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BACKGROUND

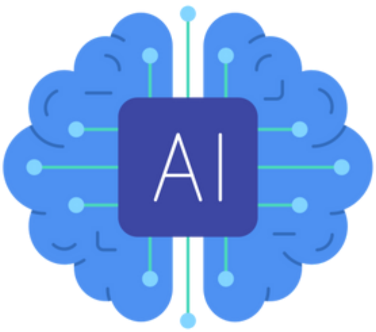
Metallic glass, a unique solid material, is synthesized from a liquid state without crystallization during cooling, resulting in a non-crystalline structure with random atomic arrangement. This material exhibits exceptional properties such as strength, flexibility, and corrosion resistance, making it promising for various applications. However, its susceptibility to weakening through deformation poses a challenge.

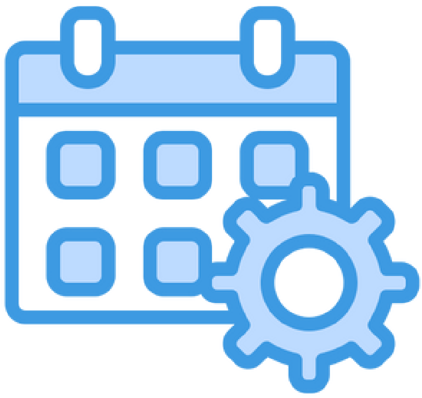
Historically, metallic glass was first synthesized in 1960 by W. Klement Jr., Willens, and Duwez at Caltech, using an alloy ($Au_{75}Si_{25}$). Early formulations required rapid cooling rates to prevent crystallization, limiting production to specific forms like ribbons and foils. In 1969, an alloy containing palladium, copper, and silicon demonstrated improved properties, leading to expanded applications.

Metallic glass, synthesized without crystallization, boasts a non-crystalline structure with exceptional properties like strength, flexibility, and corrosion resistance. First produced in 1960, it faced challenges due to rapid cooling requirements. Later alloys improved its properties, expanding its applications. Despite its promise, processing hurdles remain. Yet, its unique attributes make it invaluable in aerospace, electronics, and beyond.

OBJECTIVES

- Accurate Prediction: Develop a machine learning model to accurately predict the Glass-Forming Ability (GFA), represented by Dmax (in mm), using relevant features.
- Robustness Testing: Conduct repeated training-testing splits to ensure the model's robustness and reliability in different data partitions.
- Performance Assessment: Calculate the average predictive performance across multiple training-testing splits to gauge the model's overall effectiveness in predicting GFA.
- Uncertainty Estimation: Determine the standard deviation of predictive performances to quantify the variability and uncertainty associated with the model's predictions.
- Insight Generation: Gain insights into the influential factors affecting GFA by analyzing feature importance and model behavior, contributing to a deeper understanding of metallic glass properties and manufacturing processes.





The dataset contains 8 parameters (including the 1 output variable (Dmax)) which are all related to the Glass Forming Ability (GFA) of the metallic alloys. These 8 parameters are discussed in brief below:

Tg (Glass-Transition Temperature)

- This is the temperature at which an amorphous solid (glass) transitions into a supercooled liquid state upon heating.
- It is a critical parameter in determining the stability of the glassy phase.

Tl (Liquidus Temperature)

- The temperature at which a crystalline material fully melts into a liquid phase.
- For metallic alloys, this is relevant because it indicates the temperature range within which the alloy remains in a liquid state before solidifying upon cooling.

Tx (Onset Crystallization Temperature)

- This is the temperature at which the first signs of crystallization appear in an amorphous material upon heating.
- It's significant in understanding the thermal stability of the glassy phase.

TEN (Total Electronegativity)

- The total electronegativity of the alloy's constituent elements. It reflects the overall tendency of the elements to attract bonding electrons.
- It is relevant to the alloy's atomic interactions, which influence its glass-forming ability.

VA (Average Atomic Volume)

- This parameter represents the average volume occupied by atoms in the alloy.
- It's relevant because atomic packing density affects the ease of glass formation and thereby affects the GFA.

Sm (Entropy of Mixing)

- The entropy change associated with mixing the constituent elements to form the alloy.
- It influences the alloy's phase stability and propensity for glass formation.

d (Atomic Size Difference)

- The difference in atomic sizes between the constituent elements of the alloy.
- This parameter influences the alloy's ability to form a glassy structure by affecting atomic packing and the likelihood of crystal nucleation.

Dmax (Critical Casting Diameter)

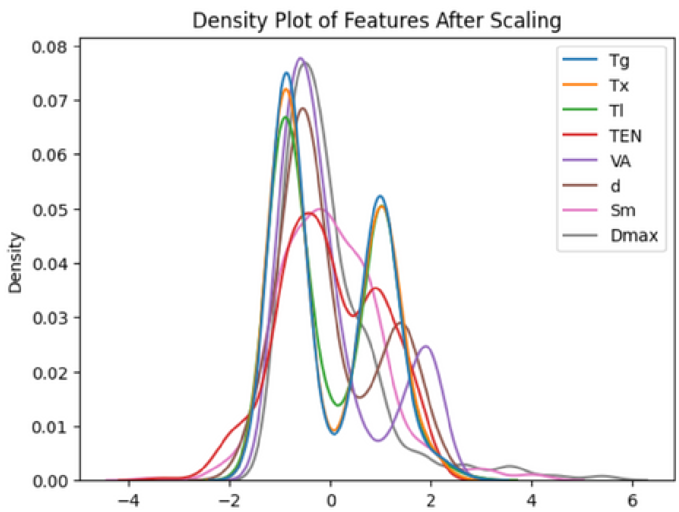
- This is the maximum diameter of a bulk metallic glass (BMG) rod that can be successfully cast without crystallization during rapid solidification processes.
- It's a practical measure of the alloy's glass-forming ability and is directly related to the cooling rate achievable during casting.

STEP 1: TESTING FOR NAN VALUES

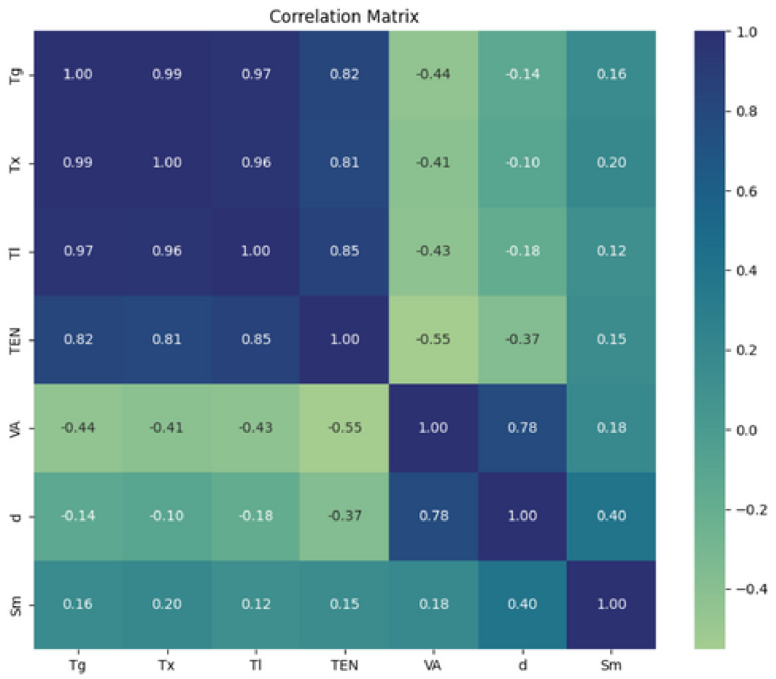
We have found that there were no NaN values in the data set.

STEP 2: NORMALIZATION

- We have implemented normalization techniques to ensure that all the features in our dataset are on a homogeneous scale, which facilitates the learning and interpretation of the data.
- We have used StandardScaler technique for normalization.
- The StandardScaler is a tool for standardizing features in machine learning. It rescales features to have a mean of 0 and a standard deviation of 1, making them comparable and easier for models to interpret.



DATA VISUALISATION

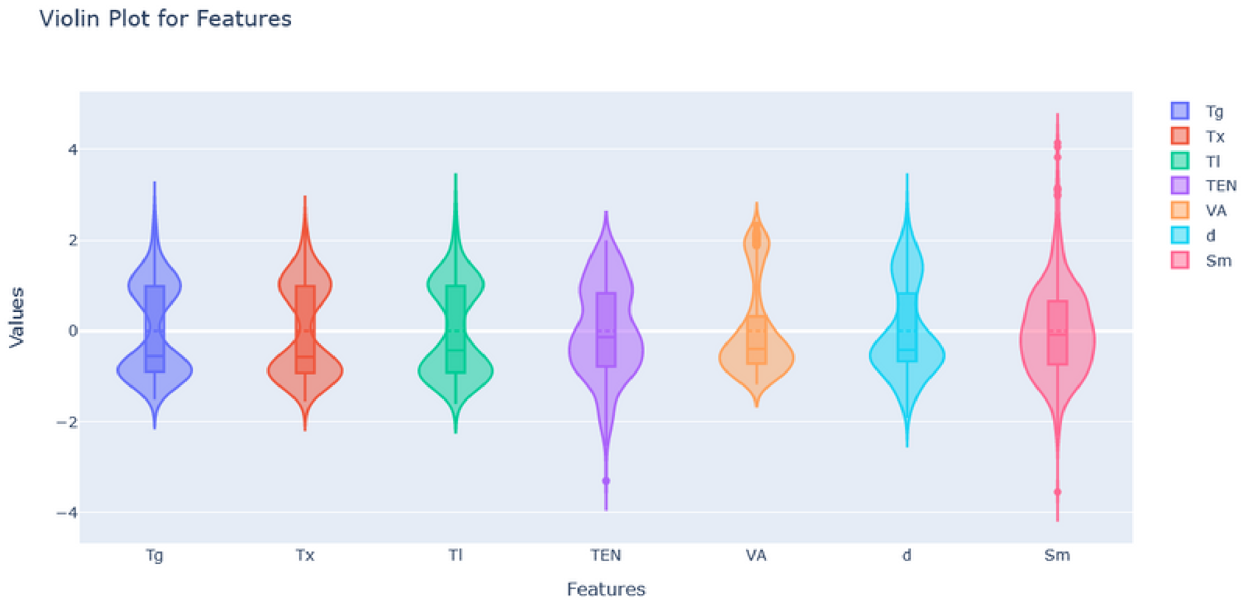


1

From the correlation matrix, we have observed and considered the correlation values above 0.85 to be highly correlated. Considering this, we find that the features Tx, Tl and Tg are highly correlated .

2

The violin plots have been plotted to get an idea about the outliers and distribution of the data. We have used the scaled data to plot the distributions for uniform subplots in all variables. We note the bimodal distributions of all the variables except Sm.

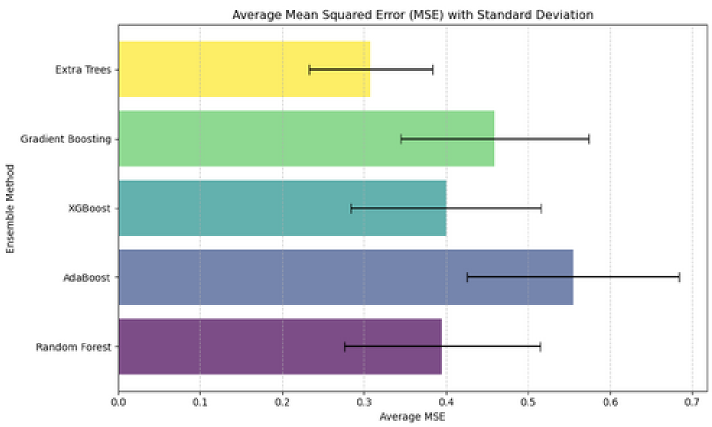


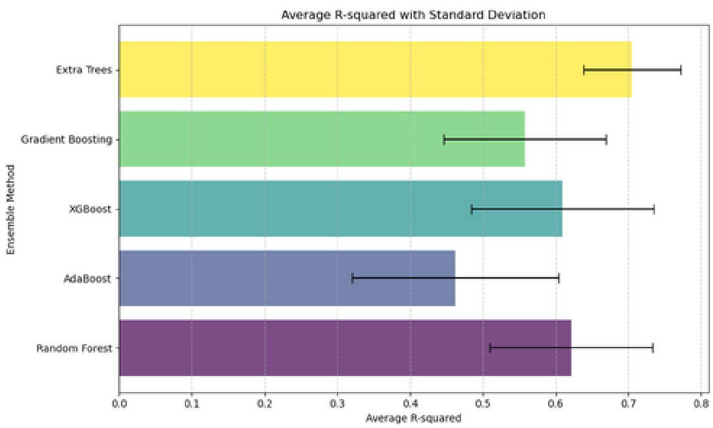
APPROACH

- Curated a selection of regression models including Random Forest, AdaBoost, Extra Trees, Gradient Boosting and XGBoost
- Employed Mean Squared Error (MSE) and R-squared (R2) as primary evaluation metrics.
- Implemented K-fold cross-validation to ensure robust model evaluation.
- Trained and evaluated each model on training and testing sets iteratively.
- Calculated average and standard deviation of evaluation metrics across multiple runs.
- Compared models based on average performance and variability.
- Selected the model(s) with the best average performance and lowest variability for further consideration or deployment.

$$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \bar{y})^2}$$

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$$



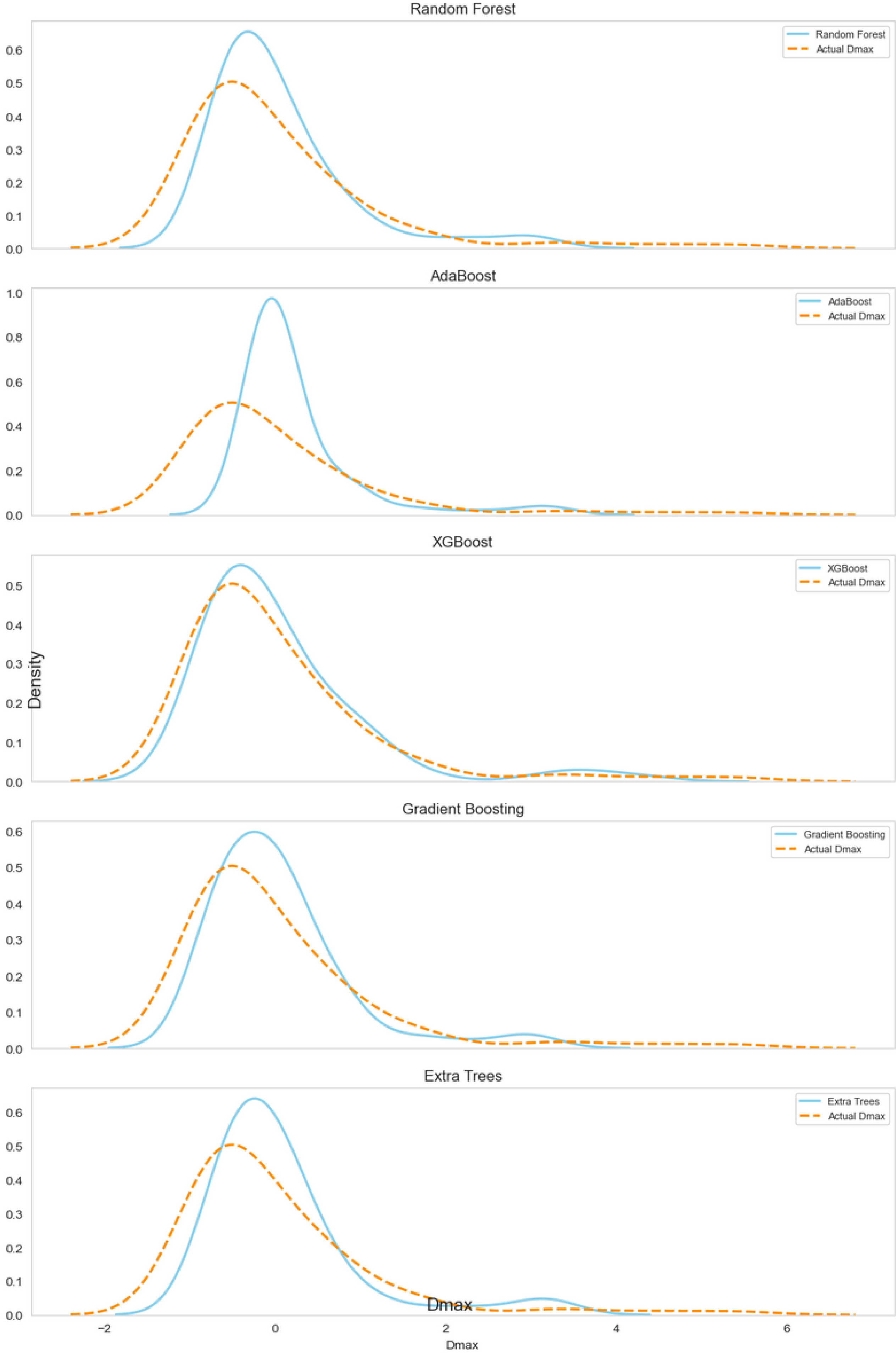


CONCLUSION

In conclusion, after thorough evaluation of various regression models including Random Forest, AdaBoost, Extra Trees, Gradient Boosting, XGBoost, and Polynomial Regression, the Extra Trees model emerged as the top performer. With the highest average R-squared (R2) score and lowest Mean Squared Error (MSE) among the evaluated models, it demonstrated superior predictive performance on our dataset. **Therefore, Extra Trees was selected as the base model for further analysis or deployment in our predictive modeling task.**

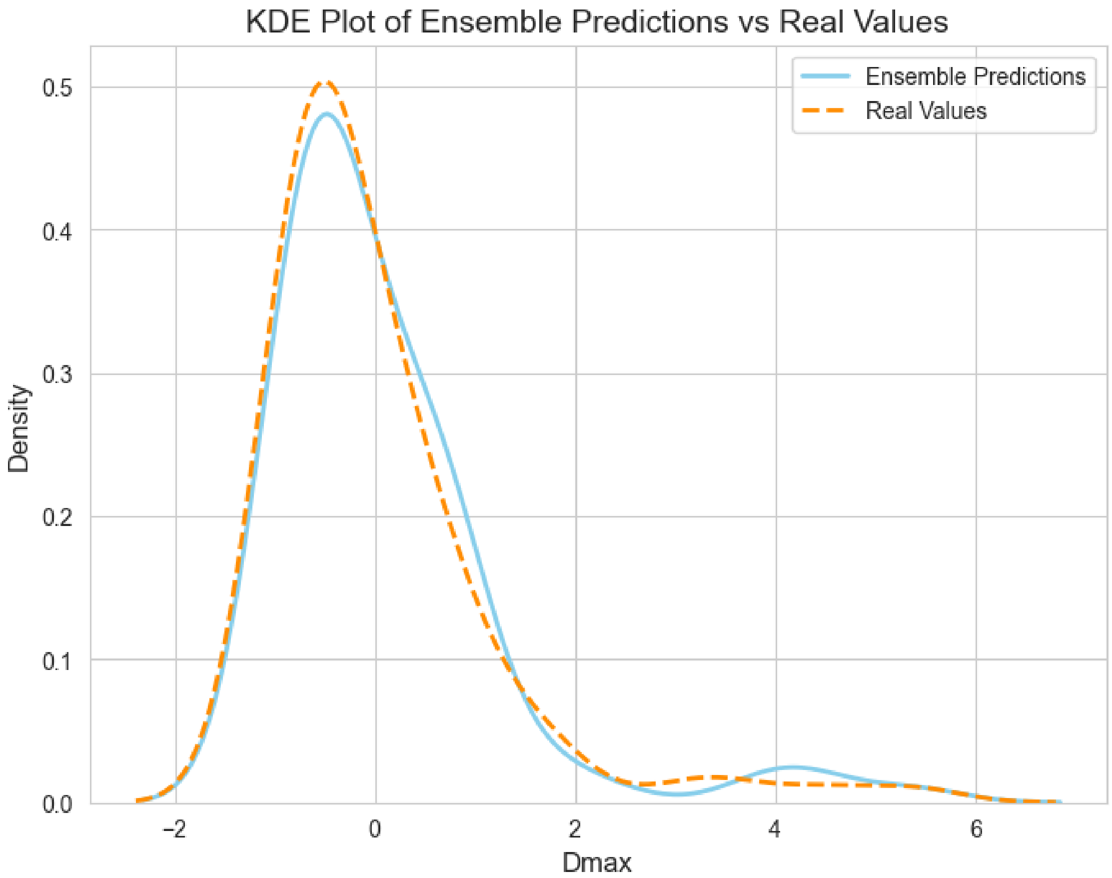
BASE MODEL SELECTION

GRAPHICAL REPRESENTATION OF VARIOUS MODELS AND HOW THEY FIT THE TRUE DATA



APPROACH

- Imported necessary libraries for the experiment, including scikit-learn, TensorFlow, and NumPy.
- Set seed for reproducibility to ensure consistent results across runs.
- Initialized base models and meta-learner outside the loop, including an Extra Trees Regressor and a neural network model implemented using Keras
- Used 10-fold cross-validation with shuffling to evaluate model performance robustly.
- Split the training data into training and validation sets for the base models within each fold of the cross-validation loop.
- Trained both the Extra Trees Regressor and the neural network model on the training data.
- Generated predictions from the base models for the validation set and stacked them horizontally to create the input for the meta-learner.
- Trained the meta-learner, a clone of the Extra Trees Regressor, using the stacked predictions as input.
- Generated predictions from the base models for the test set and stacked them horizontally to create the input for the meta-learner.
- Calculated the R-squared score for the ensemble predictions from the meta-learner compared to the ground truth on the test set for each fold of the cross-validation.
- Calculated the average R-squared score over all 10 folds to summarize the model's performance.



CONCLUSION

The achieved average **R-squared score of 0.822** highlights the effectiveness of the stacking ensemble technique in improving predictive performance. By combining predictions from diverse base models, such as the Extra Trees Regressor and a neural network model, the ensemble model can leverage the strengths of each individual model while mitigating their weaknesses.

The stacking ensemble approach allows the meta-learner to learn how to best combine the predictions from the base models, ultimately yielding more accurate predictions than any single model alone. This adaptability and flexibility make stacking particularly powerful in scenarios where different models excel at capturing different aspects of the underlying data patterns.

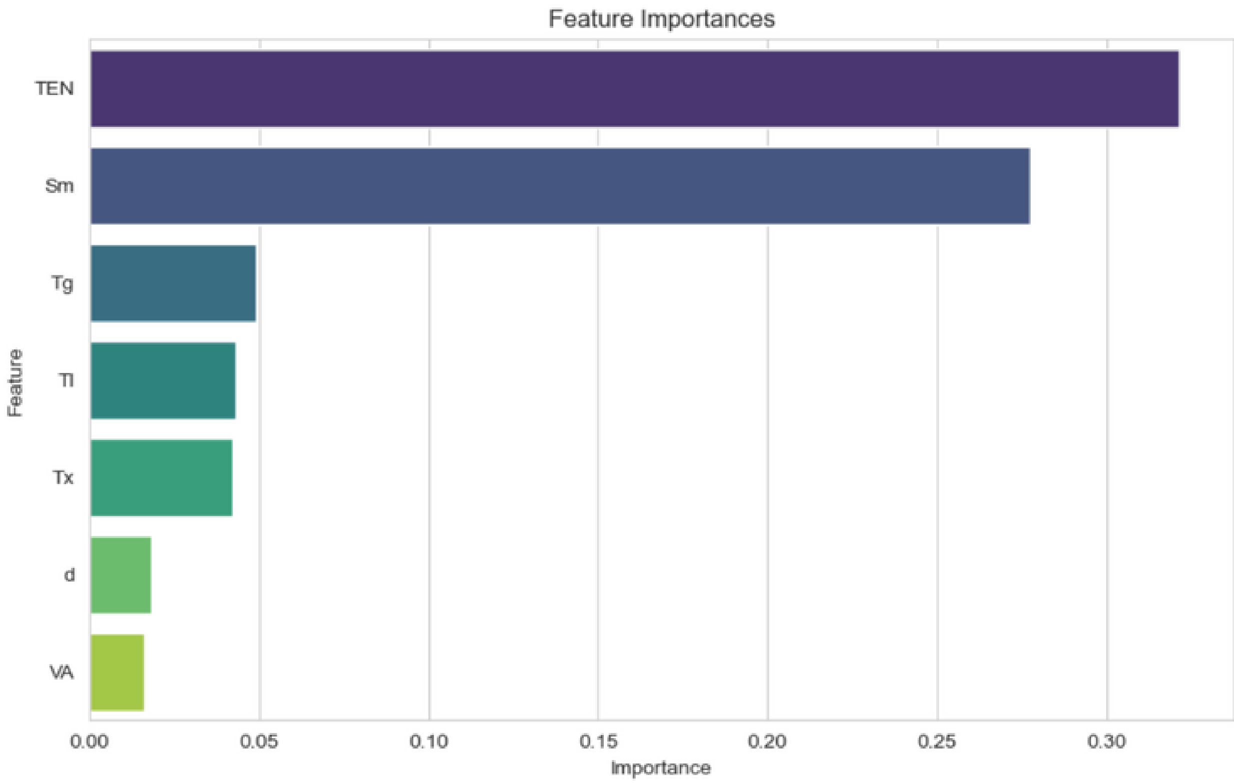
Additionally, the use of cross-validation ensures robust evaluation of the stacking ensemble's performance across multiple folds of the data, reducing the risk of overfitting and providing a more reliable estimate of its generalization ability.

Overall, the achieved average R-squared score underscores the utility of ensemble learning techniques like stacking in enhancing predictive performance and underscores their value in practical machine learning applications.

FINAL SCORE

Standard Deviation of R2-Scores= 0.0664 (6.64%)

FEATURE IMPORTANCE



We used the Extra Trees regressor model to find out which thermodynamic variable had the maximum impact on the value of the Dmax. From the results, it has been inferred that the TEN is the variable having the maximum impact.

Reported Feature Importances

```
TEN: 0.32145259891661354
Sm: 0.27733694579269214
Tg: 0.04933094853830799
Tl: 0.04303414345866305б
Tx: 0.04238178693647974
d: 0.018179925151822762
VA: 0.016201226533786042
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EVALUATING SOME OTHER PARAMETERS

Glass forming ability (GFA) is defined as the ease of vitrification for a material. In the case of cooling from liquid state, a higher GFA suggests a lower critical cooling rate and a higher section thickness for the glass. There has been extensive research to identify alloys with higher GFA with the help of various parameters. In the case of cooling from liquid state, a higher GFA suggests a lower critical cooling rate and a higher section thickness for the glass.

Several parameters [reference 1] have been defined with different combinations of the critical temperatures of the alloy. The parameters are reduced values/functions of Tx, Tl,Tg which help to show a better dependency of GFA on these criteria.

Parameters

$T_{rg} = T_g/T_l$
ΔTx = Tl-Tx
α *parameter* = T_x/T_l
β_1 *parameter* = $T_x/T_g + T_g/T_l$
β_2 *parameter* = $(T_xT_g)/(T_x + T_l)^2$
δ *parameter* = $T_x/(T_l - T_g)$
ϕ *parameter* = $\Delta T_{rg}(T_xT_g)^{0.143}$
ω *parameter* = $(T_l*(T_l + T_x)/(T_x*(T_l - T_x))$
γ_c *parameter* = $(3T_x - 2T_g)/(T_l)$

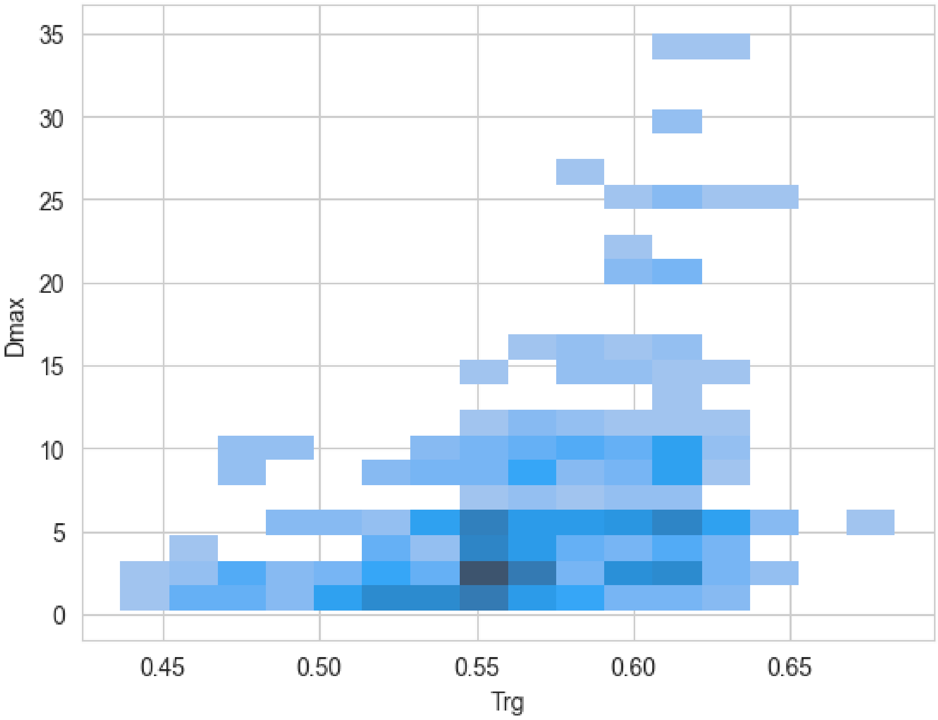
We have analysed the first two parameters.

T_{rg} : Turnbull[3] has first shown that the ease of formation of glass can relate to critical temperatures of the glass. It has been observed that the higher the T_g and the lower the T_l of a glassy alloy, the better is its GFA. Since GFA α T_g and GFA α $1/T_l$, a combination of these two produces GFA / $T_g/T_l(T_{rg})$. It has been shown that, if$T_{rg} > 0.6$, the alloy can be considered to have higher GFA.

ΔTx :It has been shown that the tendency of devitrification increases with the decrease in T_x, i.e. the higher the T_x, the more is the chance of a glassy alloy to retain its amorphous nature. Thus, the range of stability of a glass is from T_g to T_x. Inoue proposed that the GFA can be correlated to the glass stability range, i.e.T_x - T_g, which has been termed as ΔTx. A larger ΔTx indicates higher GFA.

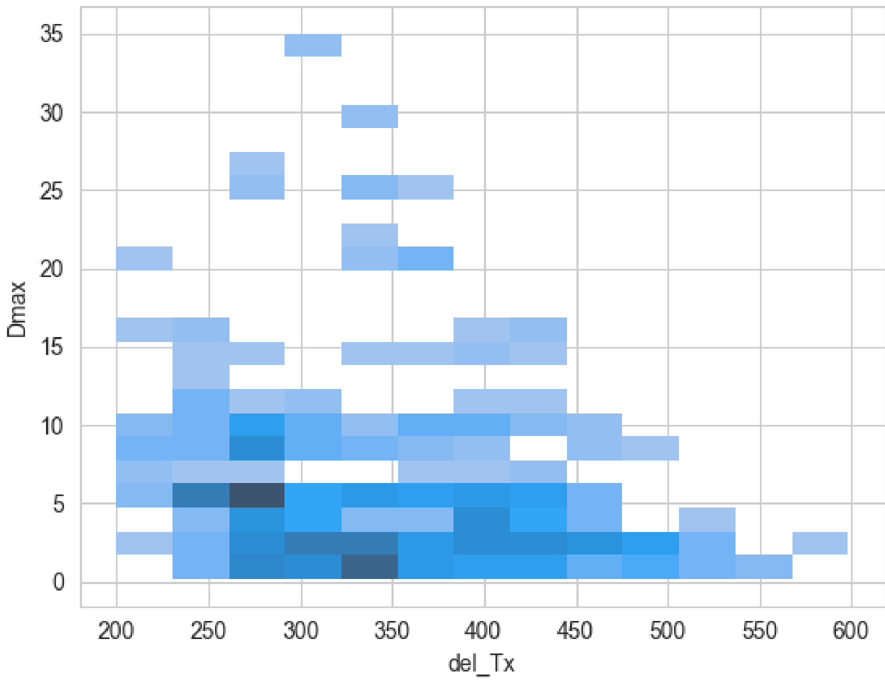
SOME OTHER PARAMETERS

We know, higher Dmax values indicate higher GFA.



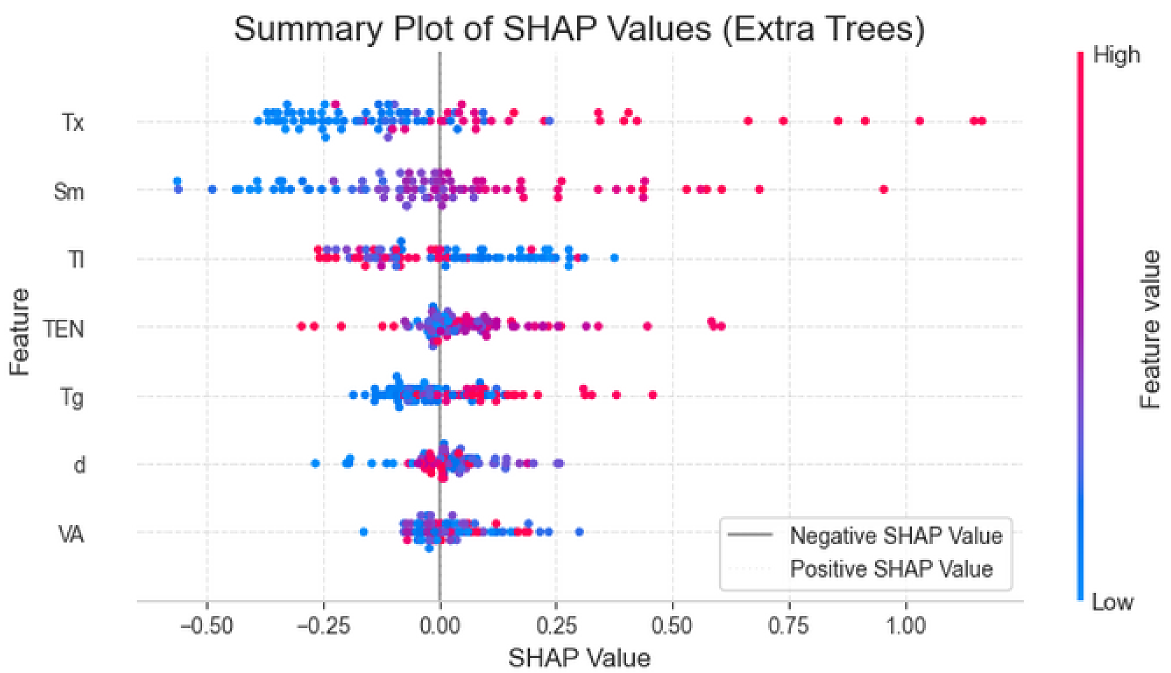
We can see, as Dmax increases ie GFA increases, the Trg value also tends to be larger than 0.6. This is in line with the expected prediction of Trg.

With the increase in value of Dmax ie increasing GFA, the values of tend to be higher as well, as expected from predictions.



Hence, our models are **in line** with the study [reference 1].

USE OF SHAP VALUES



1. **Magnitude of SHAP Values**:
   - The magnitude of SHAP values indicates the impact of a feature on the model's prediction for a specific instance.
   - Large positive SHAP values indicate that the feature pushes the prediction higher, whil large negative SHAP values indicate the opposite.
   - Features with SHAP values close to zero have little impact on the prediction.
2. **Direction of Impact**:
   - Positive SHAP values indicate that the feature contributes to increasing the prediction.
   - Negative SHAP values indicate that the feature contributes to decreasing the prediction.
3. **Feature Importance**:
   - Features with consistently large SHAP values across multiple instances are considered important for the model's predictions.
   - Conversely, features with SHAP values close to zero or fluctuating around zero may have less importance.
4. **Interaction Effects**:
   - SHAP values can also reveal interaction effects between features. For example, if the SHAP value of one feature changes depending on the value of another feature, it suggests an interaction between the two features.
5. **Global vs. Local Importance**:
   - Global SHAP values provide an overall understanding of feature importance across all instances in the dataset.
   - Local SHAP values are specific to individual instances and provide insights into why a particular prediction was made for that instance.
6. **Consistency of Impact**:
   - It's essential to assess the consistency of a feature's impact across different instances. Features with inconsistent impacts may indicate model instability or noise in the data.
7. **Model Interpretability**:
   - SHAP values can help make complex models interpretable by providing insights into the contribution of each feature to individual predictions.

REFERENCES

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