Ensemble of Artificial Neural Networks and AutoML for Predicting Steel Properties

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***Abstract*—The design of new steel grades is a continuous pursuit in the metallurgical industry, aiming to develop lighter and stronger materials for diverse industries. This study explores the use of an ensemble of artificial neural networks, named E-ANN, to model the relationships between chemical composition, process parameters, and mechanical properties of five types of steels. Auto-Keras, an automated machine learning framework, is employed to identify the best configurations for the ANNs and create the ensemble model. The best ANN, named B-ANN, obtained through the same AutoML process, and the one model ANN generated by Auto-Keras, named ANN, are used as a benchmark to evaluate the E-ANN performance. The results obtained show that the E-ANN model is competitive in terms of predictive capability. Sensitivity analysis provides insights into the influence of input parameters on mechanical properties, while Shapley Value analysis highlights the relative importance of these parameters. The findings contribute to the understanding of steel behavior and provide guidance for steel design processes. This study demonstrates the effectiveness of E-ANN in predicting mechanical properties and emphasizes the value of data-driven techniques and automated machine learning in steel design.**

***Index Terms*—Steel, Prediction of mechanical properties, Data-driven model, Automated Machine Learning**

I. Introduction

The design of new grades of steel is a recurring theme in the metallurgical industry, with researchers relentlessly seeking to create lighter and stronger steel to meet the requirements of various industries. Achieving the desired characteristics involves altering the chemical composition and process temperatures, which can be a complex and challenging task [23]. As a result of the intricate nature of variable relationships in the field, many insights and mathematical equations have been derived from experimental data. While vast amounts of data are available from production lines and testing, interpreting this data can be difficult due to the erratic and highly variable environments in which it is collected [3].

When it comes to the choice or development of steel, it is essential to consider the desired mechanical behavior, as it determines how the steel will respond to the applied forces. In this work, the properties of tensile resistance (TS), yield strength (YS), and elongation (EL) will be addressed. As these mechanical properties are directly related to the internal organization of steels, they are dependent on the chemical composition and process parameters employed in their production [20]. Each type of steel has unique characteristics regarding its internal structure, hardening mechanisms, and alloy element adhesion [7], which increases the complexity of predicting their mechanical properties. In this study, data from five types of steels were considered, namely: Interstitial Free (IF), Bake Hardening (BH), Dual-Phase (DP), Transformation Induced Plasticity (TRIP), and High Strength Low-Alloy (HSLA), which requires a careful and detailed analysis of the specific characteristics of each material for a reliable design model.

To overcome these challenges, data-driven techniques such as Artificial Neural Networks (ANNs) have become increasingly popular. ANNs have the ability to learn and generalize from large datasets, enabling them to capture both linear and nonlinear patterns that traditional modeling techniques may not discern [1]. Therefore, to ensure the best generalization of the data, it is essential to find the most appropriate set of parameters and architecture for the problem [23]. Failure to do so can result in poor performance, overfitting, or underfitting of the model, leading to inaccurate predictions and unreliable results.

To assist in the choice of hyperparameters, a field has stood out in the machine learning area, namely Automated Machine Learning (AutoML). Its objective is to automate the entire process of model creation, training, and deployment. One of the main techniques used in AutoML is Neural Architecture Search (NAS), which seeks the best neural network architecture through search space exploration and performance evaluation. The use of NAS has presented promising results in various areas, especially in image recognition [5].

Even after optimizing the ANN parameters depending on the complexity of the input data and therefore their relationships, the results generated by the ANN can suffer from the poor generalization of input space regions, resulting in considerable errors. To reduce this problem, some authors [2], [8] have resorted to using ensembles of ANN, with this structure formed by ANNs already trained, and the final result as a function of each of the networks. Thus, the combination of these networks with different parameters can distribute errors throughout the input space and give the model better accuracy, resulting in better predictions [2]. It is important to highlight that the TS, YS, and EL mechanical properties being predicted are in a continuous domain. Thus, a multivariate regression problem is characterized.

The objective of this paper is to apply and evaluate the performance of an ensemble of ANNs, named E-ANN, created based on the best configurations of multiple runs of Auto-Keras [10], an open-source AutoML framework developed in Python. The ensemble will be used to model the relationships between the chemical composition, process parameters, and mechanical properties of IF, BH, DP, HSLA, and TRIP steels. To establish a benchmark for comparison, it will be used two models, the best ANN model, named B-ANN, obtained through the same parameter optimization process employed to create the ensemble, and an ANN model which is the first neural network generated by Auto-Keras.

In a recent study, [21] proposed the modeling of IF steels using ANNs. Different activation functions were used, and the hyperparameters were optimized using the Auto-Keras library as NAS. The best ANN for each activation function was selected and compared using the performance metrics mean absolute error (MAE) and mean squared error (MSE). In the present study, instead of using only the best configuration found by Auto-Keras, the top five ANNs were selected to form an ensemble of ANNs. Additionally, the data generalization was performed for five different types of steels: IF, BH, HSLA, DP, and TRIP.

The remainder of this paper is organized as follows: Section II and III discuss the theory and background related to this paper. Section V presents the proposed method and the experimental setup used. Section VI presents the proposed experiments considered for this study. Section VII shows the results achieved and its analysis and discussion, and finally, the conclusion is shown in Section VIII.

II. Background

A. Artificial Neural Networks and Ensemble

ANNs have emerged as a powerful tool for data analysis and decision-making in various fields. ANNs are inspired by the structure of biological neural networks and are composed of multiple layers of interconnected artificial neurons, where their effectiveness highly depends on the proper selection of model parameters, such as the number of layers, the number of neurons per layer, and activation functions [1].

These structures can be used to capture complex patterns and relationships between input and output, using a large amount of data [3]. However, they are also susceptible to problems such as overfitting and learning instability, which can result in a low capacity for model generalization and accuracy [22].

Ensemble techniques aim to improve the performance of machine learning models by combining multiple individual models and providing a single result. Typically, these models are trained independently and then combined to generate the final result. For classification problems, the most common technique is to follow the majority of results, while for regression problems, the technique used is usually the arithmetic mean of the results [13].

The combination of multiple ANNs can be beneficial for improving the final model. Each ANN has its own parameters, structures, or datasets and therefore its own way of generalizing patterns in relation to the database [18]. The techniques employed in crafting these ANNs are strategically designed to impart a broad spectrum of diversity to the resultant models.

As a result, each ANN with its own characteristic might exhibit a more significant error concerning specific regions within the input space [8]. By forming an ensemble, it is possible to balance these errors and use the information contained in each ANN to generate an average response with higher accuracy and better overall model performance.

III. Steels

Steels are renowned for their exceptional strength, durability, and versatility, making them a widely utilized group of alloys in various industries. Steel can be classified into different types, each possessing unique characteristics, including distinct forms of hardening. These forms of hardening play a crucial role in enhancing the mechanical properties of steel, allowing it to meet specific performance requirements in diverse applications [7].

1) Interstitial Free Steels (IF): Are known for their high formability. This is due to their chemical composition, which does not contain interstitial elements such as carbon and nitrogen, resulting in a highly ductile material that can be molded into complex shapes without cracking or rupturing [19]. Thus, the absence of these interstitial elements makes IF steels highly malleable, making them widely used in the automotive industry for external body components.

During the IF steel manufacturing process, the addition of niobium or titanium is common to minimize the presence of carbon and nitrogen as interstitial solutes. These elements have the ability to stabilize the carbon and nitrogen atoms, preventing them from being incorporated into the crystal structure of the steel [17]. Additionally, it is crucial to maintain tight temperature control during the reheating and hot rolling phases. These steps are critical in determining the crystallographic structure and grain size of the material [19], which directly influence the final properties of the steel.

2) Bake Hardening Steels (BH): This is a type of low-carbon steel that has its strength and hardness increased through a heat treatment process, due to the diffusion of carbon atoms to form an atmosphere around dislocations which will result in fixing these dislocations and, in turn, increasing the strength [15].

The addition of alloying elements such as niobium, titanium, molybdenum, and vanadium can affect the dissolution of carbides during annealing, which in turn can have a significant effect on the amount of carbon present in the solution. However, the impact of these elements on carbide formation depends on both the carbide dissolution temperature and the strength of the carbon bonding energy [16]. The balance between these factors can lead to a variety of microstructures and final material properties.

3) High Strength Low-Alloy Steels (HSLA): It is a type of steel that aims to provide improved mechanical properties and/or greater resistance to atmospheric corrosion compared to conventional carbon steels. These properties are achieved through various hardening techniques such as grain refinement and precipitation strengthening [11], which are further enhanced through the addition of small amounts of alloying elements in their composition, such as aluminum, vanadium, niobium, or titanium.

4) Dual-Phase Steels (DP): It is a type of steel known for its high combinations of tensile strength, elongation as well as higher fatigue resistance.

The manufacturing process of dual-phase steels necessitates high control over phase transformations, which represent distinct states characterized by specific chemical compositions, types of atomic bonds, and arrangements of elements. These phase transformations are strongly influenced by the steel's heat treatment history. Each phase within the steel exhibits distinct and unique properties, contributing to the overall performance of the material [12].

5) Transformation Induced Plasticity Steels (TRIP): Are a class of advanced metallic materials with superior mechanical properties due to their ability to undergo phase transformations during plastic deformation, resulting in a unique combination of high strength and ductility [7].

This phase transformation takes place as a result of the alloying elements redistributing within the material, leading to the formation of a stable crystalline structure that enhances its strength. Additionally, the presence of a stable austenitic phase imparts TRIP steels with increased energy absorption capacity during deformation, making them well-suited for applications demanding high strength and toughness [6].

IV. Mechanical Properties

The range of available steel types, along with various composition approaches, is primarily motivated by the pursuit of enhancing their unique properties. In the context of this study, we focus our attention on essential mechanical properties, namely: yield strength (YS), tensile strength (TS), and elongation (EL).

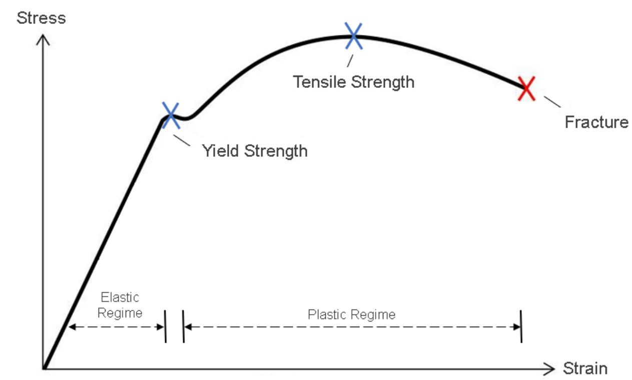

Fig. 1: Stress-Strain Curve.

To better comprehend the investigated properties, we can utilize Fig. 1, which depicts a standard stress-strain curve for steel testing.

1) Yield Strength: It can be defined as the maximum stress value within the material's elastic regime [4]. In other words, up to this stress level, any deformation experienced by the material is reversible upon the removal of the applied load.

2) Tensile Strength: It can be defined as the maximum stress point required to further deform the material, which is now in the plastic regime [4], resulting in permanent deformations that do not revert to the original size upon load removal.

3) Elongation: It can be defined as the amount of deformation sustained by the material in the plastic regime until its complete fracture.

Each of these properties holds significance within a project. In mechanical forming, for example, tensile strength and elongation are important, since they are necessary for the material to undergo maximum deformation [9], thus operating within the plastic regime. However, in most other engineering applications, Yield Strength takes precedence in design, as the aim is to work within the material's elastic range [4], without inducing significant deformations.

V. Proposed Approach and Dataset

An overview of the proposed approach is shown in Fig. 2. Initially, data is extracted from the steel production process and subsequently stored in a database including all relevant data points. Next, the data is processed and balanced so that every type of steel has a considerable representation in the dataset. Then, hyperparameter tuning is performed using AutoML with the Auto-Keras framework. This process leads to the creation of a multivariate ensemble regression model composed of the 5 best ANNs generated by the Auto-Keras. The number of ANN models that will be part of the final ensemble model was defined empirically. After creating the ensemble model, named E-ANN, the next step is to determine the methodology for merging the individual predictions into a single value for each mechanical property. In this work, the fusion decision is to average the output of all ANN models present in the ensemble. Finally, the accuracy of the model is measured.

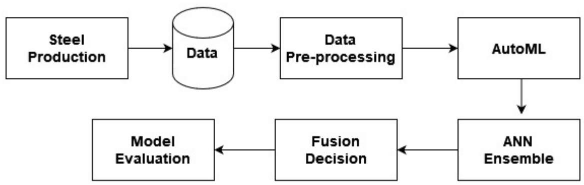

Fig. 2: Proposed Approach Flowchart.

The database was collected using real data from the steel production process. To ensure that every type of steel had adequate representation in the dataset, the authors utilized an ad-hoc filter method suggested by steel specialists. Despite the unequal distribution of steel types, the ANNs should be capable of generalizing the data, given that each steel type has a sufficient amount of representative data.

In order to perform a fair and unbiased comparison of different neural network models, it is necessary to evaluate the models on an impartial dataset. To accomplish this, a cross-validation procedure was performed in conjunction with the Auto-Keras library. The procedure involved randomly dividing the dataset into k parts (or ”folds”). In each iteration of the cross-validation, one fold was used as the test set, and the others were used as the training set.

For each fold, an E-ANN model was created and the results were aggregated and statistically analyzed to evaluate the robustness of the observed differences between the models.

The consolidated dataset contains 27160 rows and 29 columns, including process parameters and chemical composition that have a direct impact on the prediction outcomes and are shown in detail in Table II. In this case, we are dealing with a multivariate problem, as we are predicting multiple mechanical properties: yield strength (YS), tensile strength (TS), and elongation (EL). Table I provides an overview of the current distribution of data for each steel type after the consolidation process. In the above-mentioned table, DP and TRIP steel types have been grouped together due to the remarkable similarity in their chemical properties.

VI. Protocol of Experiments

In this study, we aim to assess the effectiveness of utilizing an ensemble of ANNs in predicting the mechanical properties of 5 types of steel, BH, DP, TRIP, HSLA, and IF.

Steel Type	Count
BH	9223
DP-TRIP	4529
HSLA	7569
IF	5839

TABLE I: Distribution of Steel Types

Variable	Description
Esp Real	Actual Thickness
Red Frio	Cold Reduction
Larg Real	Actual Width
TRPL	Reduction Temperature
TB	Outlet Temperature Hot-Rolling
TA	Inlet Temperature Hot-Rolling
C	Carbon
Mn	Manganese
P	Phosphor
Si	Silicon
S	Sulfur
Ni	Nickel
Al	Aluminium
Cr	Cromium
Nb	Niobium
Mo	Molybdenum
Ti	Titanium
V	Vanadium
B	Boron
N	Nitrogenium
Forno-Veloc	Oven Speed
SPM Med	Skin Pass Medium
P3 Med	Pyrometer Medium Temperature (Point 3)
P4 Med	Pyrometer Medium Temperature (Point 4)
P10 Med	Pyrometer Medium Temperature (Point 10)
P12 Med	Pyrometer Medium Temperature (Point 12)
P13 Med	Pyrometer Medium Temperature (Point 13)
P15 Med	Pyrometer Medium Temperature (Point 15)
P16 Med	Pyrometer Medium Temperature (Point 16)

TABLE II: Input Variables

The E-ANN model represents an ensemble of the top five neural networks selected from a total of 100 neural networks generated by Auto-Keras. The selection process for the five best neural networks was based on their MAE performance.

The proposed model is evaluated against two other models, all generated using AutoML. The B-ANN model uses the best neural network chosen from the 100 neural networks generated by Auto-Keras. This selection is based on the model's performance, considering the MAE metric. The ANN model, in turn, is built for each fold of the cross-validation, being one neural network generated by Auto-Keras.

Two performance metrics, namely Mean Absolute Error (MAE) and Mean Squared Error (MSE), were calculated to evaluate the model's performance on the validation dataset. The Mean Absolute Error measures the average absolute difference between the predicted and actual values, providing an indication of the average magnitude of the errors. On the other hand, the Mean Squared Error calculates the average squared difference between the predicted and actual values, giving more weight to larger errors.

By analyzing these metrics, and comparing all models presented, it is possible to comprehensively evaluate the performance of the ensemble of ANNs in predicting the mechanical properties of different steel types.

VII. Results and Analysis

This project was developed on Python3 with Tensor-Flow and Auto-Keras as the main libraries. An Intel(R) Core(TM) i9-9900K CPU @3.60 GHz, 62 GB RAM, equipped with an NVIDIA Geforce Titan V 12 GB, was used in experiments.

In this section, the authors intend to compare performance, sensitivity, and interpretability in order to better understand the behavior of the algorithms. The results were taken from the exact same test dataset for all models and the training of all models was conducted by harnessing the maximum processing power of available GPUs, thereby parallelizing the process effectively. For this study, the cross-validation procedure was conducted considering the dataset divided into 10 parts (or "olds").

Figure 3 shows one example of E-ANN hyperparameters for the five best ANNs configurations suggested by Auto-keras for one cross-validation fold. The best configuration is used as the B-ANN model.

A. Model Performance

Concerning the model loss of the ANN for the training and validation data, Figure 4 illustrates that the best ANN does not suffer from overfitting or underfitting. Even though Figure 4 only displays the performance of the B-ANN model, it is important to note that the other ANNs used to form the ensemble exhibit similar behavior.

The results for the cross-validation experiment can be seen in Figure5. This graph depicts the progression of MAE and MSE metrics for each model in a 10-fold cross-validation experiment.

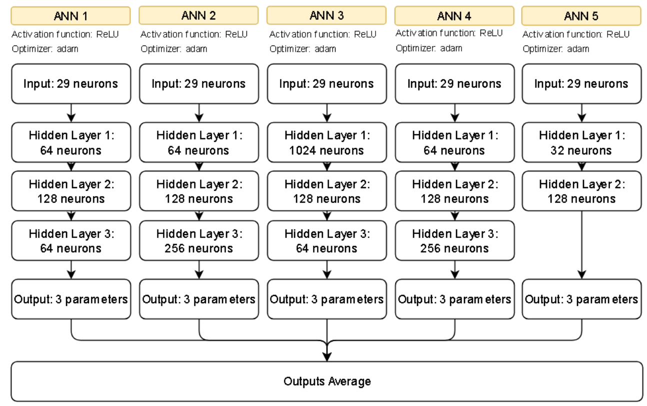

Fig. 3: Example of E-ANN hyperparameters for the five best Artificial Neural Networks suggested by Auto-Keras.

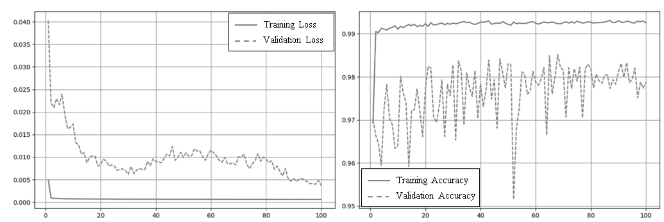

Fig. 4: Training and validation loss/accuracy of training epochs using the NAS architecture.

When evaluating the selected metrics (MAE and MSE), it becomes evident that the E-ANN model outperforms the other two models in terms of performance. The results consistently demonstrate a reduction in mean absolute error (MAE) and mean squared error (MSE) compared to the B-ANN and ANN models. This improvement can be attributed to the weighted combination of the outputs from the top five neural networks in the E-ANN model, enabling a better capture of data nuances and patterns.

On the other hand, the ANN model proves to be unques-

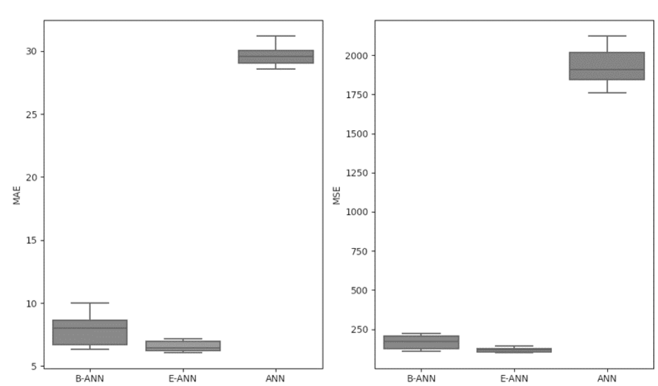

Fig. 5: Performance Comparison of Models in 10-Fold Cross-Validation

tionably inferior to the other two models. This is because the ANN model is based on a single execution of Auto-Keras, whereas the E-ANN and B-ANN models are created from multiple executions. This inferiority highlights the importance of performing multiple Auto-Keras runs and exploring different initializations to obtain a more reliable and generally better result.

B. Sensitivity Analysis

To gain insights into the relationship between input parameters and mechanical properties, numerical experiments were performed using sensitivity analysis. This analytical technique evaluates how uncertainties in model inputs contribute to the variability in the output, facilitating a deeper understanding of the factors influencing the results. By systematically modifying one parameter while keeping all other variables unchanged, the effects of different input parameter combinations can be compared across multiple models. This systematic approach allows for a comprehensive assessment of how individual variables impact the overall mechanical behavior of the materials under study.

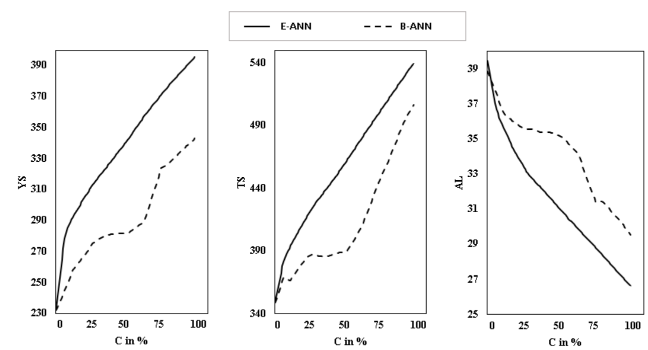

Fig. 6: Sensitivity analysis of 'C' for the E-ANN and B-ANN models

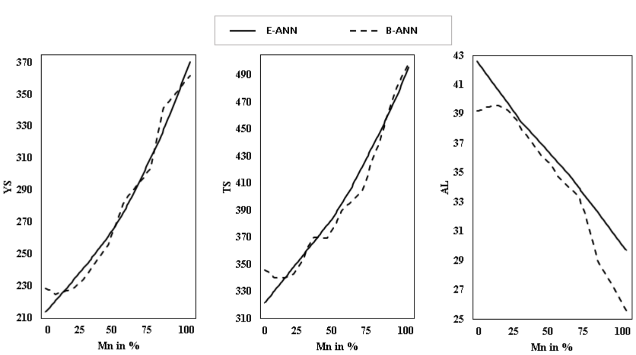

Fig. 7: Sensitivity analysis of 'Mn' for the E-ANN and B-ANN models

Figure 6 illustrates the relationship between the percentage of Carbon in the steel composition and the corresponding mechanical properties. The graph shows a clear trend where an increase in carbon percentage results in higher values of tensile resistance and yield strength and a decrease of elongation, which is expected by the literature [20]. This indicates that a higher carbon content contributes to the steel's overall strength.

Figure 7 illustrates the relationship between the percentage of Manganese in the steel composition and the corresponding mechanical properties. Which is also supposed to have an increase in the steel strength according to the literature [19].

Although the graphs demonstrate the expected behaviors for the analyzed properties, it is crucial to emphasize that the magnitude of variations for each chemical element depends significantly on the other chemical elements present in the system, as well as the process parameters. However, it is noticeable that both models exhibit similar patterns for the majority of the considered range of values. Despite being a local analysis, this comparison between the prediction models can be considered valid and helpful in understanding the relationships between the chemical elements and the mechanical properties.

C. Importance of Input Parameters

To gain a deeper understanding of the overall influence of input parameters on the mechanical properties, a tool derived from cooperative game theory was applied, known as Shapley Value analysis (SHAP) [14]. This approach allows us to calculate the contribution of each feature to the model output by assessing their distributional impact. By applying SHAP, we can discern the relative importance of each input parameter in determining the resulting mechanical properties, providing valuable insights into the global impact of these parameters.

Based on Figure 8, it is clear that in the B-ANN model, manganese emerges as one of the most influential elements, whereas carbon does not appear among the top influential features. However, in the case of the E-ANN model, manganese retains its high importance, and carbon is included in the list of most influential features.

Figure 8 shows only the top 20 most influential features out of a total of 29 features.

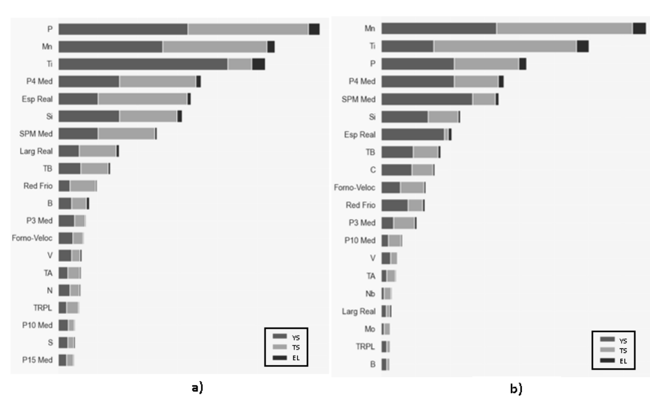

Fig. 8: SHAP values for a) B-ANN Model, b) E-ANN Model

When comparing these findings with those presented in [21], a noteworthy reduction in the significance of carbon is observed in both models. This decline can be attributed to the inclusion of additional steel types, such as DP, BH, TRIP, and HSLA, alongside IF. Consequently, the combination of steels with different levels of complexity assigns greater importance to alloy elements and process temperatures, which play a crucial role in hardening and phase transformation, ultimately defining the specific type of steel under consideration. As a result, these factors exert a greater influence on the model, superseding the relative importance of carbon.

VIII. Conclusion and Future Work

The utilization of AutoML frameworks, such as Auto-Keras, revolutionizes machine learning applications by enabling efficient exploration of the vast search space of neural network architectures. Additionally, AutoML facilitates the creation of ensembles, where multiple trained models are combined to enhance performance and accuracy. By automating the entire process, from model creation to training and deployment, AutoML optimizes the workflow and contributes to its growing popularity, making it accessible and applicable in a wide range of real-world scenarios.

Overall, our study provides compelling evidence of the effectiveness of using an ensemble of ANNs to predict the mechanical properties of various steel types. The ensemble model surpassed the performance of the single ANN model, as evidenced by superior performance metrics in the testing dataset.

Furthermore, the ensemble approach provided valuable insights into the intricate relationships between input parameters and mechanical properties, demonstrating that the model is sensitive to the inclusion of new types of both simple and complex steels, each with distinct hardening mechanisms.

Future works involve the analysis of different fusion decisions in the ensemble output.

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