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Evaluating the effect of salinity on corn grain yield using multilayer perceptron neural network

O. M. Ibrahim
Plant Production Department, Arid Lands Cultivation Research Institute,
City of Scientific Research and Technological Applications (SRTA-City),
New Borg El-Arab, Alexandria 21934,
Egypt

Abstract

Multilayer perceptron neural network (MLP) is a powerful statistical modeling technique in the agricultural sciences. The aim of the relative importance analysis is to separate explained variance among multiple predictors to better understand the role played by each predictor or independent variable in relation to the dependent variable. To assess the relative importance of independent variables (Na^+, K^+, Ca^{2+}, and Mg^{2+}) which have negative relationship with the dependent variable (corn grain yield) in multilayer perceptron neural network the current study was carried out to make a comparison among different algorithms, the Connection Weights Algorithm, Modified Connection Weights Algorithm, Most Squares Algorithm, Dominance Analysis, Garson's Algorithm, Partial Derivatives, Profile Method, and Multiple Linear Regression. The performance of these algorithms is studied for empirical data. The Most Squares Algorithm was found to be a better algorithm in comparison to the above mentioned algorithms and seem to perform much better, and agree with the results of multiple linear regression in terms of the partial R^2 and seem to be more reliable, Most Squares Algorithm cleared that Na^+ had the main impact on corn grain yield followed by Mg^{2+}, K^+, and Ca^{2+}, respectively.

Keywords: salinity, relative importance, multilayer perceptron neural network

1. INTRODUCTION

The nature of the relationships between independent and dependent variables in agriculture are almost very complicated. One of the most successful methods to illustrate these relationships is multilayer perceptron neural network. A number of authors have shown the interest of using Artificial Neural Networks (ANNs) instead of linear statistical models **(Özesmi and Özesmi, 1999, Ibrahim, 2012, Ibrahim, 2013, Ibrahim *et al*., 2013, Ibrahim *et al*., 2014).** The main application of ANNs is to develop predictive models to predict future values of a dependent variable from a set of independent variables. The study of the contributions of input variables in ANNs models has been attempted only by few authors. **(Ibrahim, 2013)** has presented a new method to understand how yield components of corn as inputs are correlated to the grain yield as output by the MLP. He has tested this new method on empirical dataset and has shown that the results correspond well to the partial least squares method interpretation for multiple linear regression 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

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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).**

2. MATERIALS AND METHODS

An experiment was set up during the summer seasons of 2012 and 2013 to investigate the effect of three levels of water salinity (0.5, 2.75, 5.5 dS/m.) on yield and yield components of Maize as well as the relative importance of Calcium (Ca^{2+}), Magnesium (Mg^{2+}), Sodium (Na^{+}), and Potassium (K^{+}) as the major cations. Grain of Maize cultivar (Gemmeiza 12) was obtained from Field Crops Research Institute, Agricultural Research Center, Egypt. The soil was analyzed according to **(Chapman and Pratt, 1978)** before sowing and had the following mechanical and chemical characters. Soil texture was sandy loam where Sand (74%), silt (10.4%), and clay (15.6%). Electrical conductivity (1.82 dS/m), pH (7.53), Saturation percent (43.3%). 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 sowing in first May and before sowing the cemented plot 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 of 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 grain/row, 100 kernel weight (g), and grain yield (g/plot).

The data was subjected to analysis of standardized and stepwise multiple linear regression according to **(Snedecor and Cochran, 1982)** and dominance analysis using SAS computer software v.9.1.3 SP4, 2003. A program was written 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 multilayer perceptron neural network is considered and 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 4 neurons corresponding to 4 independent variables, Ca^{2+}, Mg^{2+}, Na^{+}, K^{+} and the output layer contains one neuron corresponding to one dependent variable, corn grain yield (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).

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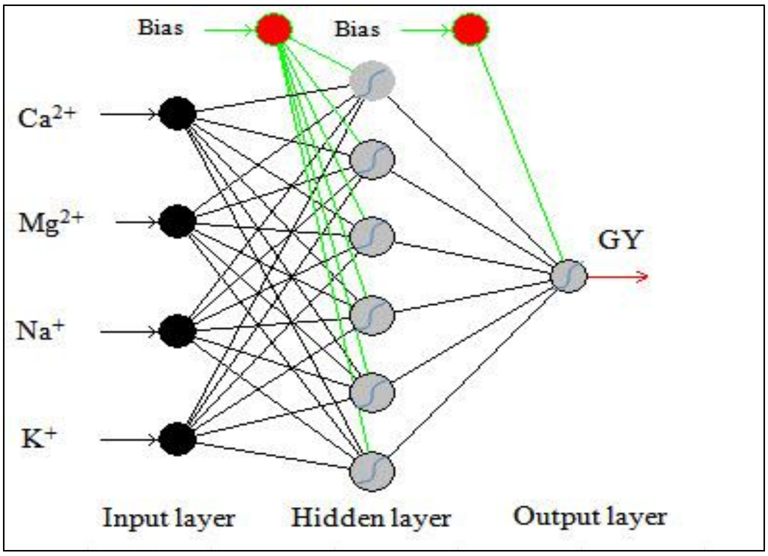

Fig.1. Structure of the multilayer perceptron neural network used in this study.

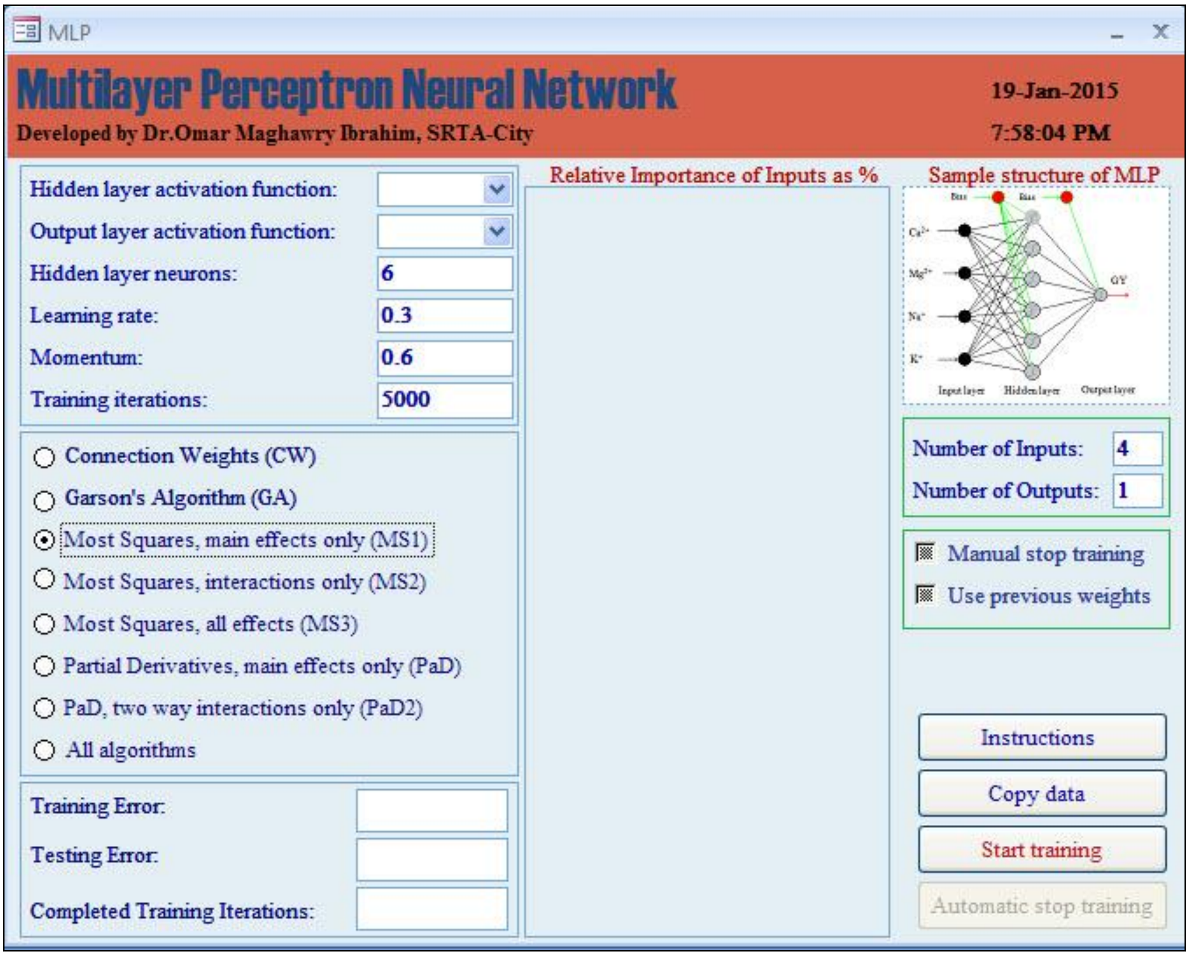

Fig.2. Interface of the program used to perform the comparison among the studied methods.

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3. RESULTS AND DISCUSSION

Relative importance of independent variables methods

The relative importance of a predictor or input variables is the contribution of each of the variables for predicting the dependent variable.

1- Connection weights algorithm (CW)

The connection weights algorithm **(Olden and Jackson, 2002)** calculates the sum of products (Table 3) of final weights of the connections from input neurons to hidden neurons (Table 1) with the connections from hidden neurons to output neuron (Table 2) 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 (1). Input-hidden final connection weights

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6
Ca^{2+}	-0.511	-0.068	-0.188	-0.273	0.385	-0.106
Mg^{2+}	-1.101	2.723	0.505	0.203	1.425	-0.504
Na^{+}	1.261	-3.402	-0.831	-1.348	6.157	0.140
K^{+}	0.139	-0.630	-0.055	0.132	-0.978	-0.304

Table (2). Hidden-output final connection weights

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6
GY	-1.136	2.802	0.563	0.753	-3.790	-0.315

Table (3). Connection weights products, relative importance and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6	Sum	Absolute sum	Relative importance	Rank
Ca^{2+}	0.580	-0.191	-0.106	-0.206	-1.461	0.034	-1.350	1.350	3.12%	4
Mg^{2+}	1.250	7.632	0.285	0.153	-5.401	0.159	4.077	4.077	9.44%	2
Na^{+}	-1.433	-9.535	-0.468	-1.015	-23.331	-0.044	-35.826	35.826	82.93%	1
K^{+}	-0.158	-1.764	-0.031	0.099	3.706	0.096	1.947	1.947	4.51%	3
Sum	0.240	-3.858	-0.321	-0.968	-26.488	0.244	-31.150	43.200	100%	

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2- Modified Connection Weights (MCW)

This method was proposed by (**Ibrahim, 2013)**. In this 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 4), 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 from both.

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 (4). Absolute corrected sum and relative importance of inputs.

Inputs	Sum	partial correlation	Absolute corrected Sum	Relative importance	Rank
Ca^{2+}	-1.350	0.044	0.0596	0.174%	3
Mg^{2+}	4.077	0.648	2.6417	7.73%	2
Na^{+}	-35.826	-0.877	31.4089	91.93%	1
K^{+}	1.947	0.029	0.0570	0.167%	4
Total	-31.150		34.1672	100%	

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3- Most Squares (MS)

This method was proposed by (**Ibrahim, 2013**). In this 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 5) and the final weights after training the network (Table 1). 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 6). 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 (5). Input-hidden initial connection weights

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6
Ca^{2+}	0.0236	-0.3437	-0.0608	0.2627	0.1889	0.0868
Mg^{2+}	0.0562	0.1844	0.2564	-0.3138	-0.3158	0.1045
Na^{+}	-0.1488	0.2224	0.2054	0.3179	0.0654	-0.1670
K^{+}	-0.1401	0.1478	-0.0894	-0.0962	-0.0221	-0.1560

Table (6). Squared difference between initial and final connection weights, relative importance, and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6	Sum	Relative importance	Rank
Ca^{2+}	0.2859	0.0759	0.0162	0.2872	0.0386	0.0373	0.7412	1.06%	4
Mg^{2+}	1.3381	6.4470	0.0620	0.2671	3.0310	0.3708	11.5161	16.43%	2
Na^{+}	1.9889	13.1394	1.0742	2.7754	37.1024	0.0943	56.1746	80.13%	1
K^{+}	0.0779	0.6044	0.0012	0.0521	0.9133	0.0220	1.6708	2.38%	3
Sum							70.1027	100.00%	

4- Multiple linear regression (MLR)

A comparison between MLR and the other methods was made in order to judge their predictive capacities. The stepwise multiple regression technique **(Tomassone *et al*., 1983)** was computed especially to define the significant variables and their contribution. In fact the influence of each input variable can be 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 authors **(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 regression is carried out. The results of multiple linear regression are shown in (Table 7). The results revealed that Na^{+} was the most important variable with a partial R^2 of 0.7067 followed by Mg^{2+} (0.1531), Ca^{2+} (0.0003), and K^{+} (0.0001). 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 (86.01), for example the relative importance of Na^{+} is computed as: RI= (0.7067/0.8601)*100 = 82.16 %.

Table (7). 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	577.479	0					
Ca^{2+}	2.693	0.0240	0.75970 ns	0.0003	0.03%	-0.300	0.044
Mg^{2+}	50.148	0.7767	0.00010 **	0.1531	17.80%	-0.540	0.648
Na^{+}	-14.798	-1.5387	0.00010 **	0.7067	82.16%	-0.841	-0.877
K^{+}	11.845	0.0126	0.85160 ns	0.0001	0.01%	-0.522	0.029

5- Dominance analysis (DA)

Dominance analysis determines the dominance of one input over another by comparing their additional contributions across all subset models. Dominance analysis **(Azen and Budescu, 2003)** 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 8). 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 (86.01), for example the relative importance (RI) of Na^{+} is computed as follows:
RI = (0.5571/0.8601)*100 = 64.78%.

Table (8). Relative importance and rank of inputs.

Inputs	Overall average contributions of inputs	Relative importance based on contribution to regression R^2	Rank
Ca^{2+}	0.0353	4.10%	4
Mg^{2+}	0.1684	19.58%	2
Na^{+}	0.5571	64.78%	1
K^{+}	0.0993	11.55%	3
Total	0.8601	100%	

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.

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

where RI_x is the relative importance of neuron *x*, $\sum_{y=1}^{m} w_{xy} w_{yz}$ is sum of product of final weights of the connections from input neurons to hidden neurons with the connections from hidden neurons to output neurons. (Table 9) shows the contribution of each input to each hidden neuron, for example the contribution of Ca^{2+} is (2.421) resulted from dividing its products (0.580) on the sum of products of all inputs (0.240) in (Table 3) and take the absolute result.

Table (9). Relative contribution of each input neuron to each hidden neuron, relative importance, and rank of inputs.

	Hidden1	Hidden2	Hidden3	Hidden4	Hidden5	Hidden6	Sum	Relative importance	Rank
Ca^{2+}	2.421	0.050	0.331	0.212	0.055	0.137	3.206	12.25%	3
Mg^{2+}	5.213	1.978	0.888	0.158	0.204	0.651	9.092	34.75%	2
Na^{+}	5.975	2.471	1.460	1.048	0.881	0.181	12.016	45.93%	1
K^{+}	0.659	0.457	0.097	0.103	0.140	0.393	1.848	7.06%	4
							26.16	100%	

The results in (Table 10) reveal that Garson's algorithm produced inaccurate results where it tends to under estimate the most important input and over estimate the lowest important input.

7- Partial derivatives (PD)

To obtain the relative importance of each input, the partial derivatives of the MLP 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 that 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 10).

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8- Profile Method (PM)

Profile method involves varying each input variable across its entire range while holding all other input variables constant; so that the individual contributions of each variable are assessed. This approach is somewhat cumbersome, however, because there may be an overwhelming number of variable combinations to examine. As a result, it is common first to calculate a series of summary measures for each of the input variables (minimum, maximum, quartiles, percentiles), and then vary each input variable from its minimum to maximum value, in turn, while all other variables are held constant at each of these measures **(Özesmi and Özesmi, 1999)**. The results of profile method are shown in (Table 10).

Table (10). Relative importance and rank of inputs.

	Partial derivatives		Profile Method	
Inputs	Relative importance	Rank	Relative importance	Rank
Ca^{2+}	0.00005%	4	7.36%	3
Mg^{2+}	1.74%	2	19.18%	2
Na^{+}	98.26%	1	71.13%	1
K^{+}	0.00007%	3	2.33%	4
Total	100%		100%	

Comparison of the 8 methods used for quantifying relative importance of input variables:

According to 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, 0.4949 (Table 11), they were in the same cluster (Fig. 4), and produced comparable results (Fig. 3). The performance of Modified Connection Weights (MCW) was less than MS where the degree of dissimilarity coefficient between MCW and MLR was 1.1563, Connection Weights (CW), Partial Derivatives (PD), **(Gervey *et al*., 2003)**, and Profile Method (PM) showed moderate performance (dissimilarity 1.2750, 1.8706, and 2.1446 respectively), whereas Garson's Algorithm (GA), and Dominance Analysis (DA) performed poorly (dissimilarity 3.9906 and 3.3219 respectively). Furthermore, MS exhibits acceptable precision compared to the other methods, as indicated by the small variation around its mean (Fig. 3). In contrast, CW, GA, and PM exhibit large variation around their means. MS method was found to accurately quantifying the relative importance of input variables and should be favored over the other methods tested in this study. This method successfully identified 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. GA was the poorest performing method, because it uses absolute connection weights to calculate variable relative importance, and therefore does not account for negative connection weights. However, all other methods used raw connection weights to calculate variable relative importance. Fig.2 provides an illustration about the key difference among the methods and shows how GA can result in incorrect estimates of variable relative importance.

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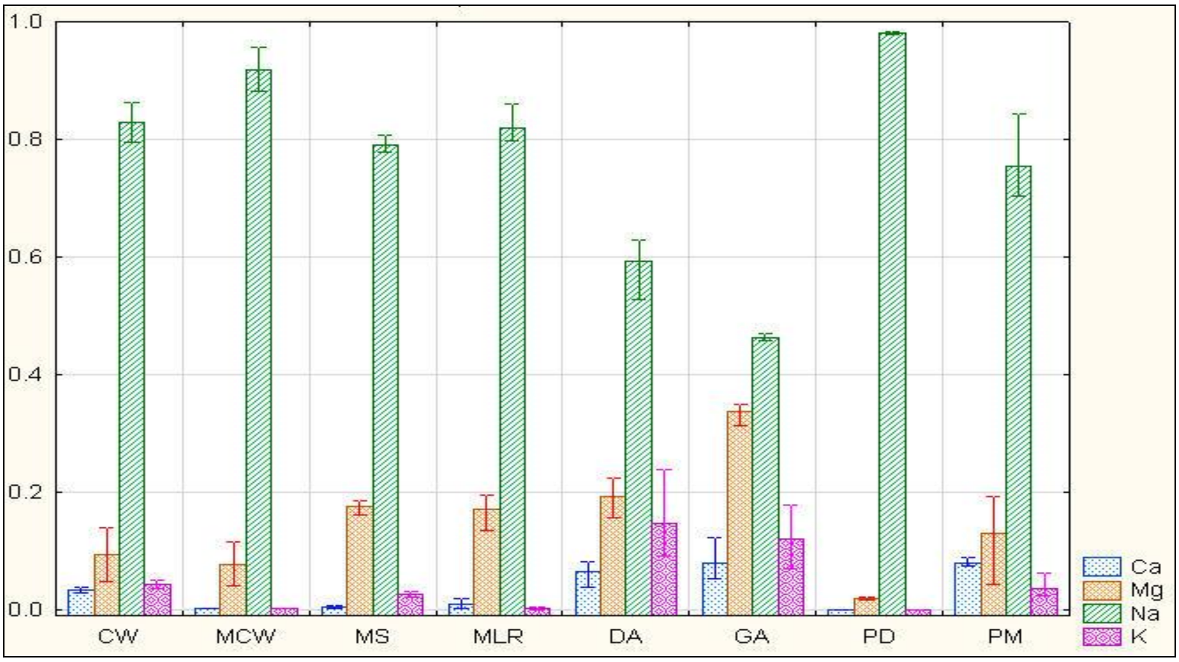
Table (11). Distance matrix based on Euclidian dissimilarity coefficient for the 8 relative importance methods.

	CW							
CW	0.0000	MCW						
MCW	1.2843	0.0000	MS					
MS	1.2338	1.3704	0.0000	MLR				
MLR	1.2750	1.1563	0.4949	0.0000	DA			
DA	2.7004	3.8893	2.9784	3.3219	0.0000	GA		
GA	3.8470	4.9006	3.7125	3.9906	1.7984	0.0000	PD	
PD	1.7047	0.7172	2.0648	1.8706	4.3443	5.4951	0.0000	PM
PM	1.4142	2.5363	2.1604	2.1446	2.2922	3.1369	2.9355	0.0000

CW=connection weight, MCW=Modified connection weight, MS= most squares, MLR=multiple linear regression, DA=dominance analysis, GA=garson's algorithm, PD=partial derivatives, PM=profile method



CW=connection weight, MCW=Modified connection weight, MS= most squares, MLR=multiple linear regression, DA=dominance analysis, GA=garson's algorithm, PD=partial derivatives, PM=profile method

Fig.3. Relative importance of the inputs according to each of the 8 methods.

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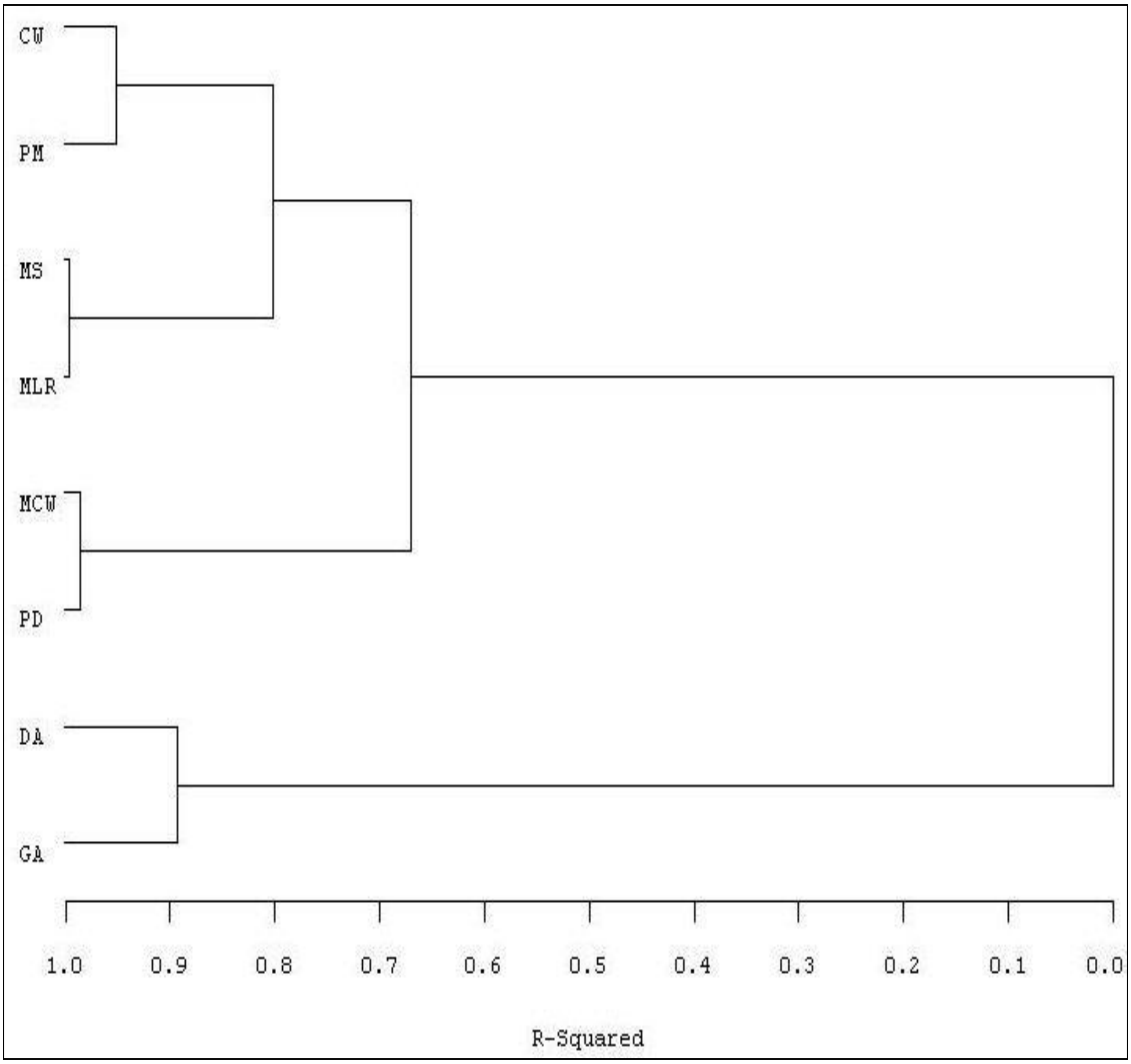

CW=connection weight, MCW=Modified connection weight, MS= most squares, MLR=multiple linear regression, DA=dominance analysis, GA=garson's algorithm, PD=partial derivatives, PM=profile method

Fig.4. Dendrogram showing cluster analysis (Ward method) of the 8 relative importance methods.

4. CONCLUSION

The current study provides a comparison of the performance of 8 different methods for assessing variable relative importance. The performance of the algorithms are studied using empirical data sets having negative relationships between one or/and more of the independent variables with the output. 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. Most Squares Algorithm cleared that Na^+ had the main impact on corn grain yield followed by Mg^{2+}, K^+, and Ca^{2+}.

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