MSE643 – Artificial Intelligence and Machine Learning in Materials Engineering
Course Instructor – Prof. Dr. Krishanu Biswas

Term Project

ML-Driven Predictive Modeling of Steel Heat Treatment for Desired Mechanical Properties

Neural Nexus

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Problem Statement

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- Different grades of Steel
- Unavailability of steel grade with desired mechanical properties
- Heat Treatment affects steel’s mechanical properties
- Traditional Selection is time-consuming and based on trial and error

Objective

- To develop an Artificial Neural Network (ANN) model that predicts the probability of achieving desired mechanical properties based on various heat treatment processes.
- Reduce the time spent on selecting the heat treatment process
- Reduce the wastage of resources

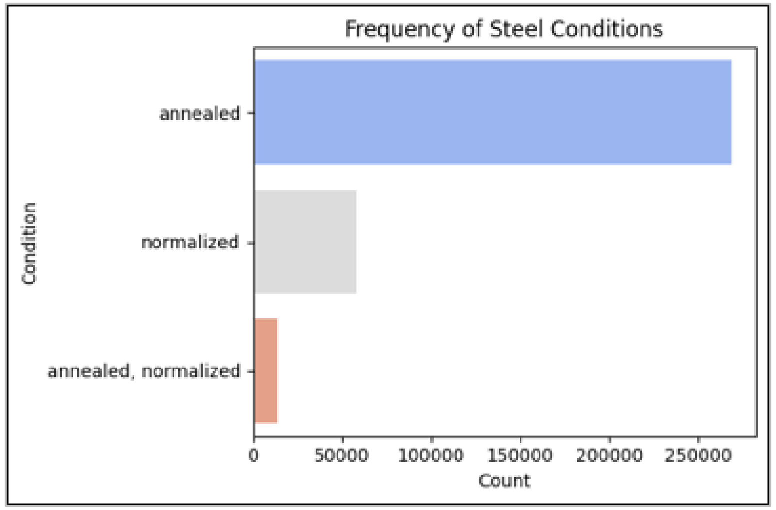
Data Collection

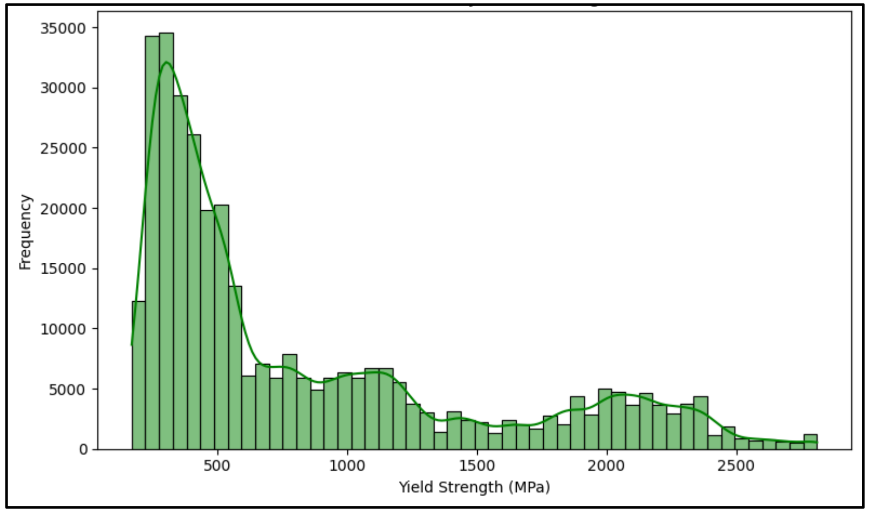
- **Data collection** is the foundational step to gather information for training, validating, and testing ML models.
- **Influence:** Quality, quantity, and diversity of data directly impact model accuracy and reliability.
- **Method:** ANSYS Granta Selector 2024 R1 software utilized to generate various steel data.
- **Steel Data:** Over 650 steel grades available in Granta Selector 2024 R1.
- Software creates data for 20 steel grades at a time, resulting in approximately 33 datasets.
- **Properties:** Each steel grade data includes diverse properties: Mechanical, H.T, electrical, chemical, composition, etc.
- **Focus:** Mechanical properties (Yield strength) and heat treatment data consolidated into a single dataset.

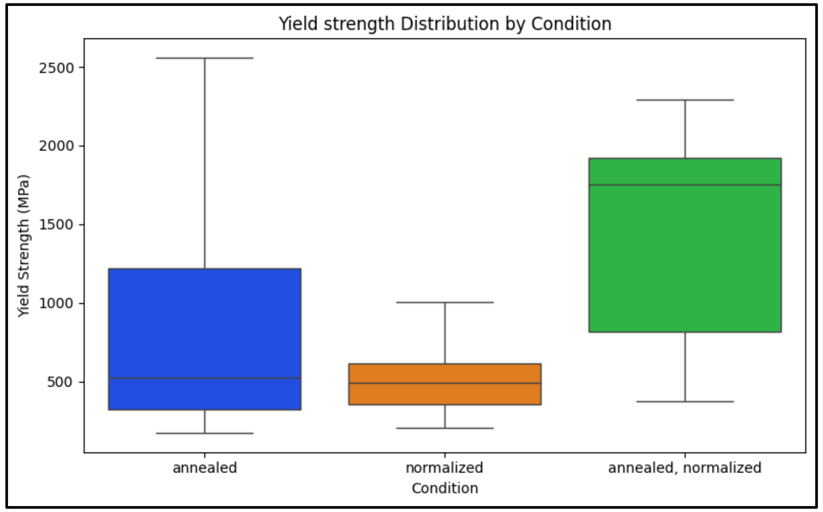
Data Pre-Processing

- Clean real-world noisy steel data from Excel "Steel_Data_Noisy.xlsx"
- Extract relevant fields: *Steel Grade*, *Condition*, *Yield Strength*
- Extracted keywords in Condition using regex (e.g., "annealed", "normalized")
- Parsed modulus ranges (e.g., 200–210 GPa) into mean and std deviation
- Generated 1000 synthetic samples per record using Normal Distribution (±std)
- Export to new Excel file "Synthetic_Steel_Yield_Strength.xlsx".

Data Visualization

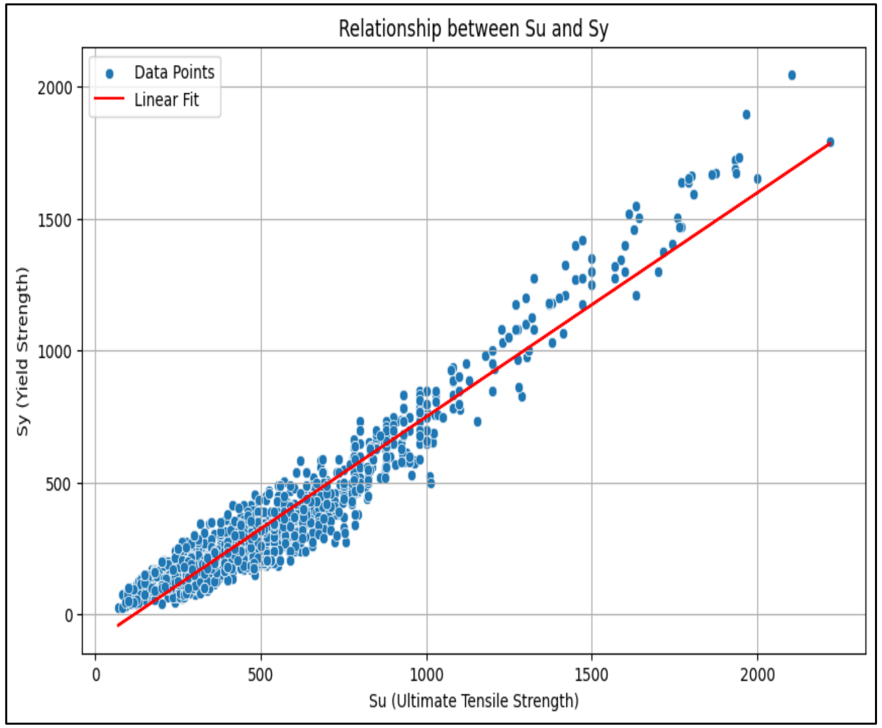






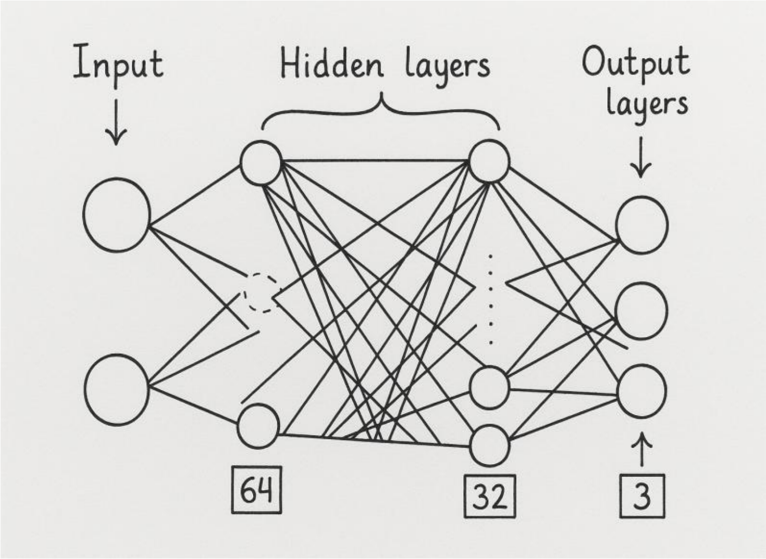
Sy and Su Relationship

- Sy - Yield strength; Su - Ultimate Tensile strength
- Plot Sy and Sy values from a different dataset that has direct values. "Data_Su_Sy.csv"
- Fitting a linear regression model.
- **Sy ≈ 0.849 * Su - 100.119** (Linear)
- R^2 score: **0.9170**
- This model helps if the desired feature is UTS



Model Training & Testing

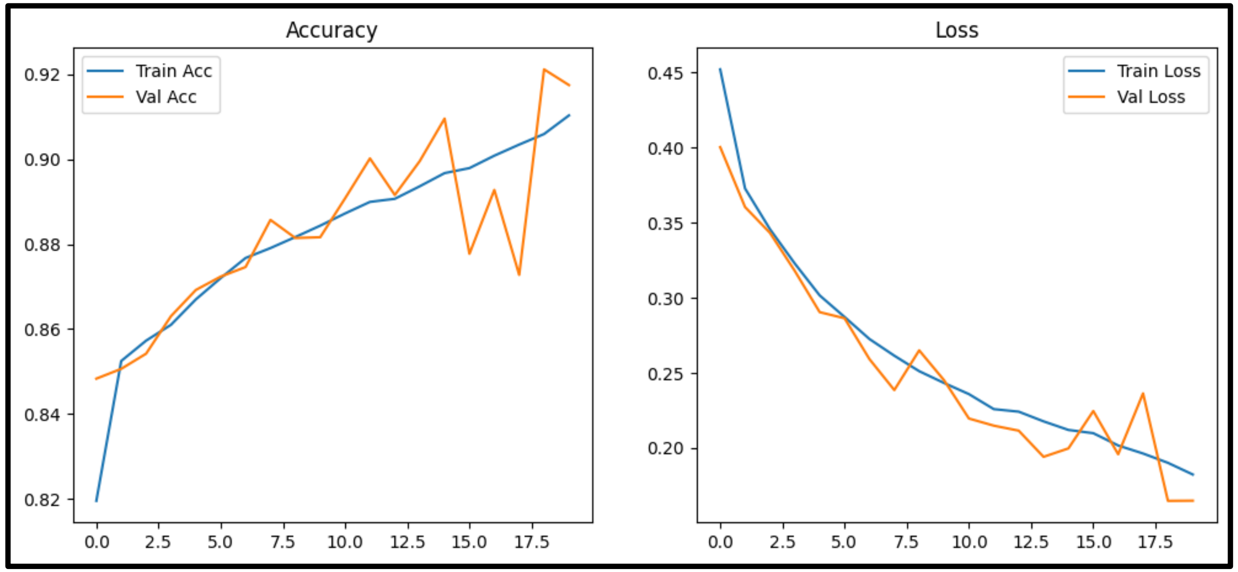
Model Training	Model Testing
Label Encoding & Scaling Prepares features	Train-Test Split – Ensures fair evaluation
One-Hot Encoding of Target– Softmax compatibility	Evaluate on Test Set – Measures generalization
ModelCheckpoint – Saves best model	Save Model & Preprocessors – For future inference
Validation Split + Deep Layers – Prevents overfitting	Plot Accuracy/Loss – Diagnoses model performance



ANN Model:

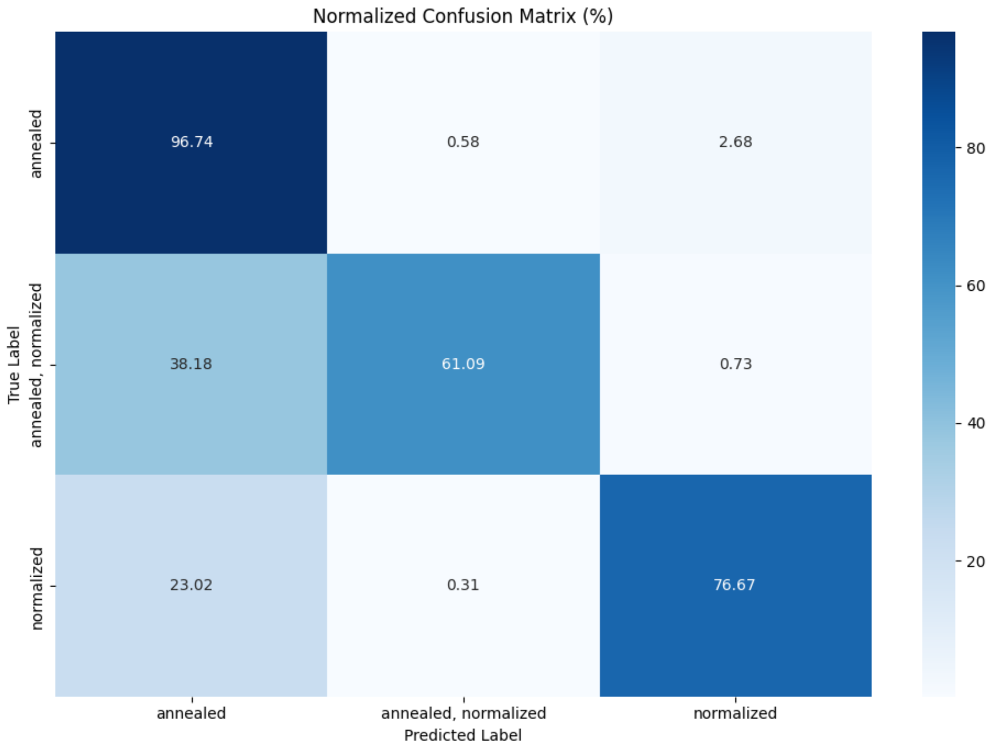
- 1 input layer,
- 4 hidden layer(Activation='Relu’),
- 1 output layer (Activation='softmax')

Model Evaluation



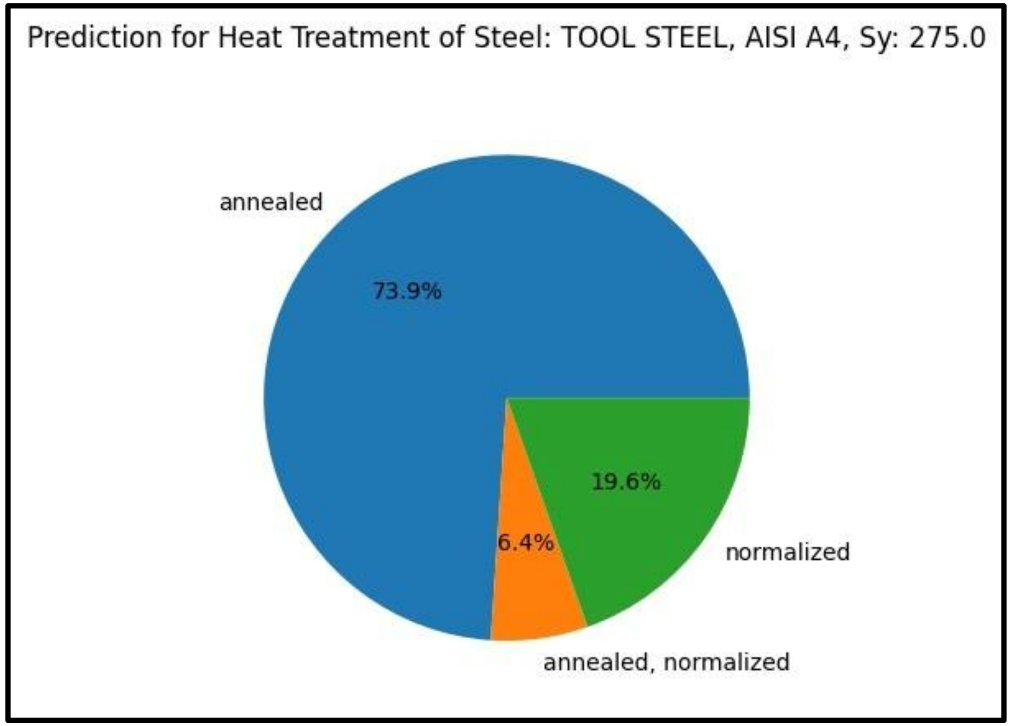
- No major overfitting
- Accuracy steadily increases, and loss decreases across epochs
- Validation accuracy fluctuates slightly due to class imbalance

Model Evaluation



- The confusion matrix highlights model performance across the three classes
- The model:
  - Performs well for Annealed and Normalized classes
  - struggles with annealed, normalized

Results



Prediction:

- Annealed: 73.9%
- Normalized: 19.6%
- Annealed & Normalized: 6.4%

Limitations

The model generalizes well to known data and provides high-confidence predictions.

However, the following limitations are encountered:

- Class imbalance,
- Reliance on a single feature (Sy), and
- Occasional misclassifications between overlapping treatment classes.

Future Scope

- Improvement can be done on various aspects
  - **Input Feature addition**
  - Composition, Different mechanical properties , Thermal properties
  - **Prediction features addition ,**Other heat treatment processes .etc

Conclusion

- Built an ANN model to predict heat treatment from steel grade and yield strength
- Achieved 90% accuracy on clean synthetic data
- Accurate for 'Annealed' and 'Normalized' treatments
- It demonstrates the use of ML in predicting the right heat treatment process for steel

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