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Hyperparameter Importance: Rethinking Bias-Variance with Meta-features

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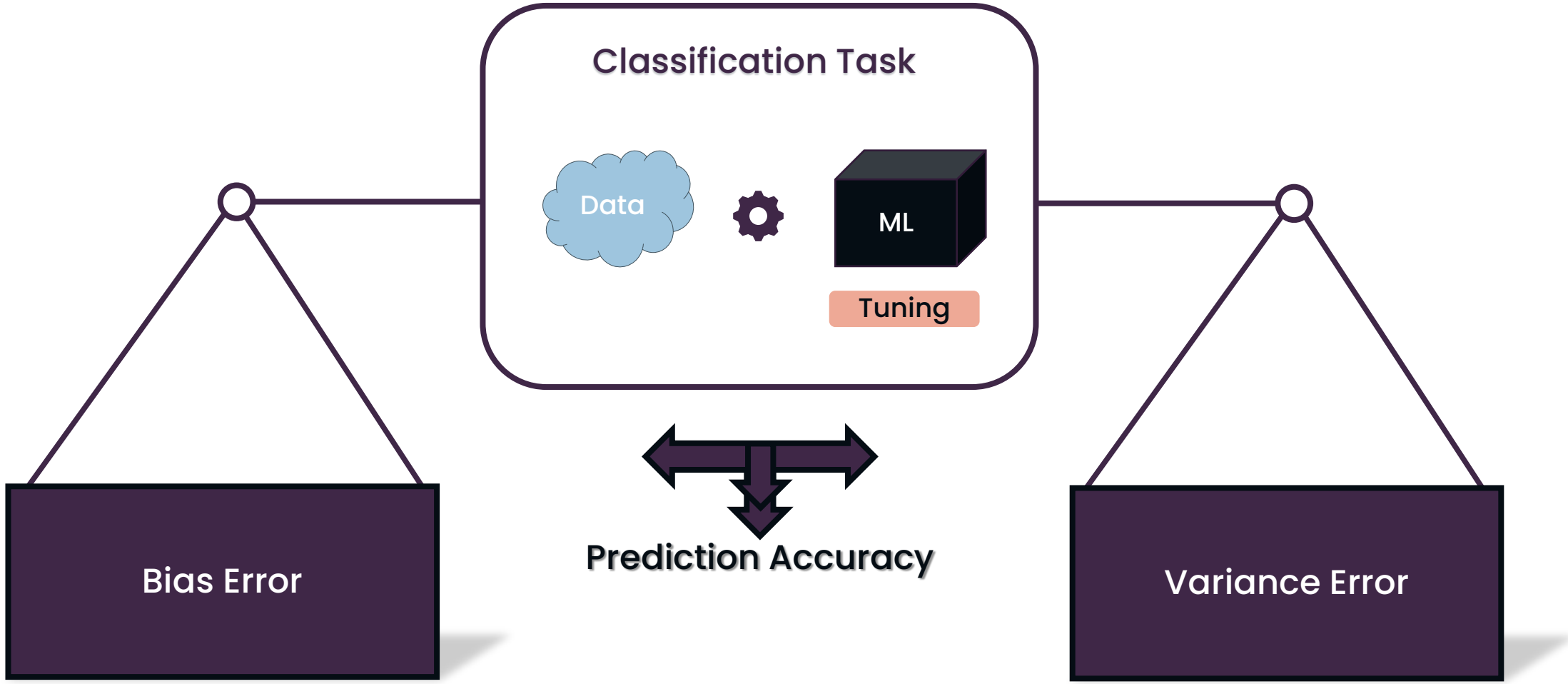
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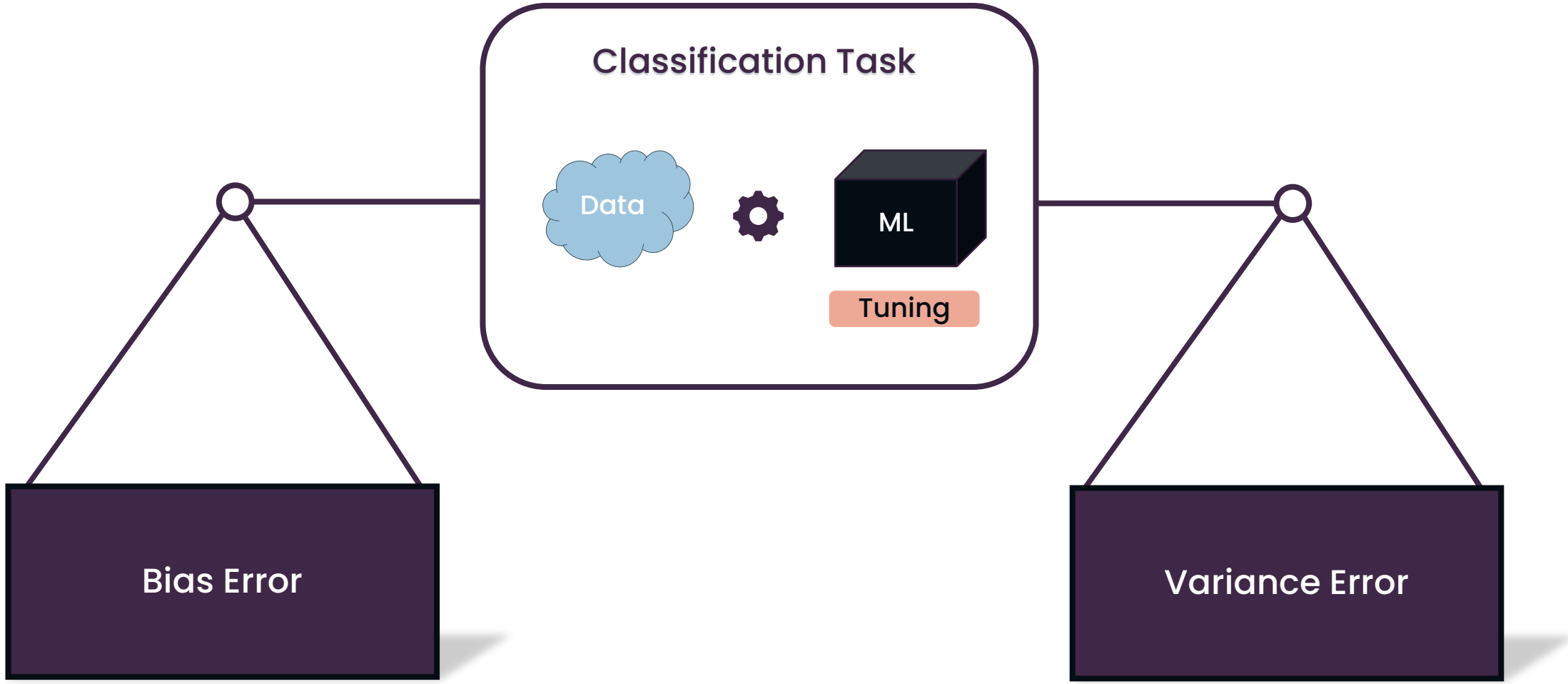
Tuning
Bias Error
Prediction Accuracy
Variance Error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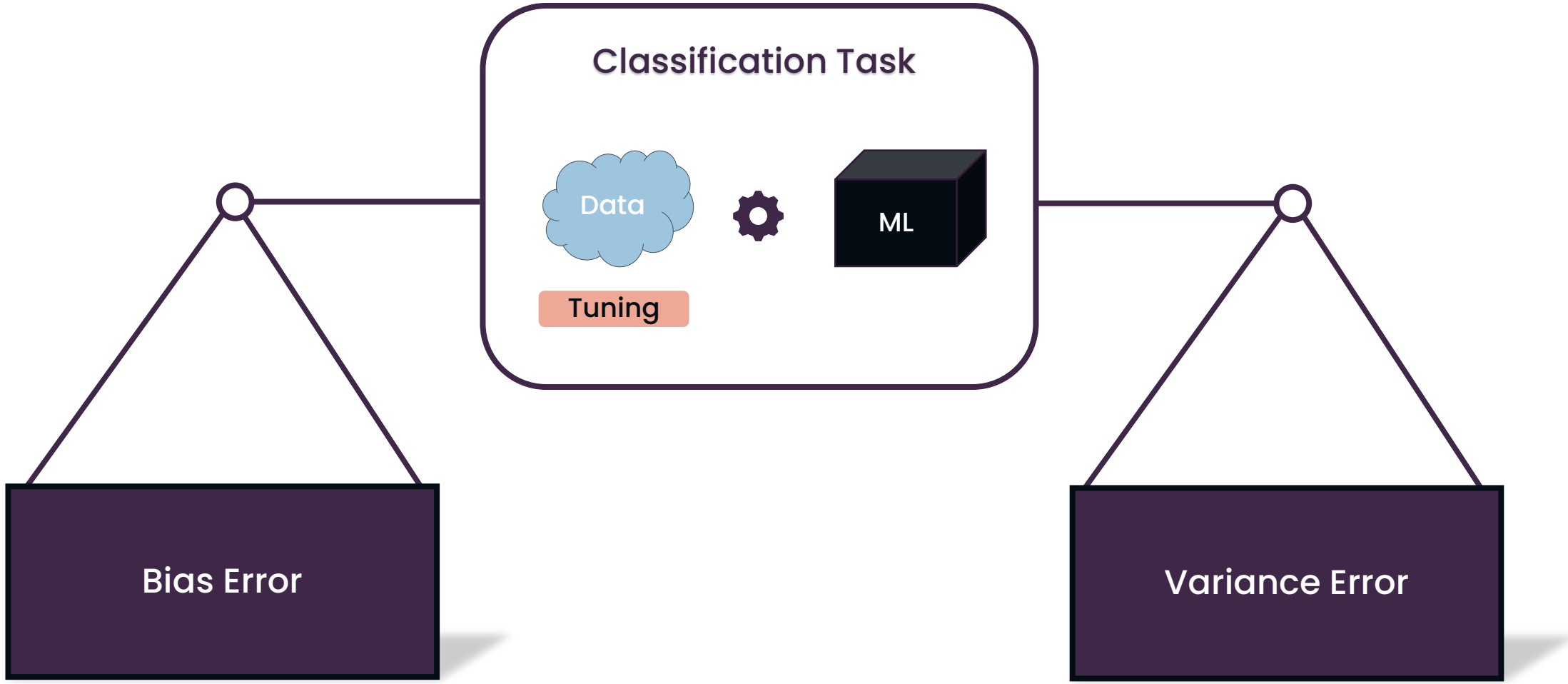
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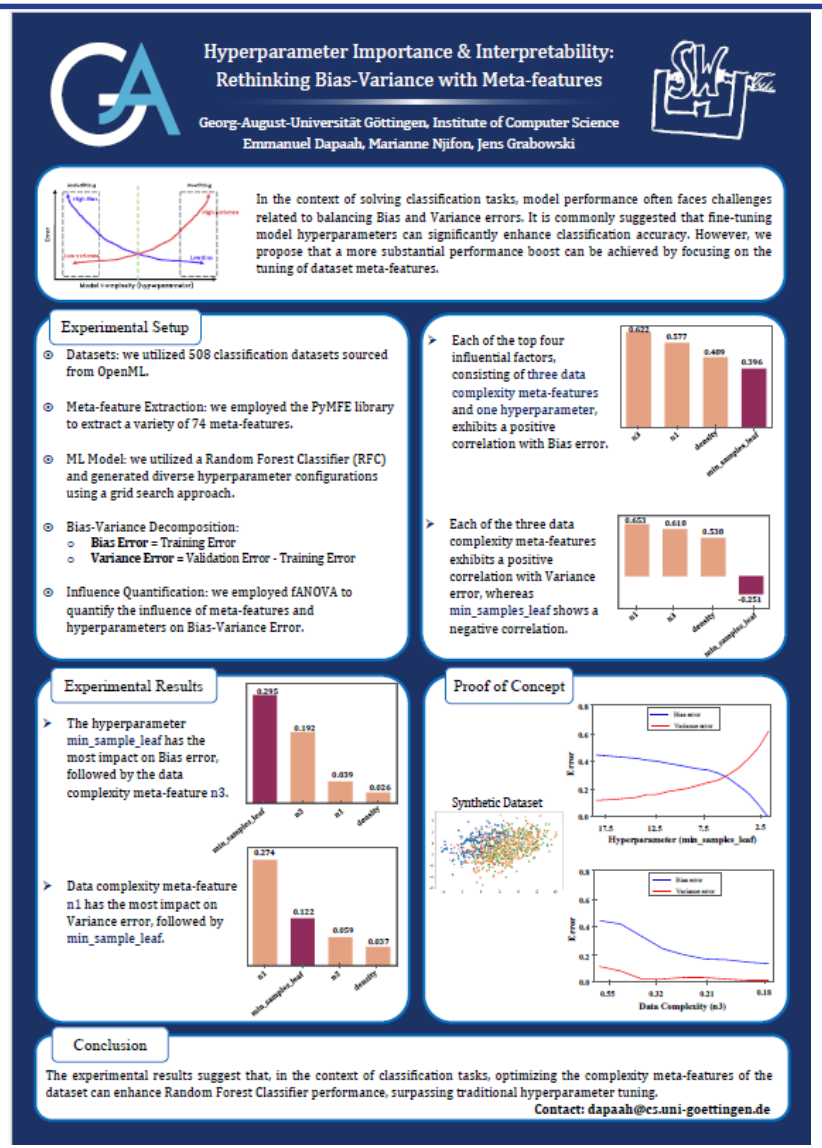

Hyperparameter Importance & Interpretability: Rethinking Bias-Variance with Meta-features

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In the context of solving classification tasks, model performance often faces challenges related to balancing Bias and Variance errors. It is commonly suggested that fine-tuning model hyperparameters can significantly enhance classification accuracy. However, we propose that a more substantial performance boost can be achieved by focusing on the tuning of dataset meta-features.

Experimental Setup

- Datasets: we utilized 508 classification datasets sourced from OpenML.
- Meta-feature Extraction: we employed the PyMFE library to extract a variety of 74 meta-features.
- ML Model: we utilized a Random Forest Classifier (RFC) and generated diverse hyperparameter configurations using a grid search approach.
- Bias-Variance Decomposition:
  - **Bias Error** = Training Error
  - **Variance Error** = Validation Error - Training Error
- Influence Quantification: we employed fANOVA to quantify the influence of meta-features and hyperparameters on Bias-Variance Error.

- Each of the top four influential factors, consisting of three data complexity meta-features and one hyperparameter, exhibits a positive correlation with Bias error.

- Each of the three data complexity meta-features exhibits a positive correlation with Variance error, whereas min_samples_leaf shows a negative correlation.

Experimental Results

- The hyperparameter min_sample_leaf has the most impact on Bias error, followed by the data complexity meta-feature n3.

- Data complexity meta-feature n1 has the most impact on Variance error, followed by min_sample_leaf.

Proof of Concept

Synthetic Dataset

Conclusion

The experimental results suggest that, in the context of classification tasks, optimizing the complexity meta-features of the dataset can enhance Random Forest Classifier performance, surpassing traditional hyperparameter tuning.

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