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.

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.

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 ScikitLearn.
- 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 yield strength).

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.

<table>
<thead>
<tr>
<th>Feature</th>
<th>Importance</th>
<th>Yield Strength</th>
<th>Tensile Strength</th>
<th>Elongation</th>
<th>Grain Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Reduction</td>
<td>0.04</td>
<td>0.18</td>
<td>0.09</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>Average Rolling Speed</td>
<td>0.04</td>
<td>0.03</td>
<td>0.05</td>
<td>0.07</td>
<td></td>
</tr>
<tr>
<td># of Passes</td>
<td>0.04</td>
<td>0.02</td>
<td>0.04</td>
<td>0.04</td>
<td></td>
</tr>
<tr>
<td>Overall Heating Time</td>
<td>0.00</td>
<td>0.02</td>
<td>0.03</td>
<td>0.00</td>
<td></td>
</tr>
<tr>
<td>Final Rolling Tempative</td>
<td>0.02</td>
<td>0.02</td>
<td>0.04</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>Annealing Time</td>
<td>0.06</td>
<td>0.02</td>
<td>0.14</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>Mill Furnace #</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td></td>
</tr>
</tbody>
</table>

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.

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
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References