Vomitoxin Prediction from Spectral Data: Analysis Report

1. Preprocessing Steps and Rationale

Data Standardization

- Standard Scaling: Applied to normalize the spectral bands, ensuring all features contribute equally to the model regardless of their original scale.
- Rationale: Spectral data typically varies across different wavelengths, and standardization prevents features with larger magnitudes from dominating the model training process.

Target Variable Treatment

- Distribution Analysis: Initial analysis revealed a skewed distribution of the vomitoxin_ppb variable.
- Log Transformation: Applied log transformation (np.log1p) to address the skewness and make the target distribution more normal.
- Outlier Handling:
    - Identified outliers using IQR (Interquartile Range) and Z-score methods
    - Applied capping at 1st and 99th percentiles to mitigate outlier influence without removing data points
    - Implemented Robust Scaling to further reduce sensitivity to extreme values
- Rationale: These treatments improve model performance by creating a more balanced target distribution that better satisfies regression model assumptions.

Feature Engineering

- Label Encoding: Applied to transform categorical 'hsi_id' values into numerical representations.
- Rationale: Converting text-based identifiers into numerical values allows machine learning algorithms to process this information.

2. Insights from Dimensionality Reduction

Principal Component Analysis (PCA)

- Implementation: Reduced the high-dimensional spectral data to 2 principal components for visualization.
- Visualization: The PCA scatter plot revealed patterns in the data with color coding based on vomitoxin levels.
- Insights:
    - The data points showed some clustering patterns related to vomitoxin levels
    - This suggests that the spectral data contains meaningful information for predicting vomitoxin concentration
    - The visualization helped identify potential structure in the high-dimensional spectral space

3. Model Selection, Training, and Evaluation

Model Selection

Three regression models were evaluated:

- Random Forest Regressor: Ensemble method using multiple decision trees
- Gradient Boosting Regressor: Sequential ensemble technique building trees to correct errors
- XGBoost Regressor: Optimized implementation of gradient boosting

Hyperparameter Optimization

- Grid Search Cross Validation: Implemented to systematically explore hyperparameter combinations
- Parameters Tuned:
    - Tree count (n_estimators): [100, 200]
    - Tree depth (max_depth): Various options per model
    - Learning rate: [0.01, 0.1] for boosting models
    - Minimum samples parameters for tree construction

Evaluation Metrics

Models were assessed using:

- Root Mean Squared Error (RMSE): Measure of prediction error magnitude
- Mean Absolute Error (MAE): Average absolute differences between predictions and actual values
- R^2 Score: Proportion of variance explained by the model

4. Key Findings and Suggestions for Improvement

Performance Comparison

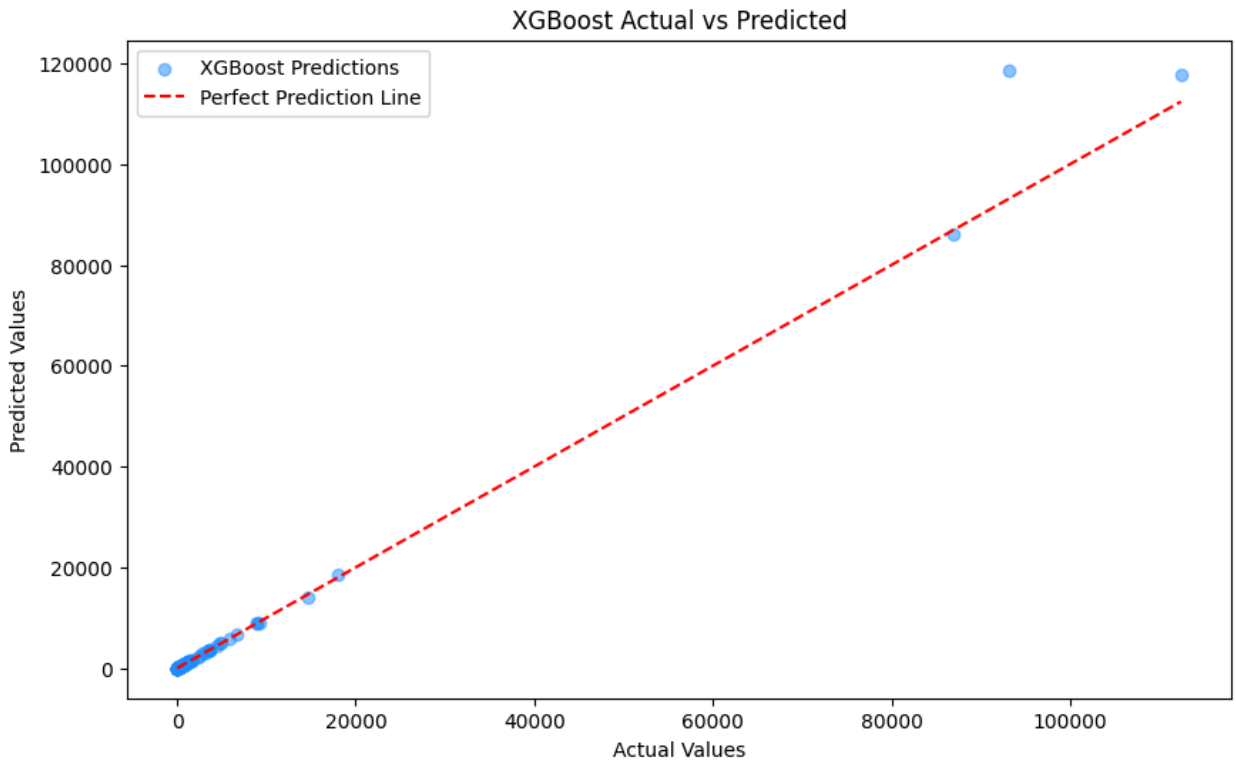
- Based on the model training results, the XGBoost model demonstrated the best overall performance with:
    - Higher R^2 score
    - Lower prediction errors (RMSE and MAE)
    - Better prediction alignment in actual vs. predicted plots

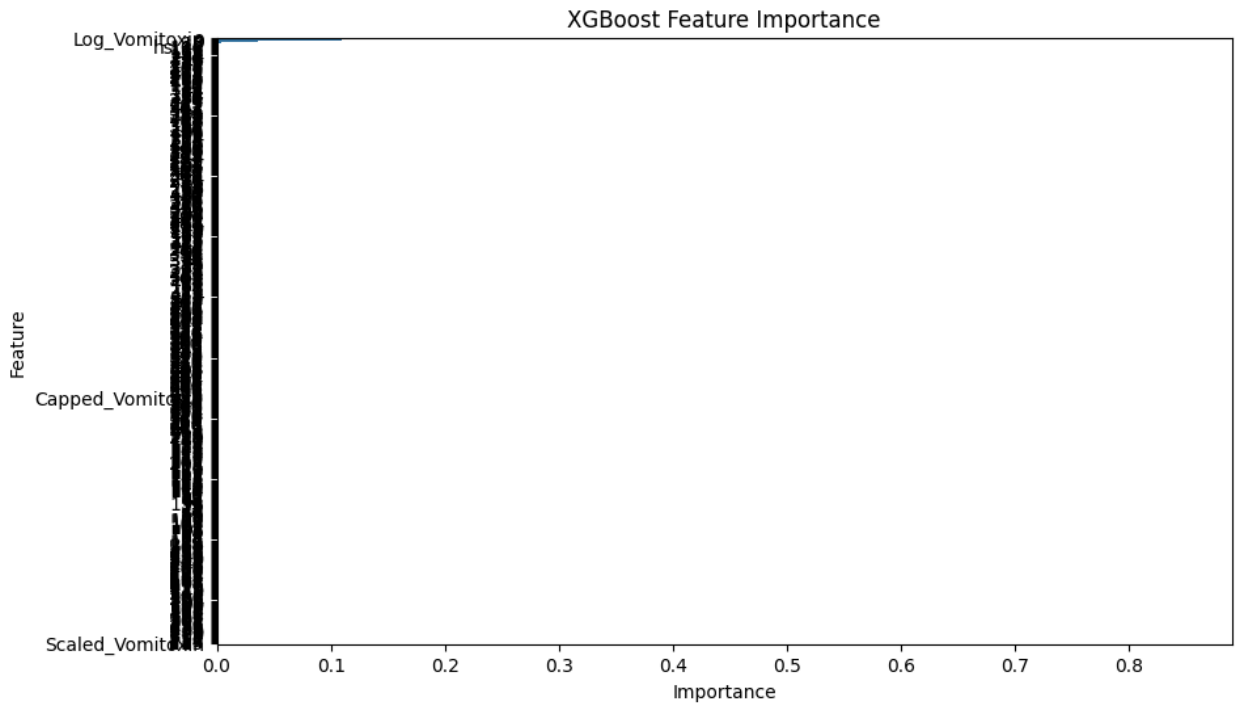
Feature Importance

- Analysis of feature importance across models revealed specific spectral bands that consistently contribute to vomitoxin prediction.
- These high-importance wavelengths could be prioritized in future data collection or analysis.

Results and Discussion (Graph):

Model	RMSE	MAE	R Squared
XGBoost	2612.54	350.33	0.9756
Gradient Boosting	3170.04	391.03	0.9641
Random Forest	2198.96	256.76	0.9827
Attention Model	17318.59	—	-0.0722
Transformer Model	17291.26	—	-0.0692




XGBoost Feature Importance
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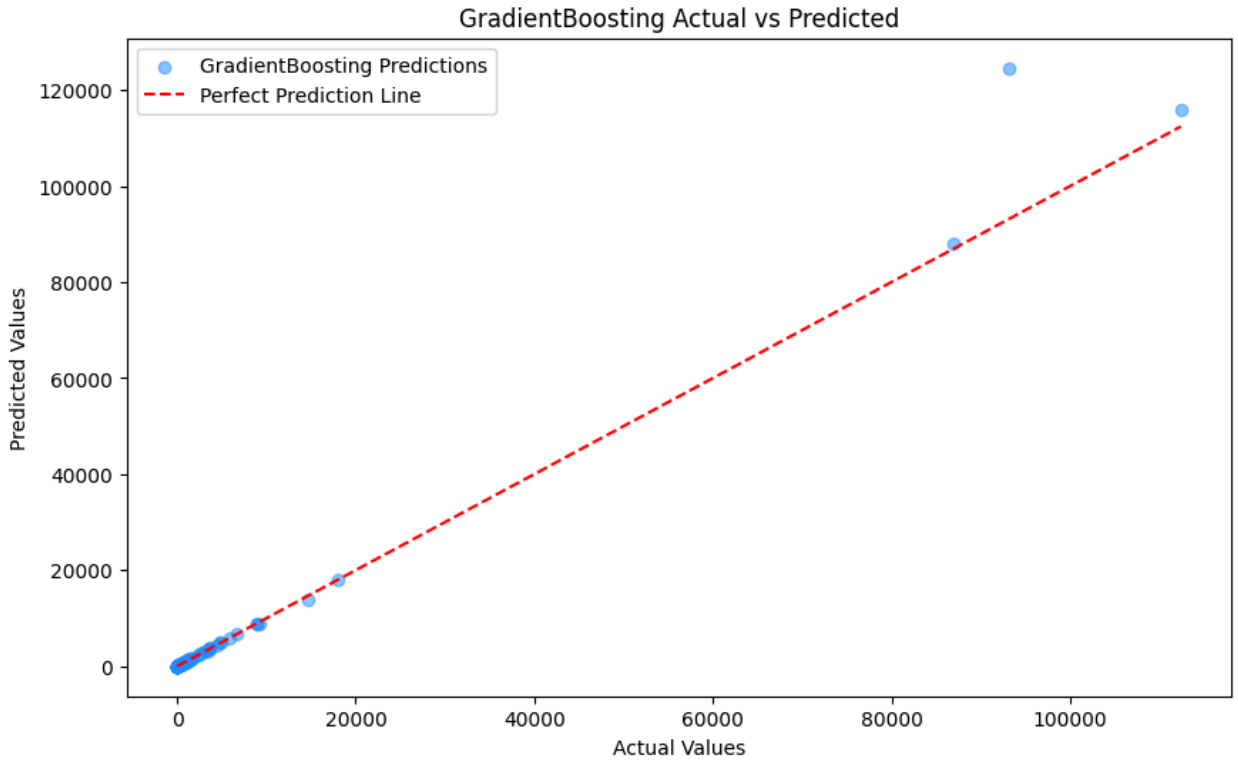
GradientBoosting Actual vs Predicted
GradientBoosting Predictions
Perfect Prediction Line
Predicted Values
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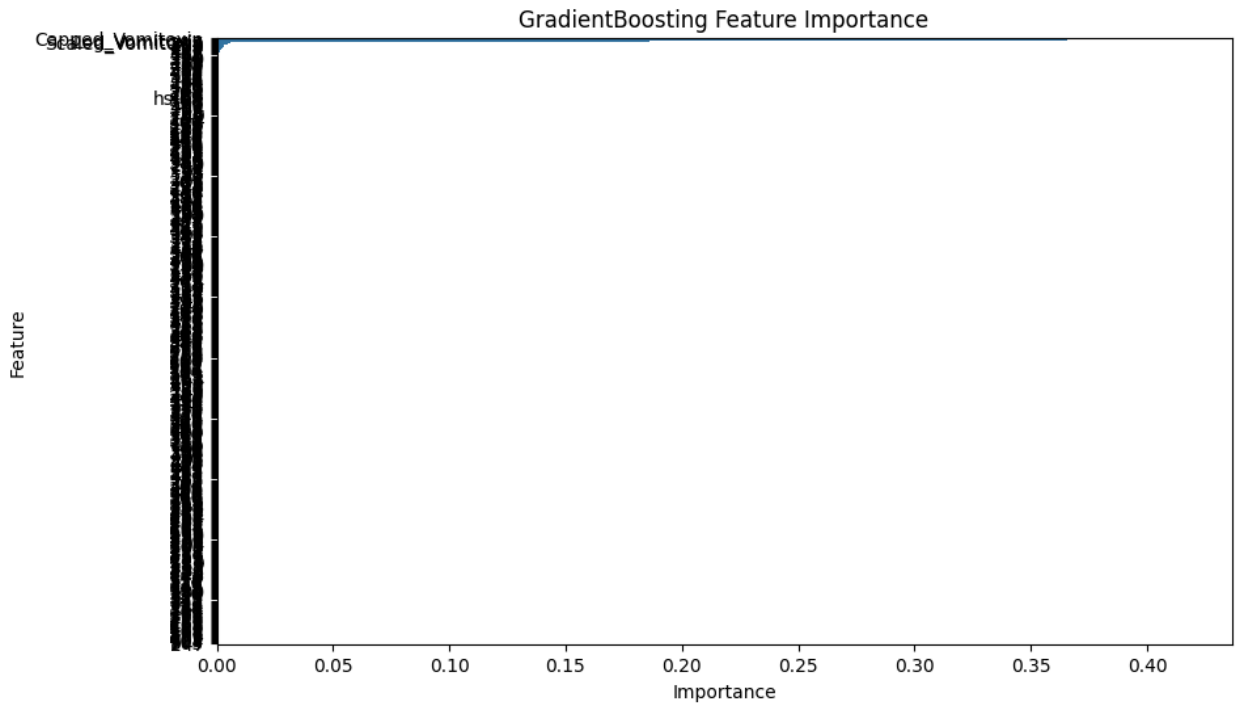
GradientBoosting Feature Importance
Feature
Importance
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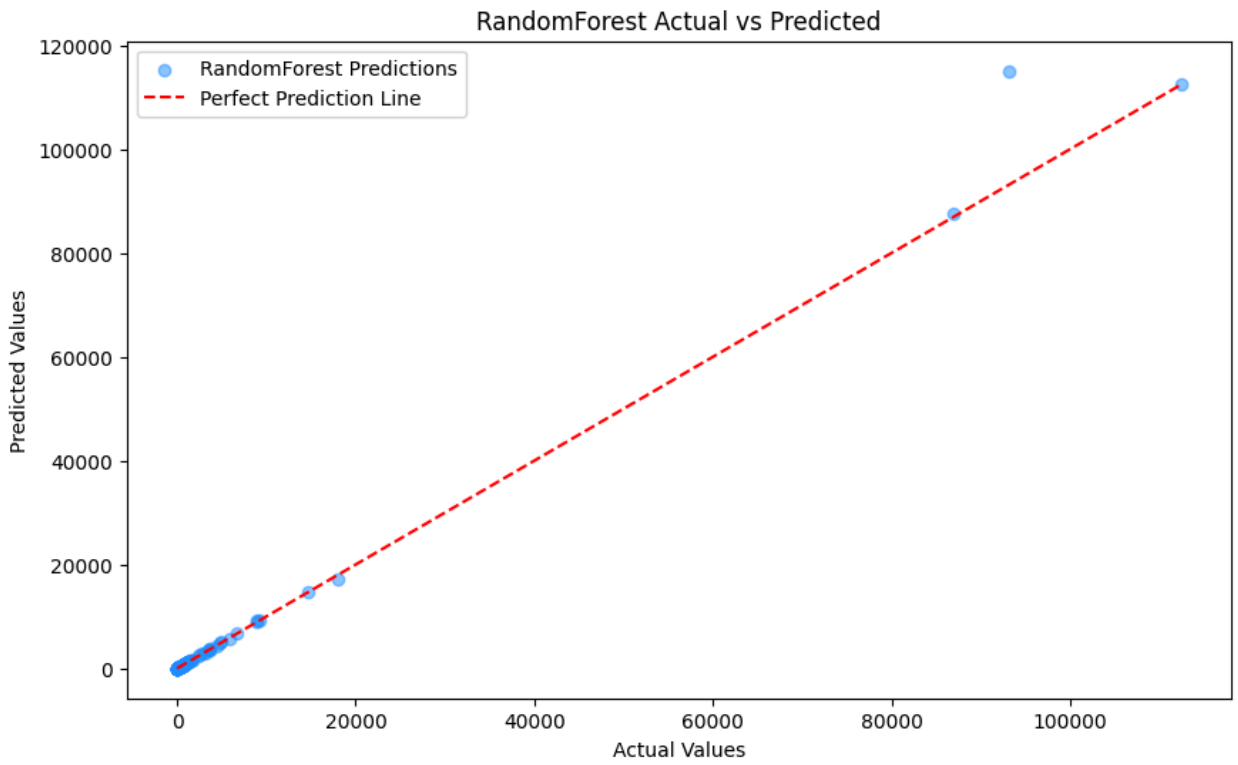

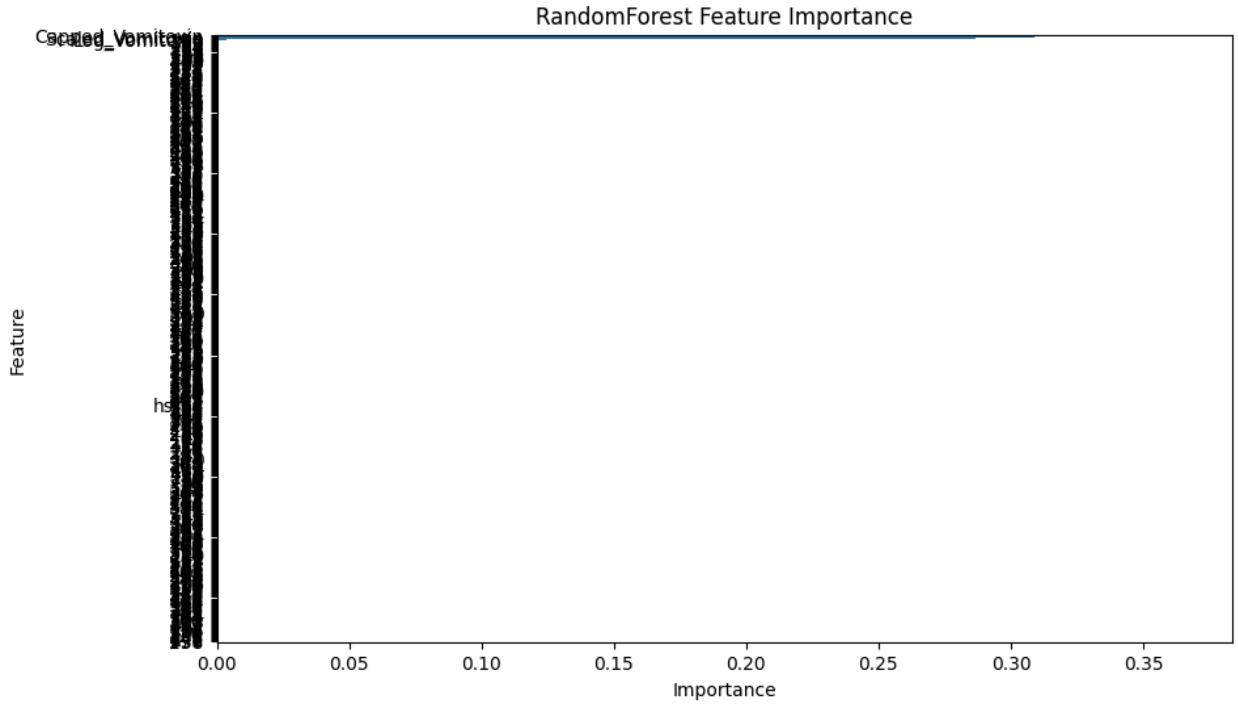

Discussion about Attention and Transformer Model

Attention and transformer models are underperforming. we might have to fine-tune the architecture or hyperparameters for better results