

Applying Explainable AI to Understand How Stellar and Planetary Parameters Impact Exoplanet Habitability

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Abstract

The study of exoplanet habitability has been an active research area in astrophysics, with the ultimate goal of finding a suitable second home for humanity. As the massive amount of exoplanetary data continues to grow, machine learning has been increasingly adopted to predict exoplanet habitability. This research applied explainable AI on exoplanet habitability studies, not only predicting habitability, but also interpreting the models to understand prediction reasoning. High-quality tree-based models, specifically a Random Forest and an XGBoost, were trained to predict habitability based on combined exoplanet data joined from the NASA Exoplanet Archive and the Habitable World Catalog, PHL @ UPR Arecibo. Additionally, SHAP (SHapley Additive exPlanations), an explainable machine learning technique, was applied to interpret the models, identifying the most influential stellar and planetary parameters for habitability, including stellar radius, stellar effective temperature, stellar mass, planet radius, and planet orbit semi-major axis. Furthermore, SHAP analysis quantitatively revealed how high or low values of these parameters move an exoplanet towards or away from habitability, offering an insight on how these parameters impact exoplanet habitability. Finally, these SHAP analysis results were cross-validated with direct observations in the raw dataset. This research sets a foundation for more in-depth analysis and study of exoplanet habitability through explainable AI. The findings of this study can be used by scientists in aiding the design of next-generation telescopes and guiding exoplanet searches to focus on only the most promising candidates, accelerating the search of habitable worlds so that we might be able to find a second Earth within our lifespans.

1 | Introduction

The search and discovery of potentially habitable exoplanets beyond our solar system has been an active research field in the past decade. Thousands of exoplanets have been discovered and confirmed, and this number continues to grow with enhanced observational technologies and capabilities. To study exoplanet habitability through this ever-growing exoplanet dataset, machine learning has been increasingly adopted in the community. Saha et al. (2018) [1] trained an XGBoost [2] model based on the dataset from PHL @ UPR Arecibo [3] to predict exoplanet habitability. The model was evaluated against Proxima b and the TRAPPIST-1 system. Ghadekar et al. (2024) [4] applied causal learning to learn the most influential factors in the dataset and trained a Recurrent Neural Network (RNN) model and a Long Short-Term Memory (LSTM) model for habitability classification. Basak et al. (2021) [5] built a novel neural network model for the task of exoplanet habitability classification.

In this study, a Random Forest [6] classifier and an XGBoost [2] classifier were trained based on combined data from the NASA Exoplanet Archive [7] and the Habitable Worlds Catalog (HWC), PHL @ UPR Arecibo [3] to predict exoplanet habitability with high precision. These decision tree-based models were chosen since their underlying machine learning libraries (sklearn for Random Forest and xgboost for XGBoost) expose the importance of each feature's contribution to the model's predictions, providing insights for identifying the most influential stellar and planetary parameters to exoplanet habitability. Another reason that decision tree-based models were chosen in this study is that they fit the datasets well. The data used in this study consisted entirely of tabular datasets. Several recent studies in machine learning found that tree-based models often outperform deep learning models on tabular data. Grinsztajn et al. (2022) [8] evaluated the performance of three tree-based models (Random Forest, Gradient Boosting Trees, and XGBoost) against 45 tabular datasets from various domains and compared the performance with three deep learning models (MLP, Resnet, and FT_Transformer). They found that for tabular data, tree-based models tend to yield good predictions more easily compared to the deep learning models with much less computational cost, and in general outperform deep learning models. Additionally, Shwartz-Ziv et al. (2022) [9] compared the XGBoost model performance on 11 tabular datasets against several deep learning models and reached similar conclusions.

Understanding why models make certain predictions can be as important as building models with high performance, and is an underexplored facet of exoplanet habitability analysis. Lundberg et al. (2017) [10] presented SHAP (SHapley Additive exPlanations), a unified framework for intercepting model predictions based on cooperative game theory. SHAP has been extensively used in other fields, such as healthcare, computer vision, and finance, to much success. In this study, SHAP was leveraged through an astrophysical lens to understand features' impact on the model outputs, and how their different values contribute towards either habitable or non-habitable prediction outcomes.

While machine learning has been applied in many previous research works to study exoplanet habitability, much of such work has focused on analysis of the datasets and constructing high-quality machine learning models with different model architectures and techniques. This work distinguishes itself by leveraging SHAP to understand the stellar and planetary parameters' influence on exoplanet habitability, not only identifying the most influential parameters, but also providing insightful information on how different values of these parameters lead the model prediction output toward either positive (habitable) or negative (non-habitable) outcomes. This study provides insight on the most influential stellar and planetary parameters to exoplanet habitability through the lens of explainable machine learning.

The remainder of this paper is structured as follows: In Section 2, the methodology of the study is described in detail, including the data sources of the study, the data preprocessing, and feature engineering, followed by the detailed information of the model training. The steps of data preprocessing and feature engineering are discussed in detail, covering data cleaning, missing value handling, imbalanced dataset handling through a combination of oversampling and undersampling, and data correlation analysis to identify and remove redundant data fields. Section 3 presents the Random Forest and XGBoost models' evaluation results, followed by feature importance analysis on both models. SHAP results are also presented with detailed analysis on how different feature values influence model prediction outcomes, and cross-validated against direct observations from the raw dataset. Finally, Section 4 concludes this study with a summarization of findings.

2 | Methods

2.1 | Data Sources

The primary dataset of this study was downloaded from the Planetary Systems Composite Data at the NASA Exoplanet Archive [7] as of 04 October 2025, which contains a compilation of system, stellar, and planetary parameters of 6,022 confirmed exoplanets. Each of these exoplanets comes with 172 data fields, resulting in a dataset with over 1.03 million data fields. This dataset was joined with data from the Habitable Worlds Catalog (HWC), PHL @ UPR Arecibo [3]. The HWC dataset contains 5,599 exoplanets as of 04 October 2025, with a *P_HABITABLE* data field to indicate the habitability status for each exoplanet based on the research community's aggregated consensus. *P_HABITABLE* = 1 indicates conservative habitable (more likely a rocky planet with surface liquid water) and *P_HABITABLE* = 2 indicates optimistic habitable (might include water worlds or mini-Neptunes), while *P_HABITABLE* = 0 indicates non-habitable. After joining the datasets, the *P_HABITABLE* data field was used to mark the labels in the dataset for supervised machine learning model training. Exoplanets with *P_HABITABLE* = 1 or 2 were labeled as positive samples (habitable) and ones with *P_HABITABLE* = 0 were labeled as

negative samples (non-habitable). Through this process, 57 exoplanets in the dataset were labeled as habitable, while the remaining 4,987 were labeled as non-habitable.

2.2 | Data Preprocessing

The Planetary Systems Composite Data from the NASA Exoplanet Archive contains a *pl_controv_flag* data field that indicates whether the existence of an exoplanet has ever been questioned in the published literature. The first step of data preprocessing was to filter out any exoplanets with *pl_controv_flag* equaling 1 so the model training and analysis were based on confirmed exoplanets without question. Then, the dataset was limited to only planetary systems with a single host star in order to reduce complexity due to stellar multiplicity. Afterwards, the data fields that were irrelevant to model training were removed from the dataset, for instance, *pl_name* (planet name), *disc_year* (planet discovery year), etc.

Some of the data fields in the dataset were missing values. The percentage of missing value for each data field was computed. Then any data fields with more than 23% values missing were removed from the dataset. Afterwards, one-hot encoding was applied to the remaining categorical data fields to convert them into numerical values.

The next step involved dealing with highly-correlated data fields in the dataset. These redundant data fields do not bring in additional information, instead, they cause unnecessary complexity and introduce the risk of degrading model performance. Furthermore, removing redundant data fields is beneficial to obtaining reliable and interpretable feature importance analysis for the tree-based models. To handle this, data correlation analysis was applied on the dataset to identify highly-correlated data fields and remove redundant fields. Figure 1 shows the correlation matrix of the dataset. As shown in the figure, *pl_orbper* (planet orbital period [days]), *pl_angsep* (planet angular separation [mas]), *st_lum* (stellar luminosity [$\log_{10}(\text{Solar})$]), *st_logg* (stellar surface gravity [$\log_{10}(\text{cm/s}^{**2})$]), *sy_bmag* (stellar B (Johnson) magnitude), *sy_vmag* (stellar V (Johnson) magnitude), *sy_gaiamag* (stellar Gaia magnitude), and *sy_tmag* (stellar TESS magnitude) were highly correlated with other data fields and thus removed. Eventually, seventeen data fields were left in the final dataset as the feature set for the model training.

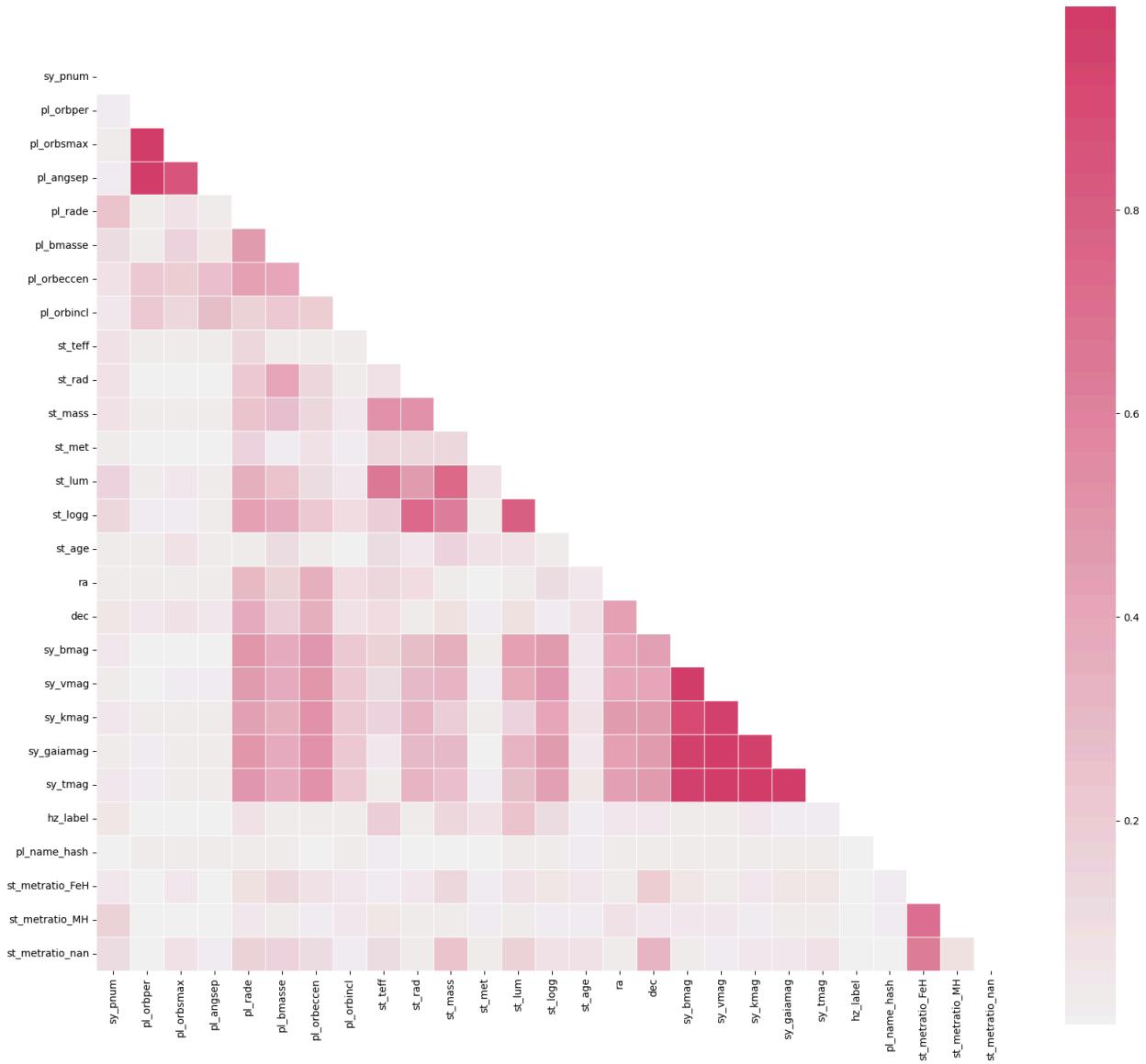


Figure 1. Correlation matrix for the dataset. Highly correlated data fields have high values in the corresponding slots in the matrix. This graph was created by the student researcher using the Seaborn library in a Google Colab notebook, 2025.

2.3 | Model Training

A Random Forest model and an XGBoost model were trained based on the dataset obtained from the process above to predict exoplanet habitability. The sklearn library was used for the Random Forest model while the xgboost library was utilized for the XGBoost model. Model training and hyperparameter tuning were implemented with Python in Google Colab notebooks and executed in Google Cloud to utilize its free computing resources.

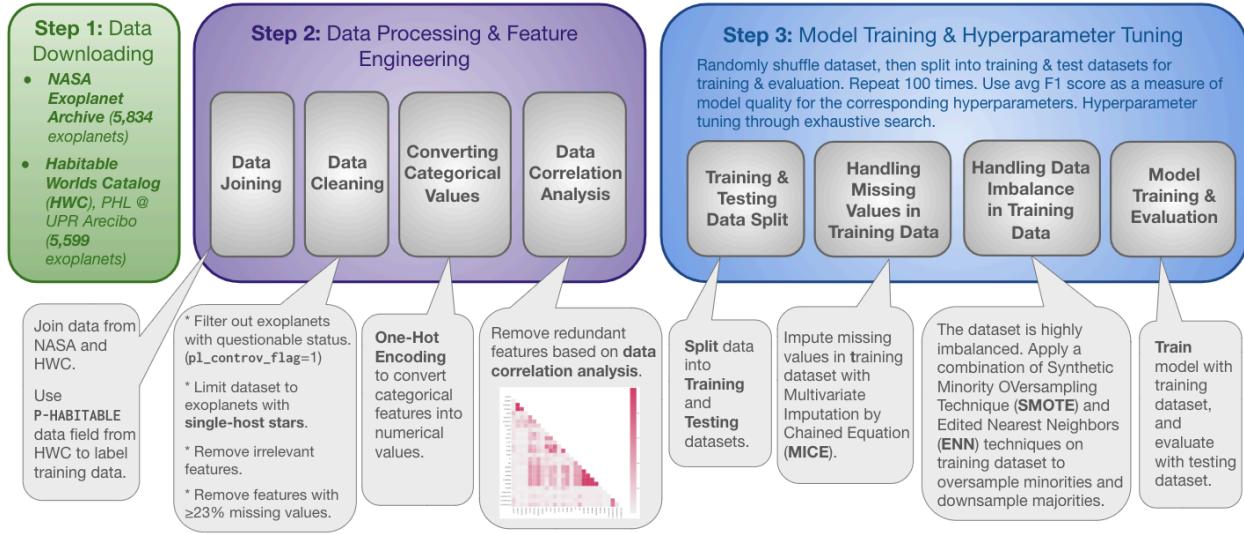


Figure 2. Data processing, feature engineering, and model training & hyperparameter tuning pipelines. This graph was created by the student researcher using Google Slides, 2025.

Figure 2 shows a comprehensive diagram illustrating the data processing, feature engineering, and model training & hyperparameter tuning pipelines. To maximize model performance, systematical exhaustive searches of optimal hyperparameter configurations were executed. One particular challenge for hyperparameter tuning was the intensive computation involved in the search due to the large search space of hyperparameter combinations. The Random Forest training and tuning process alone involved iterating through nearly 10k different hyperparameter combinations. To accelerate the tuning process, the search space was split into multiple chunks and then several training and tuning instances were executed in parallel on Google Cloud.

Within the model training and tuning processes for each hyperparameter configuration, the dataset was first randomly shuffled, then split into training and testing datasets for model training and evaluation. The split was conducted with a stratifying strategy to ensure both the training and testing datasets maintained the same ratio of positive-to-negative samples as the original dataset.

To handle missing values in the training dataset, the Multivariate Imputation by Chained Equation (MICE) technique [11] was applied to impute the missing values.

The training dataset was highly imbalanced and was dominated by negative samples (i.e., non-habitable exoplanets). The entire dataset only contained 57 positive samples (habitable), of which only 31 were allocated into the training dataset. This high data imbalance could be challenging for model training and may lead to poor model performance. To counter this problem, a combination of the Synthetic Minority Oversampling Technique (SMOTE) [12] and the Edited Nearest Neighbors (ENN)

technique were applied to oversample the minorities and undersample the majorities to balance the training dataset.

After implementing the above process, the training dataset was ready for model training. The trained model was then applied on the reserved testing dataset for model performance evaluation. Since the dataset was highly-imbalanced, the F1 score (harmonic mean of precision and recall) was chosen as the metric to evaluate the model's performance.

The above feature engineering and model training & evaluation processes were repeated for 100 rounds for each hyperparameter combination, and the average F1 score was used as the metric to represent the model's performance for the specific hyperparameter combination.

During the exhaustive search, the hyperparameter configuration resulting in the best model F1 scope was recorded and the optimal configuration was used for the model with the best performance.

3 | Results and Analysis

3.1 | Model Evaluation

Both the Random Forest and the XGBoost classifiers achieved high precisions of 0.95. Table 1 shows a further breakdown of the model performance for each classifier, including their precision, recall, and F1 score.

Table 1. Random Forest and XGBoost model evaluation results (precision, recall, F1 score). This table was created by the student researcher using Google Docs, 2025.

	Precision	Recall	F1 Score
Random Forest	0.95	0.93	0.94
XGBoost	0.95	0.90	0.93

As shown in Table 1, both the Random Forest classifier and the XGBoost classifier performed exoplanet habitability classification well, with similar model performance.

Through exhaustive hyperparameter searching, the optimal configurations for the best model performance were identified. The optimal Random Forest model achieved peak performance with 37 trees, a maximum tree depth of 15, and 17 maximum leaf nodes, alongside four other tuned hyperparameters. Meanwhile, for XGBoost, 16 trees with a maximum tree depth of 10 and 16 maximum leaves (along with three other hyperparameter settings) resulted in the best model performance.

Figure 3 visualizes an example of one of the trees from the optimal Random Forest classifier. As shown in the figure, host stellar radius is the most influential factor for this tree and thus sits at the root, followed by host stellar effective temperature, then planet orbit semi-major axis, and so on.

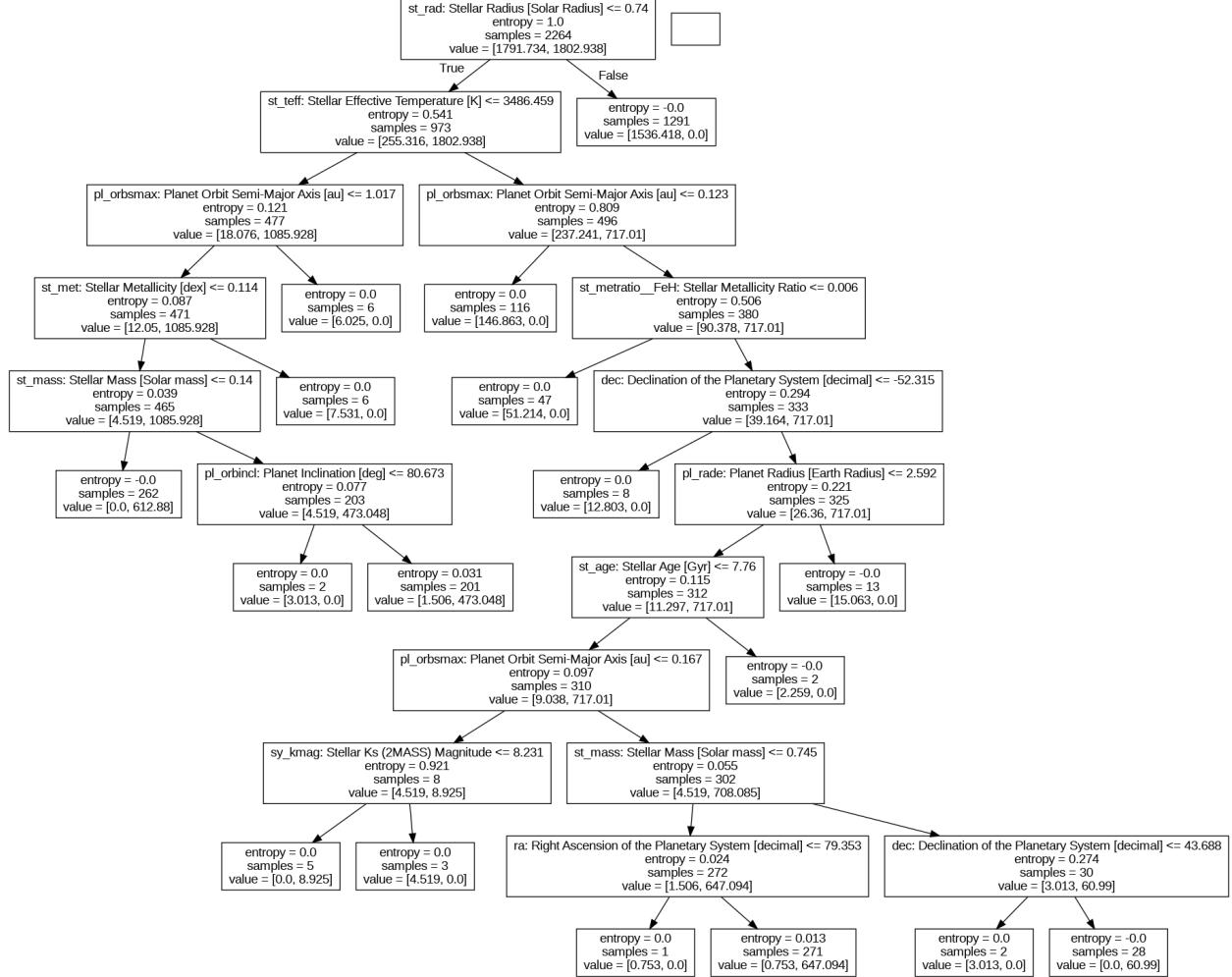


Figure 3. Example of one of trees from the optimal Random Forest classifier. This graph was created by the student researcher using the sklearn library in a Google Colab notebook, 2025.

3.2 | Feature Importance Analysis through SHAP and sklearn

The rest of this section mainly focuses on the Random Forest classifier to showcase the power of SHAP analysis in understanding model prediction and studying exoplanet habitability. SHAP analysis on XGBoost yielded similar results with some slight differences, which is covered in the Appendices.

To understand which stellar and planetary parameters most influence exoplanet habitability, feature importance analysis was conducted on both classifiers. The SHAP (SHapley Additive exPlanations) [10] technique was applied on both classifiers to intercept the importance of the contribution of each feature to the predictions, as well as to gain insights on how different feature values

lead the model prediction toward either positive (habitable) or negative (non-habitable) outcomes. Additionally, the machine learning libraries underneath the Random Forest and XGBoost classifiers (sklearn and xgboost respectively) provide functionalities to expose feature importance for models, which were used to cross-verify the SHAP analysis outcomes.

Figure 4 shows the feature important analysis results for the Random Forest classifier. Figure 4 (a) shows the global effect of each feature on model predictions (i.e. feature importance) by the mean of absolute SHAP values across all the exoplanets, and Figure 4 (b) shows the feature importance of the Random Forest classifier exposed from the sklearn library.

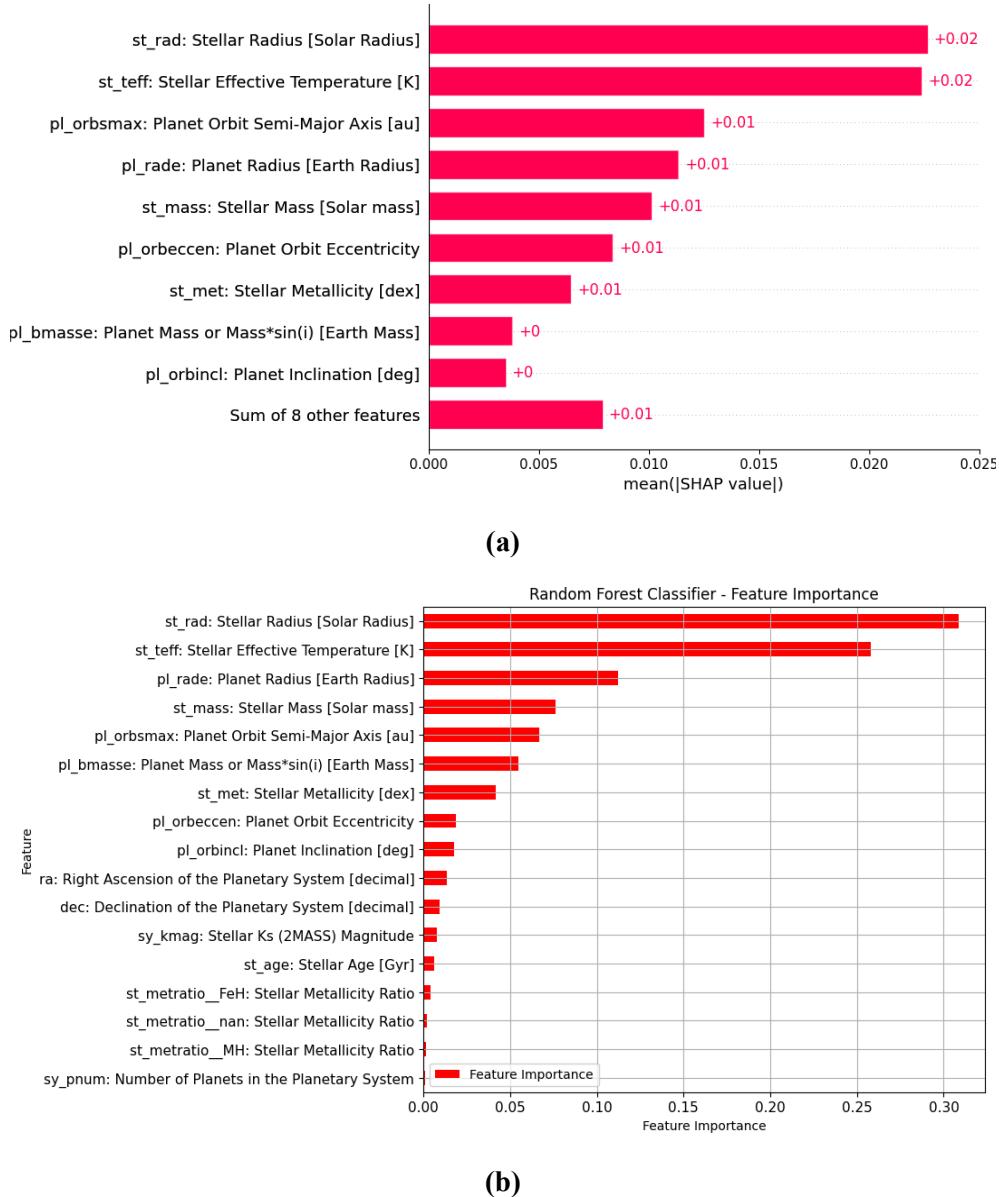


Figure 4. (a) Global effect of each feature on the Random Forest model prediction outcome (i.e. feature importance), represented by the mean(|SHAP value|); **(b)** Feature importance of the Random Forest model

by sklearn library. These graphs were created by the student researcher using the sklearn library in a Google Colab notebook, 2025.

In Figure 4 (a), the importance of each feature's contribution in the model prediction is represented by a numerical value, with a high value indicating a larger feature importance. The features are sorted in descending order by feature importance. As shown in the figure, stellar radius, stellar effective temperature, planet orbit semi-major axis, planet radius, and stellar mass are the top parameters in terms of influencing habitability prediction.

The SHAP value for each feature in each sample (i.e., the exoplanet in the context of this study) essentially represents the specific feature's contribution to the model's prediction for that specific exoplanet. In the context of this study, a negative SHAP value means that the feature contributes towards a negative prediction outcome (non-habitable) for the exoplanet, while a positive SHAP value means that the feature contributes towards a positive prediction outcome (habitable). SHAP values are specific for exoplanets and thus will be different for different exoplanets. To understand the global effect of each feature on the model prediction outcome (i.e., feature importance), the mean of the absolute value of SHAP values across all the exoplanets is used. This is essentially what is shown in Figure 4 (a).

Comparing Figure 4 (a) with Figure 4 (b) (the feature importance exposed from the sklearn library), the same set of stellar and planetary parameters were identified as the top influential factors for the habitability prediction (with some slight differences in the ordering), indicating strong alignment between the two approaches.

3.3 | Deep Dive on Random Forest through SHAP

More SHAP analysis was conducted on the Random Forest classifier to understand how stellar and planetary parameters impact exoplanet habitability.

Figure 5 shows how different feature values influence Random Forest model prediction outputs by displaying SHAP values through a beeswarm plot. Each singular dot in the figure represents a single feature (labelled to the left of the diagram) of a single sample (exoplanet). The horizontal axis represents the SHAP value, while the color of each dot indicates whether the corresponding feature of that exoplanet has a higher or a lower value compared to other exoplanets. Lower feature value is represented with a blue color while higher feature value is represented with a red color. The features in the figure are ordered by their effect on model habitability prediction. From the figure, one can determine how higher and lower values of a feature will affect the model prediction outcome.

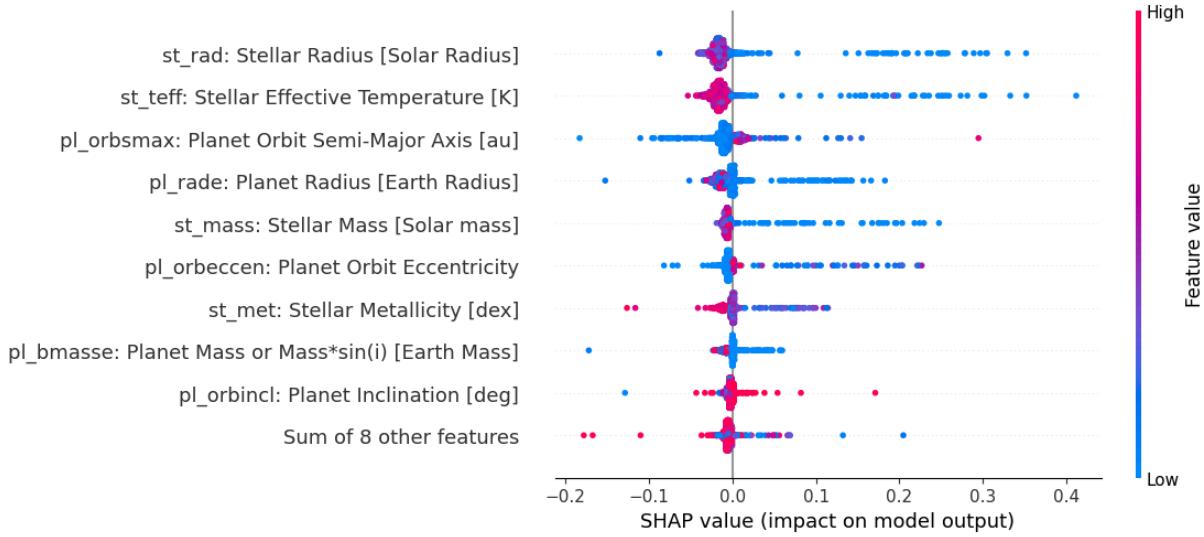


Figure 5. SHAP beeswarm plot – SHAP values (impact on model output) of each feature for the Random Forest classifier. This graph was created by the student researcher using the SHAP library in a Google Colab notebook, 2025.

As shown in Figure 5, higher host stellar radius, host stellar effective temperature, and host stellar mass values have a negative impact on model prediction (leading model output towards non-habitable), while lower values have a positive impact (leading model output towards habitable). Planetary radius shares a similar pattern. On the other hand, the planet orbit semi-major axis has the opposite impact, with higher values leading the model towards positive predictions (habitable) while lower values lead towards negative predictions (non-habitable).

Figure 6 shows the SHAP heatmap plot of the Random Forest model, which groups exoplanets that have the same prediction outcomes and with similar feature impacts together. The heatmap has instances (individual exoplanets) along its x-axis, model inputs (features) along the y-axis, and encodes SHAP values for features of individual exoplanets on a color-graded scale (again, with red positive, and blue negative). The $f(x)$ function at the top demonstrates whether or not the exoplanet in question is predicted to be habitable (higher bar) or not (lower bar). From the overwhelming presence of vividly saturated red colors in stellar effective temperature, stellar radius, planet radius, and stellar mass, as well as the saturated blue colors in planet orbit semi-major axis, we can deduce that these features were very important for the exoplanet habitability.

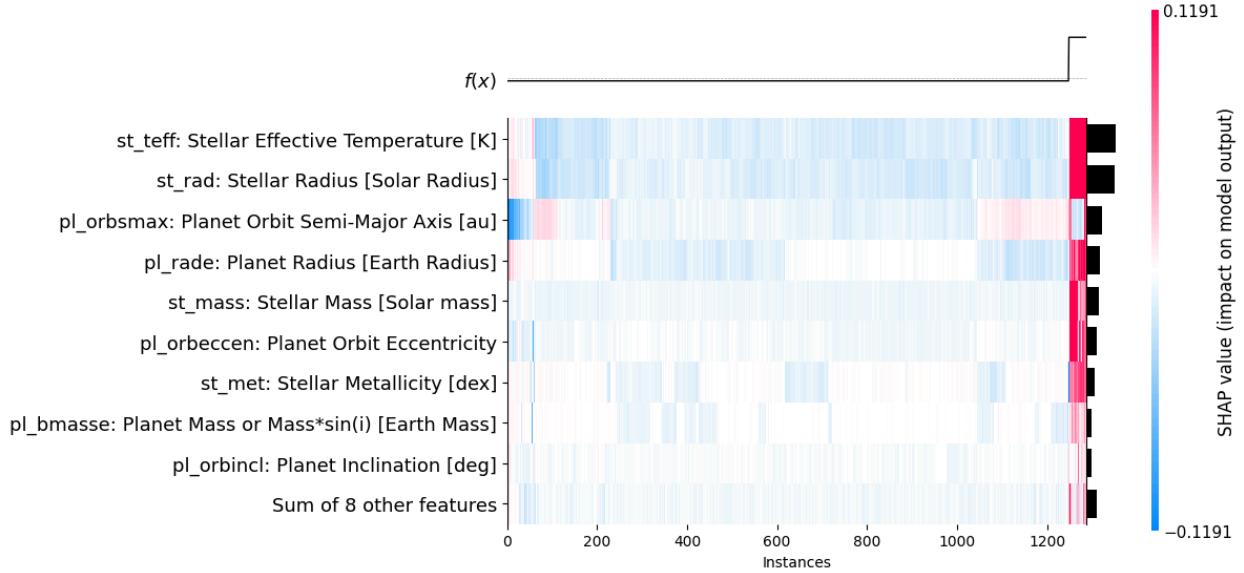
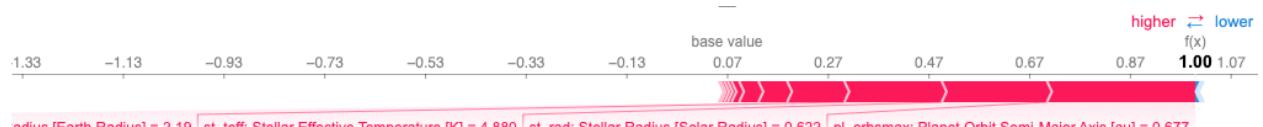


Figure 6. SHAP heatmap plot – grouping exoplanets that have the same prediction outcomes and with the similar feature impacts together. This graph was created by the student researcher using the SHAP library in a Google Colab notebook, 2025.

The bar charts, beeswarm, and heatmap plots above are fantastic for determining general trends in the global dataset, but SHAP also allows us to dig deeper and analyze the impacts of each feature on individual exoplanets as well. Figure 7 shows how different feature values influence the Random Forest model prediction output for a specific exoplanet, known as the SHAP force plot. Figure 7 (a) shows an exoplanet with a positive (habitable) prediction outcome, while Figure 7 (b) shows an exoplanet with a negative (non-habitable) prediction outcome. In the force plots, each exoplanet starts with an expected SHAP value of 0.07, which is the expectation estimation among the testing dataset. Each layered arrow represents the amount – red for positive and blue for negative – that the specific value for a given feature influences the habitability of the exoplanet. The longer the bar, the more impactful it is relative to other features. When all the features are added together on top of the base value, they sum to either 1, meaning the planet is habitable, or 0, meaning the planet is non-habitable.



(a)

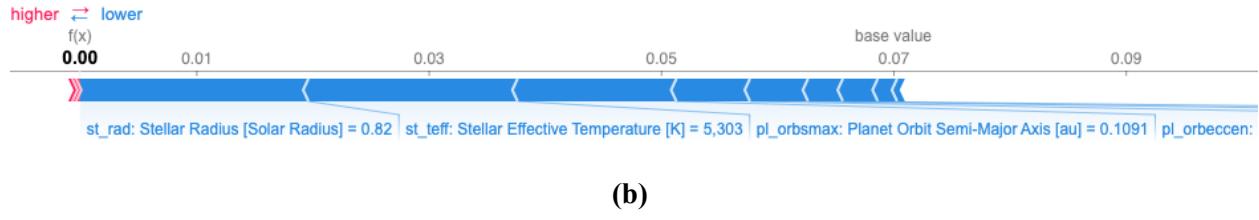
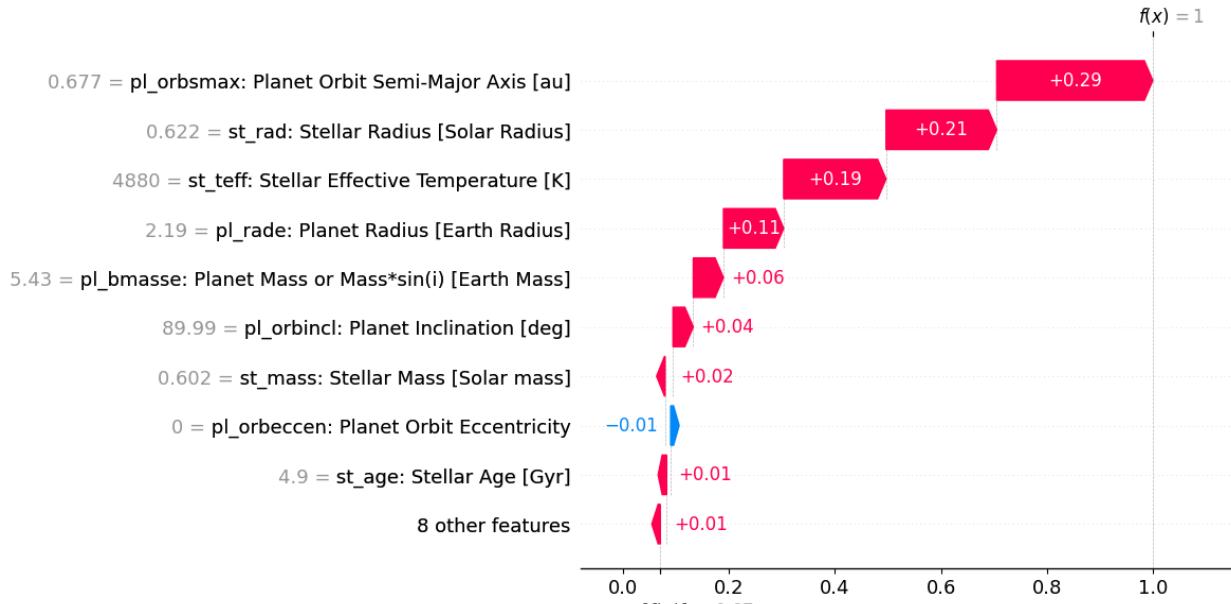


Figure 7. (a) SHAP force plot for an exoplanet with a positive (habitable) prediction outcome; (b) SHAP force plot for an exoplanet with a negative (non-habitable) prediction outcome. These graphs were created by the student researcher using the SHAP library in a Google Colab notebook, 2025.

Figure 8 shows how different feature values influence the Random Forest model prediction output for a specific exoplanet, known as the SHAP waterfall plot. Figure 8 (a) shows an exoplanet with a positive (habitable) prediction outcome, while Figure 8 (b) shows an exoplanet with a negative (non-habitable) prediction outcome. In the waterfall plots, each exoplanet similarly starts with an expected habitability value of 0.07, which is the expectation estimation among the testing dataset. Similarly to force plots, each bar represents the amount – red for positive and blue for negative – that the specific value for a given feature influences the habitability of the exoplanet. The longer the bar, the more impactful. When all the features are added together on top of the base value, they sum to either 1, meaning the planet is habitable, or 0, meaning the planet is non-habitable.



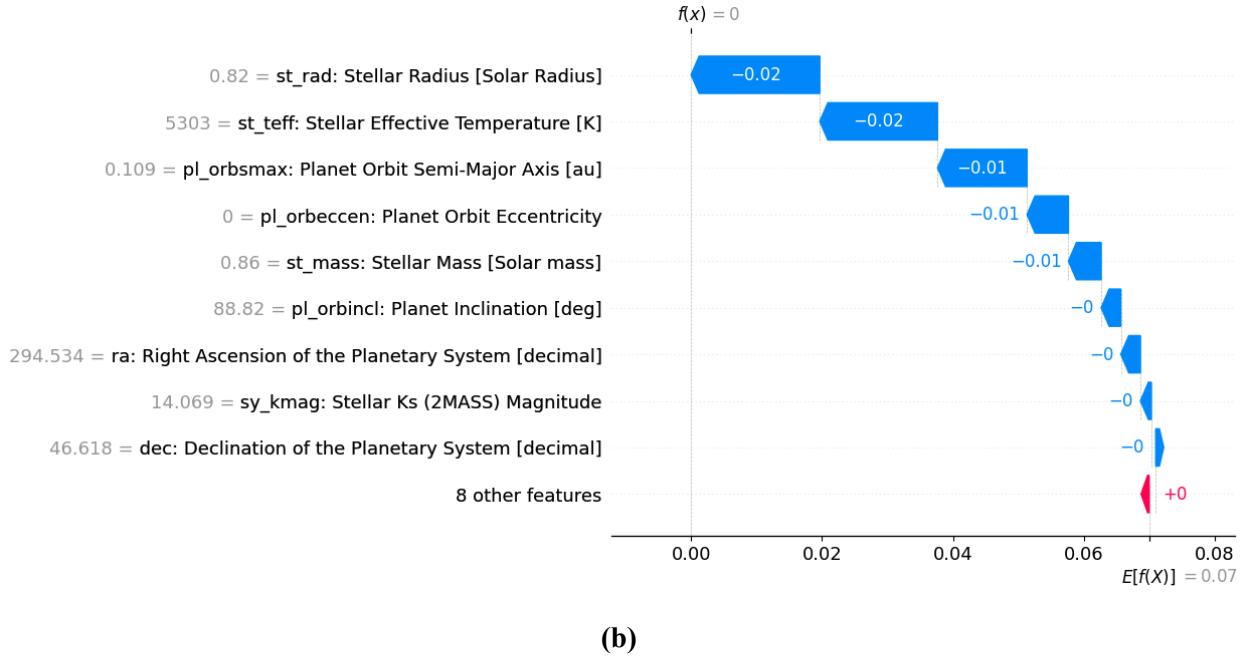
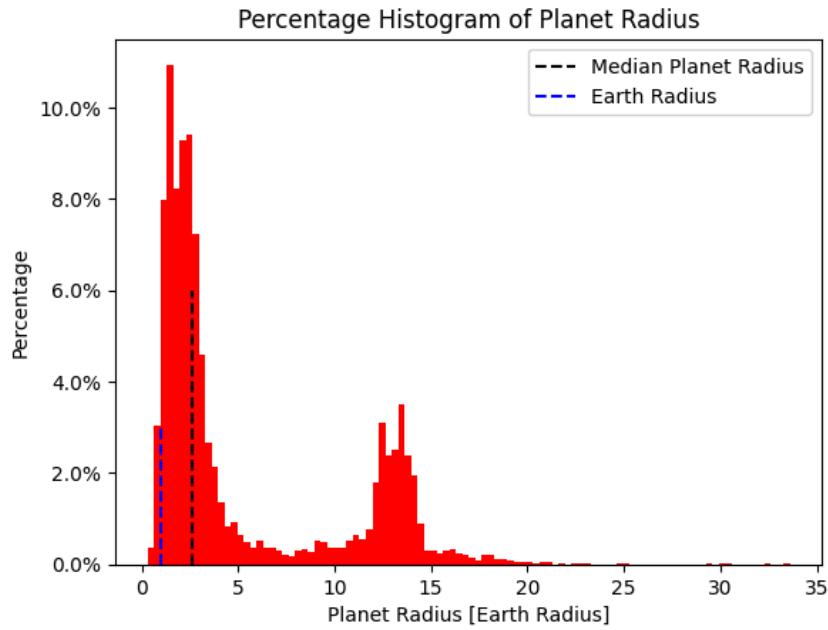


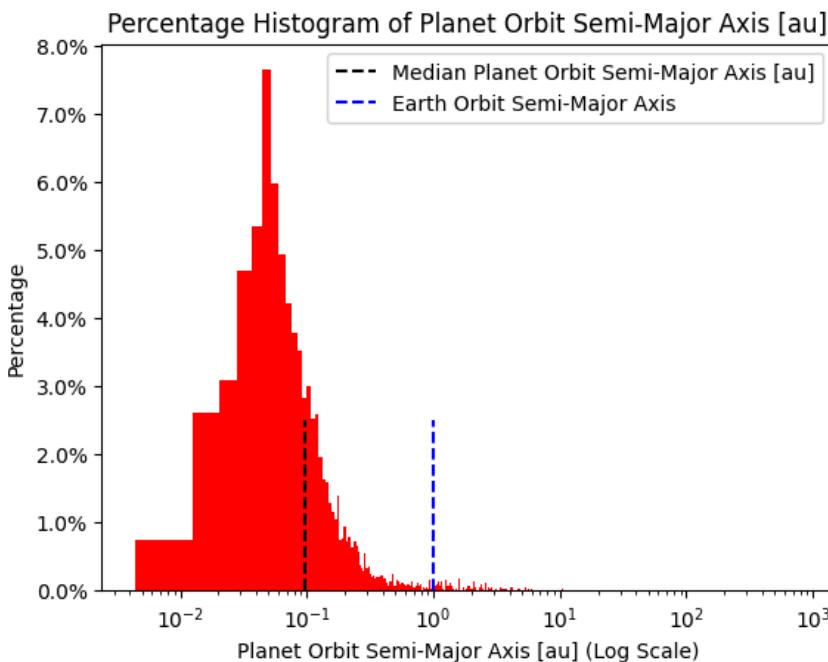
Figure 8. (a) SHAP waterfall plot for an exoplanet with a positive (habitable) prediction outcome; (b) SHAP waterfall plot for an exoplanet with a negative (non-habitable) prediction outcome. These graphs were created by the student researcher using the SHAP library in a Google Colab notebook, 2025.

3.4 | Cross-Validation of SHAP Analysis

Figure 9 (a) and (b) show the percentage histogram of planet radius and planet semi-major axis respectively for the dataset used in this study, with the median values represented by a black dashed line and the values of our Earth represented by a blue dashed line.



(a)



(b)

Figure 9. (a) Percentage histogram of planet radius; (b) Percentage histogram of planet semi-major axis [au]. These graphs were created by the student researcher using the Matplotlib library in a Google Colab notebook, 2025.

Based on the SHAP value analysis, exoplanets with a higher radius compared to others within the dataset tend to be non-habitable, while ones with a relatively lower radius are more likely to be habitable. This indeed is the case as shown by Figure 9 (a). Terrestrial planets (including our Earth) have a lower radius than the median and are thus more likely habitable, while exoplanets with higher radii (for instance, Gas Giants) are more likely non-habitable.

Similarly, the SHAP value analysis indicates that exoplanets with a relatively higher semi-major axis are more likely to be habitable while ones with relatively lower values are not. As shown in Figure 9 (b), the median of the exoplanet orbit semi-major axis is about 0.1 au (the average distance between the Earth and Sun). Any exoplanets with orbit semi-major axes smaller than that are not likely habitable – they are too close to their host star and thus are too hot for life. Our Earth, as a reference, is to the far right (with au at 1) of the median in Figure 9 (b), resulting in a large positive SHAP value and leading towards a positive prediction outcome (habitable).

4 | Conclusion

Machine learning has been increasingly adopted in exoplanet habitability study. Much of previous research work has focused on constructing high-quality machine learning models with various model architectures and techniques to predict exoplanet habitability. While this is important for habitability studies, an equally important task is to understand and identify the influential stellar and planetary parameters to habitability and how they impact habitability.

In this study, a Random Forest classifier and an XGBoost classifier were trained against the joined dataset from the NASA Exoplanet Archive and the Habitable Worlds Catalog (HWC), PHL @ UPR Arecibo with high F1 score (both at 0.95). Based on feature importance analysis through machine learning libraries (sklearn for Random Forest model and xgboost for XGboost model) and the SHAP (SHapley Additive exPlanations) technique, several influential stellar and planetary parameters to habitability were identified, including host stellar effective temperature, host stellar radius, host stellar mass, planet radius, and planet orbit semi-major axis. Furthermore, the SHAP technique exposed more information on how different feature values lead model prediction towards either positive (habitable) or negative (non-habitable) outcomes, providing insights on the stellar and planetary parameters that influence exoplanet habitability.

By using machine learning to predict habitable exoplanets among a large number of candidates, this research can guide scientists to focus their study and analysis on the most promising ones, instead of casting limited resources on the aimless vastness of space. Furthermore, understanding of the most influential stellar and planetary parameters for habitability and how they impact habitability can be very informative for designing telescopes. It can be used to guide the designs of the next-generation of future

telescopes, identifying crucial onboard, feature-specific instruments to include and optimizing flight paths to analyze and search for the most promising candidate exoplanets with specific properties.

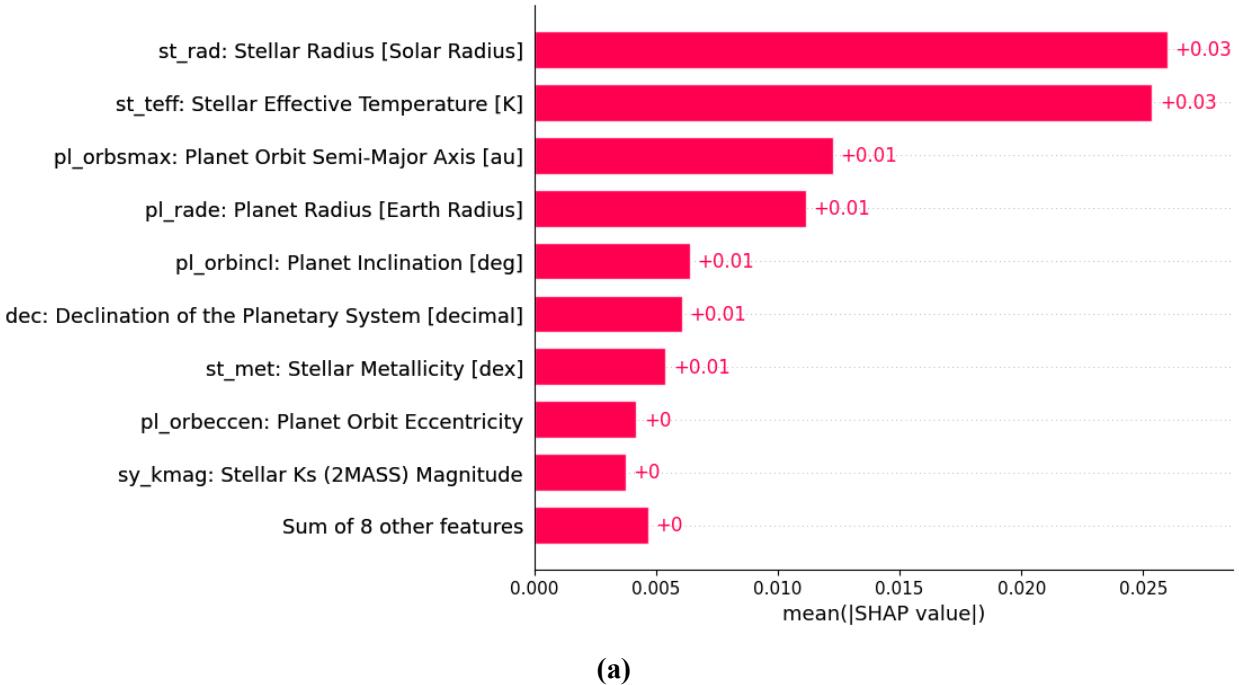
Potential avenues for future work include explorations into using simulated data from the Generation III Bern model [13] – which creates synthetic exoplanets by simulating their entire lifespans starting from their birth in an accretion disk – to create larger datasets to test the limits of our method. One of the biggest current challenges in exoplanet habitability studies is the lack of data; creating high-quality synthetic data points might be helpful in giving us a better view of how my models and methods will perform at a higher-level scale in the interim before the new influx of data.

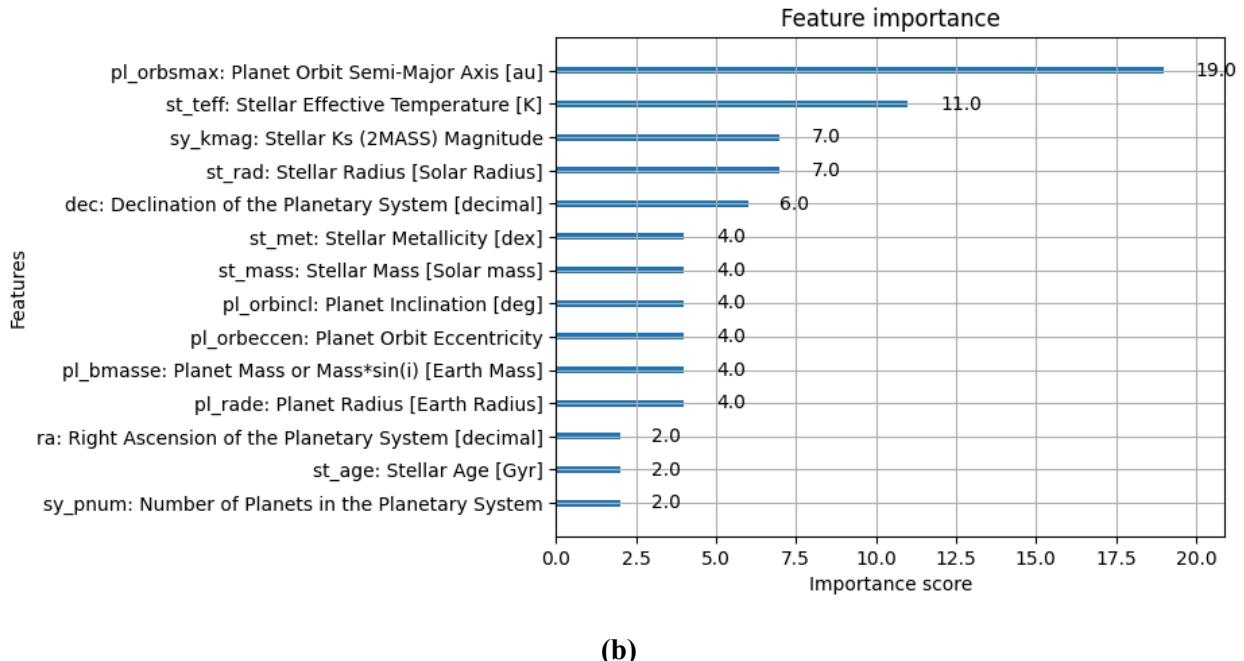
Due to the fact that SHAP is model-agnostic, we can also apply the framework to other models, even including those that do not possess pre-existing feature importance libraries like Random Forest or XGBoost. This means that even as the exoplanetary dataset grows and models evolve, we can still apply the SHAP framework to determine the direction and magnitude of the influence of different features.

5 | Appendices

5.1 | SHAP Analysis for XGBoost

Figure 10 shows the feature importance analysis results for the XGBoost classifier. Figure 10 (a) shows the global effect of each feature on the model prediction (i.e. feature importance) by the mean of absolute SHAP values across all exoplanets, and Figure 10 (b) shows the feature importance exposed from the `xgboost` library. Figure 11 shows how different feature values influence XGBoost model prediction outputs through the SHAP beeswarm plot.





(b)

Figure 10. (a) Global effect of each feature on XGBoost model prediction outcome (i.e. feature importance), represented by $\text{mean}(|\text{SHAP value}|)$; (b) Feature importance of the XGBoost classifier by xgboost library. These graphs were created by the student researcher using SHAP and xgboost libraries in a Google Colab notebook, 2025.

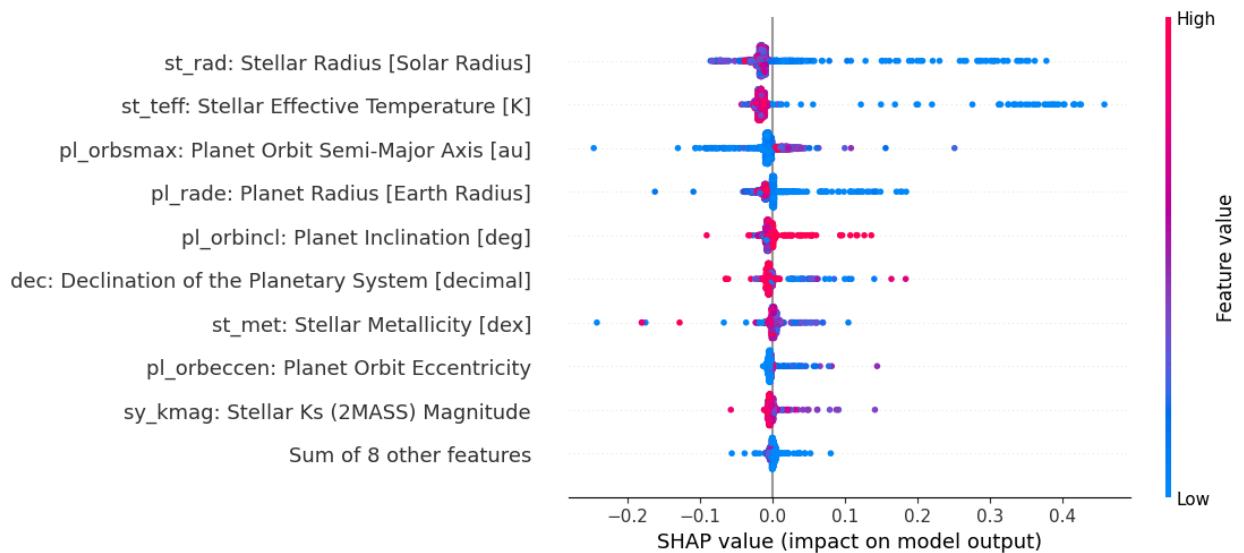


Figure 11. SHAP beeswarm plot - SHAP values (impact on model output) of each feature for the XGBoost classifier. This graph was created by the student researcher using SHAP library in a Google Colab notebook, 2025.

The feature importance analysis results of the XGBoost classifier were similar to the Random Forest, with one noticeable difference. Unlike the Random Forest, host stellar mass was not among the top 5 influential parameters to the exoplanet habitability in the SHAP analysis outcomes. Further study is needed to understand the causes of these differences.

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