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The accuracy of the prediction models for surface roughness and micro hardness of denture teeth

Sule Tugba DENIZ[1], Pelin OZKAN[2] and Gulay OZKAN[3]

[1] *Department of Prosthodontics, School of Dentistry, Bezmialem Vakıf University, Istanbul, Turkey*
[2] *Department of Prosthodontics, School of Dentistry, Ankara University, Ankara, Turkey*
[3] *Department of Chemical Engineering, School of Engineering, Ankara University, Ankara, Turkey*
Corresponding author, Sule Tugba DENIZ; E-mail: suletugba@yahoo.com

The paper aimed to compare the performance of artificial neural network (ANN) model with the results of *in vitro* experiments. For these experiments, maxillary molars of four different denture teeth were subjected to tea, coffee, cola, cherry juice, distilled water. Vickers microhardness and surface roughness values were measured. Subsequently, ANN model for the prediction of microhardness and surface roughness of different denture teeth were examined. A back-propagation ANN has been used to develop a model relating to the amount of microhardness and surface roughness. The independent variables of the model are distilled water, tea, filtered coffee, cola, cherry juice, time and denture teeth. Microhardness and surface roughness were chosen as the dependent variables. According to the results, a neural network architecture having one input layer with ten neurons, two hidden layers with six neurons, one output layer with two neurons and an epoch size of 48 gives better prediction. Prediction models for dental materials could also be supportive for *in vitro* studies.

Keywords: Microhardness, Surface roughness, Denture teeth, Neural networks, Prediction

INTRODUCTION

Artificial teeth are the most important components of a removable denture in restoring function, phonation and aesthetics[1,2]. Acrylic resins and porcelains have been used for the fabrication of artificial teeth; however, neither type completely accomplishes the requirements for an ideal prosthetic tooth[3]. Good mechanical and physical properties are required of materials used for artificial teeth[4]. New types of artificial teeth using modified acrylic resin that incorporate cross linking agents and composite resin containing different type of filler have become increasingly common[5-8]. However, evidence-based information regarding composition and properties is lacking[6].

An artificial neural network (ANN) has the capability of relating the input and output parameters, learning from process data, without requiring a prior knowledge of the relationships of the process parameters[9]. Its algorithm which needs short computing time connects neurons. Its structure has a high potential of robustness and adaptive performance. ANN models were evaluated as potential alternatives to physical-based models for bioprocessing. ANNs were used successfully as a modeling tool in several bioprocessing applications like sensory analysis and quality control[10].

The simplest definition of ANNs is the modelling of human brain and its building blocks are neurons. There is an average of 100 billion neurons in the human brain. A neuron has a connection point between 1,000 and 100,000. The information in the human brain is distributed to this server and when needed we can use them more than one at the same time. So this means the human brain is consist of thousands of very powerful parallel processors. ANNs have neurons similar to the human brain. Each neuron connects to the other neurons with certain coefficients.

A neural network consists of three layers; the input layer, the hidden layer and the output layer. The data set for training in the input layer is displayed to the network. The network assigns the weights of events that it learns to the connection points on the hidden layer. Each connection point does not have to have a value, besides some points may have a value of zero. A threshold value is added between the layers so that the zero values on the ports are not zero. Finally, we need to test our network. Unlike the data set, a test set without output results is shown to the network and the network gives us an output value for each event of this test set. The results are obtained by interpreting these output values.

There are rapid improvements in ANN approach for the last 30 years. The ability of learning from the previously acquainted pattern is the most important feature of ANN. Predictions based on the previous learning can be made once the processing of the network is achieved with enough sample data sets. This make the technique being used in lots of studies. By using simple input parameters, the prediction of various complex parameters can be achieved. Training must be achieved before the new information is interpreted. Researchers from many scientific fields are devising ANNs to bring solution to the difficult problems such as optimization, reduction and pattern recognition. Neural networks

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have been proven to successfully predict the results of complex non-linear problems in a variety of research fields, including medical research such as creating predictive models of core body temperature and local skin temperature (specifically at forehead, chest, upper arms, abdomen, knees and calves)[11,12].

To control the properties of artificial teeth, adequate precision in estimating variables from incomplete information are desirable among the various techniques. Neural networks do not require any prior knowledge about the relationships that exist between the states of the parameters. There is now extensive literature showing how neural networks may be used for classification, estimation and prediction[13-18]. However, their implementations are new for denture materials. To make it common for denture materials, the neural network must be trained off-line as achieving all possible predictions for different conditions can take a very long time. Any update about the weights of the neural network should be recorded simultaneously, so that it can learn in real time. It would then be effective for real time applications[19].

Surface properties such as hardness, roughness, contact angle, surface free energy and wettability are releated to denture pellicle property composition and initial adherence of microorganisms to denture surfaces. Dental materials with rough surfaces are more inclined to bacterial adhesion and plaque accumulation than smooth surfaces[20-22].

In order to determine the micro hardness and surface roughness of different denture teeth in different beverages, ANN has been used in this study. Standard methods generally place constraints such as continuous differentiable. However, ANN has an ability to learn and generalize any complex system without making any model assumption[13,15,18]. Development of a model, which can represent the influence of the affecting parameters on the surface roughness and micro hardness is of great importance for either economical process design and terms of time. The related literature reveals that ANN has been used for modeling purposes in the several fields of sciences. However, among dental researches, there is only one study[19] about the prediction of dental restoration material. They investigated the wear prediction model of titanium alloy and found that ensemble learning model had good stability and high precision on predicting the wear loss. Özkan *et al.*[23] investigated ANN models to predict the performance of a wastewater treatment plant (wwtp) based on past information. The ANN-based models were found to provide an efficient and a robust tool in predicting wwtp performance. Modeling of various patterns of biological activity in different beverages and their impact on the micro hardness and surface roughness of different denture teeth is essential for achievement of a satisfactory control of different denture teeth. Instead of expensive and time-consuming experiments, it is highly recommended the usage of ANN for modeling materials. So, the objectives of this study were to present a methodology designed by ANN for predicting the surface roughness and micro hardness values and to evaluate the capability of ANN in modelling the surface changes against different beverages. This study aims to evaluate the performance of a feed forward back propagation artificial neural network (BPANN) approach by using *in vitro* results of the surface roughness and hardness tests of different denture teeth in mostly consumed beverages. The effects of four different beverages and time on the micro hardness and surface roughness were studied with *in vitro* experiments. Then the BPANN was constructed and the micro hardness and surface roughness for the defined independent variables were predicted by using the *in vitro* results. The best performing architecture of neural networks was found. The null hypothesis of this study is that ANN is not able to predict the amount of surface roughness and micro hardness change of denture teeth immersed in different beverages with reasonably low prediction error.

MATERIALS AND METHODS

Conventional acrylic resin teeth (Major Dent, Major Prodotti, Dentari, Moncalieri, Italy), reinforced acrylic resin teeth (Integral, Merz Dental, Lütjenburg, Germany), microfiller composite resin teeth (SR Orthosit PE, Ivoclar Vivadent, Schaan, Lichtenstein) and nanofiller composite resin teeth (Veracia, Shofu, Kyoto, Japan) were used, for a total of four different denture teeth groups. From each group of denture teeth, 10 maxillary first and second molars for a total of 200 specimens were immersed in each of the 5 solutions. The specimens were embedded individually in a 1 cm diameter methyl methacrylate resin block (Dent Temp Set A2, GDF, Rosbach von der Höhe, Germany) prepared from a silicone impression material (Zetaplus C-Silicone Impression Material, Zhermack Clinical, Rovigo, Italy) so that the buccal sites of the denture teeth were exposed. Each specimen was stored in 5 mL plastic tubes individually and subjected to four beverages (tea, filtered coffee, coke and cherry juice) and distilled water (as control) for a total of 6 days at 37±1°C. This test period simulates the effects of 6 months of denture usage and normal beverage consumption[24]. According to this simulation 5.6, 24 h and 3 days storage periods simulate 1 week, 1 month and 3 months denture usage respectively. Vickers microhardness and surface roughness of denture teeth were measured for baseline and each test period. Before immersing each set of denture teeth into the solution, they were stored in distilled water for 24 h. Solutions were refreshed every day.

Microhardness measurements were obtained for all specimens with a Vickers hardness tester (HSV 1000, Bulut Makine, Istanbul, Turkey) at 300 g load for 15 s. Three readings were recorded for each specimen and the mean value was calculated. A profilometer (Mahr Perthometer M2, Mahr, Germany) was used to measure average roughness (Ra) values. Three repeated measurements were recorded for each specimen. The analysis of all the data and calculated values obtained from the measurements was done using the statistical analysis program of IBM SPSS Statistics 19 (SPSS for Windows, Version 19.0, IBM, Armonk, NY, USA). For the results of microhardness and surface roughness one-way analysis of variance (ANOVA) with a significance level of p<0.01 was used to determine the differences between artificial teeth and different storage solutions.

Design of the ANN is composed of two sections (Fig. 1).

Neural network training includes selection of ANN structure, training function and algorithm. The ANN architecture used for the modeling of microhardness and surface roughness was shown in. We selected the feed forward algorithms (BPANN). The BPANN was categorized as 10+6+6+2, which means one input layer with 10 neurons which are the values from time, water, tea, filtered coffee, cola, cherry juice and four denture teeth material (Integral, Major, Veracia, Orthosit) two hidden layer with six neurons and one output layer with 2 neuron which are the values from microhardness and surface roughness. The transfer functions in the two hidden layers and the output layer were Log sing, differentiable tan-sigmoid function (tansig), linear function (purelin), respectively. Data obtained from experimentally was used for training of the ANN and the data of other experimental was used for testing the trained network.

Neural network includes evaluation, simulation, prediction and validation. The training data set was given

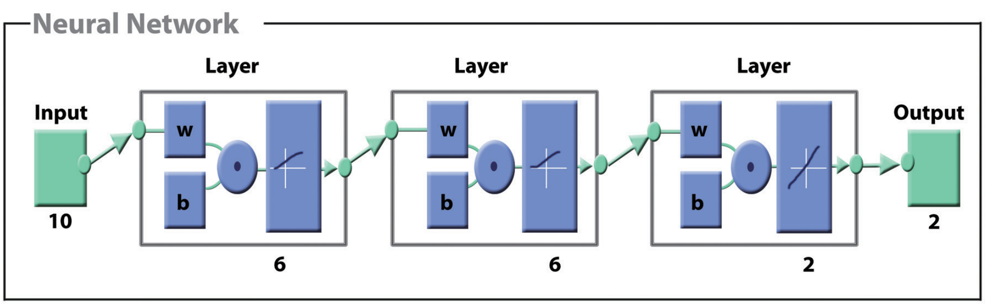

Fig. 1 ANN architecture used for the modeling of microhardness and surface roughness (W and b are weight and bias respectively).

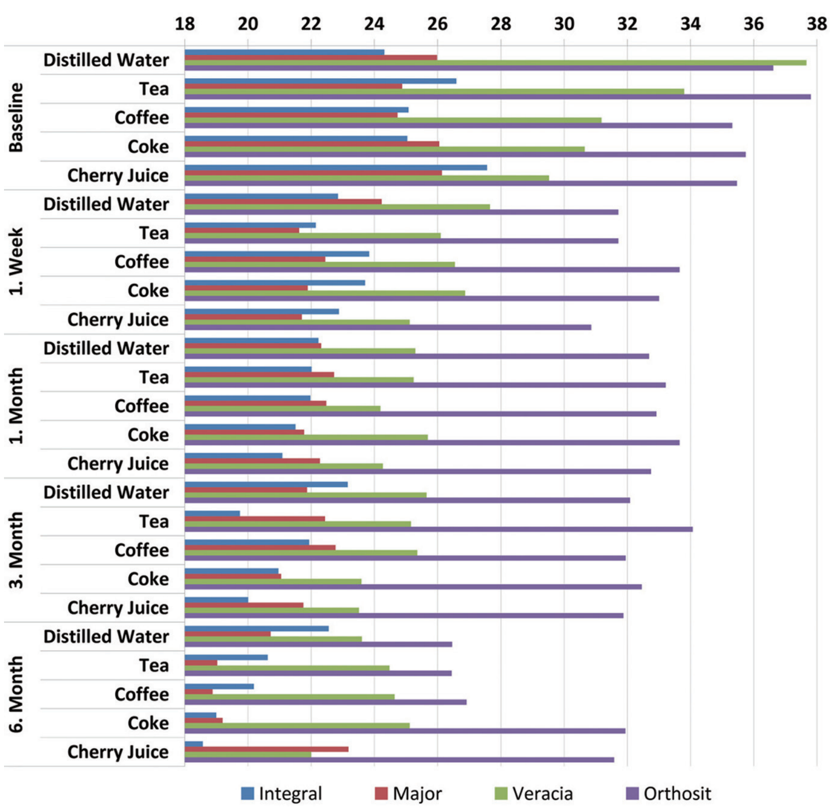

Fig. 2 Microhardness of denture teeth in different beverages (kg/mm²).

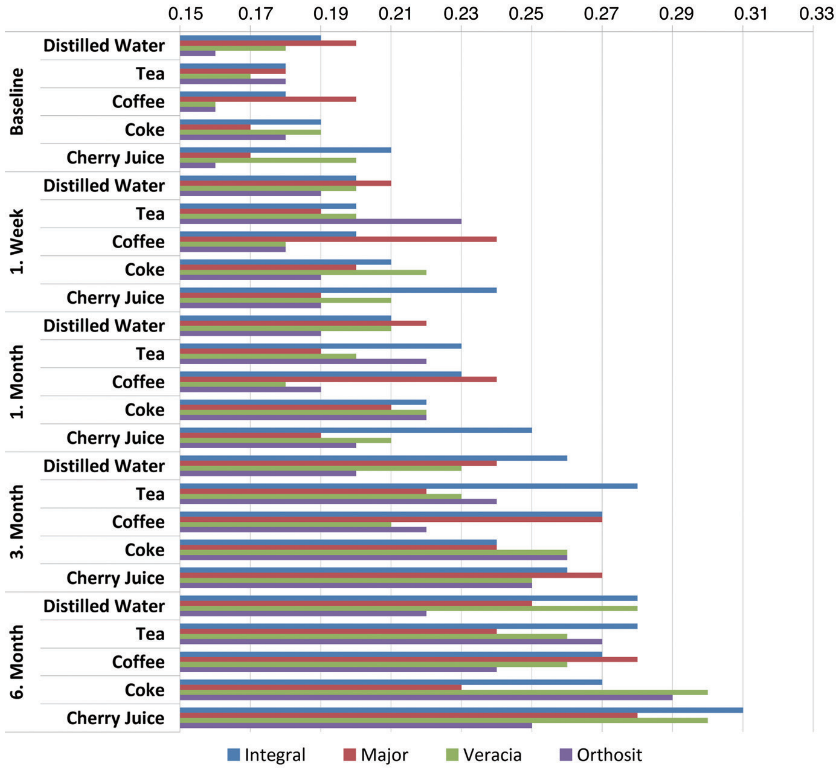

Fig. 3 Surface roughness of denture teeth in different beverages (μm).

(For example: Microhardness and surface roughness of different denture teeth in different beverages was given in Figs. 2 and 3) to the network and a feed forward algorithm automatically adjusted the weights so that the output response to input values was as close as possible to the desired response. Prediction was made and results were compared with the desired value. Then the prediction error was distributed across the network in a manner which allowed the interconnection weights to be modified according to the scheme specified by the learning rule. This process was repeated while the prediction error decreased. Two training algorithms, gradient descent (traingd) and Levenberg Marquardt (trainlm) were used to train the BPANN. These two algorithms both work by iteratively adjusting the weights and biases of the network to minimize the performance function. The performance function is the mean squared errors (MSE) between the output and the target values[25,26].

The Levenberg Marquardt algorithm was selected to retain in ANN training and prediction.

RESULTS

Statistical technique results

The differences of each value were calculated by one-way ANOVA statistically.

Distilled water, tea and cherry juice decreased the microhardness values from 1st week ($p<0.01$). The microhardness values of the specimens immersed in cola decreased from 1st month whereas the ones immersed in filtered coffee decreased from 6th month significantly ($p<0.01$). The microhardness values significantly decreased in all beverages from 1st week ($p<0.01$). After 1st month there were no significant decrease until 6th month. There were no differences among the effects of beverages on microhardness values ($p>0.01$). However, the specimens of Veracia immersed in cherry juice showed a significant decrease in microhardness values ($p>0.01$) (Fig. 2).

The surface roughness values increased significantly in all beverages ($p<0.01$) especially from 3rd month. The surface roughness values for 6th month and 3rd month were nearly the same. There were no significant differences among the beverages for the specimens of İntegral ($p>0.01$). The highest surface roughness values for Major teeth were found in filtered coffee, for Veracia and Orthosit teeth were found in cola ($p<0.05$) (Fig. 3).

ANN technique results

For the model predictions, the output of the ANN was compared with the trained and tests data sets. They were shown in Figs. 4, 5 and 6. In these graphs, the mean square errors of ANN model for test data set is 7.6596 (for microhardness) and 4.0012 (for surface roughness), respectively. Experimental data are distributed along the ANN predicted line which indicates the ANN prediction has reasonably low prediction error.

In order to create an ANN structure, training data is used firstly. Figure 4 shows the comparison of the ANN

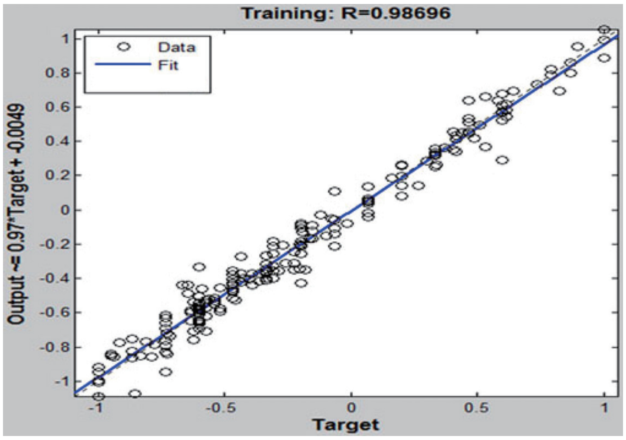

Fig. 4 The comparison of the performance of ANN model with target data (training data set).
The spheres indicate the training data and the line indicates the data estimated by ANN. Target means actual values and Output means predicted values of surface roughness with the unit of µm.

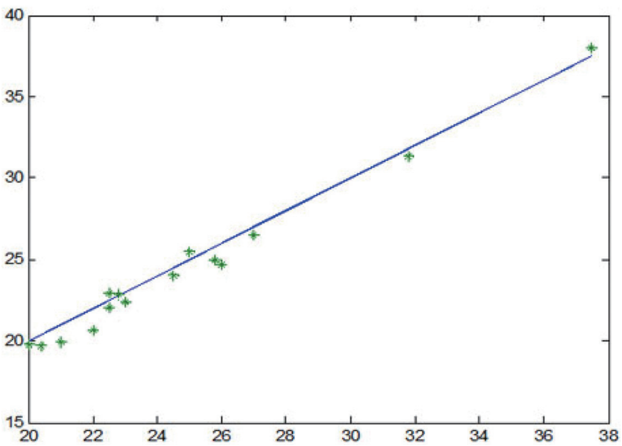

Fig. 5 The comparison of the performance of microhardness ANN model (line) with test data (*). Vertical and horizontal axes indicate microhardness values with the unit of kg/mm^2.

structure and the training data for the roughness test results. The graphic also indicates the error between them. This comparison was also made for the hardness test and a similar curve was found.

In Figs. 5 and 6, performance of microhardness and surface roughness ANN models were compared with the test data respectively and they indicated the error. So that the predicted and experimentally measured values were compared. Experimental data are distributed along the ANN predicted line.

DISCUSSION

The null hypothesis of this study was rejected since the obtained experimental values were in good agreement

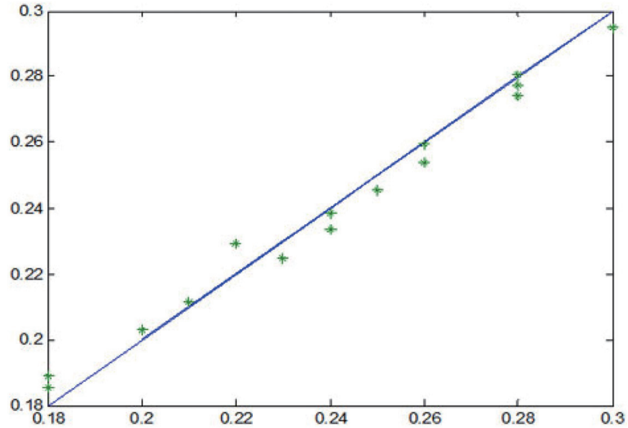

Fig. 6 The comparison of the performance of surface roughness ANN model (line) with test data (*). Vertical and horizontal axes indicate surface roughness values with the unit of µm.

with the values predicted by ANN model. This good agreement with low error confirmed that surface characteristics of denture teeth can be successfully modeled by using ANN system.

Daily intake of common beverages may change the surface characteristics and microhardness of denture teeth[27-30]. To improve these mechanical and physical properties new artificial teeth have been developed by controlling the filler particles and polymer matrix. According to the results of this study, microfiller composite resin denture teeth had the most ideal mechanical properties. The detected surface roughness values were smaller than the plaque accumulation level (0.2 µm)[31] and the high microhardness values indicated high wear resistance[32]. The obtained accuracy of surface roughness and microhardness prediction was also acceptable like the other studies[13-15,18]. The experimental and model prediction results demonstrated that the microhardness of denture teeth decreased during the immersion period while the surface roughness increased. This situation could be attributed to the composition and pH values of the beverages and also the filler type of the denture teeth. Beverages can lead surface defects on denture teeth depending on the exposure time, pH values and the quality of the saliva. The size of the filler in composite resin denture teeth can also affect the surface irregularities which are induced by the fillers separating from the matrix. The microfiller resin denture tooth used in this study is composed of inorganic micro filler and urethan methacrylate matrix. Nano fillers did not give any mechanical advantage for surface roughness and micro hardness. This could be due to the lower wear resistance of the nano fillers and the polymethylmethacrylate matrix. The addition of inorganic filler particles to the high crosslinked polymer structures of the composite resin teeth with micro-filler gave them higher hardness values. The softening of the resin matrix results in the separation of the filler particles from the surface, resulting in a rough surface. In our study, there was no significant difference between the roughness values of the nanocomposite denture teeth and the microfiller resin denture teeth. Saliva can reduce the adverse effects of the pH values of beverages, however artificial saliva was not used in this study.

ANN provide to learn system properties of many chemical applications. Although the history of ANN is old, studies have shown how neural networks can be used for classification, estimation and prediction of bioprocesses since the late of 1980s[10,16]. The structure of ANN, consisting of layers made of neurons, simulates the functioning of human brain[15]. There are many neural network applications in bioprocesses, such as surface roughness, surface hardness and wear prediction of materials[10]. However, no research on the surface roughness and hardness prediction model of dental materials has been reported. There is only one study on wear prediction model of dental restoration material[19]. Since the resulting wear mechanisms differ according to the adjustment of the simulator, the study figured out that it is not correct to compare the wear results, unless the wear devices are identical. Using machine learning method for wear prediction studies is preferred with an increasing trend in recent years[19].

Besides the advantages of ANN system, the model may suffer the level of sensitivity.

Due to their structure, ANNs are hardware-dependent. When they produce a solution to a problem, they do not give a clue for the reason and the method. This is a factor that reduces trust in the network. There is no specific rule in determining the structure of ANNs. The appropriate network structure is obtained by experience and trial and error. ANNs can work with numerical information. Problems must be converted to numerical values before being introduced to ANNs. The display mechanism to be determined here will directly affect the performance of the network. This depends on the user's ability. Lowering the network's error on the samples below a certain value means that the training is complete. This value does not give us optimal results.

The rates mentioned in the present work were predicted by utilizing ANN without using a model of the system. This method can be used as an alternative method to conventional ones because of high accuracy of results. In addition, this work uses only experimental data; therefore, it does not include error arising from the assumptions which are made for creating a model. For the cases which have modeling difficulty, ANN can be proposed because of their simple structure and rapid solution ability. Long training period is not required in order to predict the rates. Reducing the number of sampling saves time and money spent. To get high realizable results, it helps to focus on investigating the best value by finding which factor is effective on rate.

The usage of ANN for modeling composite materials is recommended rather than an *in vitro* study which is time consuming and expensive[18]. ANN is more successful when there is nonlinearity among the variables, mathematical formulas are not able to describe the function of various factors precisely[16,19,33].

Studies about the prediction of surface roughness of various materials obtained high accuracy between the model results and experimental values[14]. It was shown by the study results that the prediction of surface roughness can be made through back propagation neural network together with ANN algorithm[14]. The prediction models may also be used to predict the surface hardness of alloys very accurately[14,15].

In this study, ANN architecture was created for 6-month data and it was indicated that ANN model output could be used instead of actual experimental output in the absence of experimental data. ANN could give results also for the 1-year period or for a longer time period, however the accuracy should be discussed.

It is indicated in many related studies that the properties can be predicted with negligible error by the ANN[13,16,18,23,33]. Moreover, according to the test results of a study the experimental results and the prediction values confirmed each other in a rate of 99.999%[13].

This study opens a new way for achieving results of *in vitro* tests by using a cost and time-effective computational method. However, to apply ANN for predicting the surface roughness and microhardness values, further studies on larger dataset and more variables may be needed to refine the prediction and optimization. Furthermore, the programme performance can be improved by new experiments and different materials.

CONCLUSIONS

ANNs model was developed to predict the performance of microhardness and surface roughness for artificial teeth based on experimental data. The performance of ANN model has been compared with the statistical model. ANN is able to predict the properties with reasonably low prediction error. The surface roughness values increased with time significantly in all beverages and microfiller composite resin denture teeth had the most ideal mechanical and physical properties. It was concluded that the efficiency of the mechanical and physical properties was increased by microfiller composite resin denture teeth which were obtained by utilizing ANN directly.

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