ARTIFICIAL INTELLIGENCE FOR METALLURGICAL PROPERTIES PREDICTION OF STEEL ROLLED PRODUCTS: A REVIEW*

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Abstract
This work aims to review the advanced tools, based on Artificial Intelligence resources, used in rolled product development projects and in the optimization of steel processes. These tools have been widely used because they allow to determine, with an excellent degree of precision, the understanding of the various metallurgical phenomena involved in characteristics of interest of steel products as well as in their forecast. With the advent of a series of new technologies, including new architectures of Artificial Neural Networks, Deep Learning, Machine Learning, Genetic Algorithms, among others, these tools have become quite reliable, even allowing to design new products and new processes, yet not known. Numerous recent examples of uses of these tools are displayed as well as the results regarding the use of new technologies. These technologies are already being used on site, for microstructure prediction, for example. In the end, it is demonstrated that Artificial Neural Networks, the basis of many of these technologies, are able to predict with a high degree of precision the historically established metallurgical trends, which proves their effectiveness as tools for studying and understanding the phenomena involved.

Keywords: Artificial Intelligence, Artificial Neural Networks; Deep Learning.

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1 INTRODUCTION

Steel processes today are capable to generate a huge amount of data, which has been growing at an exponential rate. Such an advent will drive the evolution of scientific methods towards online databases [1]. With the consequent increase in the volume of data, there is an important demand to obtain information efficiently and that is scientifically sustainable, that is, that reflects the known mechanisms and that brings knowledge of new mechanisms. The tools based on Artificial Intelligence can extract information from a large amount of data in a fast way, being able to discover relations not yet known, leading to new material discoveries, for example [2]. In traditional development processes, a new material is designed from a set of information related to the chemical composition as well as processing conditions, which is followed by a microstructural analysis and property evaluation. Such an approach has a high cost, low efficiency and is not enough to design an unprecedented material with the desired properties [3]. Among the technologies explored in this article are: Artificial Neural Networks, Genetic Algorithms, PSO, BFO, Machine Learning, Deep Learning, Convolutional Neural Networks, Random forest, Support Vector Machine (SVM), Decision Tree, Ensemble Method and K-Nearest Neighbor (K-NN). As an example of using these technologies, we have the following approach of developing new materials using machine learning methods, which can be divided into approximately four stages: 1) Construction of the database from the literature or from own experimental observations, 2) Development of the Machine Learning model linking the input parameters and output properties based on the data set, 3) Search and first evaluation of a new set of input data, aiming at superior outputs in the vast candidate space and 4) Identification of newly designed candidate solutions for experimental validation. For step 1, the size and quality of the data set is essential, and the inputs and outputs must be properly defined. For step 2, a reliable and available Machine Learning model is needed to maximize learning capacity. For step 3, an appropriate search algorithm should be employed to explore the vast candidate space and find good candidate solutions. For step 4, the search methodology generally yields many good solutions, and an intelligent separation methodology may be necessary to select or identify the most promising solution, which will be subjected to an expensive experimental validation step [4]. In the following sections, these tools will be explored and later some use cases and the results obtained.

1.1 ARTIFICIAL NEURAL NETWORKS

The concept of artificial neural networks was inspired by the study of the central nervous system of human beings. In the artificial neural network, simple artificial nodes, known as neurons, processing elements, or units, are connected to build a network that mimics the biological neural network of human beings. The backpropagation neural network is a well-known type of neural network, with multi-layered perceptron architecture with error backpropagation for supervised learning and is particularly powerful for nonlinear forecasting. It uses error back propagation to calculate the gradient of the loss function and modify the model parameters (such as weights and activation limits) by the descending gradient method for each specific observation [5]. The interactions between neurons characterize the transmission and processing of information and artificial neural networks have the advantage of strong adaptability, fault tolerance and anti-noise capability. These merits have enabled neural networks to be applied successfully in numerous fields [6]. As an analytical tool,

artificial neural networks consist of numerous connections of artificial neurons, or nodes. Each node represents a specific output function called an activation function. The connection between each two nodes represents a weighted value for the signal that passes through the connection, called weight, which is equivalent to the memory (or learning) of the artificial neural network. The network output differs depending on the network connection path, the weighted value, and the activation function. The network is usually an approximation of a certain algorithm or function, or it can be an expression of a logical strategy. The neural networks of backpropagation can include three layers: The input layer, the hidden layer, and the output layer, as can be seen in figure 1. The model is trained by comparing the differences between the network outputs and the outputs of reference and minimizing its error by adjusting the connection weights. Then the neural network of reverse propagation is constructed with acceptable errors through the continuous adjustment of their weights [7].

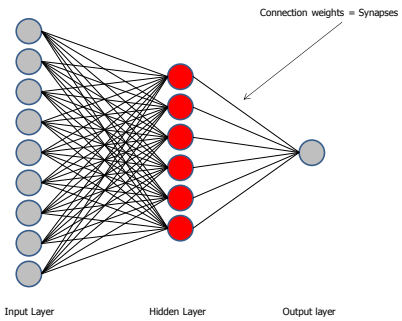

Figure 1: Basic architecture of a three-layer reverse propagation neural network.

1.2 DEEP LEARNING AND MACHINE LEARNING

In a simple definition machine learning or deep learning refers to the use of an artificial neural network with multiple layers of hidden nodes between the exit and the entrance, see figure 2, where the deep architectures are built by various levels of operations nonlinear. The deep network has the same architecture as a traditional neural network, but with a greater number of hidden layers. The main difference between a deep network and a traditional neural network are the algorithms developed for the training of deep architecture which are faster and generate more solid results. Deep learning includes representation learning algorithms that transform raw features into high-level abstractions using a deep network made up of multiple hidden layers. In other words, deep learning applies computational approaches, which have multiple nonlinear transformations, to train data representation through various levels of abstraction [8].

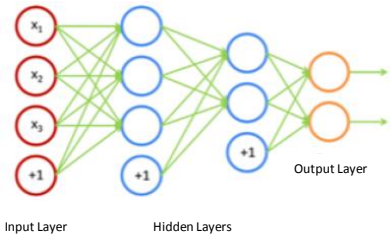

Figure 2: Multilayer Artificial Neural Network (Deep Network). Adapted from [8].

Recently, the automatic extraction of features and representations has become an emerging area of research in recognition of human activity. To reduce the dependence on human resources in engineering and the time spent for specific activities and applications, deep learning has become highly sought after for this purpose. Deep learning uses appropriate machine learning techniques to present and model high-level representational resources in sensor data using multiple layers of neural networks that represent hierarchical characteristics from low to high level. Deep learning often provides flexibility, robustness and performance improvement using the power of multiple layers of neural networks [9]. Deep learning is essentially a redesign of artificial neural networks. In theory, a neural network with more than two layers, input, and output, can be classified as deep architecture. However, it is not just about the number of layers, but about the idea of automated construction of more complex features at each stage. This means that stacking other algorithms multiple times, using probabilities instead of class labels, can be considered as deep learning as well [10].

1.3 GENETIC ALGORITHMS

The genetic algorithm is a Machine Learning model based on the mechanism of natural selection and natural genetics. This is accomplished through the random creation of a population of individuals, represented by chromosomes. These individuals are evaluated and undergo an evolutionary process starting with natural selection, inspired by Darwin's Theory of Evolution: The best individuals in a population are selected. Then a biological process occurs: Some recombination, such as crossing and mutation, is carried out to create a new generation of individuals with the hope that this new individual will be better. The process is interrupted when a target value is reached. Genetic algorithms are optimization tools and allow solving problems for which an extreme solution is sought [11]. In this process, one looks for a set of inputs (x1, x2, x3, ..., xj) which will generate a desired output y. This mechanism is illustrated in figure 3, below [12].

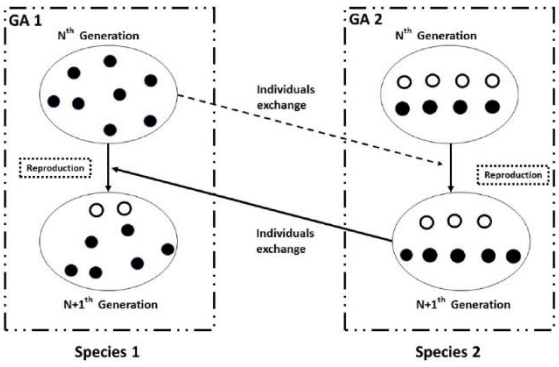

Figure 3: Example of co-evolutionary mechanism.

1.4 PSO (PARTICLE SWARM OPTIMIZATION)

This technique is considered as stochastic (undetermined state, originating from random events) and generates the optimization process through a biological structure, such as a group of birds, for example. It contains some generalizations of the genetic algorithms; however, it does not consider the classical genetic operator which is based on crossing and mutation. The PSO handles internal speed and an appropriate

memory, generating better autonomy for updating the algorithm during processing. In addition, PSO offers massive potential because it includes specific characteristics of Evolution Strategies and / or Genetic Algorithms. During PSO processing the algorithm reproduces the movement of birds as a group in a natural environment. Considering a simple vector, it is possible to reproduce the grouping and the movement of each individual bird that forms the grouping of birds. However, intelligent agents or particles allow the production of different numbers of iterations that are determined at random [13].

1.5 BFO (BACTERIA FORAGING OPTIMIZATION)

The BFO strategy mimics the process produced by mobile biological bacteria (such as E. Coli and Salmonella). These bacteria are usually guided by the help of locomotive scourges when they produce demand in the space in which they collect nutrients and avoid harmful substances. The movements occur in a clockwise or counterclockwise rotation of the flagellum when they try to locate the best nutrient, moving in a systematic way (swimming or running) or colliding chaotically. In addition, their movements are derived from the concentration of nutrients in space. Its generality has been demonstrated to swim more than to bump in a random direction once the nutrients are more concentrated [13].

1.6 CONVOLUTIONAL NEURAL NETWORKS, CNN

Convolutional Neural Networks are the Deep Learning method most widely used to represent characteristics, as they provide invariant, automatic, salient, and translational resources for different areas of application. Convolutional Neural Networks use deeply interconnected structures to perform convolutional operation on sensor data using several hidden layers. These networks are subdivided into different components, which include: Convolutional layer, pooling layer and fully connected layers merged to form deep architectures for local extraction of correlated characteristics from data. Convolutional layers capture the feature map using various kernel sizes and feeds, and then group them to minimize the number of connections between the convolutional layer and the cluster layer. In the same way, the components of the grouping layer reduce the map of characteristics, the number of parameters and makes the translation of the network invariant to changes and distortions. Another vital component of Convolutional Neural Networks is the values of the activation unit, derived in each region for learning patterns from data using the adjustment terms and feature map [9]. Figure 4 illustrates the structure of a forecast model for mechanical properties [14].

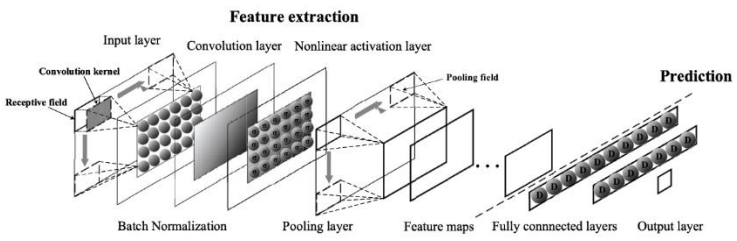

Figure 4: Forecast model for mechanical properties using CNN.

1.7 RANDOM FOREST

A supervised machine learning algorithm that is an extension for decision trees and similar to the set method called bagging. It can be used for classification and regression tasks. It creates multiple decision trees during a training phase, where each data point is fed into all trees and generates statistics for all trees and combines all changes to provide its own forecast. It also avoids tree overfitting problems. In this approach to predicting mechanical properties, a random forest regression is chosen to train the model and predict the target variables. In the data collected, 85% of the data is used for training the models and 15% of the data for the is used for testing models. The performance of the trained model is evaluated by the correlation coefficient of the real values and estimated values of the test data [15].

1.8 SUPPORT VECTOR MACHINE

SVM performs classification and regression tasks and is a supervised technique that handles multiple continuous and categorical variables. In regression, there are two types of SVM models: epsilon-SVM regression, nu-SVM regression. The different types of SVM kernels are sigmoid, radial basis function (RBF), polynomial and linear. In the proposed approach nu-SVM regression model with radial kernel is selected. Coefficient of Correlation is calculated for actual test data values and predicted test data values for trained model performance evaluation [15].

1.9 DECISION TREE

This is a supervised technique that performs both classification and regression techniques. Decision trees work well for categorical and continuous input, output variables. It develops an associated decision tree by splitting the dataset into smaller subsets. In the proposed approach 85% of data is used for training the decision tree model and 15% of data is used to test the trained decision tree model. Further, the trained and tested decision tree model is evaluated by correlation coefficient of test data values and predicted data values [15].

1.10 ENSEMBLE METHOD

Ensemble methods are the combination of multiple models to improve the prediction accuracy and yields better results. This model is mainly used to decrease variance and increase bias. The various methods in ensemble methods are: Bagging, Boosting, stacking, simple average, weighted average, majority voting, weighted voting. In this proposed method to predict the mechanical properties tensile strength boosting method is employed. Boosting is the method which boosts up the performance of the weak models. It converts weak models to strong models. There are three different types of boosting techniques: Ada Boost (Adaptive Boosting), Gradient Boosting, XGBoost [15].

1.11 K-NEAREST NEIGHBOR (K-NN)

K-NN is the algorithm which is used for both classification and regression. In regression K-NN algorithm will evaluate all the suitable cases to predict numerical target based

on similarity measure. This algorithm is widely used in applications like pattern recognition and statistical estimation. The K-NN regression calculates average of numerical targets of k-nearest neighbors. K-NN uses three types of distance functions they are: Euclidean, Manhattan, Minkowski [15].

1.12 LINEAR REGRESSION

Linear regression finds relationship between continuous variables i.e., between dependent and independent variables by fitting a linear equation for the data. Usually, the relationships between variables can be either linear or non-linear. Linear relationships between the variables are represented by using straight lines and non-linear relationships between the variables are represented by curved lines. Two types of linear regression are simple linear and multiple linear regressions. When a single independent predicts a dependent variable then it is called as simple linear regression. When two or more independent variables predict a dependent variable then it is called as multiple linear regression [15].

2 DEVELOPMENT

Some selected technical papers, covering both Hot and Cold Rolling, for many metallurgical knowledge areas, will be shown below. The information is listed according to: Publishing Date, Paper Title, Rolling Process, AI Methodology and Author's Perceptions:

- 2019: "Property prediction and **properties-to-microstructure** inverse analysis of steels by a machine-learning approach" [3], Cold-Rolling, Machine Learning: "*The results presented in this work are expected to provide a new approach in materials design to accelerate the materials discovery process.*";
- 2019: "Physical metallurgy-guided machine learning and artificial intelligent **design of ultrahigh-strength stainless steel**" [4], Hot-Rolling, Machine Learning + Genetic Algorithm: *"The results illustrate that the ML model shows promise in the ability to capture the characteristics closely related to targeted outputs.*";
- 2019: "Improvement of **tribological behavior of H-13 steel** by optimizing the cryogenic-treatment process using evolutionary algorithms" [13], Hot-Rolling, Particle Swarm Optimization + Bacteria Foraging Optimization: "*The adaptation of intelligent evolutionary algorithms in the domains of critical engineering opens the possibility of sophisticated advanced optimum results that is hardly achievable by implementing traditional statistical methods.*";
- 2019: "**Mechanical Properties Prediction for Hot Rolled Alloy Steel** Using Convolutional Neural Network" [14], Hot-Rolling, Convolutional Neural Networks: "*The results show that the prediction accuracy of the proposed CNN model for predicting hot rolled steel mechanical properties is greatly improved.*";
- 2019: "**Prediction of Mechanical Properties of Steel** using Data Science Techniques [15], Hot-Rolling, Random Forest, Support Vector Machine, Artificial Neural Network, Decision Tree, Ensemble Method, Linear Regression, K-Nearest Neighbor: "*The current material sciences will definitely be affected by Data science and analytics by exaggerating accuracy and reliability in predicting mechanical properties.*";
- 2018: "**Design Optimization of Microalloyed Steels** Using Thermodynamics Principles and Neural-Network-Based Modeling" [16], Hot-Rolling, Artificial Neural

Networks + Genetic Algorithm: "*The neural network model helps quantify the impact of excess or reduced addition of microalloying elements in steel. Thus, the findings can be used directly while designing any new steel grade for commercial production.*";

- 2019: "**Designing dual-phase steels** with improved performance using ANN and GA in tandem" [17], Cold-Rolling, Artificial Neural Networks + Genetic Algorithm: "*The ANN models could be used successfully to understand the role of the compositional and processing variables of DP steel, individually and in combination, through sensitivity analyses and simulation studies.*";
- 2019: "Evaluation of **ratcheting behaviour in cyclically stable steels** through use of a combined kinematic-isotropic hardening rule and a genetic algorithm optimization technique" [18], Hot-Rolling, Genetic Algorithm: "*Finally, it is demonstrated that the predicted results by the proposed methodology, in general, are in better agreement with the reported experimental results than that by the available predictions in the literature.*";
- 2020: "Design of **alumina-forming austenitic stainless steel** using genetic algorithms" [19], Hot-Rolling, Genetic Algorithm: "*Using GA, the process becomes computationally more affordable for alloy discovery and optimization.*";
- 2017: "Incorporation of prior knowledge in neural network model for **continuous cooling of steel** using genetic algorithm" [20], Hot-Rolling, Artificial Neural Networks + Genetic Algorithm: "*When the concept of multi objective optimization method is employed to reduce the prediction error and the average temperature difference simultaneously though adjustment of the neural network the chosen model is found to have even better predictability.*";
- 2019: "**Microstructural diagram for steel based on crystallography** with machine learning" [21], Hot-Rolling, Machine Learning: "*The recent progress in microstructural observations with the aid of AI technology is paving the way for automatic recognition of steel microstructures. The present scheme can serve as an effective tool for obtaining a deep understanding and control of the microstructures of steel.*";
- 2020: "Design of **Comprehensive Mechanical Properties** by machine learning and high-throughput optimization algorithm **in RAFM steels**" [22], Machine Learning + Genetic Algorithm: "*A design system based on ML and high-throughput optimization algorithm was established to obtain the optimal solutions of RAFM steels with both composition and treatment process modification for the improvement of both yield strength and impact toughness.*";
- 2020: "**Tensile property prediction** by feature engineering guided machine learning in **reduced activation ferritic/martensitic steels**" [23], Hot-Rolling, Machine Learning + Random Forests Regressors (RFRs): "*The trained models showed significantly higher accuracy and universality than traditional physical metallurgical model. It could provide a guidance for the further design of the new generation of RAFM steels with better comprehensive properties.*";
- 2020: "Quantifying **Mechanical Properties of Automotive Steels** with Deep Learning Based Computer Vision Algorithms" [24], Cold-Rolling, Artificial Neural Networks: "*The presented results show that the ANN trained with data of deformed surface profiles or force–indentation curves can predict the material behavior of the welded high strength steels with a very high accuracy. It was observed that this method is strongly robust for the determination of the yield strength.*".

From the results obtained in the selected articles the following author's perceptions are highlighted:

- **Disruption**: These are disruptive tools that bring a new way of interpreting processes;
- **Understanding**: Such tools allow a greater understanding of the phenomena involved in the production of steel as well as other materials;
- **Superior results**: When compared to traditional methodologies, these tools allow superior results, with better precision, reliability, and forecasting capacity;
- **Practicality**: The tools can be implemented in systems that are easy to access and use by production and development teams;
- **Research and Development**: R&D teams can use the tools to simulate new processes as well as in the discovery of products and processes not yet developed;
- **Predictability**: It is possible to forecast the final characteristics of products still in the production phase. Modifications to the process aimed at optimizing results can be carried out online aiming at superior results as well as reuse in other standards and / or conditions;
- **Agility**: These tools allow quick assessment of process data and impacts on product data;
- **Optimization**: Extraordinary cost reductions can be obtained with the possibility of simulating scenarios for new alloys and new processes.

Given the unique influence of each of the process and product variables on the physical characteristics of the materials, a sensitivity analysis of the influence of these variables as well as their metallurgical coherence is necessary. This is due to the "Black Box" nature of Artificial Neural Networks, which have limited ability to explicitly identify possible cause relationships: It may not be easy to determine which input variables are the most important for the final output. Researchers have developed techniques to increase understanding of the internal logic of RNA's. Studies show that it is possible to verify the influence of the input variables on the final results, reflecting the expected metallurgical trends, according to the figure 5, where the influence of Carbon and Manganese on Tensile Strength, for HSLA Wide Flange Beam are shown [25].

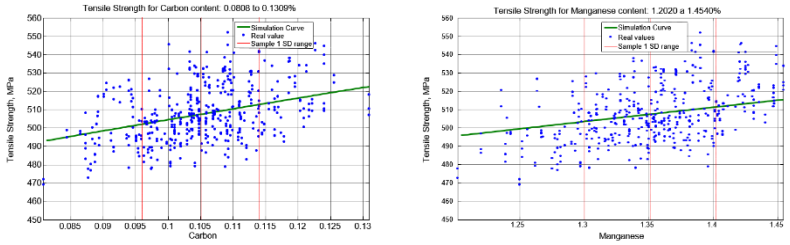

Figure 5: Tensile Strength for WFB produced from HSLA Steel [25].

An example of industrial use of the technology of Artificial Neural Networks is one developed for monitoring the microstructure from furnace to cooling and predict the mechanical properties. According to the manufacturer the advantages of this system is to save costs, to improve material quality, to continuously control the quality and to diagnose irregularities on the process. The entire steel production process can be optimized using this technology [26].

3 CONCLUSIONS

Such tools based on Artificial Intelligence technologies represent a disruptive factor in the way in which the influence of the various variables involved in the processing of materials, steel for example, is understood and explored. New forms of research and product development can be implemented with the achievement of results never seen before, with precision, reliability, and practicality beyond that obtained with current techniques, many of which are based on trial and error. There are countless works being done and several techniques being explored. Artificial Neural Networks, the basis of the so-called Deep Learning and Machine Learning, together with the Genetic Algorithms, represent a turning point in the understanding of the phenomena involved as well as in R&D since they allow determining the values of the product parameters aiming at obtaining desired characteristics. It is a highly valuable tool for the R&D areas, and it has already been used by some steelmakers around the world, with good results.

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