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Application of Bayesian Neural Networks to Predict Strength and Grain Size of Hot Strip Low Carbon Steels

Mohammad Reza Toroghinejad and Mohsen Botlani Esfahani

Dept. of Materials Engineering, Isfahan University of Technology, Isfahan, 84156-83111, Iran

1. Introduction

Low alloy steels are the most demanding materials that are used in industrial processes such as hot stripping. Hot stripping is a severe plastic deformation which is applied on cast steels for a variety of shapes and sizes. A hot strip mill consists of, from start to finish, reheat furnaces, roughing mill, finishing mill, runout table with accelerated cooling and finally a coiler, as shown in Figure 1.

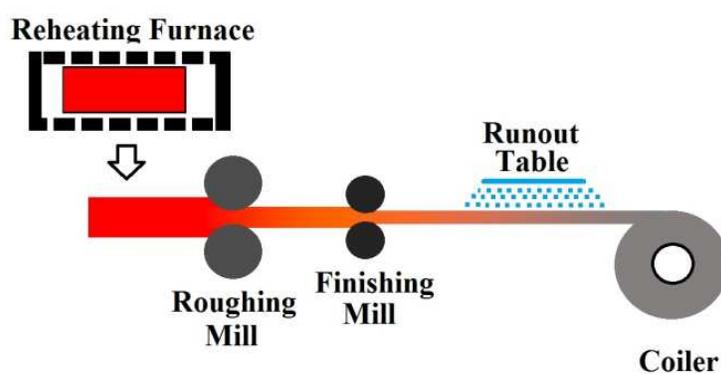


Fig. 1. Schematic illustration of hot strip mill.

The process enhances the properties of steels by several metallurgical mechanisms which take place in different parts of the hot strip mill. This process is illustrated in Figure 2 which includes following metallurgical phenomena:

1. Austenitization, dissolution of microalloy compounds and homogenization of the chemical segregation in the reheating furnace.
2. Deformation and reduction of reheated slab to intermediate thickness which is accompanied with recrystallization, grain growth and precipitation of alloying and microalloy elements in roughing and finishing mills.
3. Phase transformation and precipitation during cooling and decreasing the heat to room temperature (Ryu, 2008), (Gonzalez, 2002).

These mechanisms by refinement of structure bring about a simultaneous improvement in strength and toughness (Singh et al., 1998).

1.1 Grain size effect on mechanical properties

Grain size is an important aspect of microstructure with respect to mechanical properties of steels. The ferrite in low carbon steels is typically strengthened by grain refinement, precipitation hardening, and, to a lesser extent, solid-solution strengthening. Grain refinement is the most desirable strengthening mechanism because as mentioned earlier it improves not only strength but also toughness. According to equation (1) indicating the Hall-Petch relation, fine grain size produces higher yield strength, (σ_{yield}) (Parker, 1997):

$$\sigma_{\text{yield}} = \sigma_{\text{init}} + k_y d_{\alpha}^{-1/2} \quad (1)$$

where σ_{init} is the yield strength for a polycrystalline material, k_y is a constant, and d_{α} is a measure of the ferrite grain size. Grain size also has an effect on the ultimate tensile strength by changing work-hardening rate. Work-hardening takes place within the grains during plastic deformation according to Morrison (Ryu, 2008):

$$n = 5 / (10 + d_{\alpha}^{-1/2}) \quad (2)$$

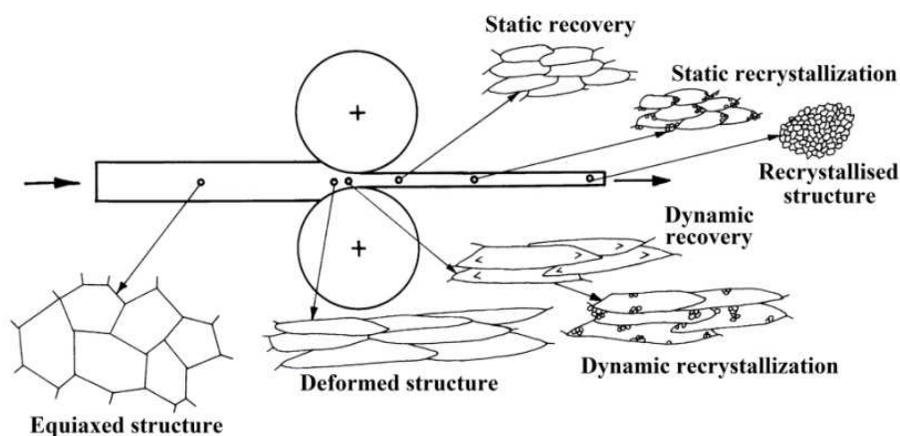


Fig. 2. Related metallurgical phenomena.

where n is work-hardening exponent and d_{α} is grain size. Ferrite mainly nucleates at the austenite grain boundaries and thus a finer austenite grains produces fine ferrite grains. Further ferrite refinement can be achieved by transformation from deformed austenite grains because, deformation increases ferrite nucleation rate (Parker, 1997). The effects of chemical composition on these properties are an important parameter as well as thermo-mechanical processing features such as temperature and final dimensions (Ryu, 2008). The additions of some alloying elements affect ferrite transformation and thus control the amount of phases present in the final matrix. The presence of microalloying elements generally control the grain size and provide precipitation strengthening and have a significant impact on the strength (Singh et al., 1998). Therefore, estimating of strength and grain size of hot stripped steel products depends on thermo-mechanical behavior of steel, microstructure evolution and phase transformation, during hot rolling stages and cooling period. These are complicated metallurgical phenomena and strongly depend on chemical composition, therefore developing a physical model to analysis these parameters and predict strength as well as final grain size, is cumbersome. Also, the accuracy of the models developed so far is somehow questionable and

are not suitable for practical purposes. Traditionally, setting the tolerances is carried out by making several samples and checking the final results by trial and error approach. Generally, these procedures are expensive and time-consuming especially in such a complex metallurgical phenomena. Consequently, the overall effects of these features can have an effect on rolling design and therefore too many experimental trials are needed to achieve ideal tolerances. Since estimating these properties of low carbon steel strips in terms of chemical composition and thermo-mechanical parameters is desirable from engineering view point, several models are introduced based upon different neural network methods. These models are capable of understand very complex and unknown relationships between inputs and output data. Furthermore, the models can explore the effect of the individual input on output which can be extremely difficult in the experimental tasks. Achieved model for estimating tensile strength can be used as a quantitative tool to predict the final tensile strength of these commercial low carbon steels with different of input variables. Moreover analysis of the effect of input parameters on results may leads to design new steels with different input parameters. In the present work also, by selecting more relevant inputs and using hybrid Bayesian Artificial Neural Network (ANN) model assisted with Reversible-Jump Markov Chain Monte Carlo (RJMCMC, also known as trans-dimensional MCMC), the prediction of final grain size in low carbon steel strips is carried out.

2. Method

2.1 Artificial Neural Networks

A neural network is an interconnected network of a set of simple processing units which are connected by a set of connections called "weights". They can learn the given information by a set of examples and transfer them to their structure. The method which is inspired from studying the human brain, is capable of recognizing complex patterns of the training data and can be applied to regression and classification tasks. The training is an optimization procedure by finding a set of weights which combined with processing units, describes the data pattern. There are several advantages in this method. Firstly, there is no need to choose the behavior of the model in advance. Secondly, its need to train data, does not grow as fast as other conventional regression methods and therefore, growing the complexity and dimensionality of the problem doesn't need any further data (Botlani-Esfahani et al., 2009a). Basic ANN model with k outputs is

$$f_k(x, w) = w_{k0} + \sum_{j=1}^m w_{kj} \tanh(w_{j0} + \sum_{i=1}^d w_{ji} x_i) \quad (3)$$

where x is a d -dimensional input vector, w denotes the weights, and indices i and j correspond to input and hidden units, respectively (Lampinen & Vehtari, 2001). Arrangement of layers and units in an ANN called architecture (Doan & Yuiliong, 2004). Figure 3 sketches schematic architecture of a feed forward ANN model. In each layer, units receive their input from previous layer's units and send their output to units in the following layer. Output of each hidden unit is the transfer function response to the weighted sum of its inputs.

The number of units in input and output layers are dictated by the problem, but the number of hidden units which control the complexity of the model, must be determined.

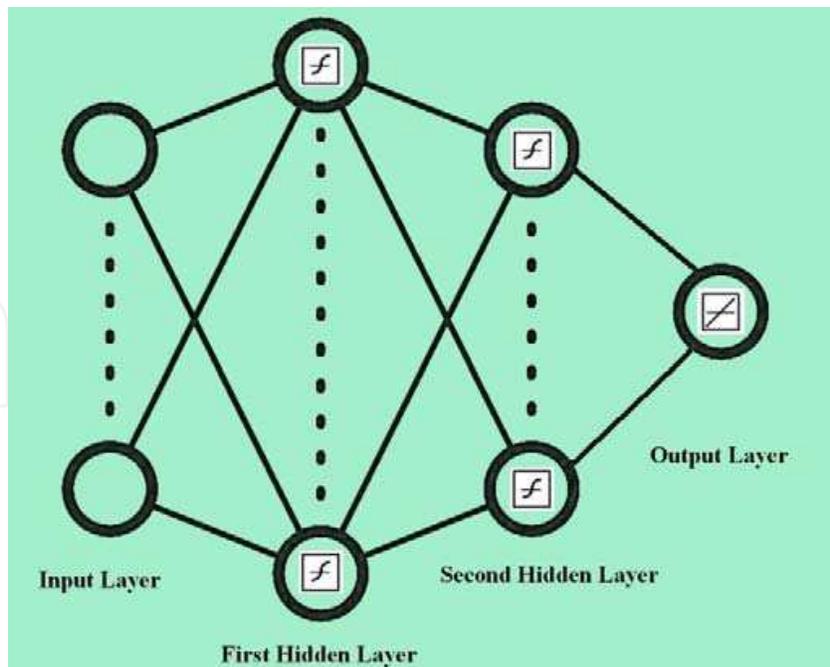


Fig. 3. Schematic architecture of Artificial Neural Network model.

The processing units for computational convenience, like nonlinear hyperbolic tangent sigmoid functions are easily differentiable, and are employed in the present model, Equation (4):

$$\tanh(x) = \frac{2}{(1 + \exp(-2x)) - 1} \quad (4)$$

Traditionally the complexity of the ANN has been controlled with early stopping. In which part of the training data is used to train the network and other part is used to control the complexity of the model. Early stopping is inefficient because the effective complexity may be much less than the number of parameters in the model. Consequently, two different Bayesian Learning paradigm for ANN was employed to train models.

2.2 Bayesian learning for ANN

In the Bayesian framework which has introduced by MacKay (MacKay, 1992) the weights of the network are considered as random variables and the posterior distribution of the weights updated according to Bayes' rule (Xu et al., 2006):

$$\text{Posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{Evidence}} \quad (5)$$

This equation in terms of Artificial Neural Networks is:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} \propto L(\theta|D)p(\theta) \quad (6)$$

where $p(\theta)$ is prior distribution for the model parameters θ , $D = \{(x(1),y(1)), \dots, (x(n),y(n))\}$ is observing data and $L(\theta|D)$ is likelihood function that gives the probability of the observed data as function of the unknown model parameters (Lampinen & Vehtari, 2001).

2.3 Reversible jump Markov Chain Monte Carlo method

Neal has introduced an implementation of Bayesian learning for ANN in which, difficult integrations accompanied with this framework are performed using Markov Chain Monte Carlo (MCMC). In this application samples (in model parameters space) are generated using a Markov Chain Monte Carlo to estimate the desired posterior distributions (Lampinen & Vehtari, 2001). In practical problems like the present study, it is usual to measure many variables, but it is not necessarily known which one of them is relevant and required to solve the problem. To make the model more explainable or to reduce the measurement cost and the computation time, it may be useful to select a model with smaller set of input variables (Lampinen & Vehtari, 2001). As a consequence, RJMCMC method is applied for this modeling. This algorithm allows jumps between models with different dimensional parameter spaces with respect to the number of inputs chosen in the model. RJMCMC visits the models according to their posterior probability which allows it to be used for model selection (Vehtari & Lampinen, 2002). The grain size model was achieved by this method.

2.4 Bayesian Regularized Neural Network (BRNN)

Conventional performance function of neural network which optimization applied on it, has general form of:

$$F = mse = \frac{1}{N} \sum_{i=1}^N (e_i)^2 = \frac{1}{N} \sum_{i=1}^N (t_i - a_i)^2 \quad (7)$$

where mse is mean of squared error. If the performance function is changed by adding a term that contains mean of squared weights (msw), yield:

$$msereg = \gamma mse + (1 - \gamma) msw \quad (8)$$

where γ is the performance ratio, and

$$msw = \frac{1}{n} \sum_{j=1}^n w_j^2 \quad (9)$$

Using this performance function leads to smaller network weights and biases, which makes the network response to be smoother and less likely to over-fit (MathWorks). The main remaining problem is to find the ideal value for the performance ratio. Choosing too large ratio increases over-fitting likelihood and too small ratio prevents network to fit adequately the training data (MacKay, 1992). To find out the best regularization, as mentioned before MacKay in his Bayesian framework suggests, assuming the weights and biases as random variables with specified distributions and related the regularization parameters to these distributions. Another approach suggested by Foresee (Botlani-Esfahani et al., 2009b) in which the Levenberg-Marquardt method that is a rapid optimization algorithm employed for training. The (BRNN) automatically can control the complexity of the model and prevent the over-fitting of training data set. As a result, this model has good prediction accuracy and according to MacKay, (MacKay, 1992) in Bayesian framework, there is no need for test data set to control the specified network architecture. The acquired model by this approach can reveal a good generalization, even if its architecture is an over optimized (MathWorks). Consequently, the trial and error approach for finding ideal architecture is reduced. This approach was applied to acquire ideal model for prediction of tensile strength of steel strips because of its good accuracy as well as fast convergence speed.

2.5 Experimental database

Since an ANN model is empirical, its performance depends on the dataset used for training. Annual products data report of Isfahan Mobarakeh Steel Company (MSC) were used for this modeling, which input parameters for tensile strength modeling consisted of:

- i. Final thickness
- ii. Initial and final weight
- iii. Initial width
- iv. Reheating furnace temperature, roughing temperature, finishing temperature and coiling temperature
- v. The chemical composition, consisting 14 different elements
- vi. The carbon equivalent according to the following formula:

$$C_{eq} = C + Si/25 + (Mn+Cr)/16 + (Cr+Ni+Mo)/20 + V/15 \quad (10)$$

where elements are expressed in weight percent.

About 70234 examples each consisting of corresponding input and output were available for modeling tensile strength. Some further information about the variables are given in Table 1. These examples were normalized so that they had zero mean and unity standard deviation before computations.

Data set that was used to model grain size consisted of 624 metallographic images. At this company, these images are classified into three groups according to ASTM (E-112), this standard assigns larger numbers to finer grain structures. Figure 4 shows an example of such a database. Further information is also given in Table 2. The input parameters are chemical composition of the strips which include 14 elements. Additional input variables are given in Table 3.

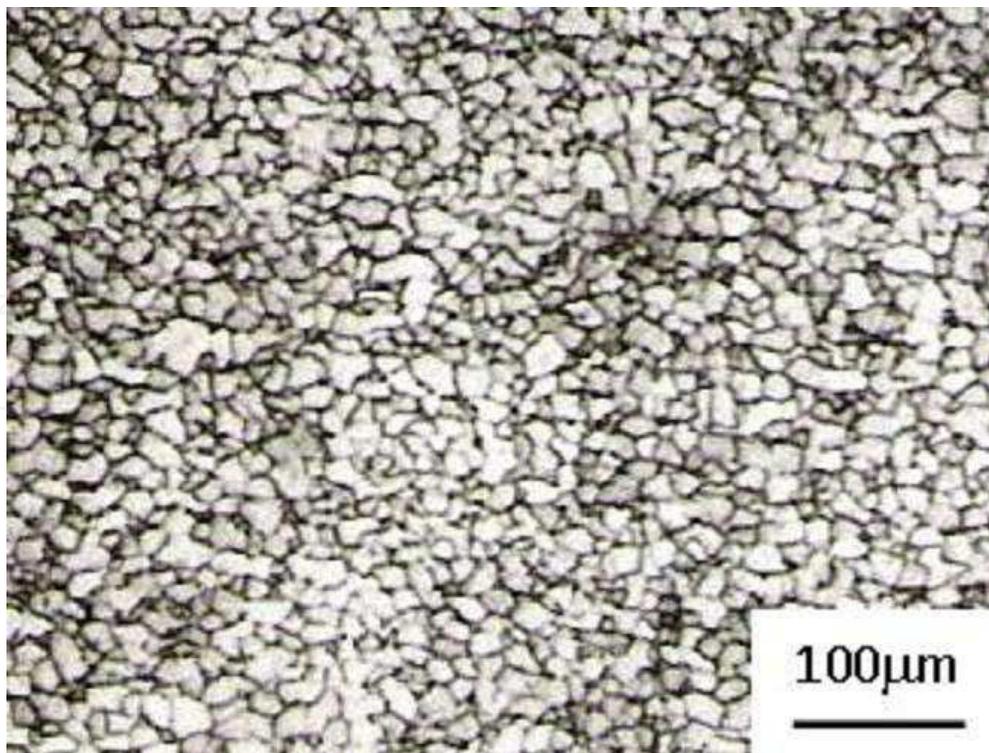


Fig. 4. One sample of data, microstructure of produced steel with ASTM grain size no. 9.0.

	Variables	min	max	mean	SD	
Inputs	Final Thickness(mm)	1.5	16	5.244903	3.155532	
	Final Weight(kg)	5097	28030	18502.91	3214.769	
	Initial Weight(kg)	5202	28660	18874.26	3264.811	
	Initial Width(mm)	650	1850	1277.022	205.7713	
	Furnace Temp(°C)	1164	1296	1229.77	23.4407	
	Roughing Temp(°C)	932	1122	1058.281	14.00645	
	Finishing Temp(°C)	782	960	881.1131	23.32006	
	Coiling Temp(°C)	517	729	610.5108	18.02052	
	C (wt %)	0.03	0.21	0.126968	0.02545	
	Si (wt %)	0	0.347	0.070235	0.084277	
	Mn (wt %)	0.175	1.38	0.658662	0.206133	
	P (wt %)	0.001	0.026	0.006786	0.002377	
	S (wt %)	0	0.02	0.008637	0.002686	
	Cu (wt %)	0	0.264	0.029318	0.011597	
	Al (wt %)	0.007	0.093	0.045926	0.010957	
	N (ppm)	15	90	39.784	9.221	
	Nb (wt %)	0	0.06	0.004854	0.009032	
	V (wt %)	0	0.043	0.003378	0.001607	
	Ti (wt %)	0	0.042	0.001654	0.002318	
	Mo (wt %)	0	0.022	0.003654	0.004104	
	Cr (wt %)	0.001	0.194	0.011992	0.008007	
	Ni (wt %)	0.016	0.243	0.028205	0.004679	
	Ceq (wt %)	0.068032	0.437799	0.2443845	0.0534388	
	Output	Strength (MPa)	299	659	444.64	48.68

SD: Standard Deviation Ceq: Carbon Equivalent

Table 1. Input and output parameter information.

Number of Samples	ASTM (E-112) grain no
162	8.5
294	9
167	9.5

Table 2. Output Data Information

2.6 Network training

As mentioned the (BRNN) models have a good predictive accuracy (generalization) and specified network architecture in Bayesian framework doesn't need of test data to adjust its

complexity. However, there is still a need for an independent set of data to evaluate the ideal network predictive accuracy on unseen data. In this respect, 10% of the total data were kept for validation. In the case of tensile strength several models were examined for finding the best network architecture. The network architecture was started with a few hidden units in a single hidden layer and as the number of hidden units increased the squared error sum on both training and test data, decreased. As expected from performance function of the BRNN, (Equation 8), when the number of training data is raised, the number of weights must also increase. When the number of hidden units is placed within one layer, the accuracy of the results is less than when two layers are used. This also indicates that more weights are needed in two layer network. Finally, the ideal network was determined with 23-60-50-1 architecture. Training stopped when the squared error sum, the squared weights sum and performance ratio (which are the criteria for training evaluation) became stable. Since network training is an optimization procedure, the calculations can become cumbersome. For example, for 4541 parameters, more than 55 hours was taken when a dual 3.2 GHz processor, with 2 gigabyte memory, was used.

For finding ideal model for grain size prediction the modeling database was divided into training and test sets, which include 60 and 40 percents of data respectively. Training was started with (14-8-3) architecture and model selection procedure was evaluated by an internal procedure of RJMCMC algorithm, as mentioned in sec. 2.3. The result of this training indicated a chain of network parameters. When this chain converged into a stable distribution, a sample of the chain (network parameters) was selected on the bases of minimum classification error of the model on test dataset.

No.	Inputs	min	max	Mean	SD
1	C (wt%)	0.032	0.179	0.1272	0.0312
2	Si (wt%)	0.008	0.218	0.0637	0.0798
3	Mn (wt%)	0.191	1.15	0.6466	0.211
4	P (wt%)	0.002	0.025	0.0072	0.0022
5	S (wt%)	0.001	0.02	0.0089	0.0029
6	Cu (wt%)	0.004	0.078	0.03	0.0109
7	Al (wt%)	0.015	0.075	0.0454	0.0119
8	N (ppm)	16	75	38	8.8
9	Nb (wt%)	0	0.045	0.0051	0.0105
10	V (wt%)	0	0.011	0.003	0.0014
11	Ti (wt%)	0	0.042	0.0017	0.0031
12	Mo (wt%)	0	0.019	0.0038	0.0045
13	Cr (wt%)	0.004	0.194	0.0131	0.012
14	Ni (wt%)	0.02	0.042	0.03	0.0034

SD: Standard Deviation

Table 3. Input parameter information

2.7 Calculation of the weights of individual input variable

Extracting effective information from a neural network model is not as easy as conventional linear regression because the discovered relationships with neural network are much more complicated. However when the output layer only consists of one neuron the dependency of

output variable on inputs is same as network dependency to input parameters (Botlani-Esfahani et al., 2009b). On the other hand, in feed-forward networks the path which the effects of the input parameters carried is straightforward from input layer to output layer. Therefore, the weights which fan out the input units can be considered as their significance, like the impact of inputs on output in linear models. The relative importance of individual input variable on output variable can be expressed as: (Xu et al., 2006)

$$I = \frac{\sum_{j=1}^S |W_{ji}|}{\sum_{i=1}^N \sum_{j=1}^S |W_{ji}|} \quad (11)$$

where W_{ji} is the connection weight from i input neuron to j hidden neuron, N , S are the number of input parameters and hidden neurons, respectively. This approach was employed to investigate the relative importance of input parameters on tensile strength however, in case of grain size such task has carried out automatically by the algorithm.

3. Results and discussion

3.1 Performance of the model

Scatter diagrams of model predictions versus experimental data for both training data and validation data are used as a means of showing the tensile strength model generalization. Figure 5, indicates that the correlation coefficients of training and validation data are close to one, and their differences are negligible. Therefore, it is clear that, the network predictions are in good agreement with experimental data.

Calculation of the misclassification error on test data is a popular way to show the prediction accuracy (generalization) of a classifier model. This error is calculated according to:

$$\text{Misclassification error} = \frac{\sum |test\ data - model\ result|}{number\ of\ test\ data} \times 100 \quad (12)$$

Therefore, grain size model revealed just 2.439 percent misclassification error, which is very low and indicates that, this model has good generalization. More information about misclassified error is available in Table 4.

Number of Misclassified	Test Target Data	Model Result
2	9	8.5
2	9.5	9

Table 4. misclassified case

3.2 Sensitivity analysis

Figure 6 shows the importance of input variable relevancies on tensile strength which were analyzed by the method mentioned in section 2.7. Figure 6 shows that silicon, carbon, manganese, copper, nickel and chromium give a large contribution to the strength. Moreover, microalloy elements such as niobium, vanadium and titanium, though less than other elements, have a similar effect of strength. Among the processing features, the width and thickness of the strip revealed remarkable influence on tensile strength (Botlani-Esfahani et al., 2009b).

The depicting effect of mentioned factors and their interactions with one another, two parameters were altered at a time and other parameters were kept on their mean values which are tabulated in Table 1. As mentioned RJMCMC method can select potentially useful inputs according to marginal probabilities of inputs. The result of this analysis indicates the importance of Si, Mn and C contents on grain refinement which is significantly greater than the concentration of other elements. The most effective element for grain refinement is recognized to be that of vanadium. However, its concentration in these steels is very low.

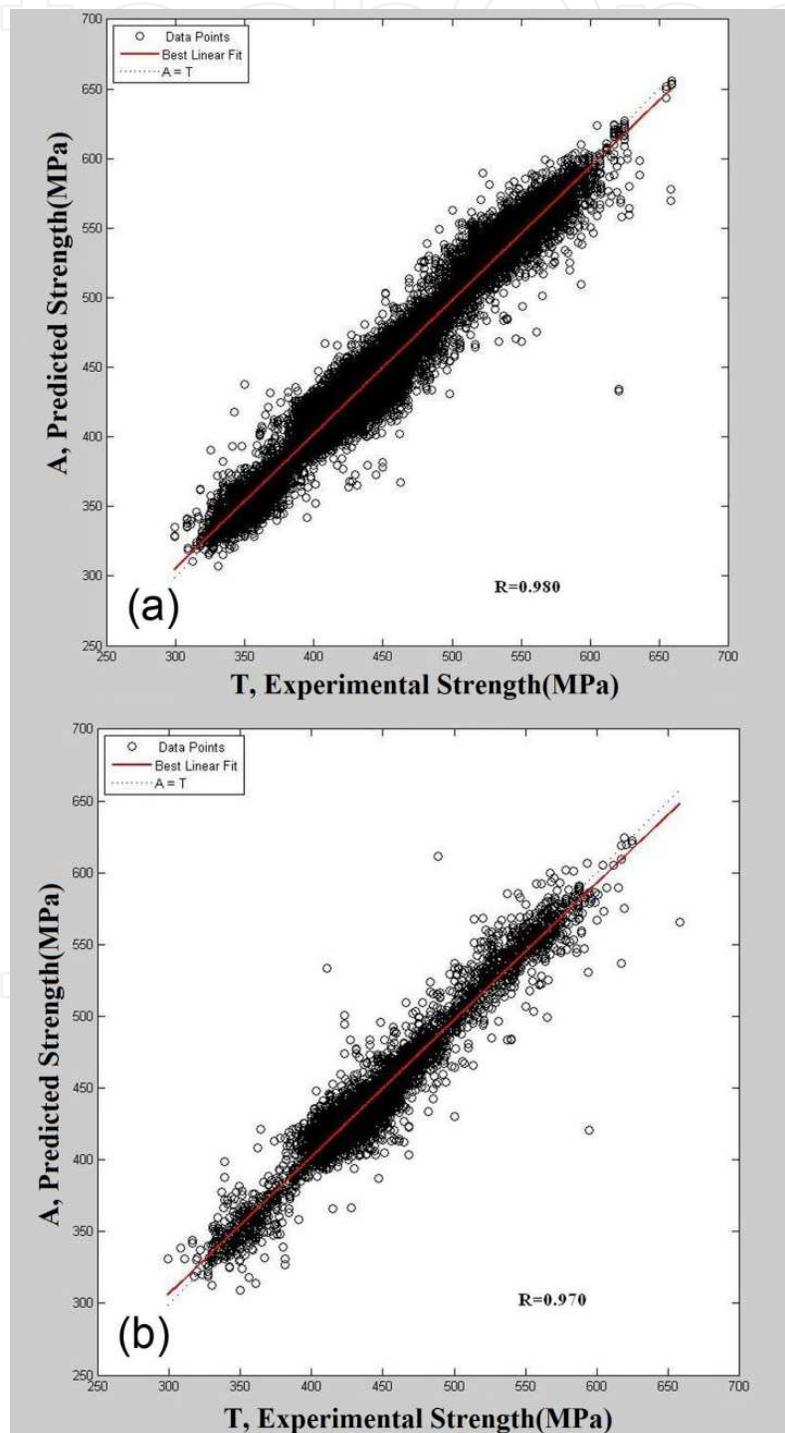


Fig. 5. Behavior of tensile strength model on (a) training data (b) test data.

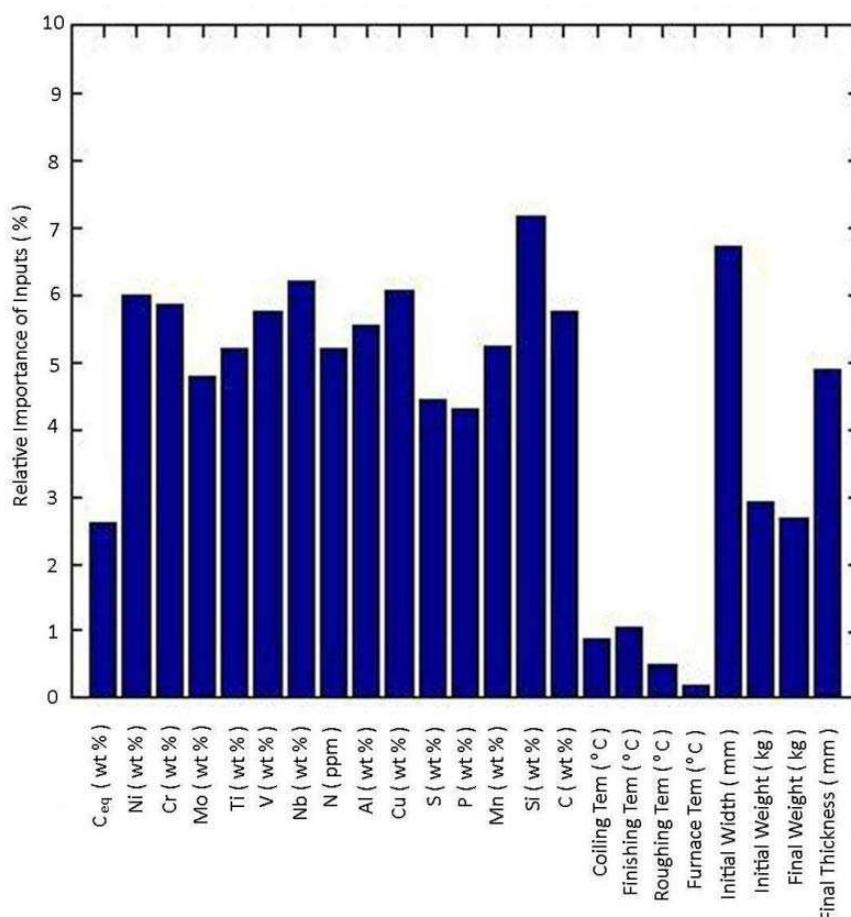


Fig. 6. Relative importance of inputs.

3.3 Tensile strength model

Carbon has a major effect on steel properties and increases the strength by interstitial solid solution strengthening. This effect is more pronounced in ferritic steels. In ferritic-pearlitic steels, the carbon content raises pearlite volume which in turn leads to the increase of alloy strength (Singh et al., 1998). Silicon is one of the principal deoxidizers used in steel-making, Figure 7a shows silicon effect which enhances the strength by suppressing precipitation of cementite from austenite. Thus carbon remains in austenite for subsequent strengthening (Bhadeshia et al., 2003). The effect is more pronounced in steels with lower carbon concentration because silicon dissolves in the ferrite. Manganese promotes stronger steels by stabilizing austenite and solid solution strengthening (Singh et al., 1998). The increase in strength is dependent upon the carbon content as is shown in Figure 7b. However the concentration of microalloy elements is low, they have a significant influence on several stages of rolling. Unlike alloying elements that alter the structure of iron, microalloy elements have a great affinity to combine with other elements such as carbon and nitrogen. This results in precipitation of several secondary phases (Meyer, 2001). Model reveals the effect of niobium concentration as the most effective microalloy. Niobium contributes towards the prevention of austenite grain coarsening during reheating period and retards the recrystallization temperature during rolling. Niobium also reduces the transformation temperature by solute drag effect (Singh et al., 1998),(Hulka, 2003). Figure 7c shows that the addition of 0.025 wt% Nb, improves tensile strength more than that of 0.04 wt%. For

instance in a steel with a carbon content of 0.15wt%, addition of 0.025% Nb increases tensile strength by 150 MPa.

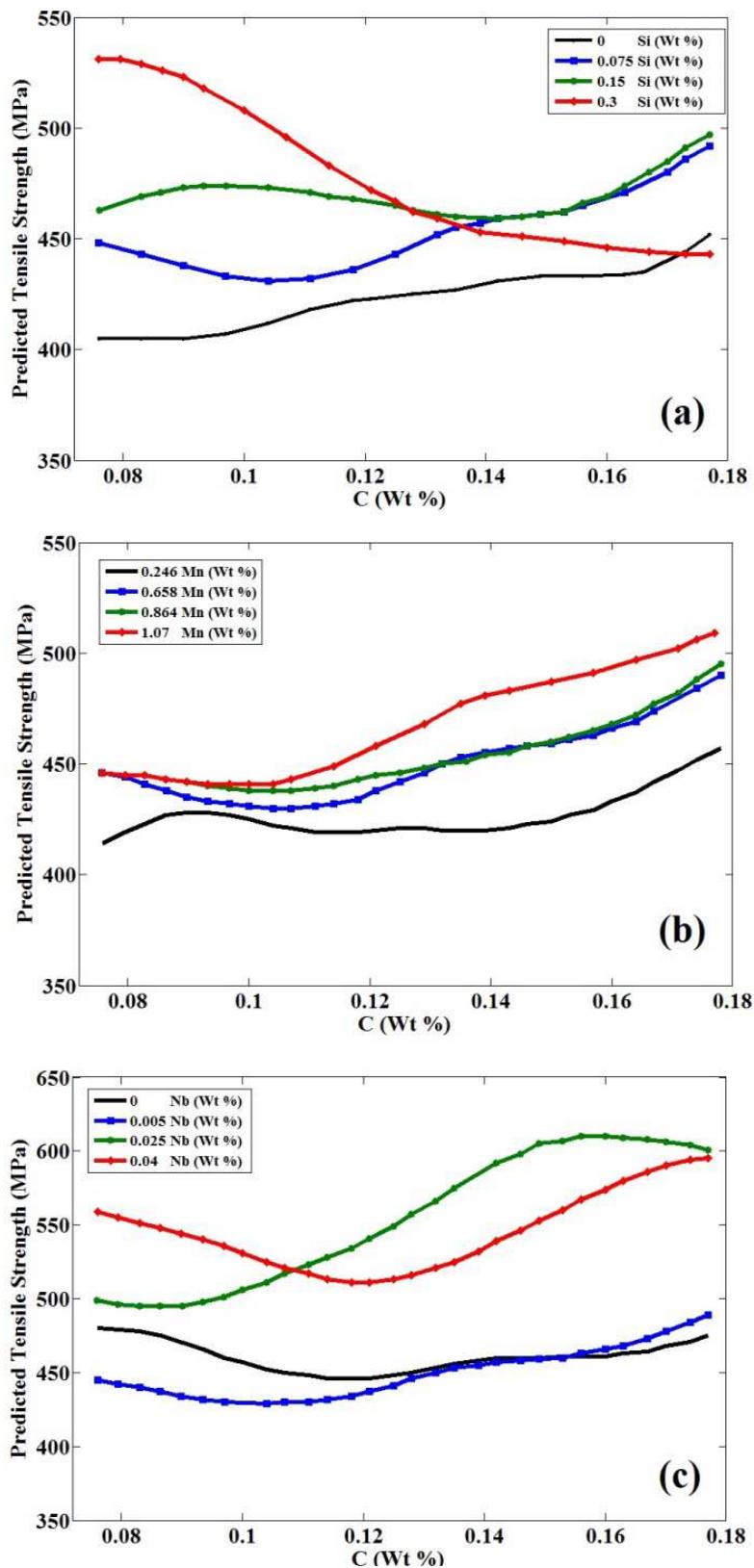


Fig. 7. Carbon concentration effect in combination with (a) Silicon (b) Manganese (c) Niobium.

Figure 8a, displays the effect of strip thickness versus manganese content on the final tensile strength. The results indicate a drop in tensile strength when final thickness is increased. This can be attributed to lower cooling rate of thicker strips. Therefore, coarsening takes place and the tensile strength decreases (Singh et al., 1998). This figure also illustrates the more influential effects of manganese on thinner strips. Figure 8b reveals the significance of finishing temperature versus the carbon concentration on tensile strength. It shows that by decreasing finishing temperature, the final tensile strength increases. Inter-pass recrystallization and grain growth prevention may causes this effect (Preloscan et al., 2002). The influence of temperatures on tensile strength is not significant when compared with that of chemical composition (in specified ranges) (Botlani-Esfahani et al., 2009b).

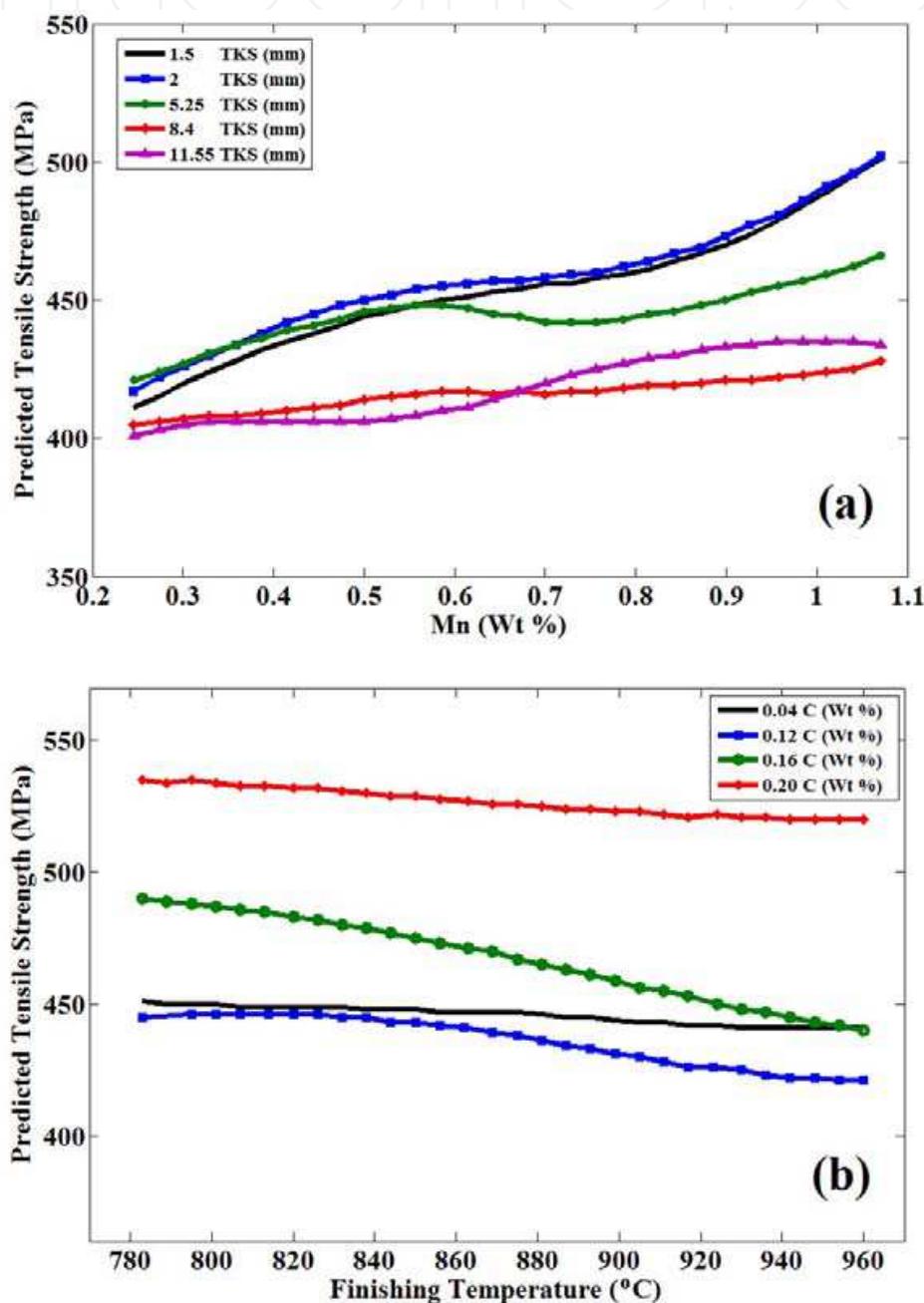


Fig. 8. Interaction of processing feature (a) Final thickness and manganese concentration, (b) Finishing temperature and carbon concentration.

3.4 Grain size model results

The result of this analysis indicates the importance of Si, Mn and C contents on grain refinement which is significantly greater than the concentration of other elements. The most effective element for grain refinement is recognized to be that of vanadium. However, its concentration in these steels is very low. For testing, the results of the model are depicted when the concentrations of elements are on their mean values which mentioned in Table 2 and the microalloying elements (i.e. Nb, Ti and V) are not present. Figure 9 shows the model result of this analysis. Manganese stabilizes austenite, therefore decreases austenite to ferrite transformation temperature and hence refines the grain structure. In addition, manganese

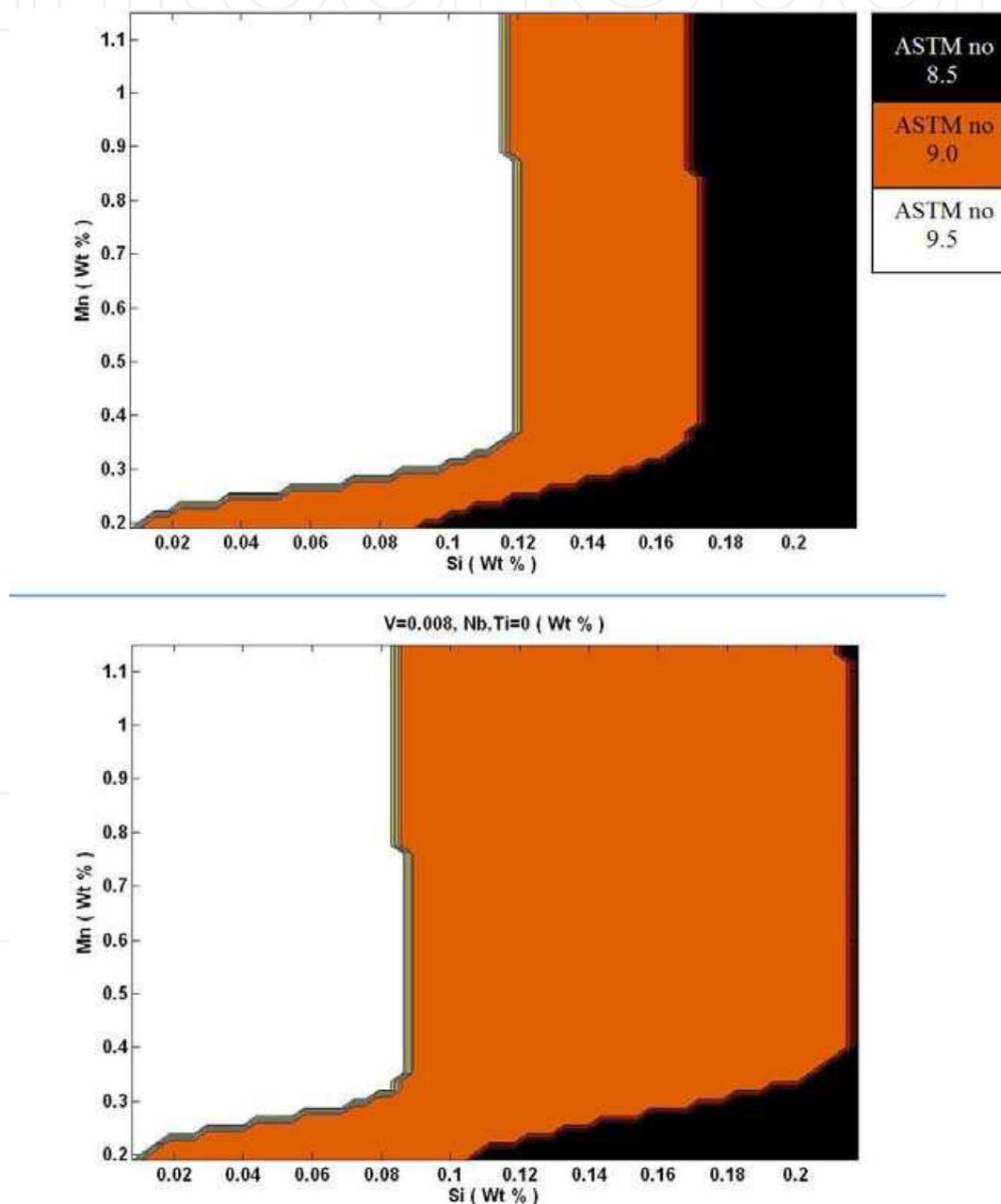


Fig. 9. Model result in respect of silicon and manganese concentration in 0.015 wt %C and 0.035 wt%Al. (a) Absence micro-alloying elements. (b) Minor addition of vanadium (0.008 wt %).

can enhance the precipitation strengthening of vanadium microalloyed steels and to a lesser extent, niobium microalloyed steels (keytosteel). Figure 9a reveals determining role of silicon on grain size in the absence of microalloying elements (i.e. Nb, Ti and V). The figure shows that silicon concentration divides the figure into three regions include finer, mild and coarser grain structures. This figure also indicates that increasing Si content, increases grain size. This is because silicon is a ferrite stabilizer and promotes ferrite grain growth (Umemoto et al., 2001). Figure 9b shows that addition of small amount of vanadium (0.008wt %) to steel severely contracts the coarser grain region. Vanadium acts as a scavenger for oxides, and forms nano-scale inter-phase precipitations. This is mainly due to the rapid rate of austenite to ferrite transformation which produces these nano-scale precipitates (Bhadeshia & Honeycombe, 2006). Furthermore, addition of vanadium also reduces the finer grain area somewhat. This is because, vanadium is strong carbide former and the majority of such elements is ferrite stabilizer and therefore, promotes ferrite grain growth (Zhang & Ren, 2003). The net effect of this minor vanadium addition is to decrease the sensitivity of grain size to silicon content, and also reduction of coarse grain area.

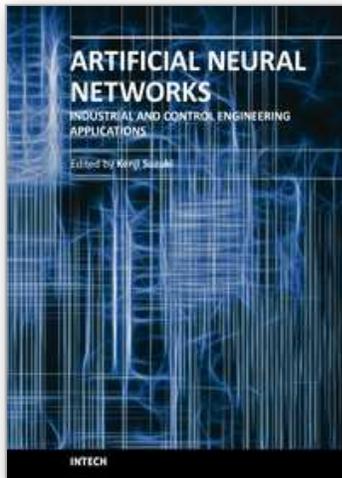
4. Conclusions

1. The effects of chemical composition and process variables on the tensile strength of hot strip mill products were modeled by Artificial Neural Network (ANN) moreover a Bayesian ANN model assisted by RJMCMC is capable of predicting the grain size of hot strip low carbon steels and can be used as a function of steel composition. The results of both models are shown to be consistent with experimental data (acquired from Mobarakeh Steel Company data).
2. The relative importance of each input variable was evaluated by sensitivity analysis for tensile strength. The influence of chemical composition on final tensile strength is much more pronounced than process parameters. Furthermore, grain size model recognizes the effects of relevant elements in grain refining. These are manganese, silicon and vanadium. Silicon concentration shows determining role this effect have not reported in the literature and vanadium reveals great impact on grain refining phenomena.
3. The results show the effects of the parameters are too complex to model with a simple linear regression technique. The developed ANN models can be used as guide to control the final mechanical properties of commercial carbon steel products. The major advantage of these methods is selection of useful inputs in complex problems with many inputs. Because many problems in materials science and engineering are similar, this method is useful for solving them.

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Artificial neural networks may probably be the single most successful technology in the last two decades which has been widely used in a large variety of applications. The purpose of this book is to provide recent advances of artificial neural networks in industrial and control engineering applications. The book begins with a review of applications of artificial neural networks in textile industries. Particular applications in textile industries follow. Parts continue with applications in materials science and industry such as material identification, and estimation of material property and state, food industry such as meat, electric and power industry such as batteries and power systems, mechanical engineering such as engines and machines, and control and robotic engineering such as system control and identification, fault diagnosis systems, and robot manipulation. Thus, this book will be a fundamental source of recent advances and applications of artificial neural networks in industrial and control engineering areas. The target audience includes professors and students in engineering schools, and researchers and engineers in industries.

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University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
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Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821

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