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COMPARATIVE STUDY ON INTELLIGENT AND CLASSICAL MODELLING AND COMPOSITION OPTIMIZATION OF STEEL ALLOYS

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Abstract

The paper considers two alternative approaches to modelling of dependence between steels alloying components quantities and their obtained after thermal treatment characteristics- nonlinear regression models and neural network

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models. The obtained two kinds of models are further applied for optimization of the steels compositions aimed at obtaining better mechanical characteristics. The optimization procedures were multiple objective mathematical programming (MOMP) approach using nonlinear regression model and gradient descent optimization procedure using neural network model. The obtained by both approaches results are compared with respect to the quality of models and characteristics of theoretically obtained steel compositions.

1. Introduction

Production of high strength steel alloys is of big importance for the modern metallurgy. The main aim is to obtain high quality materials reducing quantity of used expensive compounds. Another ecologically motivated reason to work on steels composition optimization is obtaining of ultra high strength steels (from the lower right part of the Figure 1) that will allow production of lighter machines- goal that will result finally in reduction of CO_2 emmisions in the atmosphere.

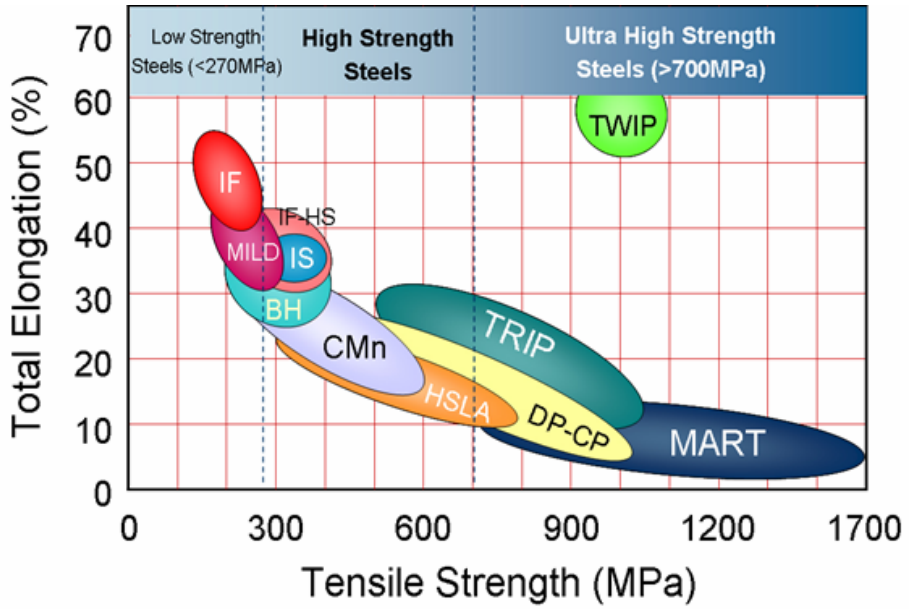

Figure 1. Steel's types dependence on their mechanical characteristics.

For achieving of this goals, first step is modelling of steels' strength characteristics in dependence on their composition. Further these models

could be user for simulation and optimization of the steels' composition. Usually, modelling in such cases uses the so-called "response surface methodology" [2] that applies regression dependences (in that case, usually nonlinear ones) between input and output variables. However, this approach can not always cope with complex nonlinear dependences in MIMO case. The application of intelligent modelling approaches such as neural networks is relatively new in this area, but there are some examples in the literature concerning other types of alloys [4, 7, 8]. From the other hand, it is known that neural networks are universal approximations of complex nonlinear dependences that apply "black-box" modelling approach [1, 3, 12]. So, they are proper candidates for modelling structure in the considered here task.

In any case, the identified high dimensional MIMO models are used further for solving of multicriteria optimization task. The multiple objective mathematical programming (MOMP) approach was usually applied in case of regression models. In the case of neural network models, another useful characteristic of them can be applied in optimization procedures: neural networks are able to accumulate knowledge by experience by using training procedures that are in fact optimization of neural network weights with respect to error at neural network output [12, 13]; thus, neural network training procedures offer a common approach to optimization tasks in process optimization and control applications [11, 12, 14].

In previous authors works, the approach described in [13] was successfully applied to dynamic optimization [5] as well as to optimization of cultural media composition and initial conditions [6] for two kind of biotechnological process that are other examples of highly nonlinear system.

In the present paper, both nonlinear regression and neural network models are applied for modelling of dependence between number of steel strength characteristics and amount of alloying elements included in that steel. These models are further applied for optimization of steel alloys composition aimed at maximization of their strength and economy of expensive alloying materials by using MOMP and gradient descent methods, respectively.

2. Strength Characteristics and Alloying Compounds of Steel

In our investigation, we have used a data base containing information about 65 steel alloys available at http://www.splav.kharkov.com/choose_type.php. There are given concentrations of eleven alloying elements included in the steels (shown in Table 1) and values of six steel strength characteristics tested after thermal treatment of the steels as follows: Rm – tensile strength; Re – yield strength; A – elongation; Z – reduction of area; KCU – impact strength; and HB – Brinell hardness (presented in Table 2). Tables 1 and 2 summarize the minimal and maximal values of the corresponding steel alloying elements and characteristics. Since the amount of sulphur and phosphorus are equal in all cases, they are considered as one variable (denoted by X_6). Further in the paper, the alloying elements are denoted as input vector X and steel characteristics – as output vector Y. Thus, our models presented further in the paper have 10 input variables and 6 outputs.

Table 1. Minimal and maximal values of the considered steel alloys compounds

		Min [%]	Max [%]
X_1	C	0.12	0.52
X_2	Si	0.27	1.4
X_3	Mn	0.35	1.75
X_4	Ni	0	4.22
X_5	B	0	0.006
X_6	S/P	0.0252	0.035
X_7	Cr	0.15	2.50
X_8	Cu	0	0.3
X_9	Mo	0	1.5
X_{10}	V	0	0.45

Table 2. Minimal and maximal values of the considered steel mechanical characteristic

		Min	Max
Y_1	Rm, [MPa]	540	1670
Y_2	Re, [MPa]	315	1375
Y_3	A,[%]	7	25
Y_4	Z, [%]	30	67
Y_5	KCU, [KJ/m²]	290	1830
Y_6	$HB^{*}10^{-1}$,[MPa]	179	541

3. Nonlinear Regression Modelling of Steel Alloys Composition

For each of the mechanical characteristics, a polynomial regression of second degree

$$Y_k = a_{00}^k + \sum_{i=1}^{10} a_{i0}^k X_i + \sum_{i=1}^{10} a_{ii}^k X_i^2 + \sum_{i=1}^{10} \sum_{j=i+1}^{10} a_{ij}^k X_i X_j, \tag{1}$$

was derived by using the regression modelling software package BMDP. Statistical evaluation of models was made with a level of significance $\alpha = 0.95$ (with the exception of the model for KCU, where $\alpha = 0.90$). The overall model equations are as follows:

$$\begin{aligned} Y_1 = {} & 922.58 - 17461.26X_6 - 3284.55X_{10} - 154.44{X_3}^2 + 39.62{X_4}^2 - 78.57{X_9}^2 \\ & - 5047.61{X_{10}}^2 - 465.49X_1X_2 + 496.46X_1X_4 + 1909.16X_1X_8 \\ & - 3020.77X_1X_9 + 9938.50X_1X_{10} + 491.27X_2X_3 + 601.62X_2X_4 \\ & - 182999.16X_2X_5 + 38414.58X_2X_6 - 5977.71X_2X_8 - 6.85X_3X_4 \\ & + 5980.11X_3X_6 + 118.85X_3X_7 + 1498.63X_3X_9 + 73546.49X_4X_5 \\ & - 5315.33X_4X_6 - 150.6X_4X_7 - 67.84X_4X_8 - 173.67X_4X_9 \\ & - 612.75X_4X_{10} + 115933.92X_5X_7 - 31798X_5X_8 + 7393.02X_6X_9 \end{aligned}$$

$$+ 1389.58X_7X_8 + 2245.49X_8X_{10} + 4803.16X_9X_{10}; \quad (2)$$

$$Y_2 = -417.10 + 2738.68X_1 + 1258.38X_7 - 8667.32X_{10} - 2846.6X_1^2 - 458X_2^2$$
$$+ 45.53X_4^2 - 312.72X_7^2 - 11693.26X_{10}^2 + 719.96X_1X_2 + 122.08X_1X_4$$
$$- 1081.15X_1X_7 + 21372.55X_1X_{10} + 700.07X_2X_4 + 171805.25X_4X_5$$
$$- 249.15X_4X_7 - 232.97X_4X_8 - 477.55X_4X_{10} - 699730X_5X_6$$
$$+ 2889.2X_5X_8 + 328.66X_7X_8 + 2378.92X_7X_{10} + 6907.67X_8X_{10}; \quad (3)$$

$$Y_3 = 30.1 - 27.41X_2 - 3.49X_4 - 16.51X_7 + 3.53X_7^2 + 6.59X_{10}^2 + 3.27X_1X_4$$
$$+ 7.91X_1X_7 - 67.35X_1X_8 - 6.8X_2X_3 + 123.1X_2X_8 - 2.7X_3X_4$$
$$- 84.85X_3X_6 + 3.78X_3X_7 + 3.01X_4X_7 + 51464.09X_5X_{10}$$
$$- 12X_7X_8 + 0.57X_7X_{10}; \quad (4)$$

$$Y_4 = 62.53 - 30.91X_1 - 6.79X_1^2 + 23.43X_2^2 + 1.08X_4^2 - 1373300X_5^2$$
$$- 903.39X_6^2 + 7473.31X_1X_5 + 66.57X_1X_8 + 209.11X_1X_{10}$$
$$- 7.15X_2X_3 + 2.31X_2X_4 - 9.36X_2X_7 - 47.57X_2X_8 + 10.57X_2X_9$$
$$- 12.47X_3X_8 - 36.54X_3X_9 - 230.93X_3X_{10} + 7040.29X_4X_5$$
$$- 95.85X_4X_6 - 2.18X_4X_7 - 4.02X_4X_{10} + 33971X_5X_6$$
$$+ 14713.5X_5X_9 + 5766.89X_6X_{10} + 54.51X_8X_9$$
$$- 348.62X_8X_{10} - 126.06X_9X_{10}; \quad (5)$$

$$Y_5 = 1078.5 + 149.71X_3 - 3613.44X_1^2 - 62413000X_5^2 - 937900X_6^2$$
$$- 419.055X_{10}^2 - 497.54X_1X_4 + 425650X_1X_5 + 84328.73X_1X_6$$
$$-1218.3X_1X_7 + 5764.8X_1X_9 + 69660X_3X_5 - 230.49X_3X_7$$
$$- 2650.3X_3X_9 - 3630.32X_3X_{10} + 321890X_4X_5 + 7010.29X_4X_6$$
$$-109.96X_4X_7 - 33.65X_4X_8 + 333.43X_4X_9 - 112380X_5X_8$$

$$+18804.16X_6X_7 + 146980X_6X_{10} + 201.35X_7X_8 - 634.5X_7X_9$$

$$- 5443.58X_8X_{10} - 4282.98X_9X_{10}; \quad (6)$$

$$Y_6 = 285.13 - 102.73X_2 + 222977.88X_5 - 4432.83X_6 + 24.49X_7 + 330.24X_{10}$$

$$- 0.23{X_3}^2 + 3.91{X_4}^2 - 83.99{X_9}^2 + 280.27{X_{10}}^2 - 58.47X_1X_4$$

$$+ 10355.06X_1X_5 + 5935.66X_1X_6 - 67.81X_1X_7 - 102.88X_1X_8$$

$$+ 625.40X_1X_9 - 1146.09X_1X_{10} - 15.64X_2X_4 + 2578.16X_2X_6$$

$$+ 36.92X_2X_7 + 52.65X_3X_4 - 3.06X_4X_7 - 28.48X_4X_8$$

$$- 6519800X_5X_6 + 884.08X_6X_8 - 1280.41X_6X_9 + 8.92X_7\mathrm{Cu}$$

$$- 74.41X_7X_9 + 41.39X_7X_{10} + 240.38X_8X_9 + 217.9386X_9X_{10}. \quad (7)$$

Table 3 below summarizes the statistical characteristics of all nonlinear regression models. Since the inequality of multiple correlations $F > F_T$ is fulfilled for all of the models, we can conclude that the coefficients obtained for all the regressions are statistically significant. From the statistical point of view, the model for HB is the best one, while that for KCU has lower level of significance and hence is the worst one.

Table 3. Mean square error and multiple regression statistical characteristics of nonlinear regression models. Here * means that this values are for level of significance $\alpha = 0.90$; the all other results are for level of significance $\alpha = 0.95$

	MSE	R	ν_1	ν_2	F	F_T
Rm	0.0927	0.8617	32	57	5.135	1.65
Re	0.1167	0.8366	22	68	7.210	1.70
A	0.1305	0.7651	17	73	6.064	1.84
Z	0.1315	0.7834	27	59	3.472	1.70
KCU	0.1159	0.6882	26	49	1.696*	1.57*
HB	0.0252	0.9804	30	47	38.765	1.74

Figure 2 presents graphical comparison of the nonlinear regression models predictions with the experimental data. All values are normalized in the range [0, 1] in order to compare them further with ANN model predictions. These normalized data are also used for mean square error (MSE) calculation that is given in Table 3 too.

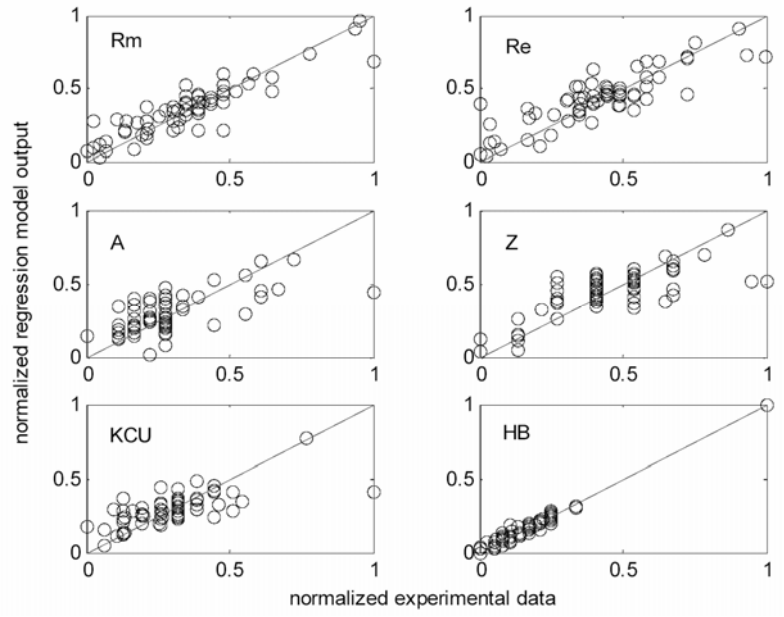

Figure 2. Nonlinear regression model fitting.

4. Neural Network Modelling of Steel Alloys Characteristics

For the modelling via neural networks, the available data are scaled in proper interval [0, 1]. The used neural network structure (presented in Figure 3) is multi-layered without feedback connections, since the modelled dependence is static. The neurons, transfer function is log sigmoid. Training procedure is resilient backpropagation. Different in number of layers and hidden neurons neural network structures were tested and the better one is chosen. It has 10:40:6 structure. The number

of input and output neurons correspond to the number of the input/output variables. The data base is separated into training and testing data sets with ratio of 90:10%. The obtained for these data sets mean square error is shown in Table 4 below. The model fitting is also shown in Figures 4 and 5. The corresponding linear regression coefficients R and mean square errors (MSE) are given in Table 4. As can be seen, the training data is approximated very well with close to 1 regression coefficient, while the testing data shows worse values especially for some of the output variables that correspond to the higher testing MSE in Table 4. This could be explained by the insufficient amount of data, because neural networks need a lot of examples to be trained properly. Moreover, some of the data are not evenly distributed over the considered interval values or contain only two or three investigated values for some of the alloying components.

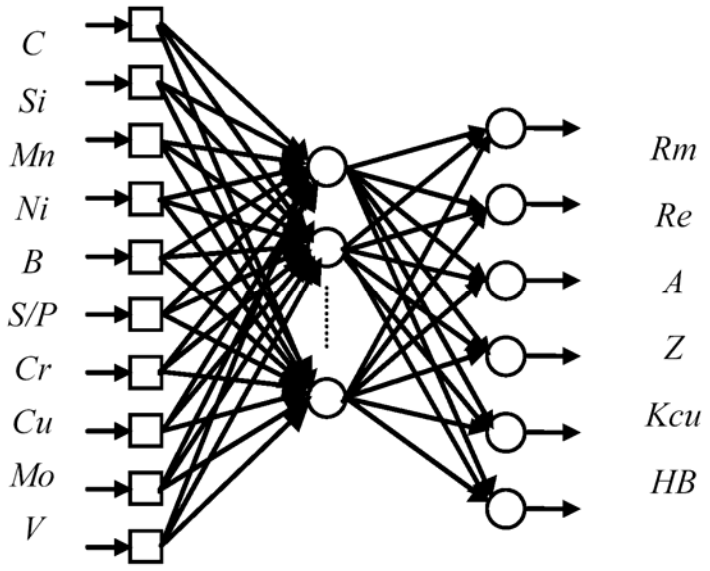

Figure 3. Neural network model structure.

Table 4. Training and testing errors and linear regression coefficient of the ANN model

	MSE		R	
	Train	Test	Train	Test
Rm	0.0058	0.1930	0.9975	0.5539
Re	0.0065	0.2611	0.9899	0.2812
A	0.0085	0.1565	0.9788	1.2510
Z	0.0135	0.2184	0.9795	0.5739
KCU	0.0110	0.1778	0.9735	1.3207
HB	0.0075	0.1417	0.9869	1.2144

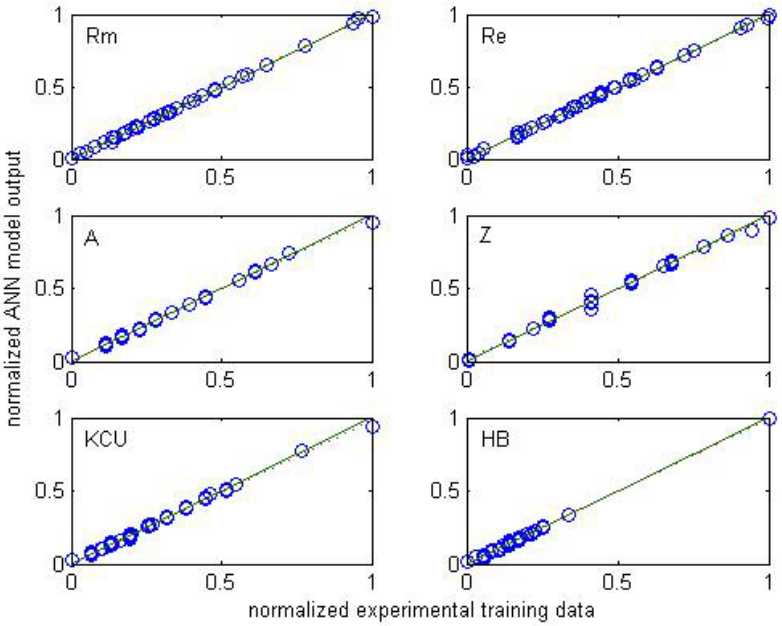

Figure 4. Training data model fitting.

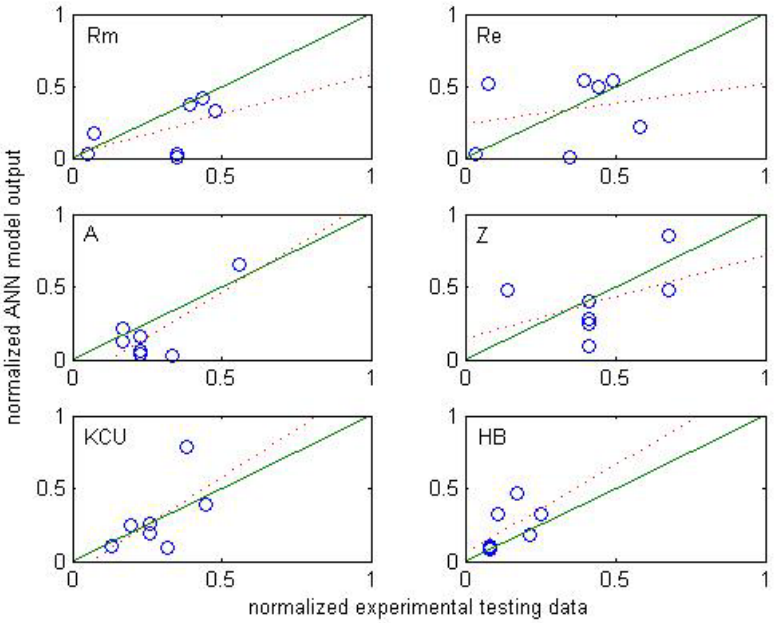

Figure 5. Testing data model fitting.

Further improvement of that model will be subject of more data collecting. However, even now the ANN model outperforms the nonlinear regression form the previous section. The results from optimization shown further also demonstrated considerably reasonable results in spite of model insufficient accuracy.

5. Solving the Optimization Problem Using Multiple Objective Mathematical Programming Approach (MOMP)

We have constructed a model, which has six nonlinear objective functions and ten decision variables. Thus, in a natural way, we derive a nonlinear multiple objective mathematical programming problem. The feasible set is one-dimensional rectangular with boundaries [–1, 1].

First, let us consider in brief the general formulation of the multiple objective mathematical programming problem (MOMP), some of its properties and how it can be solved.

Mathematically, the MOMP can be formulated as

$$\max_{x \in S: g_j(x) \le 0,\ j=1 \div m} (f_1(x), \ldots, f_k(x)), \tag{8}$$

where

$x = (x_1, \ldots, x_n) \in R^n$ is the vector of decision variables;

$f_i(\cdot),\ g_j(\cdot) : R^n \to R^1$ are real valued functions.

The symbol "max" means that all the objectives have to be maximized simultaneously. We assume also that

– at least two objectives are conflicting;

– decision point (solution) does not exist to optimize simultaneously all the objectives. MOMPs are discussed, for example, in [9, 15].

We say that a decision vector $f(y)$ dominates a decision vector $f(x)$ iff $f_i(x) \le f_i(y)$ for $i = 1, 2, \ldots, k$ and strong inequality holds for at least one index.

According to the above defined orders, (Pareto) efficient and weak (Pareto) efficient points are defined.

Definition 1. The solution of x is Pareto optimal, if and only if there do not exist another solution of y such that $f_i(x) \le f_i(y)$ for $i = 1, 2, \ldots, k$ and $f_i(x) < f_i(y)$ for at least one index $j \in I = \{1, 2, \ldots, k\}$.

Definition 2. The solution of x is weakly Pareto optimal, if and only if there do not exist another solution of y such that $f_i(x) < f_i(y)$ for $i = 1, 2, \ldots, k$.

The corresponding vector $f(x)$ is called a *non-dominated vector*.

The aim of solving MOMPs can be defined as supporting the decision maker to identify the most preferred solution in the set of efficient points. It is called final, best compromise solution. It is a compromise between conflicting objective values. To find such a solution, additional information is needed. It is usually given by a person: the expert/decision maker (DM).

As it could expect, a number of methods exist for solving MOMP [9]. A straightforward way for the DM to express preferences is to specify the aspiration levels for the objective functions. They are desirable values of the objective functions and form the so-called reference point [15, 16].

A dialogue in the form of a classification is related to reference points. In classification, the DM studies a current solution and tells what kinds of changes are desirable, in other words, which function values are satisfactory at the moment, which should improve and which could impair (and by how much). The satisfying trade-off method - STOM [10] uses such a classification. When the DM has indicated desirable aspiration levels for the objective functions that should be improved, the method calculates what kinds of impairments are necessary in the other objective functions. In this way, the DM has to specify less information. However, the method sets many mathematical assumptions for the problem. The method generates one solution for all iteration. Despite of its restrictions, method STOM is very simple and understandable to use by the DMs. Therefore, we used it to solve our problem.

In brief, STOM method consists of the following general steps:

Step 1. Generate initial Pareto or weak Pareto solution.

Step 2. The DM evaluates it and if it is not a final solution, then he/she is asked to classify the objective functions into three classes. They

are the unacceptable objective functions, whose values he/she wants to improve $(I >)$, the acceptable objective functions he/she accepts as they are $(I =)$ and objective functions he/she agrees to relax $(I <)$. The DM has to specify the aspiration levels only for the objective functions in $I >$.

Step 3. Solve the following scalarising function:

$$\min_{X} \max_{i=1,\ldots,k} [w_i^h (f_i(x) - z_i^{**})], \tag{9}$$

where X is the set of decision variables that fulfills the constraints and the weighting coefficients are

$$w_i^h = 1/(f_i^{r,h} - z_i^{**}) \quad \text{for } i = 1, 2, \ldots, k. \tag{10}$$

Here, $f^{r,h}$ is the reference point at iteration h and z^{**} is the ideal vector.

Let the solution found is x^h. Go to Step 2.

The solutions of the above scalarising problem are weak efficient solutions. Also, it is shown that the solution is satisfying (i.e., $f_i(x^h) \leq f_i^{r,h}$), if the reference point is feasible and weighting coefficients are employed.

If we cannot find exactly max f_i or f_i is unbounded over X, then we can use sufficiently large number. Also, it is necessary $f_i^{r,h} < z_i^{**}$.

The DM performed several iterations for different aspiration levels and a number of efficient solutions were generated. As a result of the study on the efficient set, 1-2 decisions have been separated as promising ones.

Applying the above described STOM for the nonlinear regression models (2)-(7), the following solution is obtained and presented in Tables 5 and 6. However, because of big MSE of the model, the results about steel strength characteristics are far from the reasonable intervals. So, the nonlinear regression model is not of quality sufficient to be applies for optimization purposes.

Table 5. The optimized composition of elements from solution obtained

Element	C	Si	Mn	Ni	B	S/P	Cr	Cu	Mo	V
%	0.5	1.25	1.645	3.95	0.006	0.02	0.15	0	0.44	0.02

Table 6. The obtained strength characteristics for the optimized steel composition

Rm	Re	A	Z	KCU	HB
6745.2	8329.0	– 38.7167	242.0310	7439.2	1094.4

6. Gradient Descent Optimization of Steel Alloys Composition

Unlike the MOMP optimization procedure used here (gradient descent) could lead to stopping in local minima, since the explored input/output space is multi-dimensional and the modelling function is highly nonlinear. So, in order to find optimal values of input variables with respect to given quality criteria that comprises output variables, there is need to explore whole region of the input space. However, because of big number of possible combinations, the exhaustive search on whole variables space will take too much time. Because of this, we applied gradient optimization technique starting from several different points of input variables surface and compare the obtained results.

Figure 6 below represents the optimization procedure scheme adopted from the so-called “backpropagation of utility” method [13].

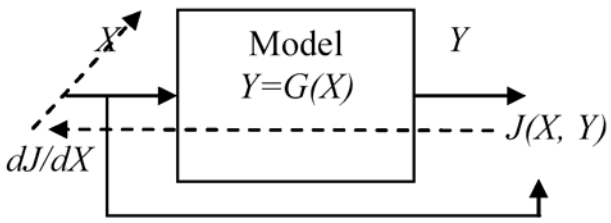

Figure 6. Optimization procedure.

The optimization task here is defined as follows: Find values of input vector X that minimize/maximize the utility function

$$J = J(X, Y), \tag{11}$$

where Y is vector of output variables that are related to the input once by a given usually nonlinear model function G as follows:

$$Y = G(X, p). \tag{12}$$

Here, p is model parameters vector.

Every optimization procedure needs calculation of performance function gradients with respect to the optimized variables as follows:

$$dX = \frac{dJ}{dX} = \frac{\partial J}{\partial X} + \frac{\partial J}{\partial Y}\frac{\partial G}{\partial X}. \tag{13}$$

In case when J does not depend explicitly on X, the first term in Equation (13) is zero and thus gradient depends only on function G.

The layered neural network structure offers a convenient way for calculating derivatives in Equation (13), because their training backpropagation method [12, 13] was developed initially as procedure for error derivatives calculation "propagation" from the output to the input of the network. From a more common point of view, it is method for a given function derivative calculations with respect to variables of an ordered system of equations [13]. Hence, it could be applied to any optimization

problem that can be described in appropriate way. So, application of neural network model trained before as function G within optimization scheme from Figure 6 allows easy gradient calculation by using backpropagation method.

Further some gradient iterative optimization procedure could be applied to find optimal values of the X variables by using calculated derivatives as follows:

$$X_i = X_{i-1} \pm \alpha \Delta X_i, \tag{14}$$

where α is parameter called *learning speed* and ΔX_i is step-change of X for the i-th iteration calculated as follows:

$$\Delta X_i = g(dX_i). \tag{15}$$

Here, g is some dependence of optimized variable derivative. Usually, it is proportional to the derivative dX_i, but can also depend on the old values of ΔX_i.

In the present study, we used simple gradient optimization procedure with identity function for g, i.e., $\Delta X_i = dX_i$. The learning speed α is set to a relatively small value and stopping criteria is very small change of performance function gradient. Since we have totally 6 output variables that represent different steel characteristics, we combine them in a single criterion by simple summation with equal weight coefficients of 1 as follows:

$$J = \sum_{k=1}^{6} Y_k. \tag{16}$$

In order to explore different input variables regions, several initial combinations of alloying components values are generated. They are shown in Table 7.

Table 7. Initial values of optimization procedure

	Case 1	Case 2	Case 3	Case 4	Case 5	Case 6	Case 7
C	0.1634	0.2426	0.3219	0.4011	0.4804	0.3417	0.4804
Si	0.3806	0.6071	0.8337	1.0602	1.2867	0.9469	1.2301
Mn	0.4869	0.7675	1.0482	1.3289	1.6097	1.2588	1.4693
Ni	0.4136	1.2576	2.1016	2.9456	3.7896	2.9456	3.1566
B	0.0005	0.0015	0.0025	0.0035	0.0045	0.0037	0.0035
S/P	0.0231	0.0257	0.0284	0.0310	0.0337	0.0324	0.0304
Cr	0.3837	0.8539	1.3243	1.7946	2.2649	2.1473	1.5594
Cu	0.0294	0.0894	0.1494	0.2094	0.2694	0.2694	0.1644
Mo	0.1470	0.4470	0.7470	1.0470	1.3470	1.4220	0.7470
V	0.0441	0.1341	0.2241	0.3141	0.4041	0.4491	0.2016

The obtained after optimization concentrations of all 10 alloying components are shown in Table 8. Table 9 presents the steel alloys strength characteristics that correspond to the optimized compositions.

Table 8. Compounds values after optimization

	Case 1	Case 2	**Case 3**	Case 4	Case 5	Case 6	Case 7
C	0.1673	0.2354	**0.2392**	0.4804	0.4470	0.2134	0.2648
Si	0.6427	0.3919	**0.3919**	1.2867	0.3919	0.3919	1.2823
Mn	0.5009	0.5009	**1.1820**	1.6097	1.6097	1.1742	1.0663
Ni	0.6178	3.7896	**3.7896**	0.4558	0.4558	3.7896	0.4558
B	0.0011	0.0045	**0.0005**	0.0021	0.0026	0.0005	0.0022
S/P	0.0245	0.0232	**0.0337**	0.0303	0.0337	0.0337	0.0337
Cr	2.2649	0.4072	**0.4072**	2.0727	2.2649	0.6727	2.2649
Cu	0.0324	0.0324	**0.0520**	0.2694	0.2694	0.0655	0.1140
Mo	0.5961	0.1620	**0.1620**	1.3470	0.8717	0.1620	1.3470
V	0.3789	0.0486	**0.0645**	0.0805	0.0486	0.0731	0.0486

Table 9. Characteristics values after optimization

	Case 1	Case 2	**Case 3**	Case 4	Case 5	Case 6	Case 7
Rm	1334.3	1621.6	**1564.6**	546.5	538.9	1559.1	536.5
Re	1072.8	1268.7	**1368.8**	1269.5	488.8	1367.3	723.6
A	19.7	16.7	**21.1**	69.0	22.1	21.2	19.6
Z	66.7	59.4	**66.5**	29.7	57.8	66.5	30.2
KCU	1719.9	1548.5	**1684.4**	292.6	1787.1	1703.0	1579.3
HB	180.7	450.2	**485.9**	406.9	369.6	481.9	416.8

Table 10 summarizes the training procedure iterations and achieved value of criterion J in normalized form. This means that maximal possible value of J is 6. The case with best results is marked in bold in all tables. The obtained results showed that the optimal values depend too much on the starting point that means that nonlinear dependence F has a lot of local optima. Of course definition of performance criterion J also is of big importance since by using weight coefficients, it can give preference to some of the strength characteristics over the others. All these will be issues of further investigations.

Table 10. Optimization procedure iterations and achieved criterion value

	Iterations number	Scaled criterion
Case 1	175	4.0569
Case 2	407	4.7620
Case 3	**952**	**5.4288**
Case 4	522	1.5472
Case 5	919	3.2619
Case 6	464	5.4245
Case 7	1109	2.6

7. Conclusion

From the presented comparative study, the following main conclusions are derived:

– The exploitation of neural network properties as universal nonlinear approximations of complex nonlinear MIMO dependences allowed to model six steel alloys characteristics in dependence on ten alloying substances with a single model structure. Lack of sufficient data did not allow perfect modelling, but nevertheless, the ANN model of steel alloys compositions in dependence on obtained strength characteristics of steels outperforms the nonlinear regression model.

– The obtained via MOMP optimization steel compound is close to spring structural steel, but with considerably bigger amount of Ni. Bigger amount of C guarantee obtaining of martensite structure that means high strength and low plasticity. However, since the nonlinear regression model approximates with bigger error, the dependence between input and output variables, the obtained via MOMP optimization steel characteristics, were not reasonable.

– The gradient optimization technique using properties of neural network layered structure for derivatives calculation allowed solving of multi-criteria optimization task with reasonable number of iterations. The newly developed composition of steel, which position among other steels is shown in Figure 7 is close to the TRIP steel in [17], but in contrast to [18], it contains two times less Ni and also lower amount of Mo, Cr, and Si.

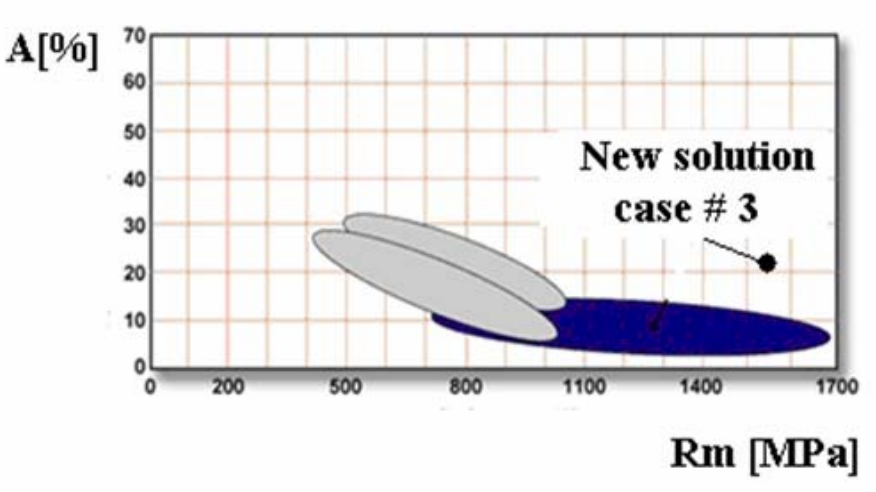

Figure 7. The obtained new steel composition position on the steels types chart.

In conclusion, the comparative study definitely showed that intelligent approach using ANN significantly outperforms the classical one by using regression models. Further investigations targeted to including more data in training data base as well as to exploring exhaustively the input variables surface will allow refinement of the proposed methodology and obtaining of more accurate results that could be tested in practice.

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