Prediction optimization of mechanical properties of ferrite stainless steels after forging treatment with use of genetic algorithms

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ABSTRACT

Purpose: The paper describes the use of artificial neural networks to research and predict the effect of chemical components and thermal treatment conditions on stainless steel's mechanical characteristics optimized by genetic algorithm.

Design/methodology/approach: The quantity of input variables of artificial neural networks has been optimized using genetic algorithms to enhance the prediction quality of artificial neural network and to enhance their efficiency. Then a computational model was trained and evaluated with optimized artificial neural networks.

Findings: Optimization, with the exception of tensile strength, has enabled the creation of artificial neural networks, which either showed a better or similar performance from base networks, as well as a decreased amount of input variables As a consequence, noise data is decreased in the computational model built with the use of these networks.

Research limitations/implications: Data analysis was required to confirm the relevance of obtaining information used for modelling to use in training procedures for artificial neural networks.

Practical implications: Using artificial intelligence enables the multi-faceted growth of stainless steel engineering, even though there is only a relatively small amount of descriptors. Built and optimized computational model building using optimized artificial neural networks enables prediction of mechanical characteristics after normalization of forged ferritic stainless steels.

Originality/value: In order to decrease production expenses of products, an introduced model can be obtained in manufacturing industry. It can also simplify the selection of materials if the engineer has to correctly choose chemical elements and appropriate plastics and/or heat processing of stainless steels, having the necessary mechanical characteristics.

Keywords: Numerical techniques, Computational Material Science, Artificial algorithms, Stainless steel

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

RESEARCH PAPER

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1. Introduction

The material mechanical properties prediction possibility is valuable for manufacturers and design engineers. That is why in [1] results of mechanical properties optimization of ferrite stainless steel after rolling treatment with the use of genetic algorithms were published. Now the author would like to present the continuation of this investigation. This paper describes the optimisation results of forged stainless steel mechanical properties. To preserve the possibility of results comparison the applied modelling methodology was identical with the methodology used in [1].

2. Material

Examples of forged ferrite stainless structural steels were selected for examinations. The chromium concentration, which for stainless steel exceeds 10.5% [2-10], was the main criterion for selecting steel types. Further criteria for minimum and maximum concentration of chemical elements, temperature and other of heat treatment were taken from literature. The selection of examined mechanical properties, was based on analysis of world biggest steel markets and studies of literature [11-16].

3. Investigation methodology

Investigation methodology was identical to the study used to investigate steel after rolling treatment [1]. Computational model build with use of artificial intelligence allow prediction of mechanical properties of ferrite stainless steels after forging treatment based on input variables such as chemical composition and treatment conditions [17-23]. First stage of researches was the development of computational model built with the use of artificial neural networks. To improve prediction quality of artificial neural network models obtained artificial networks has been optimized with use of genetic algorithms. An automatic designer was used for comparative purposes in the modelling software. Modelling data was prepared using Excel [25] from Microsoft Office. Training of artificial neural networks and optimization through genetic algorithms was carried out using Statsoft's Statistica Neural Network [26].

4. Modelling of mechanical characteristics of ferrite stainless steel after forging treatment

An adequate amount of variables influencing the network is needed to construct an artificial neural network that will yield results with a strong correlation to laboratory measured values. Too many variables can influence the acquired outputs and cause noise. It is necessary to remove these less important variables. The removal of variables, which impacts the output considerably, will lead to a major error. The "automatic designer," which selects random topologies with the lowest statistical mistake and the highest performance based on its search algorithms, is another way to select the appropriate variables. Another way to do this is to use a genetic algorithm. It shows which variables have a significant effect on output values and which have no effect of any kind.

4.1. Input data analysis

Analysis of data is required to verify whether data is suitable for use in training of artificial neural networks. At the start from the information ranges for artificial neural network model variables were acquired. The best data distribution to be used for artificial neural network training is the number of variables uniformly distributed across the entire spectrum. Unfortunately, it is difficult to achieve such distribution for all variables. Variables that have values in clustered groups, may have no effect whatsoever on the model of artificial neural network, it was recommended that such variables be removed before creating a model. It is assumed that those variables should be removed from the set of input variables by the genetic algorithm.

Then the variable distribution within these ranges was determined using the Microsoft Excel histogram tool to further illustrate the results in a graph. Based on the results of the analysis, variables were assigned to three subgroups. The most significant variables were marked as "good", "mean" means less significant variables, and "poor" means the variables with the worst results. These variables should be discarded immediately from data vectors, but they were left for later analysis using artificial neural network tools and to confirm their proper operation. For carbon (Fig. 1a) and silicon concentration (Fig. 1b), the best distribution values were observed.
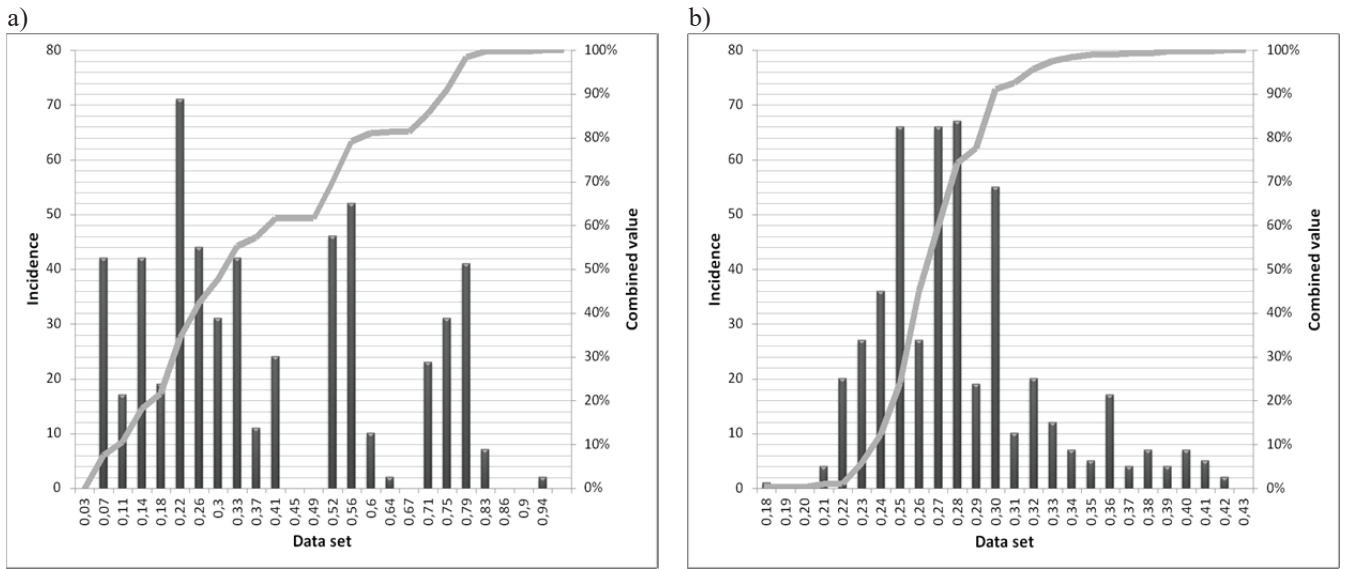
Fig. 1. Data set histograms for a) carbon concentration, b) silicon concentration

Five mechanical characteristics are estimated on the basis of input values such as concentration of chemical elements, normalizing temperature and time, rod diameter: yield strength (Rp$_{0.2}$), tensile strength (R$_m$), relative elongation (A), relative area reduction (Z) and hardness (HB).

The most significant parameters of artificial neural networks that were considered when choosing the best accessible network were the average absolute error, deviation ratio, and Pearson correlation [21].

Average absolute error E is the difference between the reference value and the value obtained at the output for the output variable:

$$E_j = \frac{1}{n} \sum_{i=1}^{n} (|x_i^z - x_i^o|)$$

where:
E_j – error of j-th property,
n – set size,
x_i^z – i-th value measured,
x_i^o – i-th calculated value.

Standard deviations ratio s for errors and for data is the main indicator of the quality of the regression model built by the network:

$$s = \sqrt{\frac{n \sum_{i=1}^{n} E_i^2 - (\sum_{i=1}^{n} E_1)^2}{n(n-1)}}$$

The correlation is determined by the standard Pearson R correlation coefficient for the set value and the value obtained at the output.

$$R = \frac{n(\sum_{i=1}^{n} x_i^z x_i^o) - (\sum_{i=1}^{n} x_i^z)(\sum_{i=1}^{n} x_i^o)}{\sqrt{(n \sum_{i=1}^{n}(x_i^z)^2 - (\sum_{i=1}^{n} x_i^z)^2)(n \sum_{i=1}^{n}(x_i^o)^2 - (\sum_{i=1}^{n} x_i^o)^2)}}$$

4.2. Construction of base artificial neural networks

The first model was constructed without optimisation using all 17 input variables. Table 1 presents the ranges of input and distribution of variables. All 1558 vectors based on laboratory data have been split into three sub-sets in relation 2-1-1. Using half of all available data, a set of vectors were created to modify the weights of the neuronal network (training set), one quarter of vectors were assigned to evaluate the prediction error during the training process (validation set). The remaining vectors was used to determine the prediction accuracy after network training process (testing set). The vectors were randomly assigned to the suitable sets.

Table 2 introduces statistics on architecture and regression for the best artificial neural networks build with use of all variables. This model was chosen for optimization with the use of genetic algorithm.

Table 1.
The range of input variable values

| range | diameter, mm | chemical composition, mass % | | | | | | | | | | | | | normalising | |
		C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al	temp., °C	time, min
min.	96	0.03	0.42	0.18	0.01	0	10.60	0.10	0	0	0	0	0	0	600	50
max.	980	0.94	1.57	0.43	0.02	0.02	20.00	2.41	2.70	0.01	0.01	0.08	0.71	0.03	980	360
distribution	good	good	good	good	poor	poor	good	mean	mean	poor	poor	poor	good	poor	mean	good

Table 2.
Parameters of non-optimized artificial neural networks

| variable | MLP network architecture | training set | | | validation set | | | testing set | | |
		average absolute error	standard deviation ratio	Pearson correla-tion	average absolute error	standard deviation ratio	Pearson correla-tion	average absolute error	standard deviation ratio	Pearson correla-tion
$R_{p0.2}$, MPa	17-3-1	19.21	0.36	0.93	24.88	0.36	0.93	20.16	0.26	0.97
R_m, MPa	17-10-1	13.11	0.24	0.97	13.53	0.22	0.98	18.50	0.28	0.96
A, %	17-5-1	0.92	0.56	0.83	0,88	0.46	0.89	0.97	0.56	0.83
Z, %	17-5-1	1.68	0.47	0.88	1.86	0.51	0.86	2.17	0.63	0.72
HB	17-5-1	9.36	0.60	0.80	11.45	0.63	0.78	13.03	0.83	0.61

4.3. Construction of the artificial neural networks using automatic designer

The next computational model has been created for verification purposes. For this model, artificial neural networks were developed using the automatic designer that promotes the critical building phases of the design. It has many instruments that make selecting the suitable network architecture automatically simple and optimizing the amount of variables input. Automatic designer also automatically stores the finest artificial neural network in which model built from these artificial neural networks will be used to assess the efficacy of a genetic algorithm. Table 3 introduces statistics on architecture and regression for the best artificial neural networks used in this model.

4.4. Optimization of artificial neural network using genetic algorithm

The last step was to use genetic algorithm to optimize the chosen artificial neural network. It consisted of creating the "mask" of variables to be used to model and examine the neural network's error. By adding to each variable penalty unit, the amount of inputs can be reduced, which can have a beneficial effect on their regression statistics. The genetic algorithm parameters in each test were the same except for the penalty unit, which increased every time the algorithm was used. With the amount of 200 generations, the algorithm population was 200 individuals. Standard values for Holland's classic genetic algorithm are the mutation probability of 0.1 and the crossover probability of 0.4. Sampling value was set to 0.3 to speed up modelling procedures. This reduced the search time for about 2 minutes and allowed to increase the number of individuals in the population and the number of generations. Then artificial neural networks were built using genetic algorithm-suggested variables. In this model, architectures and regression statistics are presented in Table 4 for the best artificial neural networks.

5. Modelling results discussion

Figure 2 introduces a comparison of mean absolute error for base, automatically constructed and optimized

neural artificial networks (testing set). Figure 3 introduces a comparison of Pearson correlation for base, automatically

constructed and optimized neural artificial networks (testing set).

Table 3.
Parameters of artificial neural networks build using the automatic designer

variable	MLP network architecture	training set			validation set			testing set		
		average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation
$R_{p0.2}$, MPa	11-6-1	12.84	0.21	0.98	15.50	0.24	0.97	23.01	0.61	0.82
R_m, MPa	11-7-1	14.68	0.25	0.98	12.37	0.19	0.98	17.61	0.34	0.94
A, %	3-4-1	1.15	0.70	0.71	1.15	0.62	0.79	1.26	0.68	0.73
Z, %	4-8-1	2.00	0.57	0.82	2.00	0.57	0.82	2.39	0.74	0.68
HB	11-7-4-1	8.27	0.55	0.83	11.04	0.60	0.80	11.48	0.74	0.68

Table 4.
Parameters of artificial neural networks optimized using genetic algorithms

variable	MLP network architecture	training set			validation set			testing set		
		average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation	average absolute error	standard deviation ratio	Pearson correlation
$R_{p0.2}$, MPa	14-4-1	23.74	0.27	0.93	18.93	0.27	0.96	16.90	0.21	0.98
R_m, MPa	8-5-1	16.15	0.29	0.96	12.58	0.19	0.98	18.50	0.35	0.94
A, %	9-4-1	0.86	0.54	0.84	0.94	0.54	0.84	0.93	0.53	0.85
Z, %	9-5-1	1.71	0.49	0.87	1.91	0.55	0.84	2.13	0.70	0.78
HB	4-8-1	9.66	0.70	0.72	12.10	0.70	0.72	10.21	0.73	0.69

Regression statistics analysis of optimized artificial neural networks built for yield strength prediction $R_{p0.2}$ showed that the optimized network with the lowest average absolute error and deviation ratio has the highest results. Pearson correlation also achieves peak value for this network. For tensile strength R_m. the optimised artificial neural network has a slightly smaller correlation, but also a much smaller error. For the relative elongation regression statistics analysis shows the best performance for artificial neural network optimised with use of genetic algorithm. The Pearson correlation is the highest with the smallest error. Very similar situation occurs for neural network optimized for the relative contraction Z. Regression statistics for automatic and optimized artificial neural

networks build for prediction of Brinell hardness HB are very similar. Again optimised network have the Pearson correlation the highest along with the smallest mean average error. Large values of the deviations ratio in the case of HB results from the method of measuring this quantity (accuracy). Even in metallurgical approvals, for the same melts, the measurement results are given as ranges with a tolerance of up to 30%.

Summarizing, for all material property, optimization improved the mean absolute error, which is the smallest in optimized networks. Only in the case of R_m, no improvement in Pearson's correlation was obtained, but the difference in neural networks is only 0.02% for the testing set.
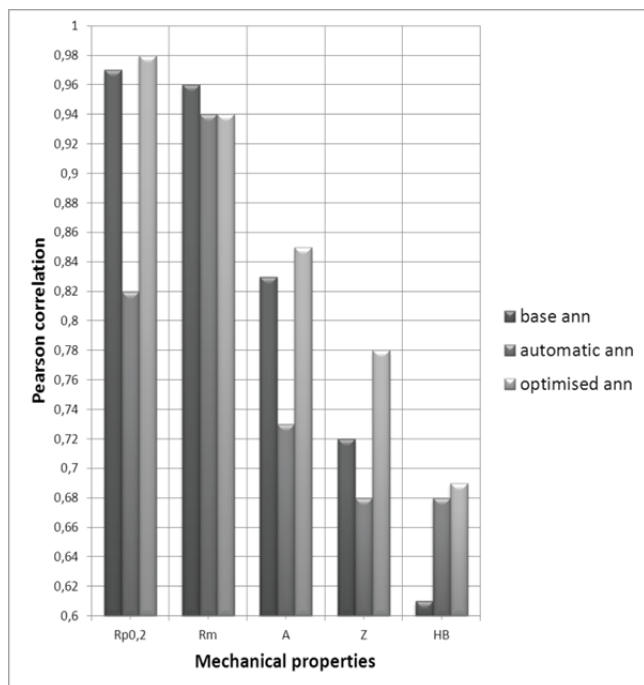
Fig. 2. Comparison of mean absolute error for base, automatic designed and genetic optimized neural artificial networks (testing set)
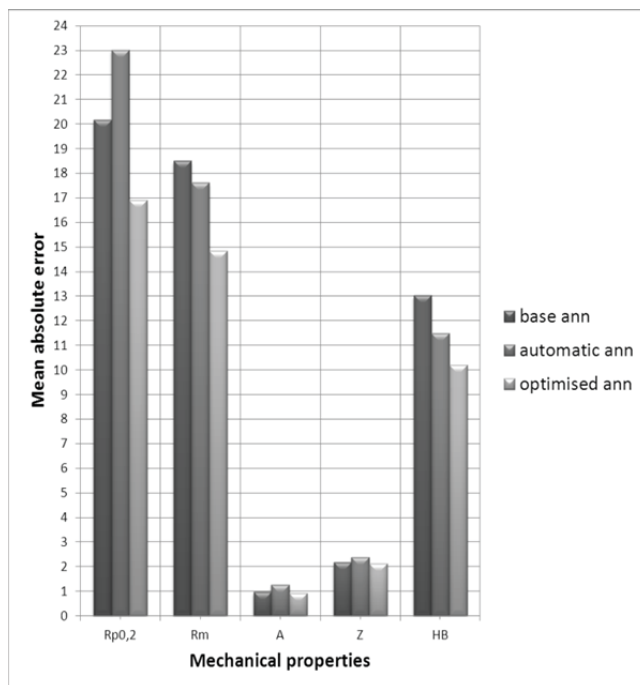

Fig. 3. Comparison of Pearson correlation for base, automatic designed and genetic optimised artificial neural networks (testing set)

Table 5.
Chemical composition, shape and heat treatment conditions of examined stainless steels used for verification purposes

| sample | diameter, mm | chemical composition, mass % | | | | | | | | | | | | | | normalising | | |
		C	Mn	Si	P	S	Cr	Ni	Mo	W	V	Ti	Cu	Al	temp., °C	time, min	medium
1	271	0.77	0.74	0.29	0.01	0.01	14.95	8.47	0.92	0	0	0	0.35	0	720	240	
2	180	0.03	0.50	0.26	0.01	0.01	14.15	1.61	2.14	0	0.01	0	0.37	0.01	980	120	air
3	50	0.11	0.46	0.22	0.01	0	12.11	1.35	2.65	0	0.23	0	0.33	0.02	960	60	

6. Experimental verification

The procedure for forged steel experimental verification was identical as for steel after rolling treatment [1]. An experimental set of three samples of ferritic stainless steel was created. Table 5 presents their chemical composition and treatment parameters. In order to minimize the variations between primary and verification results, material research was conducted in the same manner and using the same machinery used in the primary investigations. The results in a real laboratory obtained experimentally were compared to the results from

computer models. All of this is presented in Table 6. Differences between predicted and measured mechanical property values are very low and expected outcomes in all designs for the respective property did not exceed the artificial neural network tolerance values.

7. Summary

The aim of this study was to optimize the neural artificial networks to predict, following normalization, the mechanical properties of ferrite stainless steels. Using the

genetic algorithm, artificial neural networks have been optimized to obtain better regression statistics. Optimization enabled the creation of artificial neural networks, which either showed a better or similar performance from base networks, as well as a decreased amount of variables input. As a consequence, noise data is decreased in computational models built using these networks. Results of computational research conducted using these models were fully verified through experiments conducted in a real laboratory.

Table 6.
Comparison of measured and predicted mechanical properties of examined stainless steels used for verification purposes

sample	model	$R_{p0.2}$, MPa		R_m, MPa		A, %		Z, %		HB	
		measured	predicted	measured	predicted	measured	predicted	measured	predicted	measured	predicted
1	base	379	378	583	583	31.8	31.9	46,2	46.8	160	160
	automatic		378		583		30.2		43.8		157
	optimised		379		581		31.6		46.0		158
2	base	373	368	573	570	19.6	20.4	51,1	54.4	152	156
	automatic		369		581		22.8		58.6		163
	optimised		372		572		18.4		55.6		151
3	base	334	362	551	553	30.0	29.9	67,9	42.8	148	143
	automatic		342		555		31.8		61.5		147
	optimised		334		552		30.3		68.1		146

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