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Original Article

Comparison of Trial and Error and Genetic Algorithm in Neural Network Development for Estimating Farinograph Properties of Wheat-flour Dough

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ABSTRACT

Background and Objectives: Rheological characteristics of dough are important for achieving useful information about raw-material quality, dough behavior during mechanical handling, and textural characteristics of products. Our purpose in the present research is to apply soft computation tools for predicting the rheological properties of dough out of simple measurable factors.

Materials and Methods: One hundred samples of white flour were collected from different provinces of Iran. Seven physicochemical properties of flour and Farinogram parameters of dough were selected as neural network's inputs and outputs, respectively. Trial-and-error and genetic algorithm (GA) were applied for developing an artificial neural network (ANN) with an optimized structure. Feed-forward neural networks with a back-propagation learning algorithm were employed. Sensitivity analyses were conducted to explore the ability of inputs in changing the Farinograph properties of dough.

Results: The optimal neural network is an ANN-GA that evolves a four-layer network with eight nodes in the first hidden layer and seven neurons in the second hidden layer. The average of normalized mean square error, mean absolute error and correlation coefficient in estimating the test data set was 0.222, 0.124 and 0.953, respectively. According to the results of sensitivity analysis, gluten index was selected as the most important physicochemical parameter of flour in characterization of dough's Farinograph properties.

Conclusions: An ANN is a powerful method for predicting the Farinograph properties of dough. Taking advantages of performance criteria proved that the GA is more powerful than trial-and-error in determining the critical parameters of ANN's structure, and improving its performance.

Keywords: Artificial neural network, Genetic algorithm, Rheological characterization, Wheat-flour dough

Introduction

Wheat-flour dough is a unique viscoelastic material with gas-retaining ability. It is created when wheat flour and water are mixed together completely (1). Rheological characteristics of dough are important for obtaining useful information about raw material quality, behavior of dough during mechanical handling such as dividing, rounding and molding, and textural characteristics of the finished product, as well as the process efficiency (2).

Artificial neural network (ANN) is a popular learning machine that simulates living nervous systems, and makes a non-linear map between the input and output spaces (3). ANNs are effective tools for classification, optimization, modeling, prediction,

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and control of complex problems (4). Recently, ANNs have been applied in different fields of food science, such as simulating processes like drying behavior of different agricultural materials (5-6), osmotic dehydration (7), and cross-flow microfiltration (8). They have also been used in other fields of food science, including classification (9), prediction (10-11), optimization (12), or food-quality evaluation (13).

Genetic algorithm (GA) is a randomized method for procedure optimization. It is based on the Darwinian idea on survival of the fittest generation by natural selection to reach to an optimal solution (14). GA is a significantly more efficient than trial-and-error method for designing ANN structures. Many investigators have addressed the requirements of applying GA to optimizing ANN parameters (15-18). A GA can optimize several of the most important parameters in a neural network structure. The most common parameters with significant influence on the performance efficiency of ANNs are number of hidden layers, number of processing elements (PE), learning rates, and momentum coefficient. Networks need a relatively simple structure that can keep their errors within tolerance limits (17).

For satisfying consumer demands, bakery industries, like other food industries, need to design standard and reliable procedures for controlling product quality and safety. Bakery industries usually encounter raw materials with variable quality, and their processes exhibit non-linear behavior. Rheological measurements of every batch in the production line are very useful, but impractical. In contrast, assessment of the physicochemical properties of flour is feasible: wheat-milling industries can easily supply these data to the bakers. Predicting dough rheological properties from several simple measurable factors enables online process control, and helps modify subsequent process conditions for preventing economic loss and deterioration of product quality. The present study aims to apply GA to optimizing ANN structure for predicting Farinograph-measured properties of white wheat flours (82% extraction rate) from several of their accessible chemical and physical properties.

Materials and Methods

Sample preparation: One hundred samples of white flour (82% extraction rate) were collected from different provinces of Iran. Iran has been divided to 14 regions with various climatic and environment conditions. Surely, wheat varieties grown in each region are different from other areas. In milling industries, various wheat varieties are mixed together to achieve special parameters of flour. In order to remove the difference of milling procedure and qualitative properties of laboratory miller and industrial products, and also to develop practical predictive models for bakery requirements, sampling procedure was done randomly from different wheat milling plants of all provinces in order to analyze samples with extensive physiochemical and rheological properties.

Flour and dough properties: Seven physicochemical properties of flour were selected as NN inputs: total protein content, total ash content, wet gluten, gluten index, amylase activity, sedimentation value, and particle size index. They were determined according to the approved methods 46-19, 08-01, 56-81B, 38-12A, 56-60 and 50-10, respectively (19).

Rheological properties of the samples were determined with the Brabender Farinograph (Brabender, Duisburg, Germany) according to the approved method 54-21 (19). Farinogram parameters are water absorption, dough-development time, dough-stability time, degree of softening, and Farinograph quality number. All measurements were carried out in triplicate, and the results were averaged. Physico-chemical and Farinograph properties of the samples are shown in Table 1.

Table 1. Range of physicochemical and Farinograph properties of the samples

Parameters	Range
Ash (%W/W)	0.5-1.1
Protein (%W/W)	10.1-13.2
Wet gluten (%W/W)	22.7-38.2
Gluten index (%W/W)	19.2-99.1
Sedimentation value (mL)	15.0-31.5
Falling number (s)	434.8-1182.0
Particle size (%W/W)	0.7-10.4
Water absorption (%W/W)	53.1-67.9
Dough development time (min)	1.7-8.0
Dough stability (min)	1.5-18.9
Degree of softening after 12 minutes (Bu)	19.0-178.0
Farinograph quality number (-)	27.0-200.0

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Artificial neural network (ANN) model: Designing networks in trial-and-error and GA training procedures was managed in NeuroSolutions environment (version number 5.07). One hundred patterns were normalized to [-1, 1], and randomly divided in to 65, 15 and 20 data sets for training, validation (cross-validation), and testing, respectively. A feed-forward multi-layered perceptron (MLP) neural network with a back-propagation (BP) training algorithm was developed. The inputs into the first layer were physicochemical properties of flour. Farinograph-measured characteristics of the samples were set as outputs. In the first step, a three-layer neural network with one hidden layer was developed. Neuron numbers of the hidden layer were changed from 1 to 3x (where x is the number of input neurons) (15). Therefore, 21 different neural networks were achieved for the first section of trial-and-error method. The learning rate of 1 and the momentum coefficient of 0.7 for hidden layer, and the learning rate of 0.1 and the momentum coefficient of 0.7 for the output layer were considered.

In the next stage, the second hidden layer network was created. Neuron number of the first layer was set to 1 and increased one by one up to 21 neurons. Neuron numbers of the second layer were changed from 1 to 21 and at every stage, the effect of neuron numbers on the ANN performance was investigated. Transfer functions for calculating the output of neurons were applied. Therefore, 441 different NNs are achieved for the second section of trial-and-error method.

Outputs of the hidden layers' neurons were calculated using a hyperbolic tangent (tanh (x+bias)), while the output neurons were calculated using a bias axon (x+bias). The networks were trained ten times, and the validation data set was used to prevent over fitting problem. The training process of the networks was stopped after 10,000 epochs or when cross-validation MSE was not improved during 100 epochs. The optimal configuration network with minimum mean square error in the cross-validation data set was selected for testing. After optimizing the neuron numbers of the hidden layers, the quantities of momentum and step size were changed from 0.5 to 1 and 0.1 to 1, respectively, in order to determine the NN with the best performance by trial-and-error.

The developed ANNs were tested by test data set, and their performance were evaluated using different criteria such as mean square error (MSE) and mean absolute error (MAE) (20):

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(X_D - X_P)^2 \quad (1)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}\left|X_D - X_P\right| \quad (2)$$

Where, n is the number of data points, and X_D and X_P are the desired and predicted values of parameters, respectively.

Optimizing ANN parameters by using Gas: Genetic algorithm (GA) was applied to optimize the ANN structure (number of neurons in the hidden layer, coefficient of learning rate, and momentum). According to the results of previous section, a four-layer feed-forward NN was developed. An initial population of networks with different sets of parameters (genes) was randomly created. These parameters were automatically tuned through GA training in population. The range of neuron numbers in the hidden layers, step size, and momentum were set to 1-21, 0-1 and 0-1, respectively. All chromosomes in the population pool had at least one different parameter of NN. The initial setting of GA parameters such as genetic operator rates, number of generation, and population size are based on the literature review and computational experiences (16, 21-22). The GA was started with 200 randomly generated chromosomes (networks). Chromosomes in population contained three genes. The first gene represented the hidden neuron number of the network; the second and the third genes were used for learning rate and momentum in the network training process. The evolving networks were iterated through 100 generations. Every chromosome evolved into new chromosomes for all generations. The back-propagation training algorithm was used for evaluating the chromosomes. The fitness value of chromosomes in generations was calculated. Stopping criterion of training process also achieved 10,000 epochs, or was not improved in the cross-validation MSE during 100 epochs. Reproduction operator was used for extracting the chromosomes from the current population, and creating an intermediate population. The reproduction operator of this study was Roulette-wheel selection based on a ranking algorithm: the

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chromosomes were ranked in order of their fitness with the Roulette-wheel operator, selected according to their relative fitness, and placed them into the intermediate population. Application of the crossover and mutation operators to the chromosomes of the intermediate population formed the next generation, and newly created chromosomes were evaluated. One-point crossover and uniform mutation operators were used, and the probability of crossover and mutation operators was adjusted to 0.9 and 0.01, respectively. This procedure for evaluation and reproduction of all chromosomes was repeated until the completion criteria were satisfied. The fitness of the population usually improves in new generation, eventually evolving a solution close to the optimal.

Identification of sensitive input variables: Sensitivity test demonstrates how changing the physicochemical properties of flour can affect the Farinograph-measured properties of dough. For identification of sensitive input variables (sensitivity about the mean), the developed network output was computed by varying the first input between the mean±one standard deviation, while all other inputs were fixed at their respective means. This process was repeated for each input, until generating the variation of output with respect to the variation of input.

Results

Correlation coefficients: Correlation coefficients of physicochemical properties of flours as the ANN inputs and theirs Farinograph-measured properties as the ANN outputs are shown in Table 2. Total ash and protein content of flour has significant effects on water absorption and other Farinograph properties. As total protein increases, water absorption, development time, stability and Farinograph quality number increase but the degree of dough softening decreases. The mixing tolerance of dough with higher protein is more than that for dough with lower protein. These findings are in accordance with the results of Robertson and Cao (27).

Wet gluten has significant positive effects on water absorption of flour, dough development time and degree of softening, and negative effects on dough stability. While, gluten index and sedimentation tests as usual criteria for evaluating protein quality have significant positive correlations with development time, stability and Farinograph quality number, and negative significant correlation with dough softening during mixing (29-30).

Increase in amylase activity decreases the water absorption, development time, stability and Farinograph quality number of dough. Particle size index has also a positive significant correlation with dough stability, and a negative correlation with the degree of softening.

ANN modeling performance: In the first step, trial-and-error training technique was used. The inputs were protein, ash, wet gluten, gluten index, sedimentation, falling number, and particle size index. Farinograph properties of flour such as water absorption, dough-development time, dough stability, degree of softening after 12 minutes, and Farinograph quality number were selected as outputs. After developing and training the networks with different hidden layers, neuron numbers, momentum, and step size with trial-and-error, the best network with the lowest error in the test data set was chosen. The developed ANNs with three layers had less learning capacity. A four-layer network with 6 and 10 neurons in the first and second hidden layers, respectively, was selected as the best ANN. The momentum and step size were 0.6 and 0.7, respectively. The mean square errors and other useful parameters for evaluating the NN performance in estimating Farinograph properties were calculated.

Table 2. Correlation coefficients of physicochemical and Farinograph properties of the samples

	Farinograph quality number (-)	Degree of softening (Bu)	Dough stability (min)	Development time (min)	Water absorption (%W/W)
Ash (%W/W)	0.133	0.134	-0.057	0.495**	0.291**
Protein (%W/W)	0.484**	-0.329**	0.295**	0.667**	0.414**
Wet gluten (%W/W)	-0.022	0.250*	-0.200*	0.281**	0.485**
Gluten index (%W/W)	0.627**	-0.762**	0.676**	0.405**	-0.094
Sedimentation value (mL)	0.564**	-0.731**	0.639**	0.355	0.095
Falling number (s)	0.262**	-0.158	0.190	0.221*	0.225*
Particle size (%W/W)	0.130	-0.303**	0.332**	-0.088	-0.076

* = Significant P<0.05
** = Significant P<0.01

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In the next step, GA was used for ANN development. According to the result of trial-and-error training technique, a four-layer feed-forward back-propagation was employed for training and chromosome evaluating. The validation data set was applied for evaluating the fitness of chromosomes according to the MSE in the training stage. The phenotypic fitness measurement processes (selection, crossover recombination and mutation) were iterated through generations. After 43 generations, the optimal network with the lowest error was designated. The best and the average fitness value versus the number of generations are shown in Figure 1. The topology of the best neural network is demonstrated in Figure 2.

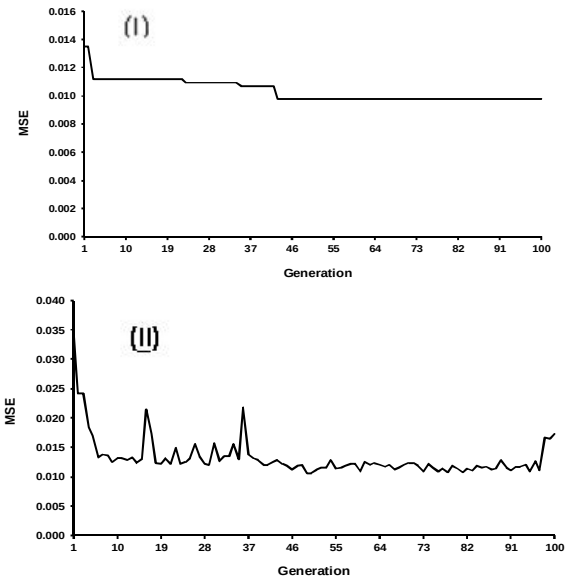

Figure 1. Best (I) and average (II) fitness (MSE) versus generation.

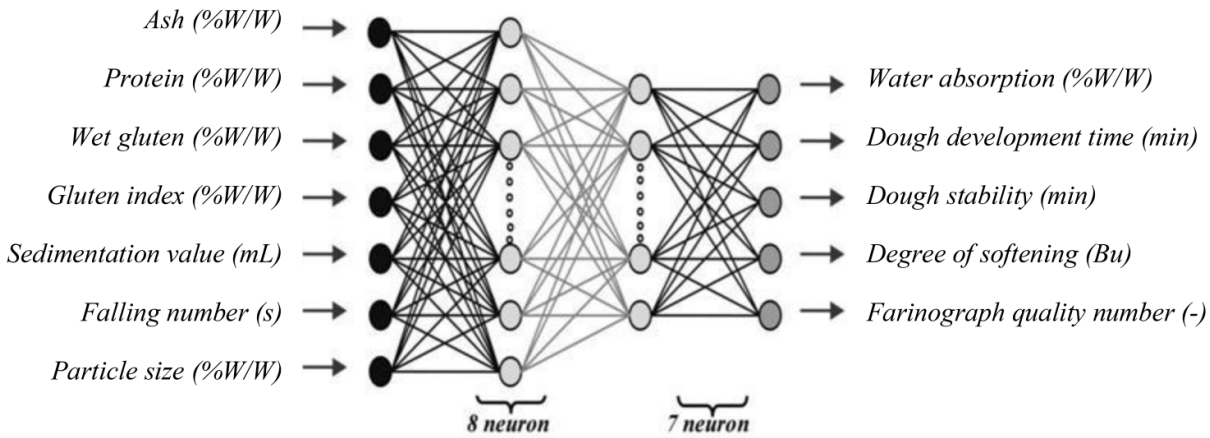

Figure 2. Schematic representation of perceptron neural network optimized with genetic algorithm.

Table 3. Performances of the developed ANNs with trial-error and GA-ANN in the test data set

	Performance	Water absorption (%W/W)	Dough development time (min)	Dough stability (min)	Degree of softening (Bu)	Farinograph quality number (-)
Trial-and-error	Mean square error	0.140	0.120	0.015	0.049	0.017
	Normalized mean square error	0.117	0.578	0.170	0.194	0.211
	Mean absolute error	0.318	0.264	0.106	0.155	0.102
	Minimum absolute error	0.070	0.024	0.023	0.032	0.009
	Maximum absolute error	0.756	0.771	0.261	0.551	0.273
	Correlation of coefficient	0.546	0.806	0.948	0.907	0.918
Genetic algorithm	Mean square error	0.037	0.029	0.010	0.015	0.035
	Normalized mean square error	0.129	0.127	0.137	0.116	0.599
	Mean absolute error	0.154	0.139	0.074	0.099	0.157
	Minimum absolute error	0.004	0.006	0.000	0.015	0.014
	Maximum absolute error	0.399	0.355	0.222	0.258	0.340
	Correlation of coefficient	0.935	0.954	0.962	0.958	0.960

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The performance of the ANNs developed by applying trial-and-error and GA on the test data set is reported in table 3. It demonstrates the MSE, MAE and other useful parameters about the prediction of Farinograph properties. Compression of normalized mean square error, mean absolute error and correlation coefficient in estimating the test data set with the developed ANN-GA and ANN- Trial-and-error show that the performance of the developed ANN with GA in estimating the Farinograph properties of dough was remarkably better than the ANN developed by trial-and-error. The GA could determine an ANN's topology (neuron number of hidden layers, momentum and step size) in less time with better performance. The predicted and measured network outputs of the test data set are plotted in Figure 3 and Table 4 summarizes the best network's architecture with GA.

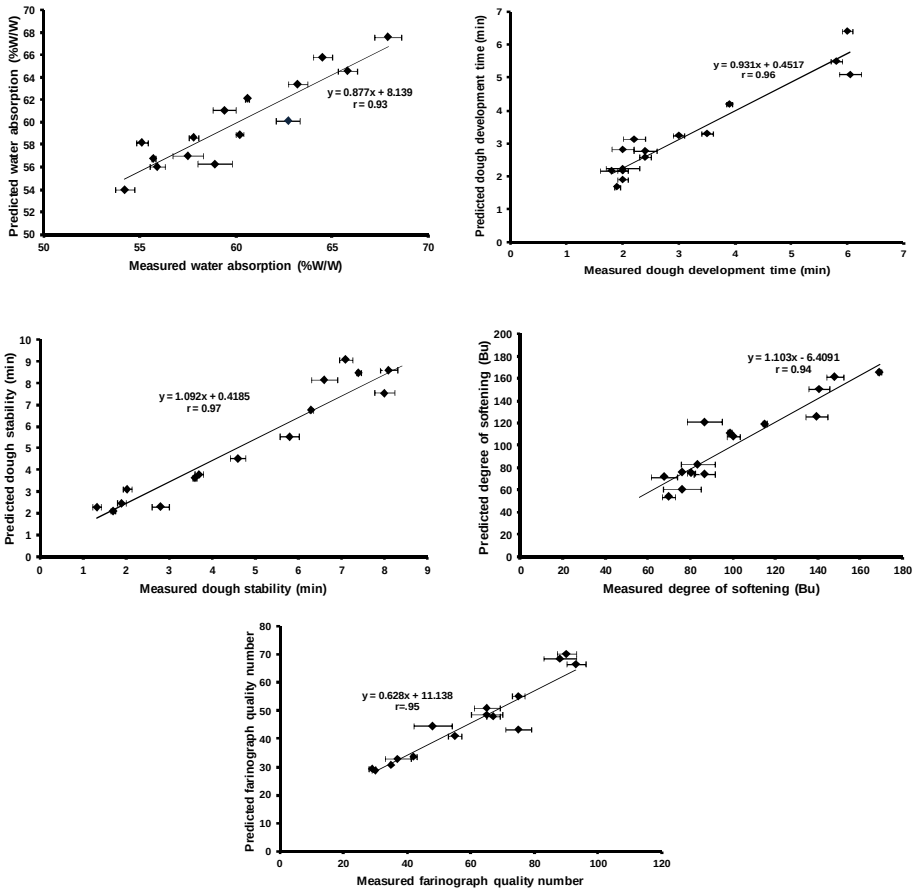

Figure 3. Desired and predicted network outputs of the test data set (Error bars represent standard error)

Table 4. Summary of the architecture of the developed network with genetic algorithm

	Number of neurons	Momentum rate (Synapse)	Step size (Synapse)	Momentum rate (Axon)	Step size (Axon)	Transfer function
Input layer	7	-	-	-	-	-
First hidden layer	8	0.192	0.046	0.061	0.457	Hyperbolic Tangent
Second hidden layer	7	0.319	0.471	0.366	0.282	Hyperbolic Tangent
Output layer	5	0.729	0.081	0.337	0.344	bias
Epoch number in training	10000 epochs or no improvement in validation error after 100 epochs					
Learning algorithm	Back propagation					

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Sensitive variables: Falling number is the most sensitive variable with positive effects on water absorption. Researchers have demonstrated the effect of amylase activity on water absorption (32). The sedimentation value is the second sensitive variable on water absorption. The sedimentation value and water absorption of flour have also significant positive correlation (0.661). Furthermore, other variables such as total ash content, wet gluten, particle size index, gluten index, and total protein content are significantly sensitive with respect to water absorption respectively.

Dough-development time gives an indication of optimum mixing time during dough formation. Wet gluten, total protein content, gluten index, total ash content, sedimentation value, falling number, and particle size index are the sensitive variables, respectively, in predicting development time.

Dough stability is the interval of arrival time and departure time. It also refers to the flour's tolerance for over-mixing. A higher value of stability means that the flour is more tolerant. Gluten index and total protein content with a positive effect are the most sensitive variables for predicting dough stability.

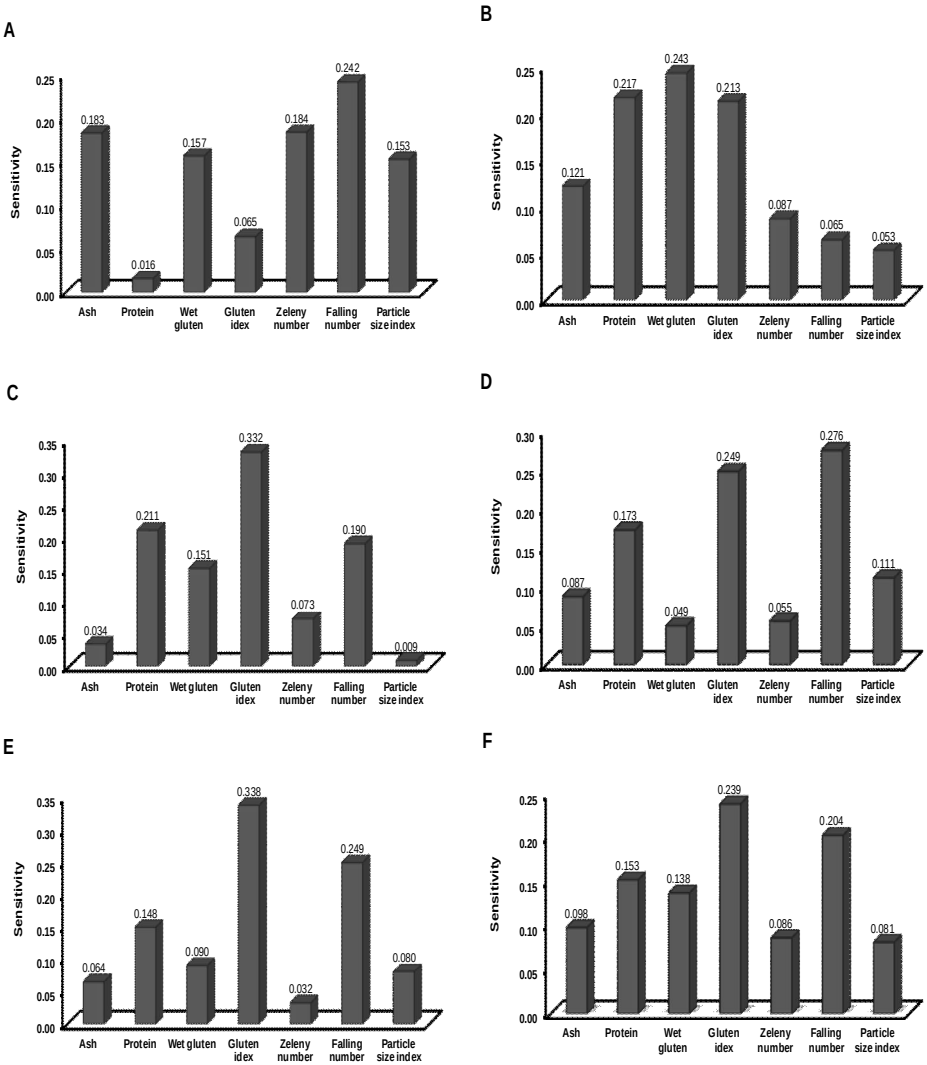

Figure 4. Sensitivity about the mean (A: Water absorption (%W/W), B: Dough development time (min), C: Dough stability (min), D: Degree of softening (Bu), E: Farinograph quality number (-), F: Farinography properties).

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According to the ICC definition, degree of softening is the difference in the top of the curve at peak time to the top of the curve twelve minutes after the peak is reached. A higher value means that the flour breaks down faster after the development. Therefore, it can serve as a criterion for dough mixing intolerance. Falling number and gluten index are the first and second most important sensitive variables in predicting the degree of softening, respectively. Total protein content is the third most sensitive variable affecting this factor. Particle size index, total ash content, sedimentation value and wet gluten have less sensitivity.

Gluten index is the most sensitive variable on Farinograph quality number. Other variables have less sensitivity. Figure 4 summarizes the variation of outputs with respect to the variation of inputs.

Discussion

Water absorption is a very important factor in the bakery industry; it influences dough-handling properties, and is related to the quality of baked products. Flour with higher water-absorption can produce products that remain soft for a long time and exhibit good texture properties (23). Complex carbohydrates such as hemicelluloses can increase water absorption. The result is supported by a research in 2006 that reported the water absorption of different extracted rate flours with various ash contents was in the range of 56 to 66% (24). Flours with higher ash content contain larger amounts of bran and dietary fiber; these substances disturb the continuous gluten network structure of dough (25). The effect of ash content on dough development time is due to the presence of bran particles, which interferes the quick development of gluten and hydration of endosperm. Therefore, ash content may require additional time for absorbing the water of flour components completely (26).

Increasing the extraction rate increases the wet gluten content and water absorption, but decreases dough stability. It is thought that during the gluten isolation, the percentage of non-gluten protein in the wet gluten increases, and dough stability is influenced (28).

Falling number is an indicator of amylase activity. This tendency is attributed to the weakening of mixed dough in the presence of low-molecular-weight dextrins, which are produced from damaged starches by amylase hydrolysis (31-32).

The milling process and the structural characteristics of wheat influence the particle size of flour. During the milling, weak protein bonds in the endosperm can easily break and produce small particles. Strong protein bonds are not easily broken, so serious middling reduction produces fine flour with a high level of damaged starch. In the present research, the higher index of particle size indicates the flour with smaller particles. In dough mixing, two water-containing phases are developed: the gluten phase and the free water phase. If the water content of dough is about 40%, 24% is bounded and the residual 16% is free water, which coats the starch granules. Therefore, the present observation is due to the better entanglement of the absorbed water in dough with higher amount of damaged starch (33).

ANN modeling performance: The best network had the lowest training error and the highest fitness value. Researchers have defined the mathematical expressions of r, MAE, and NMSE for ANNs. The predictions of an ANN are optimum if r, MAE, NMSE and MSE are close to 1, 0, 0 and 0, respectively (34). The average fitness is the average of minimum MSE taken across all of the networks within the corresponding generation. According to the evaluated criteria, the optimal ANN evolved a four layer network with eight nodes in the first hidden layer, and seven neurons in the second hidden that was train with GA. The actual Farinograph-measured properties of the test data set had never been fed into the network during the genetic training. Therefore, according to the data illustrated in Figure 3, the genetically trained network is able to predict Farinograph-measured properties with satisfactory accuracy. Dough stability is the best predicted parameter with the developed ANN-GA (MSE=0.01 and r=0.962). Development time and Farinograph quality number (FQN) are other predicted factors with high correlation coefficients. Previous researches have used FQN for investigating the rheological properties of wheat flour (35-36). There are significant correlation coefficients in the other parameters of Farinography such as development time, stability and degree of softening with FQN. Furthermore, FQN has significant correlation with

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other parameters such as mixograph, extensograph and bread quality (37). Therefore, FQN is a suitable factor in the bakery industry that predicting it with credible accuracy can be very useful for quick evaluation of flour quality.

In 2007, researchers used an ANN for predicting Iranian dough Farinograph properties. They used four chemical compositions of 132 wheat cultivars as inputs, and their Farinograph-measured properties as outputs. They trained an ANN by trial-and-error. The average of reported MAE was 8.638 (38). Ruan in 1995 also developed an NN for predicting dough rheology using the input of work during mixing. The acquired mixer torque curve and the measured rheological properties were used as inputs and outputs, respectively. The average absolute error of predicted Farinograph peak (BU) was 23.6 (39). Comparison of the results of other papers and the present research demonstrates GA's ability as a more powerful technique than trial-and-error in developing and training an ANN, even with less data set numbers. In addition, selecting useful input variables significantly improved the performance of the present study's ANN in predicting outputs.

Sensitive variables: Sensitivity analysis demonstrates the relative importance of the ANN inputs and illustrates how the outputs vary in response to variation of an input in optimized model. It was carried out to select factors that make the largest contribution to the network. According to the results of sensitivity on the best developed network, gluten index, falling number, total protein, wet gluten, total ash, sedimentation value, and particle size index were, respectively, the sensitive variables in predicting parameters of Farinography.

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