Parametric Jominy profiles predictor based on neural networks

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Abstract
The paper presents a method for the prediction of the Jominy hardness profiles of steels for microalloyed Boron steel which is based on neural networks. The Jominy profile has been parametrised and the parameters, which are a sort of "compact representation" of the profile itself, are linked to the steel chemical composition through a neural network. Numenrical results are presented and discussed.

Keywords
Neural networks. Jominy profiles. Boron.

Estimador paramétrico de perfiles de dureza "Jominy" basado en redes neuronales

Resumen
El trabajo presenta un método de estimación de perfiles de dureza Jominy para aceros microaleados al boro basado en redes neuronales. Los parámetros de perfil Jominy, que constituyen una especie de "representación compacta" del perfil mismo, son determinados y puestos en relación con la composición química del acero mediante una red neuronal. Los resultados numéricos son expuestos y discutidos.

Palabras clave
Redes neuronales. Perfiles de dureza Jominy. Boro.

1. INTRODUCTION

As it is already known from the forties, Boron may be employed in the steel production in order to obtain an high increase of the hardenability of the products destined to thermal treatments.

The economic benefits of the Boron utilization to increase hardenability, are evident: in fact an addition of about 5-30 ppm of the element allows to obtain high hardening depth characteristics without utilizing expensive ferroalloys. On the other hand, it is not always easy estimate the hardenability of the Boron steel due to the influence both of the steel chemical composition and manufacturing process.

The variability of hardenability values, depends on a number of factors:

– the Boron content is very low and comprised in rather tight range; values outside from this useful range jeopardize its effect;
– the Boron quickly reacts in presence of Nitrogen and Oxygen forming chemical compounds not suitable for an hardenability increase: thus the Boron effect depends strongly on the practice and technology of the steel manufacturing process;
– for Boron tightly controlled contents too, the effectiveness on hardenability is highly affected by the steel chemical composition and austenitic grain dimensions;
– the austenitization temperature and the previous thermal history have a strong influence on the final results.

The foregoing shows that the Boron addition may substantially affect the steel hardenability, the sole Boron addition may however have not any apparent consequence. Therefore Boron must be considered a very peculiar alloy element.

Many steel producers use computer programs to calculate the hardenability of low alloy steels based on heat composition but it is very difficult to include boron steels in sophisticated hardenability predictors.

This paper presents some more powerful methods based on a "structured network" made of two combined neural networks, where one network provides a "parametric model" of the Jominy profile, while the second "predicts the parameters" as a

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function of chemical composition. The extracted parameters do have a strong relationship with the Jominy profile, of which they are a "compact representation".

The developed predictor has been employed for Boron steels showing better results that that achievable by standard methods.

2. PREPROCESSING OF THE INPUT DATA

In our case, real industrial data were available for three particular qualities of steel (respectively, A, B and C). Figure 1 provides a few examples of their typical Jominy hardness profiles. Associated with each Jominy profile, we have the chemical analysis indicating the content of several micro-alloying elements present in the steel.

Throughout this work, we consider as input variables the content of 17 chemical components: C, Mn, Si, P, S, Cr, Ni, V, Mo, Cu, Sn, Al, Ti, B, N, and soluble Al and B. We will call:

- $Q \in \mathfrak{R}^{17}$ the vector of chemical composition;
- $Q^* \in \mathfrak{R}^{17}$ the vector of "normalized" chemical composition, namely a vector in which each component is obtained by dividing the correspondent component of Q by its maximum value computed over the whole training set; normalization avoids the problems that arise in neural networks when input variables have different physical dimensions and standard deviations;
- $J(x)$: $\mathfrak{R} \to \mathfrak{R}$ the Jominy hardness profile as a function of the distance x from the quenched end;
- $J \in \mathfrak{R}^{15}$ the vector containing the values of $J(x_i)$ at 15 predefined positions (often, $x_i=1.5, 3, 5, 7, 9$ mm, etc.).
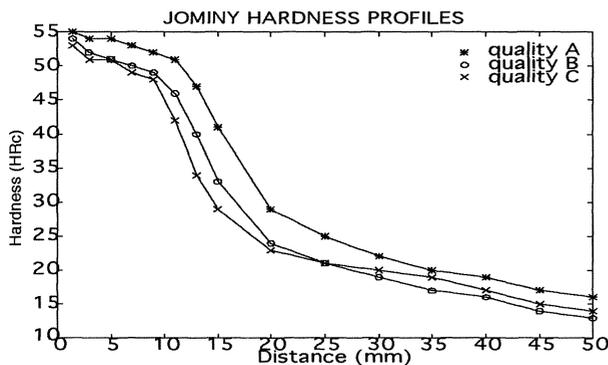
To reduce the size of the neural networks used, we tried to reduce as much as possible the number of input variables to the network, without loosing significant information. We have therefore applied Principal Component Analysis[1] namely by computing the eigenvalues and the associated eigenvectors of the covariance matrix of the vectors Q^* contained in the training set. The eigenvectors associated with the largest eigenvalues span a subspace which contains most of the information available in the training set. We have therefore decided to retain the 6 largest eigenvectors, as a good compromise between complexity and performance.

The projection of input data in the subspace spanned by these 6 vectors maintains 97 % of the original information and constitutes a new "input vector" $V \in \mathfrak{R}^6$ to be fed into the network:

$$V = M *Q*$$

where M is a matrix containing as rows the 6 principal eigenvectors.

3. THE PARAMETRIC ESTIMATOR STRUCTURE

Some preliminary considerations are needed related to traditional approaches [2 and 3]:

- the number of network outputs equals the number of measured points of the Jominy profiles, namely 15. But, from Fig.1 it can be observed that Jominy profiles are relatively slowly varying, especially in the initial and the final parts. There is usually a little difference between two neighboring points and thus the information conveyed by these values is somehow redundant. Statistical correlation of adjacent elements of J approaches unity (≈ 0.93), as well as (consequently) the correlation between weights of adjacent neurons.
- Approximation errors can produce estimates of the Jominy profiles which are physically non plausible (for instance, small local increases instead of a monotonic decrease of the hardness).
- The 15 positions where the hardness is measured are not evenly distributed and often differ among different manufacturers, therefore Jominy profiles cannot always be compared directly. In addition, even the number of points can often be varied (for instance, up to 18 or 19 points are often measured).

Figure 1. Examples of Jominy profiles for the 3 considered qualities of steel.

Figura 1. Exemplo de perfiles de dureza Jominy para las tres cualidades de acero.

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- Hardness measurements are often affected by errors, therefore the Jominy vector J usually contains a relatively large quantity of noise.

For all these and a few other reasons, we have decided to essay a completely different approach to the problem of Jominy profile estimation and classification, as sketched in figure 2. The proposed system is composed of three interacting blocks:

- The small network A is used as a "parametric model" of the Jominy profile, that is seen as a function $J(x)$, where x is the distance from the quenched end. The collection of free parameters of network A (weights, centers and biases) constitutes a vector P, which uniquely identifies an estimate of the Jominy profile and, consequently, of the Jominy vector J. For normalization purposes, the output of the network is multiplied by a fixed value of 65 HRc. As P is the set of free parameters of the NWN, it can be evaluated by simply "training" the network.

- An *a-posteriori* "model corrector" to reduce estimation error.

- The larger network B is used as a "parameter estimator" which predicts the parameter vector P (instead of the profile itself) as a function of chemical composition Q (after dimensional reduction, through vector V).

This approach has the following advantages:

- the size of the parameter vector P is smaller than that of J, therefore network B is smaller than would be a network predicting J, for comparable accuracy. As a consequence, a smaller training set will suffice and a considerable saving in computation time and memory can be achieved during both training and relaxation.

- If network A is properly chosen, P is less sensitive to measurement noise than J, therefore steel characterisation will be more robust.

- P is almost independent of the number and position of hardness measurements.

- P can be computed also when some measurements of J are missing.

- Network A can also be used to filter and reduce the effects of measurement noise.

We can therefore state that P is nothing but a more "compact representation" (with a small approximation error) of $J(x)$ and therefore of J.

4. RESULTS AND DISCUSSION

At present, we have real data from 767 manufactured commercial specimen of the three different Boron steel qualities. Additional specimen will be available in the near future.

All specimen are in the form $(Q; J) \in \Re^{17} \times \Re^{15}$ (sometimes, $\rightarrow \Re^{18,19}$). These are first preprocessed as described above to provide a more compact input-output pair $(V; J) \in \Re^6 \times \Re^{15}$ (sometimes, $\rightarrow \Re^{18,19}$) where V and J are, respectively, the input and the target vectors for network A. The collection of all specimen data is called the *data set*.

A *training set* and a *validation set* are then constructed for each of the two networks:

- As network A converts each Jominy profile into a more compact representation, each specimen contains in itself all the information required for training. From each specimen, a training set is generated containing the 15 pairs $(x_i, J(x_i))$, where $i \in [1...15]$ is the index of the measurement. The network uses fixed initialisation, where free parameters are initialised to pre-computed values which approximate an "average" profile. Training then
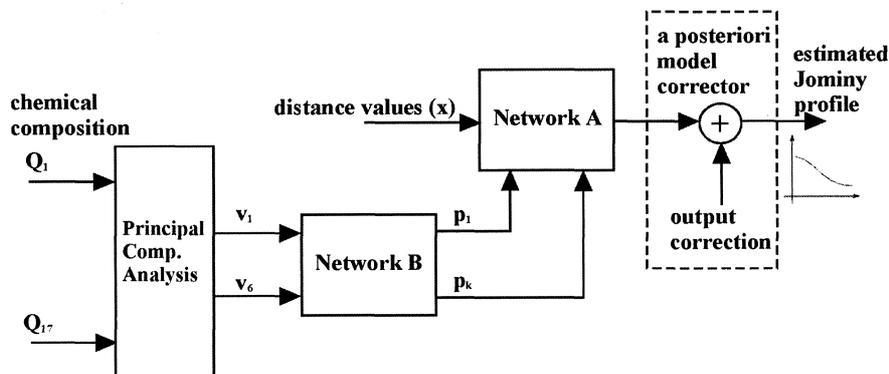

Figure 2. The parametric neural estimator.

Figura 2. Estimador paramétrico neuronal.

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takes place, using the Levemberg-Marquardt algorithm, for up to 1.000 epochs. No validation set is required, as the aim of network A is only to generate the compact parameter vector P, i.e., the most accurate representation of that particular J(x) compatible with the chosen architecture.

– Network B is a more traditional function approximator which has to be trained and tested with two independent training and validation sets. Both are obtained by first preprocessing the elements of the data set, producing input-output pairs (V;P) where P is the result of training network A from the Jominy profile J associated with that particular V. Preprocessed data points are then distributed between training and validation sets containing, respectively, 615 and 152 specimen taken evenly from the three considered steel qualities. All additional data collected in the future will only be inserted in the validation set.

As a performance index for all NWNs, we adopt the Standardized Root Mean Square Error (SRMSE) in a version suitable for multi-output networks, defined as:

$$\varepsilon = \sqrt{\frac{\sum_{n=1}^{N}\sum_{m=1}^{M}\left(\hat{j}_m^n - j_m^n\right)^2}{\sum_{n=1}^{N}\sum_{m=1}^{M}\left(\hat{j}_m^n - \bar{j}\right)^2}} \quad \text{where} \quad \bar{j} = \frac{1}{MN}\sum_{n=1}^{N}\sum_{m=1}^{M}\bar{j}_m^n$$

where N and M are, respectively, the number of samples in the training (or validation) set and the number of network outputs; j_m^n is the m-th component of the n-th output vector in the training (or validation) set, while is the corresponding network estimate.

Both network A, and network B have been chosen among a large variety of network types, by exploiting a neural unification paradigm introduced in[4], which allows to implement most neural network by means of the same general computational structure.

As far as network A is concerned, a compromise is needed among accuracy of the profile approximation and reduced dimension of the vector P of the network parameters. The best performing network is of the Multilayer Perceptron kind[5] with 1 hidden neuron and 1 output linear neuron, which corresponds to a 4-dimensional parameter vector P. A significant improvement in the system performance was obtained by adapting the activation function of the hidden neuron to

the particular task of the Jominy profiles approximation: in the improved version of the predictor, such activation function is itself obtained by means of a neural network suitably trained in order to mach as possible the classical shape of a Jominy profile.

Network B is of the Wavelet Network[6] type and contains one hidden layer with 8 neurons and a linear output layer with as many neurons as the number of entries of the vector P (4 in the final release of the system).

In its final release, the system achieved an SRMSE value of 0.0946. Such results is far better than that achievable by means of standard one-net neural predictor, such as the one presented in[3]. A similar network has been tested with the available data: many attempts have been made by essaying different numbers of neurons in the hidden layers and different kind of neurons typologies, but the final SRMSE value is never lower than 0.135.

5. CONCLUSIONS

The problem of the prediction of the Jominy hardness profiles of Boron steels has been faced through the design of a hierarchical neural system, composed of two neural networks. The parametric characterization of the Jominy profiles, namely the representation of a whole Jominy curve through a reduced set of parameters, allowed to design a neural system that associates such parameters to the chemical composition of the steel itself, by filtering out and reducing the effect of measurement errors.

Acknowledgements

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