Prediction of Mechanical Properties by Machine Learning

PURDUE UNIVERSITY
School of Materials Engineering

Student names: Bryan Adams, Amanda Guyre, Bryce McKenzie, Chad Piepenburg, Riley Plotner
Faculty Advisors: Prof. Michael Titus
Industrial Sponsors: Alex Post, Rob Christiansen

Haynes International wants to predict mechanical (yield strength, ultimate tensile strength, elongation, grain size, hardness) and corrosion properties of Haynes International Ni-Cr-Mo alloy sheets and plates using processing data and composition. This would allow Haynes to identify pieces that do not meet customer specifications and increase product yield. The goal of this project is to train a model using machine learning and compare the accuracy of a random forest and neural network. This poster highlights the process of determining the features to be used, comparing the models, and the limitations of machine learning.

This work is sponsored by Haynes International, Kokomo, IN.

HAYNES International

Project Background

The alloy used was a Ni-Cr-Mo corrosion resistant alloy. This alloy is solution heat treated, rapidly cooled by air or water quench, and further processed by hot/cold working and annealing.

Machine learning is the science of teaching a computer how to identify trends in data and create models. One type of algorithm used is a neural network (NN), which is a system of "neurons" that communicate to each other, such as that in the brain. Every neuron computes an activation value that gets sent off to the connecting neurons. Weights and biases are computed to influence the activation values, and through iterative training, the model is optimized.

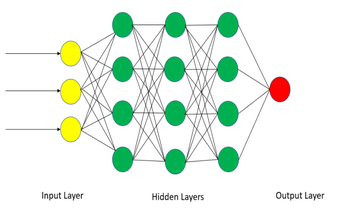

Figure 1. Neural Network Schematic

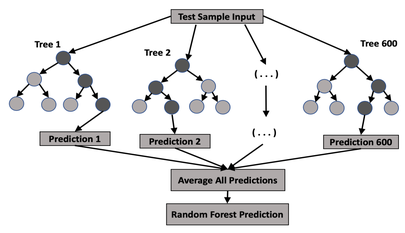

Figure 2. Random Forest Schematic

Another type of machine learning algorithm is a random forest (RF), which is a combination of different decision trees. Each decision tree makes its own predictions on the data and these predictions are averaged to provide a single output.

Experimental Procedure

Created random forest and neural network models to predict tensile strength, yield strength, percent elongation, grain size, and hardness from compositional and processing data.

- Used Python in Jupyter Notebook to create models with functions from pandas, NumPy, TensorFlow, Keras, and Sklearn.
- Compositional, processing, and calculated features were chosen using Pearson correlation and analysis of variance for property-feature relationships.
- Data sets with missing information were removed and the remaining sets were normalized before training the models.
- Data was split to use 80% for training and 20% for testing of the model.
- To avoid over fitting, features with little significance to the models were eliminated through iterative testing.
- Hyperparameters were optimized by testing different combinations until the most accurate model was created.
- Model accuracy was measured through mean absolute error (for corrosion rate) and mean squared error (for remaining properties).
- Parity plots, prediction errors, and range of predictions were compared to select the best model for each property.

Table 1. Summary of processing features used in each model. An X represents a selected feature for each predicted property.

Feature	Neural Network				Random Forest				
	TS	YS	%EL	GS	TS	YS	%EL	GS	H
Piece Gauge			X	X	X	X	X	X	X
Piece Length		X	X		X	X	X	X	X
Piece Width					X				X
Piece Weight			X	X	X	X	X	X	X
% Reduction	X	X	X	X	X	X	X	X	X
Avg Rolling Speed	X				X		X		X
Number of Passes	X	X			X		X		X
Annealing Time			X	X	X	X	X	X	X
Final Rolling Temp		X		X		X	X	X	X
Overall Heating Time (final roll)		X		X	X		X		X

Results

The strongest correlations to mechanical properties came from processing features. This was supported by the RF, which determined the reduction, annealing time, and rolling speed to be the most important features (Table 2).

Table 2. Importance of processing features in predicting mechanical properties, as determined by the RF.

Feature	Importance			
	Yield Strength	Tensile Strength	Elongation	Grain Size
% Reduction	0.04	0.18	0.09	0.08
Average Rolling Speed	0.04	0.03	0.05	0.07
# of Passes	0.04	0.02	0.04	0.04
Overall Heating Time	0	0.02	0.03	0
Final Rolling Temp	0	0	0.02	0.01
Annealing Time (min)	0.06	0.02	0.14	0.08
Mill Furnace #	0.02	0.02	0.02	0.02

The parity plots (Figure 3) give a visual representation of the model's accuracy by plotting the predicted yield strength against the measured yield strength. While the RF predictions appear to have a tighter fit around the match line than the NN, more lay outside of the acceptable error.

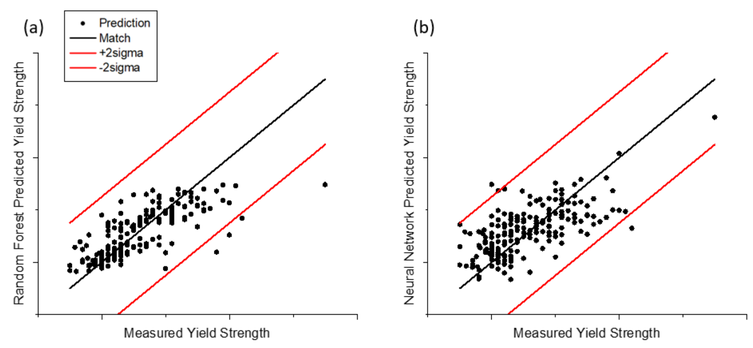

Figure 3. Parity plots for yield strength testing data predictions against measured values for (a) RF and (b) NN.

Table 3. Error analysis of the model predictions from Figure 3.

	Neural Network	Random Forest
Mean Squared Error	8.86×10^6	5.87×10^6
Number of Outliers	3	4

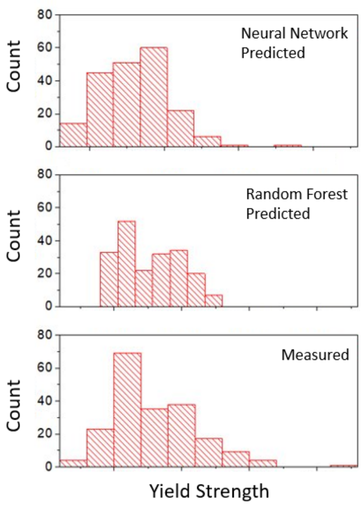

Figure 4. Distribution and range of yield strength testing data predictions by the NN and RF compared to the measured yield strengths.

Though the RF predictions yielded a smaller error (Table 3), the NN predicted a wider range of values (Figure 4). Because the final model will be used to predict the impact of changing process parameters, it must be able to identify if a change will result in an extreme difference in properties. For this tradeoff, the NN was selected as the final model for yield strength. This process of analysis was repeated for all properties (Table 4).

Table 4. Determined best model for each property.

Model	Yield Strength	Tensile Strength	Elongation	Grain Size	Hardness
Neural Network	X			X	
Random Forest		X	X		X

Discussion

Limitations of the Machine Learning Models

- The models are limited by the range of training data, therefore they cannot make new predictions outside of this range.
- The predictions the models make will only be as good as the quality of data used for training the models, therefore estimations, generalizations, and factors that cannot be accounted for in the data will weaken the accuracy of the model's predictions.
- The type of features available to be used in these models is limited to quantitative, not qualitative, data.
- The models can only learn and make predictions based on what they were exposed to. For example, our models are not capable of predicting the mechanical properties of cold worked samples due to not having exposure to enough cold worked sample data during training.
- These models do not support predictions for binary data types, such as corrosion data.

Conclusions

- Random forest models are capable of handling more features because they can establish feature importance and thus give more weight to more important features.
- Using more features in the neural networks leads to the risk of overfitting the data to the model.
- Processing data has a greater impact on mechanical properties than compositional data.
- Corrosion properties are unable to be successfully predicted by our algorithms due to the binary nature of data.

Recommendations

We recommend that Haynes International implement more processing features and increase the amount of data used in training to improve the accuracy of the machine learning algorithms. To develop a functional model for corrosion properties, more research must be done to identify other features that impact corrosion. In addition, a different model skeleton that can predict properties from binary-type data should be developed.

Acknowledgments

Special thanks to Prof. Titus for his project oversight, Alex Post and Rob Christiansen from Haynes International who helped collect data and guide our project, and Prof. Strachan for providing useful machine learning modules.

References

- Juan Carlos Verduzco Gastelum, Alejandro Strachan (2021), "Citrine Tools for Materials Informatics," https://nanohub.org/resources/citrinetools. (DOI: 10.21981/EV2W-WF04).
- Chakure, A. (2020, November 06). Random forest and its implementation. Retrieved April 29, 2021, from https://medium.com/swlh/random-forest-and-its-implementation-71824ced454f
- Navlani, A. (2019, December 9). (Tutorial) neural network models in r. Retrieved April 29, 2021, from https://www.datacamp.com/community/tutorials/neural-network-models-r