species Score Prediction - Algorithm Comparison with Composite Scoring (80-20 Split)

# Experiment Overview

This document summarizes the results of 5 machine learning algorithms for predicting species Score. Each algorithm was trained on normalized data and tuned using 5-fold cross-validation with a focus on minimizing RMSE (Root Mean Square Error). Predictions were denormalized before evaluation on a held-out test set.  
  
Data was split into 80% training and 20% testing.  
  
\*\*Hyperparameter Optimization:\*\* Parameter grids were optimized to focus on the most effective ranges, balancing comprehensive search with computational efficiency.  
  
\*\*NEW: Composite Scoring Method\*\*  
The best model is selected using a composite score that considers both R² (higher is better) and RMSE (lower is better). Both metrics are normalized to 0-1 scale and combined with equal weights (50% each) to create a comprehensive performance measure.

# Algorithm Performance Comparison (Sorted by Composite Score)

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Algorithm | Composite Score | Test R² | Test RMSE | Test MAE | Rank |
| Random Forest | 1.0000 | 0.9560 | 0.1870 | 0.0880 | 1 |
| XGBoost | 0.4840 | 0.9479 | 0.2036 | 0.0710 | 2 |
| K-Nearest Neighbors | 0.1117 | 0.9419 | 0.2151 | 0.0952 | 3 |
| Support Vector Machine | 0.0112 | 0.9402 | 0.2181 | 0.1492 | 4 |
| Neural Network | 0.0000 | 0.9400 | 0.2185 | 0.1605 | 5 |

# Feature Importance Analysis

Feature importance was calculated using a model-agnostic permutation-based approach. This method measures how much model performance decreases when each feature is randomly shuffled. The importance values are normalized to percentages that sum to 100% for each model, making it easy to interpret the relative contribution of each feature.

# Recommendation

The algorithm with the highest Composite Score (considering both R² and RMSE) was Random Forest with:  
Composite Score: 1.0000  
Test R²: 0.9560  
Test RMSE: 0.1870  
Test MAE: 0.0880  
  
This selection balances both predictive accuracy (R²) and prediction precision (RMSE), providing the most comprehensive model performance.