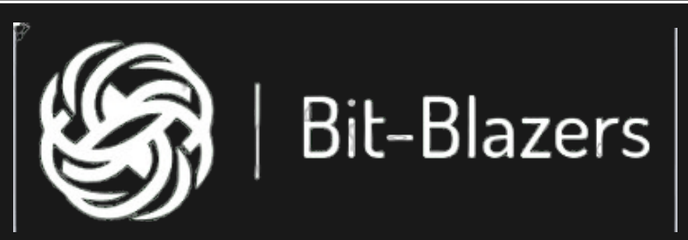
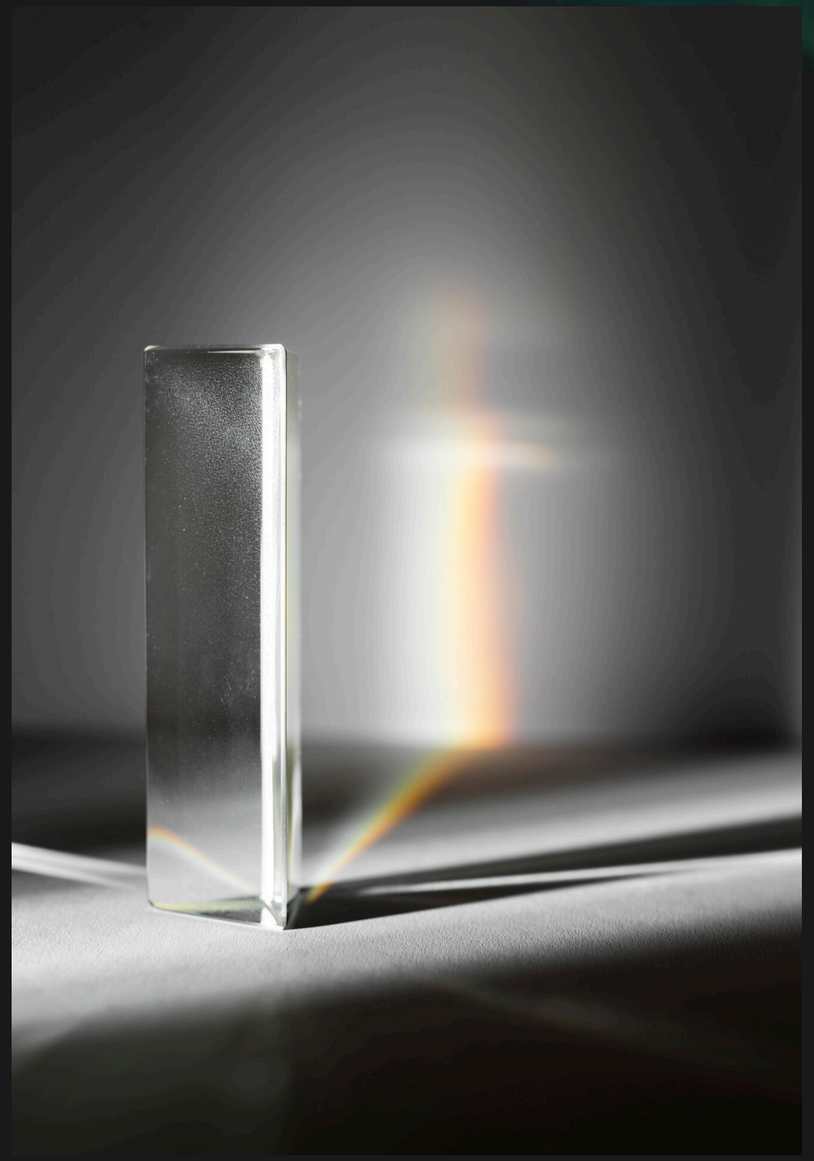
Exploring the Mysteries: Unveiling Metallic Glass Formation



Introduction

In this presentation, we will **unveil** the **glass forming ability** of **metallic glasses**. We will explore the unique properties and applications of metallic glasses in various industries. Join us as we delve into the fascinating world of amorphous materials.

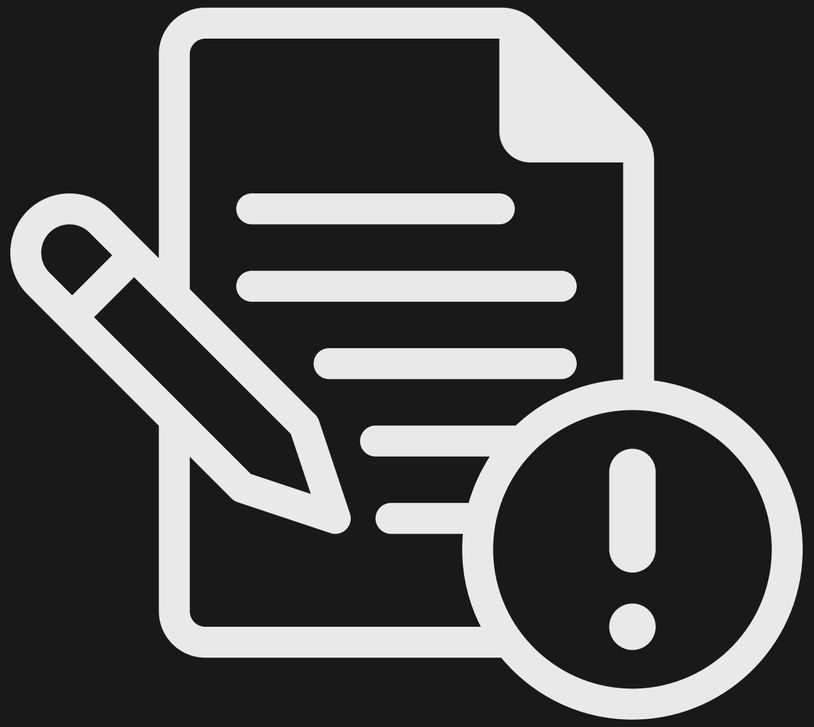


Problem Statement

The task at hand involves utilizing machine learning to predict the Gross Floor Area (GFA) expressed as Dmax (in mm) based on a dataset with seven features. The individual guiding this endeavor instructs us to partition the dataset into training and testing sets, reserving 20% for testing purposes. Moreover, we are tasked with repeating the training process ten times, each time with a random partition for training and testing. The performance of the predictive model is to be evaluated by averaging the results of these ten iterations, with the standard deviation used to gauge fluctuations in performance. Additionally, the person providing this task encourages us to delve deeper into the dataset and model, uncovering any valuable insights that may aid in understanding the relationship between the input features and GFA prediction.

Goal

The goal of this study is to develop a predictive model capable of accurately determining the glass-forming ability (GFA) of metallic glasses based on intrinsic material parameters. By employing machine learning techniques, the aim is to leverage the relationships between features such as total electronegativity, atomic size difference, and glass-transition temperature to predict the critical casting diameter (Dmax) of metallic glasses. Ultimately, the goal is to provide researchers and practitioners with a reliable tool for optimizing metallic glass synthesis processes and advancing materials science and engineering endeavors.

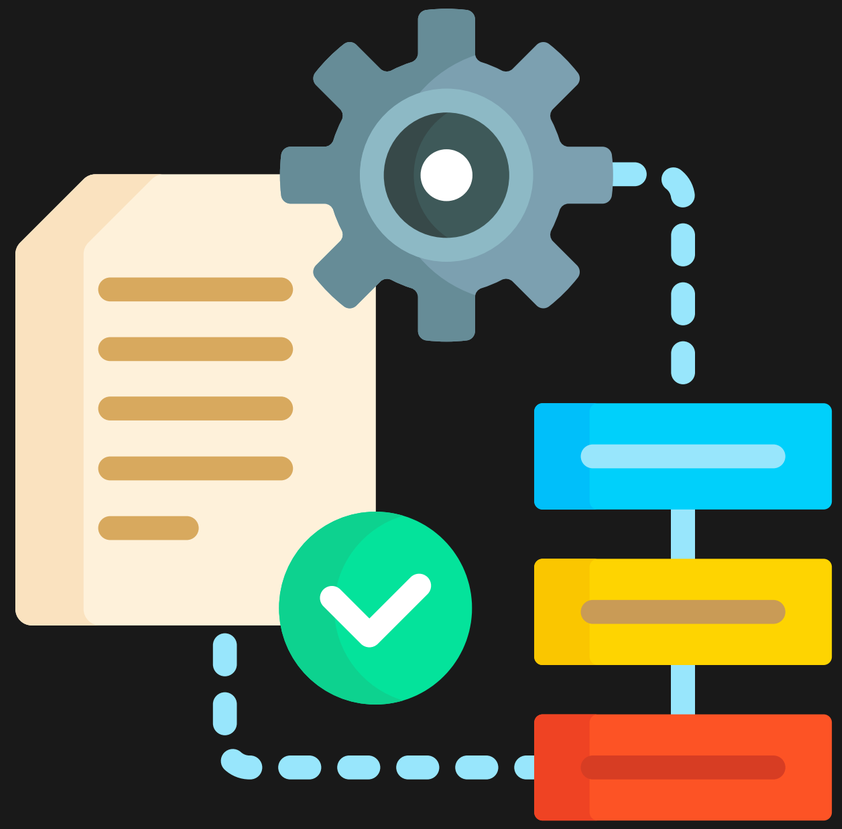


Dataset Overview

The dataset provided offers a comprehensive examination of the parameters influencing the glass-forming ability (GFA) of metallic glass. Each entry encompasses critical aspects such as total electronegativity (TEN), atomic size difference (d), average atomic volume (VA), mixing entropy (Sm), glass-transition temperature (Tg), onset crystallization temperature (Tx), and liquidus temperature (Tl). These parameters collectively elucidate the intricate interplay between material composition, structural properties, and thermal behavior crucial for synthesizing metallic glass. By systematically analyzing the dataset, researchers can uncover correlations and patterns that elucidate the mechanisms governing GFA, thus facilitating the optimization of metallic glass synthesis processes for diverse applications in materials science and engineering.

Preprocessing

In the preprocessing phase, two additional columns were incorporated into the dataset, both pivotal in determining the glass-forming ability of metallic glasses. The first, Trg, represents the ratio of the glass-transition temperature (Tg) to the liquidus temperature (Tl). The second, Rc, signifies 10 divided by the square of the atomic size difference (d). These augmentations enabled the identification of outliers within the dataset, with special attention given to the element exerting the greatest influence on the alloy's composition. Through one-hot encoding, this dominant element was appropriately represented. Subsequently, the values across all columns were normalized to ensure uniformity and comparability in subsequent analyses.

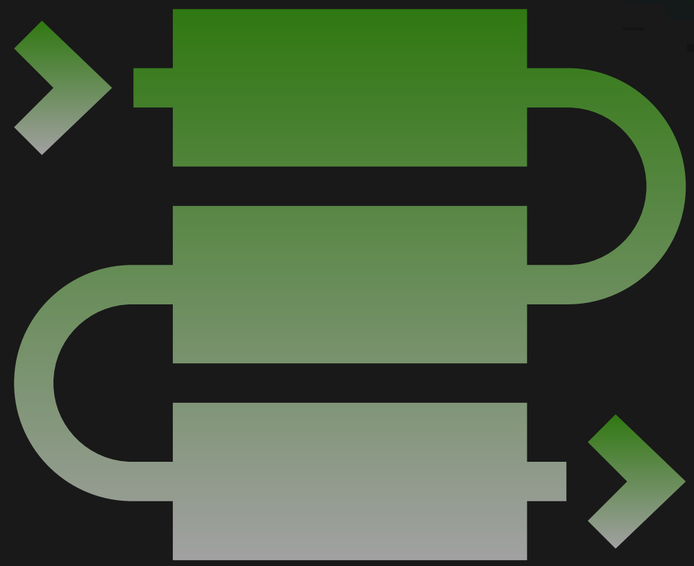


Model Architecture

During the model architecture phase, a grid search approach was employed utilizing several models: Decision Tree, Linear Regression, Support Vector Machine (SVM), and XGBoost. Among these, XGBoost emerged with the highest accuracy, showcasing its effectiveness in predicting the glass-forming ability of metallic glasses. Notably, the parameters for XGBoost were optimized through the grid search process, resulting in the following parameter configuration:

par_xgb = {"n_estimators":[100,200],
"max_depth":[3,5],
"learning_rate":[0.1,0.01] }

This fine-tuning process aimed to enhance the model's performance and ensure robustness in predicting the critical casting diameter (Dmax) of metallic glasses.



Result

After conducting tests and running all the algorithms, we have identified specific results which are being displayed here in the form of pictures. Among all the algorithms tested, XGBoost emerged as the best algorithm, consistently delivering the best results in terms of accuracy, precision, and recall. Its robust performance and ability to handle complex data sets make it a top choice for our data analysis needs. The visual representations of the results clearly showcase the superiority of XGBoost over other algorithms tested.

```
decision tree
RMSE: 0.6311006881885046
R^2: 0.3879262533715102
```

```
SVM Results:
RMSE: 4.259635872311700 5
R^2: -26.883763846680 2
```

Result

Cross Validation Scores

```
Cross-Validation Scores (XGBoost): [0.54798387 0.39511772 0.3460661  0.40082866 0.29755136 0.463424
 0.54555316 0.54913538 0.37964956 0.33879611]
Mean RMSE (XGBoost): 0.42641065681552454
```

XGBoost Results

```
XGBoost Results:
RMSE: 0.39451368814161 28
R^2: 0.7608168413924534
```

Result


Learning Curve (XGBoost)
RMSE
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
50
100
150
200
250
300
Training examples
Training score
Cross-validation score

Conclusion

In conclusion, among all the algorithms explored, XGBoost demonstrated the highest accuracy in predicting the glass-forming ability of metallic glasses. This superiority can be attributed to several factors, including XGBoost's ability to handle complex relationships within the dataset, its ensemble learning technique that combines the strengths of multiple weak learners, and its robustness against overfitting. By leveraging the optimized parameters obtained through grid search, XGBoost effectively captures the nuanced interactions between intrinsic material parameters and the resulting glass-forming ability. Consequently, XGBoost emerges as the most reliable model for acquiring insights into the glass-forming ability of metallic glasses. Its predictive power positions it as a valuable tool for researchers and practitioners seeking to optimize metallic glass synthesis processes and advance materials science and engineering endeavors.

What's our next goal?

Next, our next step involves the utilization of neural networks to significantly boost the precision of the model. Additionally, we will integrate feature extraction techniques to further elevate the model's accuracy. It is crucial to take into account various supplementary factors in order to continuously enhance the accuracy of the model.

TEAM MEMBERS

Bit-Blazers

Mukund Agarwalla

Aviral Asthana

(Team Leader)

Armaan Pant

Thanks!