MECHANICAL PROPERTIES OF DUCTILE CAST IRON DETERMINED BY NEURAL NETWORKS

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ABSTRACT

This paper presents the results of application of artificial neural networks in determination of mechanical properties of ductile cast iron. All data were collected in a Croatian foundry for 147 melts. Error back-propagation training algorithm was applied to train the multilayer networks. The optimal size of the hidden neuron layer was determined through the analysis of error parameters. The optimal slope of the tangent sigmoid activation function was investigated. Neural networks were modeled to predict each mechanical property, namely: tensile strength, yield strength, elongation, and hardness. Input parameters were 13 weight contents of chemical elements in the melt. A comprehensive analysis of errors in predicting mechanical properties of ductile cast iron was made.

1. INTRODUCTION

The world production of ductile cast iron is constantly growing, and is expected to continue to have the fastest growing rate of all ferrous materials [1]. The advantages of ductile cast iron over other types of cast iron are many, which assured the ductile iron very wide and successful fields of application. This type of cast iron has very good mechanical properties, such as high ductility, toughness, elongation and strength, and low production costs. Other iron castings may have better individual properties, but nodular cast iron has the best all-around combination of properties, which makes it very often the material of choice in many applications. Yet, the most important reason for the increasing production of ductile cast iron is a very favorable cost per unit of strength, compared to other materials [2].

The microstructure of nodular cast iron is developed from the melt. Graphite nodules are formed when magnesium or cerium or other elements are added to the iron melt. Nodularity is the ratio between volume content of spherical graphite spots and the total number of graphite spots, and in nodular cast iron it is usually above 90%. The higher the nodularity, the better mechanical properties [3]. Graphite nodules are embedded into pearlitic, ferritic or martensitic matrices, depending on the chemical composition and/ or subsequent heat treatment process of the casting.

Properties of ductile cast iron, which are most important are usually tensile strength and elongation, although the determination of other properties, such as yield strength, toughness or hardness, is sometimes required. Prediction of these properties during the melting process, and before pouring is very important in a foundry, because it allows the adequate correction of the chemical composition and/ or process parameters.

Since mechanical properties of ductile cast iron work piece depend on the chemical composition of the melt, an issue in this approach was to apply an artificial neural network for determination of these properties.

Artificial neural networks are composed of processing elements and connections [4]. Since they can be used to approximate almost any nonlinear function, neural networks have been widely used in different material science applications. Models and software products have been developed for modeling, simulation and prediction of different correlations in materials science, such as prediction of properties of existing materials, new alloys design, materials selection, and optimization of processing parameters [5]. In recent years, neural networks were used for improving the production of ductile cast iron, as well [7], [8].

2. METHODS

2.1. Experimental data

Different nodular cast iron melts were prepared and recorded at the foundry "Metalska industrija Varazdin" in Varazdin, Croatia. A total of 147 different melts was prepared. For each melt chemical composition was analyzed by spectral analysis using spectrometer GDS 400A, produced by Leco. Melt specimens were poured into a copper mould, and the weight contents of the following chemical elements were determined: C, Si, Mn, S, P, Mg, Ni, Cr, Cu, Sn, Mo, Ti and Al.

From each melt a separately cast test sample was produced. The so-called Y-blocks were cast. Shape, dimensions, mould type, methods of pouring and cooling were according to EN 1563. From the solidified Y-block, test pieces were cut out, as to EN 1563. The tensile test pieces were made as B 14 x 70, according to DIN 50125. Following mechanical properties were determined: tensile strength, R_m, N/mm^2, yield strength, $R_{p0.2}$, N/mm^2, and elongation, A_5. After the tensile test, the head of each test piece was cut off, and the Brinell hardness, *HB*, was measured on it.

2.2. Neural network model

Artificial neural networks were developed using Matlab 7's "Neural network toolbox". All networks were multilayered, with nonlinear perceptrons. Input parameters for the neural network were data on chemical composition of melts (13 chemical elements, wt.%). Output parameter for each network was one mechanical property: tensile strength, yield strength, elongation, and Brinell hardness. The hidden layer was made up by neurons with bipolar sigmoid activation functions, eq. (1):

$$y_j = \frac{2}{1+e^{-\sigma \cdot net}} - 1 \qquad (1)$$

where y_j is the output of the j^{th} hidden neuron, σ is the slope of the sigmoid function, and *net* is the weighted sum of inputs to the hidden neuron. The output layer was made up by neurons with linear activation functions. Initial weight and bias values were generated according to the Nguyen-Widrow method, since it requires less iteration steps in the learning process than training with purely random initial values [9]. All input and output data were preprocessed so that minimum was –1, and maximum was 1, eq. (2):

$$p_n = \frac{p - p_{\min}}{p_{\max} - p_{\min}} - 1 \qquad (2)$$

where p_n are normalized values of a mechanical property or chemical content, p is its actual value, p_{min} minimum value, and p_{max} maximum value.

Input and output data were divided into three data sets: one for learning, one for validation, and one for testing the network. One half of all data were a part of the learning data set, one quarter was for the validation, and the other quarter of all data was retained for the network testing. Learning data set is used during the learning process for adapting weight parameters of the selected model of neural network. The validation data set is used also during learning, but for estimating the error on data that have not been used for training. The learning process is continued until the error in the validation data set starts to increase. Finally, the testing data set is used to test the performance of the neural network after learning has been completed. The error in the testing data set is the most important parameter, which demonstrates how well the network is able to predict a certain output value, i.e. a certain mechanical property.

In order to improve generalization, and to prevent over-fitting, the early stopping method was used. This method requires all data to be divided into three data subsets: training, validation, and testing data set. The training data set was used for calculating network's weights and biases, i.e. for the network learning. The validation subset is used to stop the training early if further training would hurt generalization in the validation subset. While the network was learning, the error on the validation data set was registered. When the validation error increased for five number of iteration steps, the learning process was stopped. Finally, the performance on the test subset was used to estimate how well the network generalizes beyond training and validation data sets.

For each data subset the correlation coefficient, *R*, coefficient of determination, R^2, and normalized root mean square error, *NRMSE*, eq. (3) were registered:

$$NRMSE = \frac{\sqrt{\dfrac{\sum_{n=1}^{N}(d_n - O_n)^2}{N}}}{\sigma_{d_n}} \qquad (3)$$

where d_n, and O_n are measured values of a certain mechanical property, and values predicted by neural network, respectively. N is the total number of observations, i.e. melts, and σ_{d_n} is the standard deviation of measured values. Also, a short statistical analysis of relative errors was made.

The network was trained with the error back-propagation training algorithm. Also, the Levenberg-Marquardt algorithm was applied to neural network training, as this algorithm appears to be the fastest method for training moderate-sized feed forward neural networks [10]. Figure 1 presents the model of the neural network that was used to train the network for predicting tensile strength, with 11 hidden neurons.

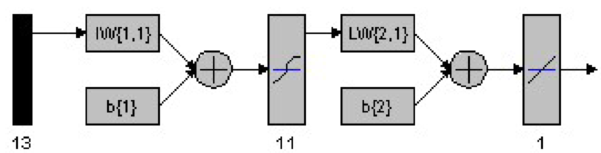

Figure 1. *Model of the applied neural network for predicting tensile strength*.

The number of neurons in the hidden layer was varied in order to find the network that is most adequate for minimizing the prediction errors, while keeping the number of iteration steps in reasonable boundaries.

3. RESULTS

Figure 2 shows how the slope of the tangent sigmoid activation function in the hidden neuron layer, σ, has influenced the ability of the neural network to predict tensile strength, R_m, in the testing data set. It can be seen that values of σ=2 and lower produced a network with best generalizing properties. For this reason, a value of σ=2 was also set when other three networks were trained to predict the other mechanical properties: $R_{p0.2}$, A_5, and *HB*.

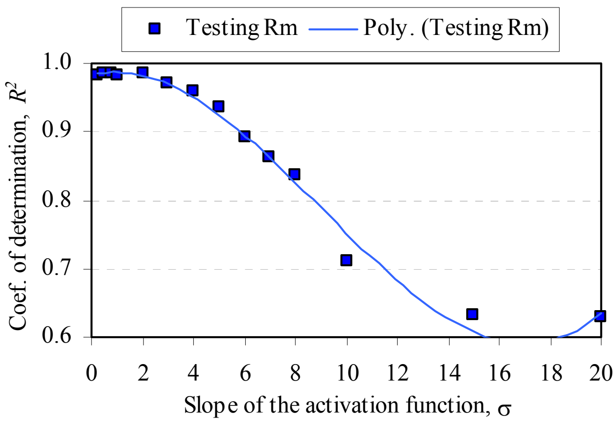

Figure 2. *Coefficient of determination in the tensile strength testing data set for different slopes of activation function.*

Figure 3 presents the influence of the number of hidden neurons onto the coefficient of determination, R^2, and onto the number of iteration steps, which were required for the network learning process, for each mechanical property. The final number of hidden neurons for each network was set to be the one that generated R^2>0.95. For predicting tensile strength, the number of hidden neurons was 11. The number of hidden neurons for predicting yield strength was 13. For predicting elongation, there were also 13 hidden neurons. And, finally, the number of hidden neurons for predicting hardness was 17.

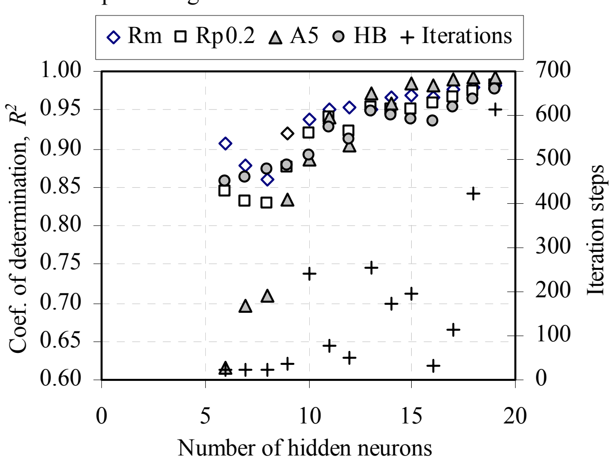

Figure 3. *Coefficient of determination in the testing data set for different number of hidden neurons.*

After each neural network was modeled with the most adequate number of neurons, the networks were retrained. Figure 4 presents distributions of relative errors for tensile strength predicted by ANN, for all three data sets (learning, validation, and testing). Acceptable relative errors in the testing data set were values under 2%. Higher relative errors occurred very seldom. Figure 5 shows the same error distribution, but for predicting yield strength. Figure 6 clearly notes that the highest errors were generated when the problem of predicting elongation was studied. Figure 7 also presents satisfactory predicting errors in the testing data set, for the case of predicting Brinell hardness of the nodular cast iron.

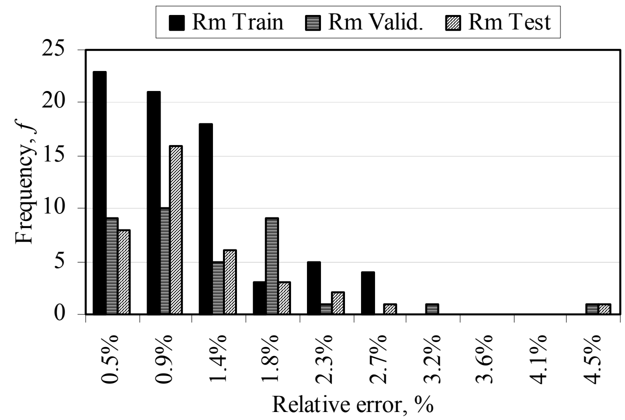

Figure 4. *Relative error distributions for tensile strength predicted by ANN.*

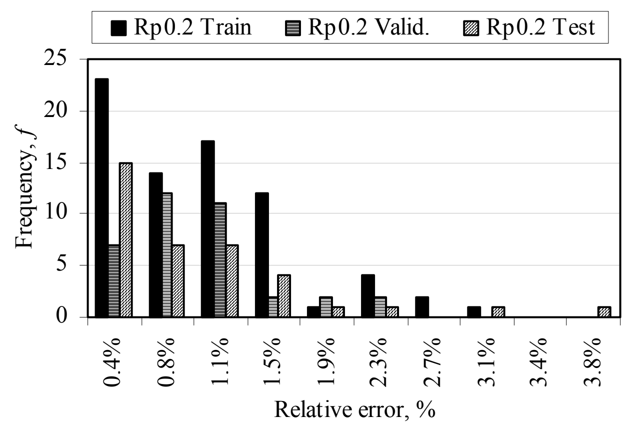

Figure 5. *Relative error distributions for yield strength predicted by ANN.*

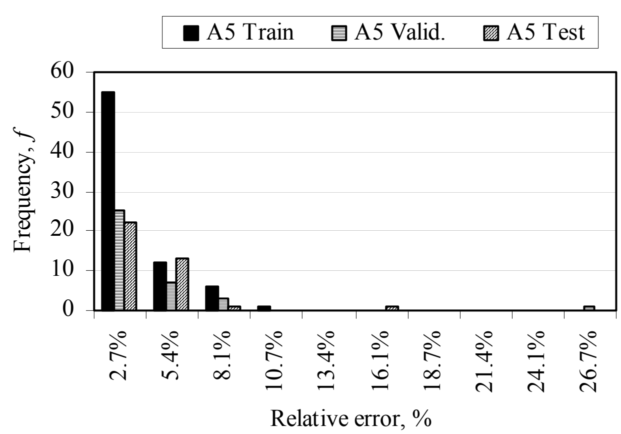

Figure 6. *Relative error distributions for elongation predicted by ANN.*

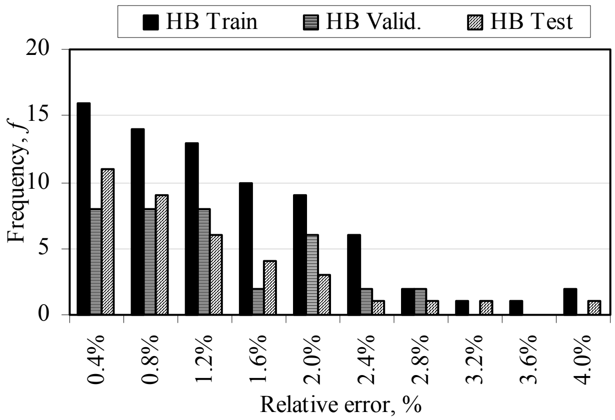

Figure 7. *Relative error distributions for Brinell hardness predicted by ANN.*

Table 1 presents the values of different error parameters in predicting tensile strength by neural network with a short statistical analysis of relative error. Also, error estimation parameter, NRMSE, and correlation coefficient, R, are given. Table 2 shows the same error parameters for predicting yield strength; Table 3 for predicting elongation; Table 4, finally, presents the errors in predicting hardness of ductile iron. All error parameters are given for each data set, i.e. learning, validation, and testing.

Table 1. *Different error parameters in predicting tensile strength.*

Rm, N/mm²		Training data set	Validation data set	Testing data set
Relative error, %	Min.	0.0%	0.0%	0.1%
	Max.	3.5%	2.6%	4.5%
	Average	1.0%	1.0%	1.1%
	St. dev.	0.8%	0.7%	1.0%
NRMSE		0.144	0.093	0.092
Correl. coef.		0.988	0.983	0.991

Table 2. *Different error parameters in predicting yield strength.*

$R_{p0.2}$ N/mm²		Training data set	Validation data set	Testing data set
Relative error, %	Min.	0.0%	0.0%	0.0%
	Max.	3.3%	2.6%	3.8%
	Average	1.0%	0.9%	1.0%
	St. dev.	0.8%	0.7%	1.0%
NRMSE		0.183	0.215	0.138
Correl. coef.		0.982	0.980	0.986

Table 3. *Different error parameters in predicting elongation.*

A_5, %		Training data set	Validation data set	Testing data set
Relative error, %	Min.	0.0%	0.4%	0.0%
	Max.	13.9%	26.7%	16.6%
	Average	3.1%	3.4%	2.9%
	St. dev.	2.8%	3.0%	3.1%
NRMSE		1.391	1.294	1.869
Correl. coef.		0.994	0.995	0.997

Table 4. *Different error parameters in predicting hardness.*

HB		Training data set	Validation data set	Testing data set
Relative error, %	Min.	0.00%	0.00%	0.00%
	Max.	4.20%	3.50%	3.40%
	Average	1.30%	1.10%	1.20%
	St. dev.	1.00%	1.00%	1.00%
NRMSE		0.312	0.427	0.287
Correl. coef.		0.968	0.983	0.985

Figure 8 shows the correlation between predicted and measured values of tensile strength for the testing data set; Figure 9 the same correlation, but for predicting yield strength; Figure 10 for elongation, and finally Figure 11 for predicting hardness. It can be seen that all four neural networks are successful in predicting corresponding mechanical properties of ductile iron, since they exhibit very high correlations in each testing data set.

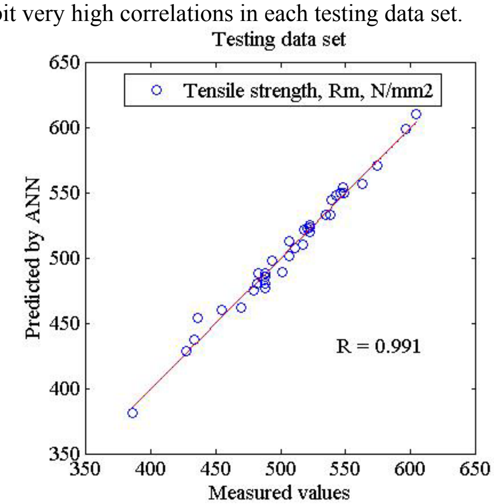

Figure 8. *Correlation of predicted and measured values of tensile strength in the testing data set.*

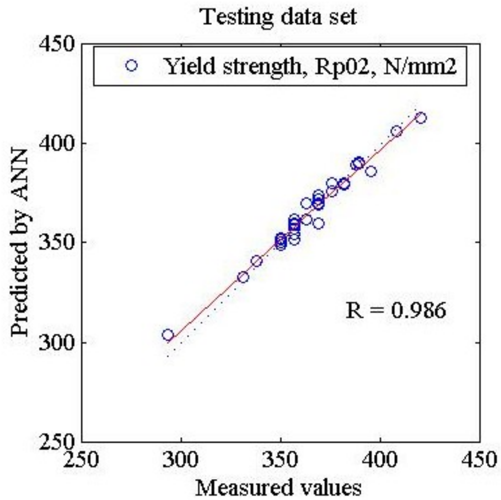

Figure 9. *Correlation of predicted and measured values of yield strength in the testing data set.*

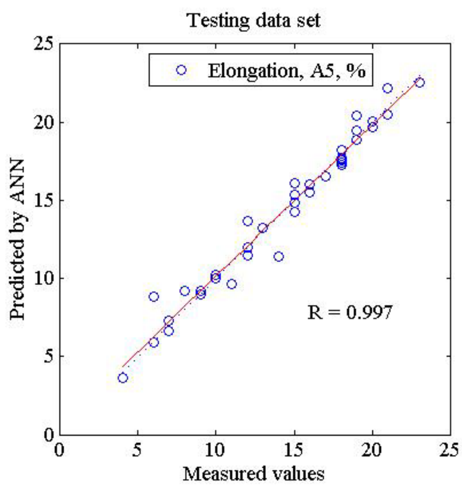

Figure 10. *Correlation of predicted and measured values of elongation in the testing data set.*

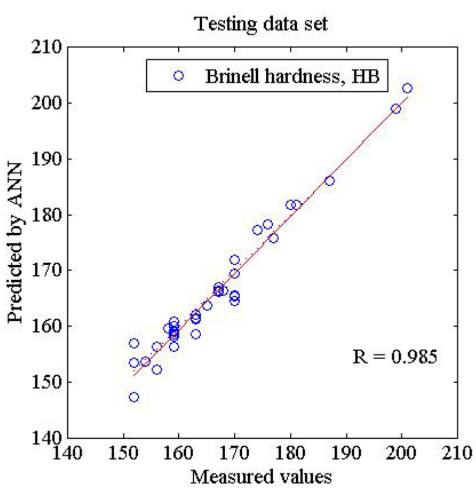

Figure 11. *Correlation of predicted and measured values of hardness in the testing data set.*

4. CONCLUSIONS

Correlation coefficients in the testing data set between measured and predicted data vs. number of neurons in the hidden layer has determined the most adequate number of hidden neurons for each of the four presented problems of predicting nodular cast iron mechanical properties.

Also, the most adequate slope of the tangent sigmoid activation function of hidden neurons was determined.

Statistical analysis of relative errors in predicting each of the specified mechanical properties, namely, tensile strength, yield strength, elongation and hardness, has showed that it is possible to successfully predict these properties by using the described models of artificial neural network, and by using chemical elements content data as input parameters. Predicted results in the testing data sets were mainly less than 2%, which is the acceptable experimental error when measuring the above-mentioned mechanical properties of ductile cast iron.

5. REFERENCES

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