear effects of the other independent variables in the model have been removed.

The partial correlation for first order is illustrated in the following equation:

$$r_{ij.k} = \frac{r_{ij} - r_{ki} \times r_{kj}}{\sqrt{\left(1 - r_{ki}^2\right) \times \left(1 - r_{kj}^2\right)}}$$

where $r_{ij.k}$ is partial correlation of input *i* with output *j* after input *k*, r_{ij} is the simple correlation between input *i* and output *j*, r_{ki} is the simple correlation between input *k* and input *i*, r_{kj} is the simple correlation between input *k* and output *j*.

Table 6: Absolute corrected sum and relative importance of inputs.

Inputs	Sum	partial correlation	Absolute corrected Sum	Relative importance	Rank
X1	8.94	0.5266	4.71	5.920%	3
X2	63.30	0.9584	60.66	76.28%	1
X3	19.46	0.7275	14.15	17.80%	2
Total	91.69		79.53	100%	

3-The second proposed algorithm (MS):

This method is referred to as Most Squares. In this proposed algorithm, the connection weights between hidden layer and the output layer were not used; however, the connection weights between input layer and hidden layer were used, both the initial weights before start training, Table (7) and the final weights after training the network, Table (4). The second step is to sum the squared difference between initial and final weights for each input. The third step is to divide the sum of squared difference for each input on the total sum of all inputs, Table (8). The following equation is used to calculate the relative importance of each input.

$$RI_x = \frac{\sum_{x=1}^{m} \left(w_{xy}^{i} - w_{xy}^{f} \right)^2}{\sum_{x=1}^{m} \sum_{y=1}^{n} \left(w_{xy}^{i} - w_{xy}^{f} \right)^2}$$

where RI_x is the relative importance of neuron *x*, $\sum_{x=1}^{m} \left(w_{xy}^{i} - w_{xy}^{f} \right)^2$ is the sum squared difference between initial connection weights and final connection weights from input layer to hidden layer, and $\sum_{x=1}^{m} \sum_{y=1}^{n} \left(w_{xy}^{i} - w_{xy}^{f} \right)^2$ is the total of sum squared difference of all inputs.

Table 7: Input-hidden initial connection weights.

	Hidden1	Hidden2	Hidden3	Hidden4
X1	0.0236	0.1943	0.1478	0.2054
X2	0.0562	-0.3437	-0.3215	-0.0894
X3	-0.1488	0.1844	-0.0608	0.3267

Table 8: Squared difference between initial and final connection weights, relative importance, and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Sum	Relative importance	Rank
X1	0.7815	0.7582	0.0824	0.7416	2.3638	2.84%	3
X2	44.5279	3.4528	24.8357	2.0313	74.8478	89.87%	1
X3	2.5121	1.5039	1.8493	0.2096	6.0749	7.29%	2
Sum					83.2865	100.00%	

4- Multiple linear regression (MLR):

A comparison between MLR and the other methods was undertaken in order to judge their predictive capabilities. The stepwise multiple regression technique (Weisberg, 1980 and Tomassone *et al*., 1983) was computed especially to define the significant variables and their contribution order. In fact the influence of each variable can be roughly assessed by checking the final values of the regression coefficients. Standardized regression coefficient has been suggested as a measure of relative importance of input variables by many investigators (Afifi and Clarke, 1990). For each input variable, standardized regression coefficient is obtained by standardizing the variable to zero mean and unit standard deviation before multiple linear regression is carried out. However, when input variables are correlated, the influence of correlations between input variables makes standardized regression coefficient not interpretable in explaining the relative importance (Johnson, 2000).

Researchers have developed other indices that accurately reflect the contribution of input variables to the prediction of a dependent variable when variables are correlated. The two most recent methodologies are dominance analysis (Budescu, 1993, and Azen and Budescu, 2003) and Johnson's epsilon (also referred to as relative weights; (Johnson, 2000). The results of multiple linear regression are shown in Table (9). The results revealed that number of grains/row (X2) was the most important variable with a partial R^2 of 0.8568 followed by 100 kernels weight (g) (X3) (0.0552), and number of rows/ear (X1) (0.0217). To make a comparison with the other methods, the relative importance of each input was computed by dividing its partial R^2 on the sum of R^2 for all inputs which is equal to regression R^2 (0.9337), for example the relative importance of number of grains/row (X2) is computed as: RI = (0.8568/0.9337)*100 = 91.76 %.

5- Dominance analysis (DA):

DA determines the dominance of one input over another by comparing their additional contributions across all subset models. Dominance analysis is chosen over other recent measures for reasons stated by (Lebreton *et al*., 2004). Dominance analysis (Budescu, 1993) approaches the problem of relative importance by examining the change in R^2 resulting from adding an input to all possible subset regression models. By averaging all of the possible models (average squared semi partial correlation), we can obtain general dominance weight of an input, which reflects the contribution by itself and in combination with the other inputs, and overcoming the problems associated with correlated inputs. The results of dominance analysis are presented in Table (10). To make a comparison with the other methods, the relative importance of each input was computed by dividing its overall average contributions on the sum of all overall average contributions for all inputs which is equal to regression R^2 (0.9337), for example the relative importance (RI) of number of grains/row (X2) is computed as follows: RI = (0.7836/0.9337)*100 = 83.92%.

Table 9: Results of multiple linear regression and correlation.

	Parameter estimates	Standardized estimates	Significance	Partial R^2	Relative importance based on contribution to regression R^2	Simple Correlation	Partial Correlation
Intercept	-547.161						
X1	21.185	0.1514	0.0001	0.0217	2.32%	0.1088	0.4965
X2	21.270	0.8622	0.0001	0.8568	91.76%	0.9256	0.9560
X3	10.452	0.2764	0.0001	0.0552	5.91%	0.4310	0.7138

Table 10: Relative importance and rank of inputs.

Inputs	Overall average contributions of inputs	Relative importance based on contribution to regression R^2	Rank
X1	0.0198	2.12%	3
X2	0.7836	83.92%	1
X3	0.1303	13.96%	2
Total		100.00%	

6- Garson's algorithm (GA):

(Garson, 1991) proposed a method for partitioning the neural network connection weights in order to determine the relative importance of each input variable in the network. It is important to note that Garson's algorithm uses the absolute values of the final connection weights when calculating variable contributions, and therefore does not provide the direction of the relationship between the input and output variables as illustrated in the following equation.

$$RI_x = \sum_{x=1}^{n} \frac{\left| w_{xy} w_{yz} \right|}{\sum_{y=1}^{m} \left| w_{xy} w_{yz} \right|}$$

where RI_x is the relative importance of neuron *x*, $\sum_{y=1}^{m} w_{xy} w_{yz}$ is sum of product of final weights of the connections from input neurons to hidden neurons with the connections from hidden neurons to output neurons. Table (11) shows the contribution of each input to each hidden neuron, for example the contribution of number of grains/row (X2) is (0.7184) resulted from dividing its products (34.4562) on the sum of products of all inputs (47.97) in Table (5) and take the absolute result.

Table 11: Relative contribution of each input neuron to each hidden neuron, relative importance, and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Sum	Relative importance	Rank
X1	0.0934	0.2669	0.0203	0.3347	0.72	17.88%	3
X2	0.7184	0.3795	0.7728	0.4192	2.29	57.25%	1
X3	0.1882	0.3535	0.2069	0.2462	0.99	24.87%	2
					4.00	100%	

7- Partial derivatives (PD):

To obtain the relative importance of each input, the partial derivatives of the ANN output with respect to the inputs were computed (Dimopoulos *et al*., 1999). In a network with n_i inputs, one hidden layer with n_h

neurons, and one output neuron, the partial derivatives of the output y_j with respect to input x_j and N total number of observations are:

$$d_{ji} = S_j \sum_{h=1}^{n_h} w_{ho} I_{hj}(1 - I_{hj}) w_{ih}$$

where S_j is the derivative of the output neuron with respect to its input, I_{hj} is the response of the h_{th} hidden neuron, w_{ho} and w_{ih} are the connection weights between the output neuron and h_{th} hidden neuron, and between the i_{th} input neuron and the h_{th} hidden neuron. If the partial derivative is negative the output variable will tend to decrease while the input variable increases. Inversely, if the partial derivatives are positive, the output variable will tend to increase while the input variable also increases. The relative importance of the ANN output is calculated by a sum of the square partial derivatives, SSD, obtained per input variable as follows:

$$\mathrm{SSD}_i = \sum_{j=1}^{N} (d_{ji})^2$$

The input variable which has the highest SSD value is the most important variable, and inversely the input variable that has the lowest SSD value is the lowest important variable. The results of partial derivatives methods are shown in Table (12).

Table 12: Relative importance and rank of inputs.

	Partial derivatives	
Inputs	Relative importance	Rank
X1	0.16%	3
X2	98.23%	1
X3	1.61%	2
Total		

Comparison of the 7 methods used for quantifying relative importance of inputs:

Based on the results of Multiple Linear Regression (MLR), the Most Squares method was found to exhibit the best overall performance compared to the other methods with regard to its accuracy, where the degree of dissimilarity coefficient between MLR and Most Squares (MS) was the lowest, 0.2242, Table (13), both were in the same cluster, Figure 4 and produced comparable results, Figure 3. The performance of Partial Derivatives (PD), (Gevrey *et al*., 2003), was less than MS where the degree of dissimilarity coefficient between PD and MLR was 0.7594. Dominance Analysis (DA) and Modified Connection Weights (MCW) showed moderate performance where dissimilarities were 1.0842 and 1.8490, respectively. Connection Weights (CW) and Garson's Algorithm (GA) performed poorly where dissimilarities were 2.6719 and 4.1282, respectively. MS method was found to accurately quantifying the relative importance of input variables and may be favored over the other methods tested in this study. Such approach could successfully identify the relative importance of all input variables in the neural network, including variables that exhibit both strong and weak partial correlations with the dependent variable.

Table 13: Distance matrix based on Euclidian dissimilarity coefficient for the 7 relative importance methods.

	CW	MCW	MS	MLR	DA	GA	PD
CW	0.0000						
MCW	0.8949	0.0000					
MS	2.4487	1.6254	0.0000				
MLR	2.6719	1.8490	0.2242	0.0000			
DA	1.8240	0.9297	0.8870	1.0842	0.0000		
GA	1.6119	2.4921	3.9144	4.1282	3.4090	0.0000	
PD	3.4312	2.6005	0.9827	0.7594	1.7773	4.8753	0.0000

J. Appl. Sci. Res., 9(11): 5692-5700, 2013

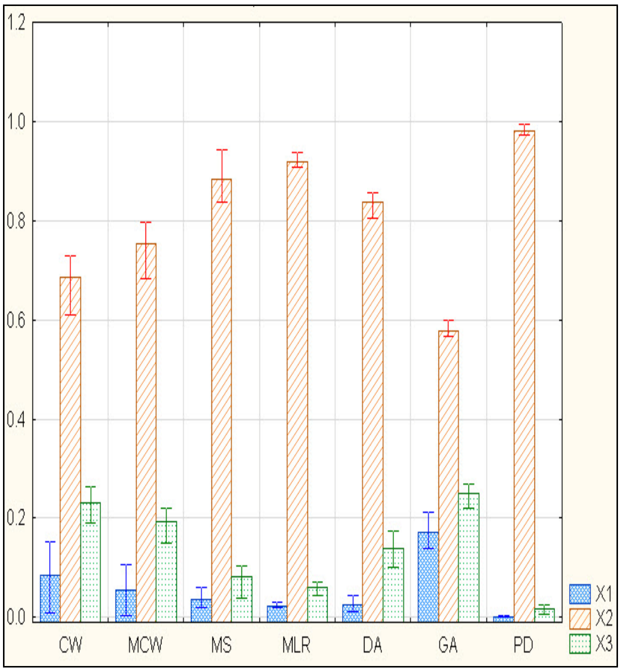

Fig. 3: Range plot showing relative importance of the inputs according to each of the 7 methods.

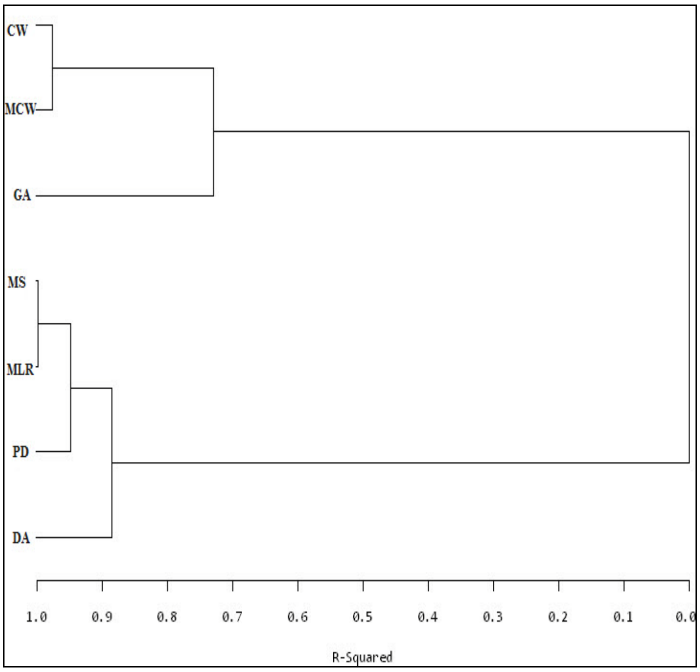

Fig. 4: Dendrogram showing cluster analysis (Ward method) of the 7 relative importance methods.

Conclusion:

The present study provides a comparison of the performance of 7 different methods for assessing variable relative importance. Two algorithms are proposed to estimate the relative importance of the independent variables. The performance of the proposed algorithms is studied using empirical data sets. Most Squares (MS) is seemed to perform much better than the other methods, and agree with the results of multiple linear regression in terms of the partial R^2 and seem to be more reliable. The application of such effective models could effectively offer better understanding of the variables govern specific crop parameter.

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