Estimation of antioxidant activity of foods using artificial neural networks

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Summary

The aim of this study was to demonstrate that artificial neural networks (ANN) is an economical and rapid method to estimate antioxidant activity of foods. Phenolic content of different food varieties (red pepper and grape seeds) was used as two input variables, and ferric ion reducing antioxidant power (FRAP) values were estimated as output. The number of total experimental data was 150 (70 % for train, 30 % for test). The developed ANN was able to reveal the relationship between phenolic compounds and antioxidant activity of food with the feed-forward model. The estimated FRAP values calculated by ANN correlated with experimental FRAP values with high correlation coefficients. In addition, error rate was found to be approximately 10 %, which corresponds to approximately 90 % of success. The relationship between antioxidant substances and antioxidant activity demonstrated that ANN can be used to determine the antioxidant properties of foods and results of this study showed that this was possible. By this way, it was demonstrated that ANN is a reliable software-based method to estimate antioxidant capacities of foods with savings of time, labour and experimental costs.

Keywords

antioxidant activity; ferric ion reducing antioxidant power; phenolic compounds; artificial neural network

It is important to estimate the future accurately for anyone who must make decisions about the future because accuracy of the decision depends on the success of the prediction. Besides many forecasting techniques that have been traditionally used, artificial intelligence technologies have come to use in recent years. Artificial neural networks (ANN) models are derived from artificial intelligence and provide successful applications for forecasting in different fields such as business, industry and science [1–6]. ANN is a system, which consists of interconnected artificial neurons. It was developed for mathematical modelling of functioning of biological neurons. The learning process is completed with the support of these artificial neurons similar to human brain. Learning process occurs between input and output variables without requiring any prior knowledge. In this way, neurons can provide linear or non-linear modelling. Therefore, as a forecasting tool, ANN is more general and flexible method than others [7].

Free radicals are highly unstable and reactive species, which contain unpaired electrons in an atomic orbital. Because of the reactivity of free radicals, they can easily interact with biologically relevant molecules such as DNA, proteins, carbohydrates or lipids. Free radicals attack these important substances, which leads to cell damage. An antioxidant compound can be defined as a substance that reduces or inhibits the adverse effects of free radicals to cellular components [8, 9]. Therefore, there has been increasing interest to determine the antioxidant potential of natural products. Antioxidants can be produced synthetically, such as butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT) tert-butylhyd-

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roquinone (TBHQ) or propyl gallate (PG). However, due to the carcinogenic and toxic effects of these compounds, consumers have interest in natural antioxidants [10, 11]. Natural antioxidants include phenolic compounds (flavonoids, phenolic acids and tannins), carotenoids, tocopherols, ascorbic acids and their derivatives. It was reported that phenolic compounds have the most important antioxidant capacity among all antioxidant substances. Therefore, they are considered as potential agents to prevent oxidative damage by mechanisms of singlet oxygen quenching, metal ion chelation and free-radical scavenging. Phenolic compounds are mainly found in plant kingdom and they form a large group of phytochemicals [12, 13].

It is important to determine the antioxidant capacity of plants due to the potential protective factors of phenolic compounds and other antioxidants against cancer and heart diseases [14]. Different chemical methods can be used to evaluate the antioxidant activity of products. One of the widely used method is ferric ion reducing antioxidant power (FRAP) assay, whose principle is the reaction of tripyridyl triazine-ferric complex (Fe(III)-TPTZ) with antioxidants. This assay was initially developed to determine the antioxidant capacity of plasma, but it has been used to measure antioxidant capacity of biological samples and foods [15, 16]. In the literature, there are studies about the strong relationship with total phenolic contents and FRAP assay. Seventy medicinal plant extracts were screened for antioxidant capacity and total phenolics, and a significant linear correlation (R = 0.9825) was found between total phenolic content and FRAP assay [17]. Other researchers also reported a high correlation of total phenolic compounds and FRAP assay [18, 19].

Artificial neural networks (ANN) have been used in food industry for modelling many processes. Guiné et al. [3] predicted the antioxidant activity and phenolic compounds of bananas from banana variety, dryness state, type and order of extract by using a simple neural network. Prediction of antioxidant activities and classification of wines using ANN were attempted with a limited set of analytical measurements, which were total phenolics, flavonoids, anthocyanins and tannins. The study reported that ANN was a reliable approach tool to predict antioxidant activity and wine characteristics [20]. Similar study was done to predict antioxidant activity and classify some teas using ANN. It was also successful in classification and prediction of antioxidant potential of tea samples [21]. In several studies, ANN was used in food engineering [22–26]. However, as far as we know, there is no study on prediction of FRAP values based on the phenolic content. The purpose of the study was to obtain a model for estimation of antioxidant activity of foods based on total phenolic content by using ANN. Phenolic content of different food varieties (red pepper and grape seeds) was used as two input variables and FRAP values were estimated as output in this research.

MATERIALS AND METHODS

Plant materials and preparation of extracts

Grape seeds were obtained from Pistachio Research Station in Gaziantep, Turkey. Red peppers were obtained from local markets in Sakarya, Turkey. Samples were taken into a tube and methanol : water mixture (70 : 30, v/v) was added as a solvent. The tubes were treated at ambient temperature in an ultrasonic water bath (Bandelin Sonorex, Berlin, Germany) for 15 min. Then, they were centrifuged (Hettich Universal 320R, Newport Pagnell, United Kingdom) at 13 130 $\times g$ at 4 °C for 10 min, and supernatant was separated for analysis [27].

Determination of total phenolic content

The amount of total phenols was determined spectrophotometrically according to Gao et al. [28]. A volume of 0.1 ml of extract was mixed with 2 ml of distilled water and 0.2 ml of Folin-Ciocalteu reagent. One milliliter of sodium carbonate solution (20%) was added after 3 min and incubated at ambient temperature for 1 h. Absorbance of samples was determined at 765 nm (UV-1240; Shimadzu, Kyoto, Japan). The results were expressed as grams of gallic acid equivalents per kilogram of sample. Precision was expressed as relative standard deviation (*RSD*) found to be lower than 2 % with $r^2 = 0.9961$.

Ferric ion reducing antioxidant power assay

FRAP assay was carried out by a modified method of Benzie and Strain [15]. The FRAP reactant was prepared by mixing (10 : 1 : 1) 300 mmol·l^{-1} acetate buffer (pH 3.6), 10 mmol·l^{-1} TPTZ and 20 mmol·l^{-1} $FeCl_3$ solutions. Volumes of 0.1 ml of the extracts were taken to tubes, followed by the addition of 1.8 ml of FRAP reactant and 1.2 ml of distilled water. Absorbance was measured at 593 nm after incubation at 37 °C for 15 min. Aqueous solutions of $FeSO_4 \cdot 7H_2O$ were used to construct the calibration curve and the results were expressed as grams of $FeSO_4$ per kilogram of sample. Precision was expressed as *RSD* found to be less than 3 % with $r^2 = 0.9947$.

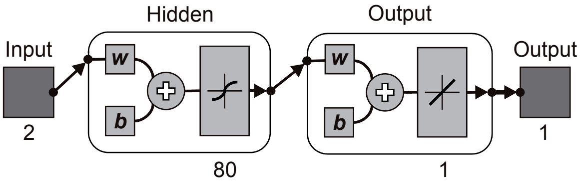

Fig. 1. Artificial neural network topology.

w – weight vector (artificial neural network learning coefficients), *b* – bias input (threshold value of artificial neural network neurons to be active).

Artificial neural network analysis

Artificial neural network is the architecture combining numbers of artificial neurons for the processing of data similar to basic biological neural networks. This architecture consists of interconnected components with one-way channels. There are three type of networks, which are feed forward, cascade connected and feedback [29].

Cascade connected network, which has at least one feedback network from previous layer, is a single or multilayer network type.

Feedback is a network in which at least one cell is also feed from next layer.

Feed-forward neural network was used in this study and it is the type of network in which the cells on the layer are fed only from the cells on the previous layer. This structure is composed of three layers, namely, input layer, intermediate layer and output layer. Data come from input layer and move towards intermediate and output layer unidirectionally. The internal structure is extremely complex and composed of several layers [30].

The working principle of network is as follows: The information from outer world is given to input layer firstly. There is one neuron for each input and processing of information is not generally performed in this layer. The received data are transmitted to the intermediate layer and this layer processes the information. The intermediate layer consists of one or more layers and information is mainly processed in this layer [30]. Most of the time, it can be also called as hidden layer. This layer has one neuron for each case in the training set. These neurons contain learning coefficients. The values reached after mathematical calculations are transferred to neurons in the output layer. Weighed values collected in the intermediate layer are compared in the output layer. The largest estimation value is generated as the output value for the target category. This type of ANN operates according to supervised learning strategy. Back propagation learning algorithm is widely used in training [31]. Levenberg-Marquardt backpropagation (LM) algorithm was used in this study.

The structure of ANN used in simulation is shown in Fig. 1. The number of input data was tested by number of data among 1–100 neurons individually and all results were recorded. Moreover, performance evaluation criteria of the network were calculated in order to evaluate the network performance.

Levenberg-Marquardt backpropagation training function

The most commonly used structure in ANN is based on Newton and back-propagation algorithm. Input data pass through hidden layer, are transmitted to output layer and let off as output. Error rate is determined by comparing the actual values and output values. Derivative of the error rate is transmitted to the hidden layer and an attempt to reduce the error rate is made by changing the weight values of neurons [32]. Error rate is calculated by the least square method. By this way, change of weight values is done to increase the performance values. However, this advantage is slowed down ANN in terms of speed this makes no sense, please correct.

The aim of using the algorithm is to achieve Hessian matrix by second order derivative of performance function with regard to weight values.

$$H(n) = J^T(n).J(n) + \mu_m.I \quad (1)$$

In this equation, H, μ_m, I express Hessian matrix, Marquardt parameter and identity matrix, respectively. J, Jokobian matrix, indicates the first order derivative of network error based on weight. n and T represent iteration number and transpose matrix, respectively.

$$J(n) = \frac{de(n)}{dw(n-1)} \quad (2)$$

where e states vector of network error, w indicates weight value.

Gradient of network (g) is calculated as

$$g(n) = J^T(n)e(n) \quad (3)$$

and obtained by Eq. 4.

$$w(n+1) = w(n) - [H(n)]^{-1}g(n) \quad (4)$$

Value of μ_m decreases at each step of getting error value. The goal is calculation of weight value which makes the performance function smallest [33].

Data processing

For ANN modeling, numbers of data for red pepper and grape seeds were 58 and 92, respectively. Variety of foods (red pepper and grape seeds) and phenolic contents were encoded in the input layer. The output layer was made of antioxidant activity of samples (FRAP value). All neurons between 1–100 were tried one by one and empirical evidence showed that the best result was obtained with 80 neurons. Therefore, all results given in this study were obtained using 80 neurons in the hidden layer. The number of total experimental data was 150 for ANN analysis. The data were randomly allocated in the MATLAB script to train (70 %) and test (30 %) for all network topologies.

The separation process was done according to the systematic sampling theorem. The first group was obtained by choosing 30 % of the total data according to this theorem. The remaining 70 % of data made up the second group. The code has been written in the MATLAB programming language for decomposition of data groups. The data were separated according to the automatic and systematic sampling theorem. The training set was used to calculate function parameters of the network and the test set was used to estimate FRAP values of samples.

Performance evaluation criteria

Mean square error (*MSE*), error rate (in percent) and Sperman correlation coefficient were used to measure the performance of the network. *MSE* was calculated by the Eq. 5 in a data set with estimated value (Y_{ANN}), real value (Y_{Real}) and size (n) [34]. There was no specific threshold value to interpret the network. However, this value close to zero meant that the system performance was high.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\left(Y_{Real}^{i} - Y_{ANN}^{i}\right)^{2} \quad (5)$$

Change between estimated value and real value (in percent) was examined. It could be said that system worked with error rate (H_{err}) expressed in percent (Eq. 6).

$$H_{err} = \frac{1}{n}\sum_{i=1}^{n}\frac{\left|Y_{Real}^{i} - Y_{ANN}^{i}\right|}{Y_{Real}^{i}} \times 100 \quad (6)$$

Correlation coefficient gives information about degree and direction of relationship between variables. Different correlation coefficients have been developed according to type of variables. While they are calculated between continuously variable data types, distribution of the data sets is important in determination of correlation coefficient. If the group shows normal distribution, Pearson correlation coefficient is calculated. However, Sperman correlation coefficient is used if the group does not show a normal distribution. In this study, Sperman correlation coefficient was used and calculated using the following equation [34]:

$$r_s = 1 - 6\sum_{i=1}^{n}\frac{d_i}{n(n^2 - 1)} \quad (7)$$

where d_{i} is the difference between sequence numbers of *i.* observation, i is calculated observation number and n is observation number.

Cases of $n < 30$ and $n > 30$ were taken into consideration for statistical decision. For $n < 30$, it was fulfilled by utilizing table of Sperman rank correlation coefficient according to error level (α) and degree of freedom ($n - 2$) [34]. t statistic is calculated in the case of $n > 30$. It is compared to t table statistic according to α and ($n - 2$). It is required that the obtained p statistical value is smaller than 0.05.

RESULTS AND DISCUSSION

The goal of this study was to estimate the antioxidant activity of foods based on phenolic contents. Red pepper and grape seeds were used as samples. Total phenolic content and antioxidant activity of red pepper and grape seeds were different. Therefore, different type of foods were used to widen the applicability of ANN model. To build the ANN-based model, total set of samples was divided into two subsets to train ANN and test the estimation capability. In order to train the subset, 105 of samples were randomly selected, while the testing subset had 45 samples. The ANN topology and parameters were selected as 2–80–1 neurons in input-hidden-output layers (Fig. 1).

The experimental and estimated results of training and testing sets are shown in Tab. 1. The errors (*Er*) between experimental ($FRAP_{\mathrm{exp}}$) and estimated ($FRAP_{\mathrm{est}}$) values of training and testing sets were calculated and average error was found to be 8.5 % and 10.1 %, respectively. This meant that estimations were accurate for the training and testing sets. Buciński et al. [23] demostrated the success of prediction of antioxidant capacity of cruciferous sprouts based on the contents of bioactive compounds. They found that mean of difference between experimental and calculated values of Trolox equivalent antioxidant capacity ($TEAC_{\mathrm{exp}}$ and $TEAC_{\mathrm{calc}}$) for testing set was 6.06 mmoles of Trolox per kilogram of dry matter. However, the difference between $TEAC_{\mathrm{exp}}$ and $TEAC_{\mathrm{calc}}$ was 12.7 % (recalculated), which was higher than in this study. Hosu et al. [20] predicted the antioxidant activity of Romanian red wines

Tab. 1. Training and testing set.

Number of sample	Training set			Testing set		
	TPC [g·kg^{-1}]	*FRAP*$_{exp}$ [g·kg^{-1}]	*FRAP*$_{est}$ [g·kg^{-1}]	*TPC* [g·kg^{-1}]	*FRAP*$_{exp}$ [g·kg^{-1}]	*FRAP*$_{est}$ [g·kg^{-1}]
1	0.62	3.02	3.31	0.64	2.57	3.38
2	0.82	3.05	4.00	1.12	3.07	4.97
3	0.75	3.07	3.74	0.78	3.21	3.87
4	0.60	3.10	3.25	0.95	3.42	4.42
5	0.71	3.31	3.61	0.68	3.55	3.51
6	0.65	3.38	3.41	0.80	3.69	3.94
7	0.76	3.44	3.78	0.74	3.79	3.71
8	0.69	3.47	3.54	0.78	4.08	3.84
9	0.78	3.62	3.84	0.87	4.13	4.17
10	0.73	3.69	3.68	0.75	4.24	3.74
11	0.62	3.70	3.31	0.77	4.29	3.81
12	1.02	3.71	4.66	0.97	4.33	4.49
13	0.78	3.84	3.84	0.84	4.61	4.07
14	0.85	4.04	4.10	0.93	4.68	4.36
15	0.69	4.08	3.54	0.95	4.94	4.42
16	0.87	4.10	4.17	1.47	5.35	6.07
17	1.14	4.15	5.03	1.54	5.65	6.30
18	0.91	4.15	4.30	1.27	5.82	5.43
19	0.72	4.25	3.64	1.34	6.16	5.68
20	1.06	4.26	4.77	1.47	6.91	6.08
21	0.74	4.29	3.71	133.62	474.89	578.59
22	0.92	4.30	4.33	93.45	482.27	544.12
23	1.07	4.44	4.80	90.95	514.66	548.43
24	0.86	4.44	4.13	109.45	536.25	515.24
25	0.93	4.65	4.36	136.45	544.20	575.97
26	0.78	4.65	3.87	100.78	557.27	509.72
27	0.97	4.82	4.49	124.78	565.23	608.12
28	1.02	4.89	4.65	112.78	570.34	537.74
29	0.93	5.20	4.36	92.45	578.30	546.91
30	1.02	5.33	4.65	184.12	585.68	673.56
31	1.16	5.48	5.08	127.28	590.23	604.68
32	0.99	5.50	4.54	201.12	603.86	649.24
33	1.30	5.68	5.55	119.62	606.14	590.95
34	1.52	5.80	6.23	113.95	619.77	547.13
35	1.16	5.88	5.09	202.12	644.20	658.03
36	1.11	6.04	4.93	131.12	658.41	588.92
37	1.53	6.44	6.24	188.12	682.84	651.60
38	1.52	6.86	6.22	181.62	691.93	684.34
39	83.12	460.68	465.01	142.12	709.55	620.61
40	137.28	461.25	578.19	212.12	720.91	780.87
41	113.78	477.16	545.76	241.28	726.59	763.20
42	162.12	482.27	595.76	208.95	761.82	741.77
43	104.78	493.64	501.94	220.12	774.32	838.68
44	131.12	512.95	588.92	214.62	777.73	805.96
45	138.45	520.91	583.95	207.12	796.48	717.35
46	131.28	522.61	588.14			
47	87.28	539.09	532.36			
48	128.45	541.36	600.81			
49	112.78	549.89	537.74			
50	124.45	555.57	608.00			
51	194.12	558.98	627.75			
52	154.45	560.11	667.35			
53	156.28	566.36	646.59			
54	143.78	569.77	642.66			

Tab. 1. *continued*

Number of sample	Training set			Testing set		
	TPC [g·kg^{-1}]	*FRAP*$_{exp}$ [g·kg^{-1}]	*FRAP*$_{est}$ [g·kg^{-1}]	*TPC* [g·kg^{-1}]	*FRAP*$_{exp}$ [g·kg^{-1}]	*FRAP*$_{est}$ [g·kg^{-1}]
55	135.62	572.05	575.25			
56	137.12	573.75	577.62			
57	92.95	580.00	545.66			
58	13.95	584.55	589.71			
59	134.62	589.09	576.13			
60	156.12	589.09	648.55			
61	135.12	598.18	575.47			
62	166.78	603.30	609.13			
63	120.62	605.00	596.65			
64	184.78	605.00	670.10			
65	159.12	610.68	615.20			
66	208.12	614.09	730.71			
67	193.28	623.18	629.41			
68	151.12	634.55	691.68			
69	143.45	650.45	638.21			
70	126.12	651.59	607.20			
71	137.95	665.23	581.09			
72	190.28	673.75	640.42			
73	239.78	684.55	766.51			
74	271.28	686.82	749.09			
75	193.95	695.91	628.02			
76	278.62	707.84	719.67			
77	142.62	714.66	627.12			
78	261.12	719.77	790.43			
79	161.12	722.61	599.95			
80	149.28	723.75	692.62			
81	275.45	727.16	729.20			
82	176.78	756.70	687.66			
83	208.95	763.52	741.77			
84	171.12	772.05	650.51			
85	200.28	774.32	642.99			
86	277.28	777.73	722.87			
87	190.28	778.86	640.42			
88	217.28	792.50	825.68			
89	220.28	796.48	839.20			
90	242.12	800.45	762.36			
91	246.45	803.86	767.33			
92	218.62	808.41	832.78			
93	236.12	810.11	783.95			
94	217.12	815.23	824.66			
95	180.78	817.50	686.85			
96	221.62	828.30	842.43			
97	233.95	832.84	798.53			
98	208.28	835.11	732.93			
99	215.28	839.09	811.59			
100	226.28	839.66	840.64			
101	212.28	841.93	782.73			
102	262.95	844.77	786.33			
103	296.28	852.16	852.83			
104	223.62	872.61	844.16			
105	263.28	906.14	785.38			

TPC – total phenolic content (expressed as grams of gallic acid equivalents), *FRAP*$_{exp}$ – experimental values of ferric ion reducing antioxidant power, *FRAP*$_{est}$ – estimated values of ferric ion reducing antioxidant power (both expressed as grams of $FeSO_4$ equivalents).

by using data on total phenolics, flavonoids, anthocyanins and tannins content. They found that relative errors between the predicted and real values of antioxidant activities of the wines were less than 3%. CIMPOIU et al. [21] also predicted the antioxidant activity of tea samples based on total flavonoids, catechins and methyl-xanthines content. They used 20 samples for training and 10 samples for testing. It was found that the relative error was less than 0.5%, which demonstrated success of training and good prediction capability of ANN models. However, when the number of data is low, ANN can memorize the results. In this work, it was out of question due to the excess of data. This was also determined with different performance criteria.

The correlations between the experimental and estimated FRAP values of training set and testing set are shown in Fig. 2. There were good correlations between the estimated and experimental values for both training and testing subsets, whose coefficients were $R = 0.9883$ and $R = 0.9925$, respectively. In the study of GUINÉ et al. [3], phenolic contents and antioxidant activity of bananas were predicted based on 4 input variables (banana variety, dryness state, type and order of extract) and correlation coefficients between antioxidant activity and phenolic contents ranged from 0.7638 to 0.8258. The authors also indicated that it was possible to predict antioxidant activity of bananas based on the phenolic content with $R = 0.90$ for whole data sets. However, they reported that predicting of phenolic contents from antioxidant activity was a harder problem because the neural network with the same characteristics could only predict it with $R = 0.85$. Antioxidant activities of Romanian red wines were predicted by using ANN and a good correlation between the calculated and experimental values was obtained ($R = 0.992$ and $R = 0.963$) [20]. Although antioxidant activity and content of total phenolic compounds of the grape seed and red pepper differed to a great extent, satisfactory results were achieved, which makes this study succesful. All

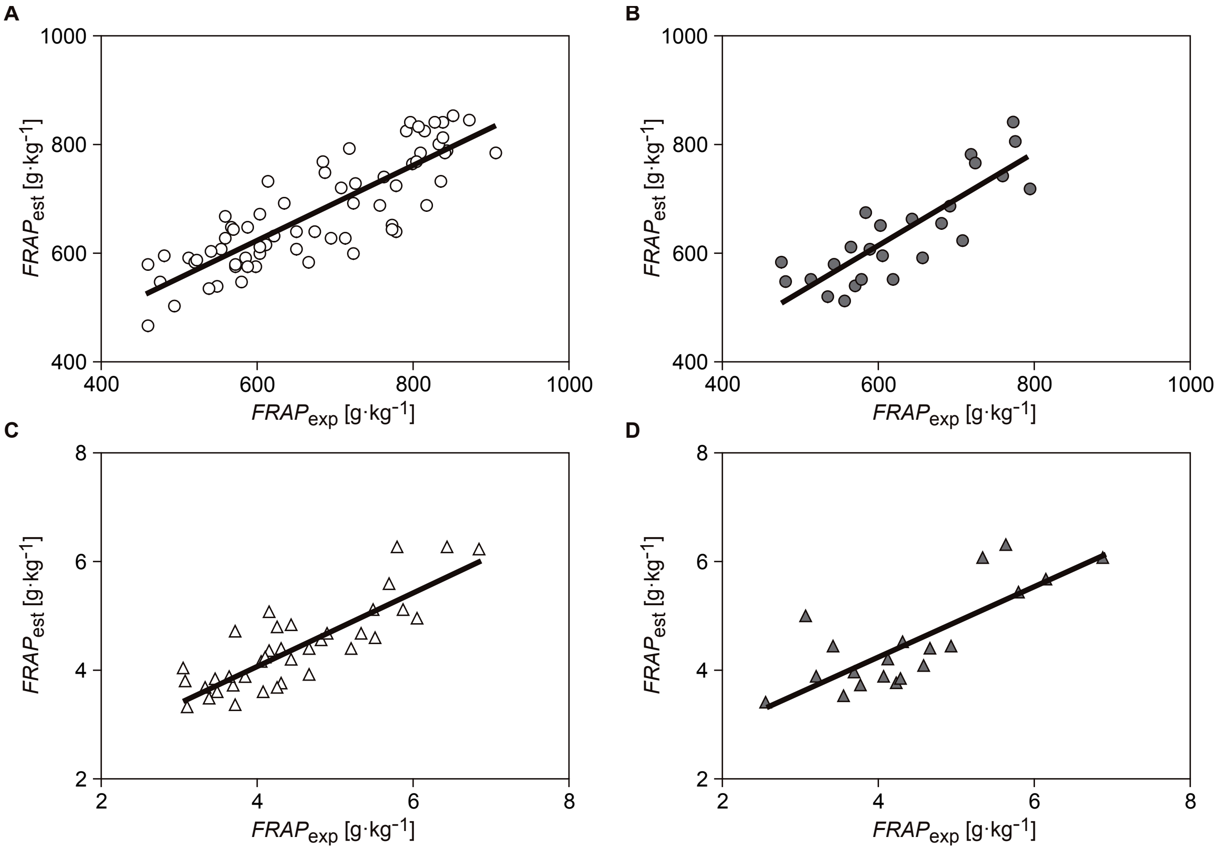

Fig. 2. Correlation between the estimated and experimental values of ferric ion reducing antioxidant power.

A – training set of grape seed, B – testing set of grape seed, C – training set of red pepper, D – testing set of red pepper. $FRAP_{exp}$ – experimental values of ferric ion reducing antioxidant power, $FRAP_{est}$ – estimated values of ferric ion reducing antioxidant power (both expressed as grams of $FeSO_4$ equivalents per kilogram of sample).

Tab. 2. Performance evaluation of training and testing data with respect to the number of neurons.

Number of neurons	Training data			Testing data		
	MSE	*AE* [%]	*R*	*MSE*	*AE* [%]	*R*
80	2660.6664	8.5	0.9518	1540.5393	10.1	0.9428
79	3010.1129	−1.6	0.9466	2045.7016	−3.4	0.9466
61	2515.1179	−0.3	0.9516	1955.5467	−4.2	0.9417
60	3263.8917	0.2	0.9478	3462.4947	−0.1	0.9403
32	3114.9557	−0.5	0.9461	1974.7900	−2.2	0.9396
43	3314.0829	−1.3	0.9410	2207.3153	−2.4	0.9391
25	2816.9782	−0.7	0.9498	1724.2495	−3.4	0.9387
10	2773.2580	−0.9	0.9486	1802.5389	−2.7	0.9386
15	3016.9883	45.3	0.9440	2273.5192	53.9	0.9384
50	2628.3754	−1.3	0.9522	2004.4673	−3.3	0.9384
13	3371.9920	−2.2	0.9435	3363.0077	−3.0	0.9382
16	2699.4588	−0.8	0.9455	2061.8949	−4.6	0.9382
42	2981.8641	0.7	0.9463	2388.1264	−0.7	0.9382
1	3586.1186	−5.4	0.9359	2466.4171	−5.9	0.9379
2	4068.8182	−254.1	0.9359	3221.8935	−316.7	0.9379
4	3318.7386	0.1	0.9359	2296.5723	−3.3	0.9379
7	3122.2174	−16.9	0.9433	2394.5744	−21.3	0.9379
14	3292.9986	−2.7	0.9400	2761.8830	−4.6	0.9379
20	3022.0772	−1.1	0.9426	2274.8811	−4.3	0.9379
21	6468.1666	0.9	0.9228	4097.2009	0.5	0.9379
71	3052.2257	−1.2	0.9433	1514.9222	−4.4	0.9376
70	2502.3210	−2.4	0.9524	2171.4548	−5.8	0.9373
9	3305.1016	2.4	0.9404	3140.7928	2.3	0.9371
56	2491.1007	0.5	0.9498	2436.4954	−3.6	0.9370
99	2983.1446	2.0	0.9482	3622.7124	−2.1	0.9370
98	2489.9948	−1.7	0.9534	3629.5881	−4.5	0.9362
83	9512.1359	−1.2	0.9463	1971.8539	−4.5	0.9353
88	2857.5629	2.2	0.9551	3131.4154	0.9	0.9351
82	2499.9597	−1.8	0.9498	2004.8857	−4.5	0.9346
86	2812.2356	17.5	0.9459	3466.1084	18.6	0.9345
29	3446.0217	−0.3	0.9289	2424.0193	−4.5	0.9337
90	2405.0568	−1.8	0.9513	2844.0623	−7.4	0.9336
67	2475.4204	−1.7	0.9519	2365.9476	−3.8	0.9334
52	3211.2984	−39.5	0.9428	2640.8802	−52.7	0.9320
64	2498.8151	−0.4	0.9542	2115.0325	−3.5	0.9316
74	2595.2082	−0.4	0.9506	2673.5251	−2.1	0.9316
89	2437.4629	−1.7	0.9515	2215.3258	−5.7	0.9312
47	2820.2671	−3.2	0.9522	3506.7080	−5.2	0.9309
95	3070.4617	59.9	0.9431	2333.4139	71.9	0.9307
63	2381.7245	−0.1	0.9517	2263.2076	−3.8	0.9305
84	2767.7731	−3.8	0.9485	2677.3215	−7.3	0.9301
48	6116.8504	−4.1	0.9405	2866.2305	−5.8	0.9296
54	2624.3261	−3.1	0.9509	2720.8881	−5.0	0.9296
77	2274.6660	−1.3	0.9545	2794.2098	−5.2	0.9296
75	2804.8744	0.2	0.9521	2276.8384	−3.6	0.9290
85	2866.7975	−1.5	0.9510	2558.3631	−3.9	0.9287
55	3681.9572	−3.6	0.9392	2759.5287	−6.2	0.9280
81	2990.0035	−2.8	0.9481	2206.8720	−4.1	0.9279
92	2971.8037	−4.8	0.9541	2386.7400	−6.7	0.9278
93	5906.5434	−44.8	0.9099	3920.3047	−60.4	0.9275
51	2540.7751	−1.2	0.9525	2361.4719	−4.8	0.9270

Tab. 2. *continued*

Number of neurons	Training data			Testing data		
	MSE	*AE* [%]	*R*	*MSE*	*AE* [%]	*R*
87	5553.6294	10.1	0.9321	7976.3525	10.3	0.9267
45	3092.5567	–1.9	0.9499	2710.9898	–2.3	0.9266
38	3088.0817	–11.0	0.9463	2205.5340	–17.8	0.9264
59	2896.2287	–0.4	0.9520	2642.3133	–3.2	0.9264
68	2383.2301	–5.4	0.9548	2795.3149	–10.5	0.9264
33	2912.1726	–2.5	0.9481	2303.3217	–6.2	0.9263
26	3200.5203	2.5	0.9450	2494.4786	2.4	0.9262
96	2598.9847	–0.8	0.9498	2418.1348	–4.9	0.9255
65	2602.2249	–2.1	0.9526	2722.0044	–5.2	0.9241
76	3756.4309	–1.4	0.9450	3060.9371	–1.7	0.9239
100	2196.2486	–2.2	0.9557	2340.5081	–4.5	0.9234
72	3040.4014	–1.9	0.9453	2871.8858	–5.0	0.9233
73	2750.6222	6.0	0.9459	2585.7146	4.9	0.9229
62	2301.1468	1.8	0.9569	2249.2635	–1.8	0.9228
31	4754.0712	64.3	0.9173	2915.1304	79.9	0.9224
44	4353.2726	–1.1	0.9284	3164.0201	–5.5	0.9218
35	3228.3771	3.2	0.9441	3564.3012	0.8	0.9201
91	2944.1054	–1.7	0.9487	2969.5571	–3.6	0.9192
27	2412.7738	–2.5	0.9490	2663.3886	–4.9	0.9188
69	4873.4710	–2.9	0.9392	3176.5238	–3.1	0.9185
46	4860.4839	2.4	0.9370	2098.3794	0.2	0.9180
57	3041.7509	–0.6	0.9449	2441.9311	–2.9	0.9176
58	2855.8841	0.6	0.9458	2828.3598	–3.2	0.9174
49	3483.5351	–4.0	0.9474	4920.2963	–8.1	0.9159
94	4512.5642	–53.4	0.9115	4739.3365	–67.8	0.9116
78	2475.7822	–1.2	0.9507	2797.1566	–4.5	0.9095
97	18592.7570	10.0	0.8966	26446.6148	10.0	0.9063
11	4771.1168	0.2	0.9211	3715.2413	–1.7	0.9062
28	4716.4043	–10.9	0.8991	2414.3349	–17.1	0.8976
66	13116.6814	–140.4	0.8849	10432.5024	–177.5	0.8722
23	17977.9129	–10.8	0.9093	30435.4724	–10.6	0.8250
30	3245.0491	0.9	0.8622	2254.9571	0.7	0.8250
22	3369.7650	–20.2	0.8676	1973.6198	–21.8	0.8189
39	3027.5782	–3.8	0.8696	2190.9543	–3.5	0.8188
24	3063.4135	–1.1	0.8681	1997.6631	0.7	0.8187
17	3116.8913	–7.5	0.8668	2378.5237	–5.1	0.8185
8	3197.0286	2.4	0.8643	2615.8734	3.0	0.8184
12	3088.6686	–3.3	0.8679	2751.0468	–3.1	0.8184
5	3472.7975	–2.7	0.8586	1942.7901	–1.6	0.8181
37	2963.2695	–19.9	0.8680	1943.2274	–23.9	0.8181
3	4704.3815	–36.1	0.8570	2742.9799	–43.0	0.8171
36	2608.2289	3.4	0.8760	1831.4884	8.4	0.8134
53	5198.2186	–7.5	0.8371	2196.9863	–8.6	0.8134
6	3346.8615	–1.9	0.8580	2250.1573	–3.0	0.8131
19	3130.9044	–2.4	0.8646	2306.1917	–3.4	0.8085
18	3440.1278	–2.5	0.8620	2075.8534	–3.3	0.8075
34	3734.9495	–90.4	0.8501	3247.8880	–106.2	0.8054
40	3727.3702	–149.5	0.8626	3426.8164	–183.1	0.8011
41	2714.3076	–5.4	0.8694	2121.9126	–6.1	0.7905
Average	4718.5907	–8.0	0.9282	3286.9967	–11.5	0.9067

MSE – mean square error, AE – average error, *R* – correlation coefficient.

this research indicated that ANN models could be used to estimate antioxidant activities of food samples with high correlation coefficients.

Data on performance evaluation of training and testing data, with respect to neuron number, are presented in Tab. 2. The study was carried out in the range of 1–100 neurons. The best result was obtained with 80 neurons. *R* values were calculated for training (0.9518) and testing sets (0.9428) using this number of neurons. As shown in Tab. 2, the percent errors were mostly single-digit, but some extreme values gave very high error rate. Average errors of training and testing were found as –8.0 % and –11.5 %, respectively.

CONCLUSIONS

This study reports on an efficient use of artificial neural network to estimate the antioxidant activity of food samples based on their phenolic contents. The feed-forward ANN-based model was designed and trained using back propagation algorithm. As shown on the training and testing subsets of data, antioxidant activity could be estimated with a high accuracy. All correlation coefficients in this study were found above 0.80, which is the value necessary for the developed system to be applicable in practice [35]. In addition, error rate was approximately 10 %, which is equivalent to 90 % of success. Therefore, it can be said that ANN is a reliable method to estimate FRAP values of foods and it may provide important savings of experimental costs and workload.

Acknowledgements

This research was supported by the Commission of Scientific Research Projects of Sakarya University (Sakarya, Turkey), Project Number 2014-50-01-027.

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Received 23 November 2016; 1st revised 10 February 2017; accepted 5 April 2017; published online 5 May 2017.