



2025 Exoplanet Research

[**Christina Liu** (Lakeside School, Seattle, WA)]

Overview of My Research

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◆ **Exoplanet Habitability Through A Machine Learning Perspective**

| Overview of My Research

- ◆ **Exoplanet Habitability** Through A **Machine Learning Perspective**
 - ◆ **Building ML Models** with High Precision

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 - ◆ Conducting **Feature Importance Analysis**

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 - ◆ **Shapley Additive Explanations (SHAP)**

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- ◆ **Exoplanet Classification**

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- ◆ Updating S. Seager's 2013 paper – *Exoplanet Habitability*

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- ◆ Planetary System Architecture

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- ◆ Updating S. Seager's 2013 paper – *Exoplanet Habitability*
- ◆ Planetary System Architecture
- ◆ Planetary Formation (Literary Studies)

Exoplanet Habitability

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Are there any other worlds where we can live?

Exoplanet Habitability

Are there any other worlds where we can live?

KEY THINGS TO LOOK FOR/AT:

| Exoplanet Habitability

Are there any other worlds where we can live?

KEY THINGS TO LOOK FOR/AT:

- ◆ Planet is within a **habitable zone**

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- ◆ Planet is within a **habitable zone**
 - ◆ Presence of liquid water

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KEY THINGS TO LOOK FOR/AT:

- ◆ Planet is within a **habitable zone**
 - ◆ Presence of liquid water
 - ◆ Planetary surface temperature

Exoplanet Habitability

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 - ◇ Stellar luminosity, variability, activity, metallicity, etc.

Exoplanet Habitability

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 - ◇ Presence of liquid water
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 - ◇ Planet atmosphere
 - ◇ Planetary orbit
- ◆ **Stellar** features + **stellar system** architecture
 - ◇ Stellar luminosity, variability, activity, metallicity, etc.
 - ◇ Other exoplanets in the system; impacts

| Exoplanet Habitability

ML is usually used in the astrophysics community to determine whether a new exoplanet should be considered habitable through comparisons to existing planets with known categorizations.

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My research instead focuses on the individual features of exoplanets, and how much they impact habitability → **feature importance analysis.**

| Exoplanet Habitability

Where do we get the features?

Where do we get the features?

◆ Planetary Systems Composite Data



Where do we get the features?

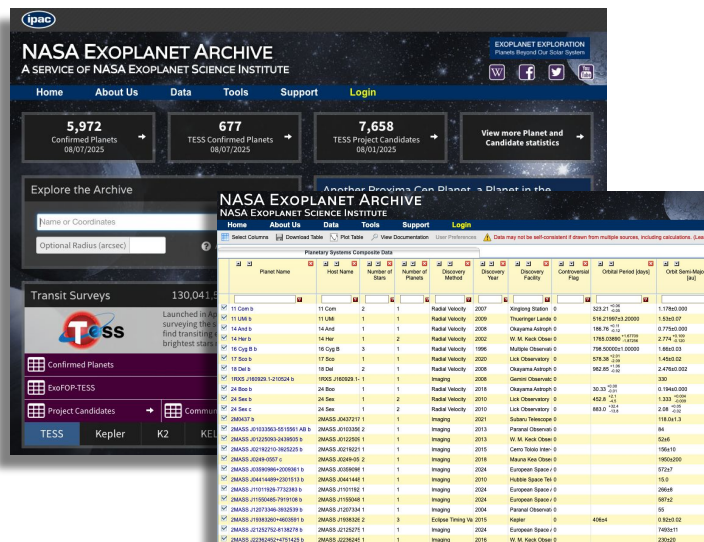
- ◆ Planetary Systems Composite Data
 - ✧ 5,834 confirmed exoplanets



Exoplanet Habitability

Where do we get the features?

NASA Exoplanet Archive



✦ Planetary Systems Composite Data

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- ✧ Features including planetary orbit semi-major axis, planet radius, planet mass, stellar effective temperature, stellar mass, etc.

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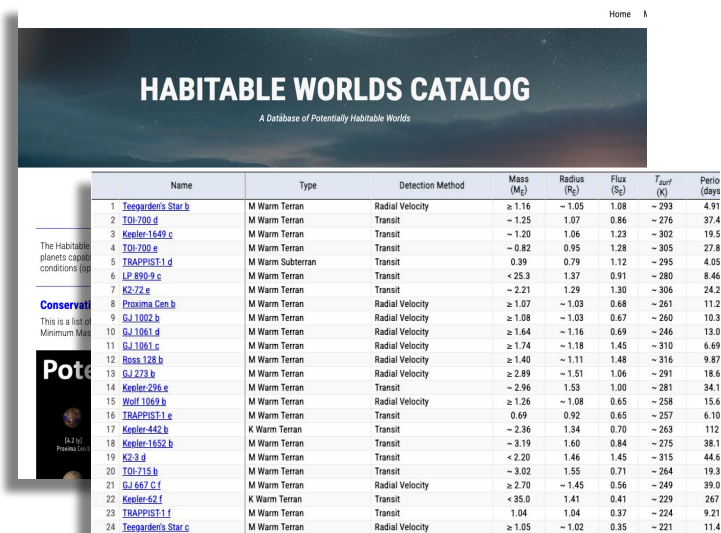
Missing a label to train our data.



Exoplanet Habitability

Where do we get the features?

Habitable Worlds Catalogue, PHL @ UPR Arecibo



The screenshot shows the 'Habitable Worlds Catalogue' website. The header features the title 'HABITABLE WORLDS CATALOG' and the subtitle 'A Database of Potentially Habitable Worlds'. Below the header is a table listing 24 exoplanets. The table columns are: Name, Type, Detection Method, Mass (M_J), Radius (R_J), Flux (S_J), T_{surf} (K), and Period (days). The planets listed include Teegarden's Star b, TOI-700 d, Kepler-1649 c, TOI-700 e, TRAPPIST-1 d, LP 899-9 c, K2-72 e, Proxima Centauri b, GJ 1002 b, GJ 1061 d, GJ 1061 c, Ross 128 b, GJ 273 b, Kepler-296 e, Wolf 1069 b, TRAPPIST-1 e, Kepler-442 b, Kepler-1652 b, K2-3 d, TOI-715 b, GJ 667 C f, Kepler-62 f, TRAPPIST-1 f, and Teegarden's Star c.

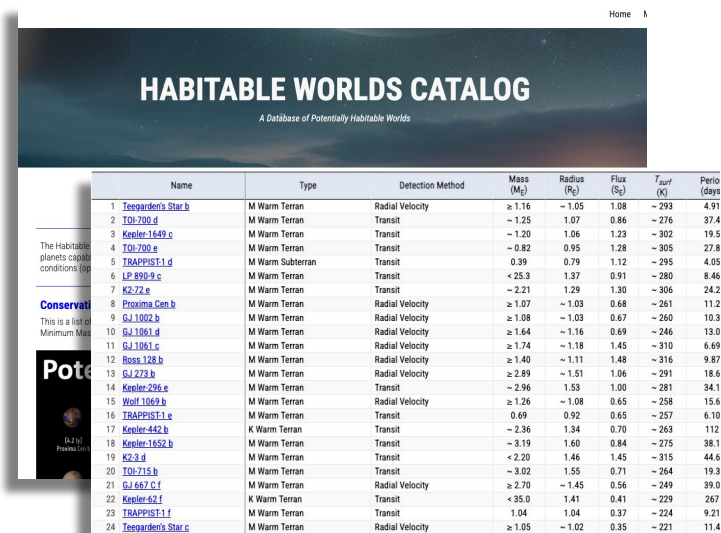
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2	TOI-700 d	M Warm Terran	Transit	~ 1.25	1.07	0.86	~ 276	37.4
3	Kepler-1649 c	M Warm Terran	Transit	~ 1.20	1.06	1.23	~ 302	19.5
4	TOI-700 e	M Warm Terran	Transit	~ 0.82	0.95	1.28	~ 305	27.8
5	TRAPPIST-1 d	M Warm Subterranean	Transit	0.39	0.79	1.12	~ 295	4.05
6	LP 899-9 c	M Warm Terran	Transit	< 25.3	1.37	0.91	~ 280	8.46
7	K2-72 e	M Warm Terran	Transit	~ 2.21	1.29	1.30	~ 306	24.2
8	Proxima Cent b	M Warm Terran	Radial Velocity	≥ 1.07	~ 1.03	0.68	~ 261	11.2
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13	GJ 273 b	M Warm Terran	Radial Velocity	≥ 2.89	~ 1.51	1.06	~ 291	18.6
14	Kepler-296 e	M Warm Terran	Transit	~ 2.96	1.53	1.00	~ 281	34.1
15	Wolf 1069 b	M Warm Terran	Radial Velocity	≥ 1.26	~ 1.08	0.65	~ 238	15.6
16	TRAPPIST-1 e	M Warm Terran	Transit	0.69	0.92	0.65	~ 257	6.10
17	Kepler-442 b	K Warm Terran	Transit	~ 2.36	1.34	0.70	~ 263	112
18	Kepler-1652 b	M Warm Terran	Transit	~ 3.19	1.60	0.84	~ 275	38.1
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21	GJ 667 C f	M Warm Terran	Radial Velocity	≥ 2.70	~ 1.45	0.56	~ 249	39.0
22	Kepler-62 f	K Warm Terran	Transit	< 35.0	1.41	0.41	~ 229	267
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◆ Habitable Worlds Catalogue

Exoplanet Habitability

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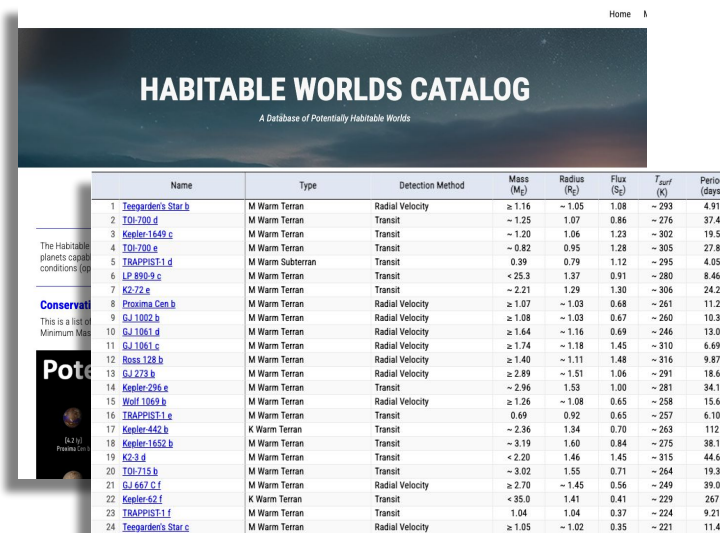
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Exoplanet Habitability

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- ◆ 5,599 confirmed exoplanets
- ◆ Includes a data field:
[pl_habitable]

Exoplanet Habitability

Choosing the models:

<https://doi.org/10.48550/arXiv.2207.08815>

Why do tree-based models still outperform deep learning on tabular data?

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Soda, Inria Saclay

Abstract

While deep learning has enabled tremendous progress on text and image datasets, its superiority on tabular data is not clear. We contribute extensive benchmarks of standard and novel deep learning methods as well as tree-based models such as XGBoost and Random Forests, across a large number of datasets and hyperparameter combinations. We define a standard set of 45 datasets from varied domains with clear characteristics of tabular data and a benchmarking methodology accounting for both fitting models and finding good hyperparameters. Results show that tree-based models remain state-of-the-art on medium-sized data (~10K samples) even without accounting for their superior speed. To understand this gap, we conduct an empirical investigation into the differing inductive biases of tree-based models and Neural Networks (NNs). This leads to a series of challenges which should guide researchers aiming to build tabular-specific NNs: 1. be robust to uninformative features, 2. preserve the orientation of the data, and 3. be able to easily learn irregular functions. To stimulate research on tabular architectures, we contribute a standard benchmark and raw data for baselines: every point of a 20 000 compute hours hyperparameter search for each learner.

1 Introduction

Deep learning has enabled tremendous progress for learning on image, language, or even audio datasets. On tabular data, however, the picture is muddier and ensemble models based on decision trees like XGBoost remain the go-to tool for most practitioners (Sta) and data science competitions [Kossen et al., 2021]. Indeed deep learning architectures have been crafted to create inductive biases matching invariances and spatial dependencies of the data. Finding corresponding invariances is hard in tabular data, made of heterogeneous features, small sample sizes, extreme values.

Creating tabular-specific deep learning architectures is a very active area of research (see section 2) given that tree-based models are not differentiable, and thus cannot be easily composed and jointly trained with other deep learning blocks. Most corresponding publications claim to beat or match tree-based models, but their claims have been put into question: a simple Resnet seems to be competitive with some of these new models [Gorishniy et al., 2021], and most of these methods seem to fail on new datasets [Shwartz-Ziv and Armon, 2021]. Indeed, the lack of an established benchmark for tabular

<https://doi.org/10.48550/arXiv.2106.03253>

TABULAR DATA: DEEP LEARNING IS NOT ALL YOU NEED

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November 24, 2021

ABSTRACT

A key element in solving real-life data science problems is selecting the types of models to use. Tree ensemble models (such as XGBoost) are usually recommended for classification and regression problems with tabular data. However, several deep learning models for tabular data have recently been proposed, claiming to outperform XGBoost for some use cases. This paper explores whether these deep models should be a recommended option for tabular data by rigorously comparing their performance to XGBoost on various datasets. In addition to systematically comparing their performance, we consider the tuning and computation they require. Our study shows that XGBoost outperforms these deep models across the datasets, including the datasets used in the papers that proposed the deep models. We also demonstrate that XGBoost requires much less tuning. On the positive side, we show that an ensemble of deep models and XGBoost performs better on these datasets than XGBoost alone.

Keywords Tabular data · Deep neural networks · Tree-based models · Hyperparameter optimization

1 Introduction

Deep neural networks have demonstrated great success across various domains, including images, audio, and text [Devlin et al., 2019, He et al., 2016, van den Oord et al., 2016]. There are several canonical architectures for encoding raw data into meaningful representations in these domains. These canonical architectures usually perform well in real-world applications.

In real-world applications, the most common data type is tabular data, comprising samples (rows) with the same set of features (columns). Tabular data is used in practical applications in many fields, including medicine, finance, manufacturing, climate science, and many other applications that are based on relational databases. During the last decade, traditional machine learning methods, such as gradient-boosted decision trees (GBDT) [Chen and Guestrin, 2016], still dominated tabular data modeling and showed superior performance over deep learning. In spite of their theoretical advantages [Shwartz-Ziv et al., 2018, Poggio et al., 2020, Piran et al., 2020], deep neural networks pose many challenges when applied to tabular data, such as lack of locality, data sparsity (missing values), mixed feature types (numerical, ordinal, and categorical), and lack of prior knowledge about the dataset structure (unlike with text or images). Moreover, deep neural networks are perceived as a “black box” approach – in other words, they lack transparency or interpretability of how input data are transformed into model outputs [Shwartz-Ziv and Tishby, 2017]. Although the “no free lunch” principle [Wolpert and Macready, 1997] always applies, tree-ensemble algorithms, such

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Choosing the models:

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Why do tree-based models still outperform deep learning on tabular data?

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November 24, 2021

ABSTRACT

A key element in solving real-life data science problems is selecting the types of models to use. Tree ensemble models (such as XGBoost) are usually recommended for classification and regression problems with tabular data. However, several deep learning models for tabular data have recently been proposed, claiming to outperform XGBoost for some use cases. This paper explores whether these deep models should be a recommended option for tabular data by rigorously comparing their performance to XGBoost on various datasets. In addition to systematically comparing their performance, we consider the tuning and computation they require. Our study shows that XGBoost outperforms these deep models across the datasets, including the datasets used in the papers that proposed the deep models. We also demonstrate that XGBoost requires much less tuning. On the positive side, we show that an ensemble of deep models and XGBoost performs better on these datasets than XGBoost alone.

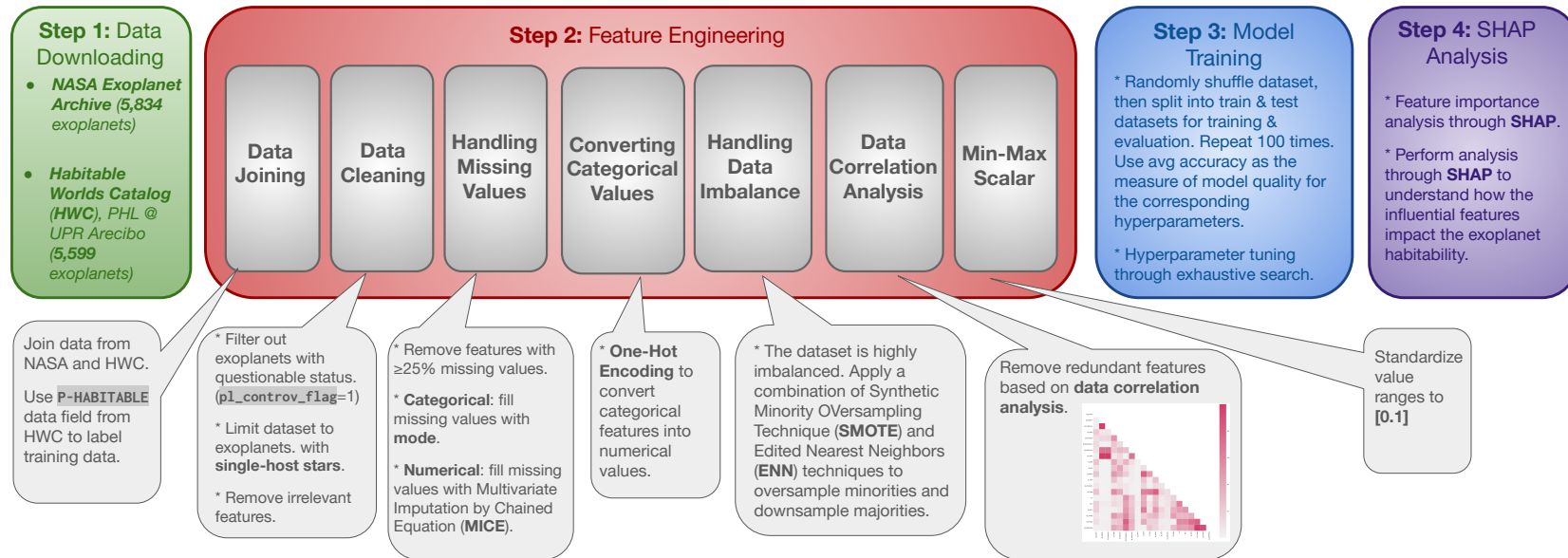
Keywords: Tabular data · Deep neural networks · Tree-based models · Hyperparameter optimization

1 Introduction

Deep neural networks have demonstrated great success across various domains, including images, audio, and text [Devlin et al., 2019, He et al., 2016, van den Oord et al., 2016]. There are several canonical architectures for encoding raw data into meaningful representations in these domains. These canonical architectures usually perform well in real-world applications.

In real-world applications, the most common data type is tabular data, comprising samples (rows) with the same set of features (columns). Tabular data is used in practical applications in many fields, including medicine, finance, manufacturing, climate science, and many other applications that are based on relational databases. During the last decade, traditional machine learning methods, such as gradient-boosted decision trees (GBDT) [Chen and Guestrin, 2016], still dominated tabular data modeling and showed superior performance over deep learning. In spite of their theoretical advantages [Shwartz-Ziv et al., 2018, Poggio et al., 2020, Piran et al., 2020], deep neural networks pose many challenges when applied to tabular data, such as lack of locality, data sparsity (missing values), mixed feature types (numerical, ordinal, and categorical), and lack of prior knowledge about the dataset structure (unlike with text or images). Moreover, deep neural networks are perceived as a “black box” approach – in other words, they lack transparency or interpretability of how input data are transformed into model outputs [Shwartz-Ziv and Tishby, 2017]. Although the “no free lunch” principle [Wolpert and Macready, 1997] always applies, tree-ensemble algorithms, such

Exoplanet Habitability



Random Forest Model Evaluation

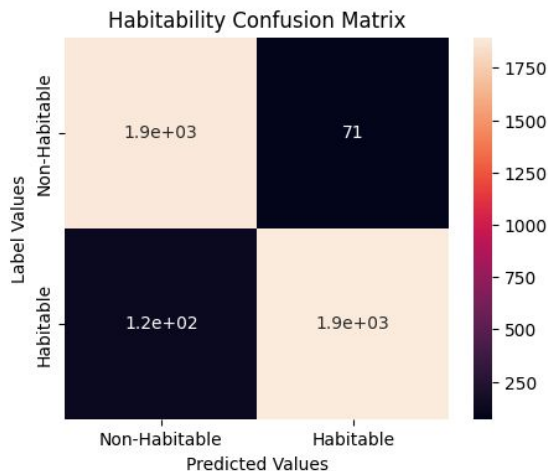
Class	Random Forest		
	Precision	Recall	F1 score
1 (Habitable)	0.96	0.94	0.95
0 (Non-Habitable)	0.94	0.96	0.95

XGBoost Model Evaluation

Class	XGBoost		
	Precision	Recall	F1 score
1 (Habitable)	0.94	0.97	0.95
0 (Non-Habitable)	0.97	0.93	0.95

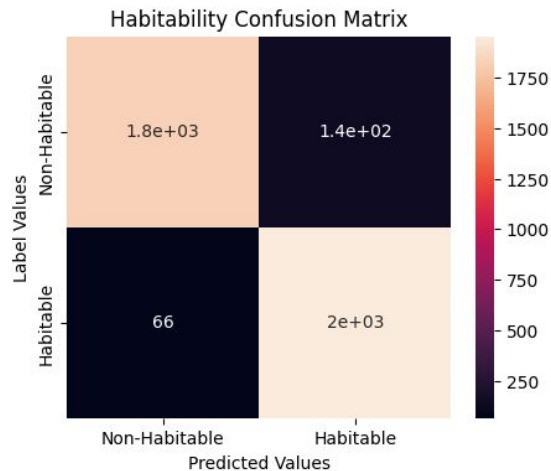
Exoplanet Habitability

Model results:



Random Forest Classifier – Classification Report:

	precision	recall	f1-score	support
0.0	0.94	0.96	0.95	1959
1.0	0.96	0.94	0.95	2020
accuracy			0.95	3979



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| Exoplanet Habitability

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Introducing **SHAP**.

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SHAP (Shapley Additive Explanations)

- ◆ A framework that helps us to recognize the impact of each individual feature positively or negatively affecting our outcome.

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| Exoplanet Habitability

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 - ✧ Look at each feature (ex. feature 1) of the dataset and train the model once with the feature and once without the feature, for each subset of the rest of the features in your training set.

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 - ✧ Find weighted average across the diff. subsets to get **feature 1's SHAP value**.

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- ◆ Apply to any model! (Because of the nature of SHAP)

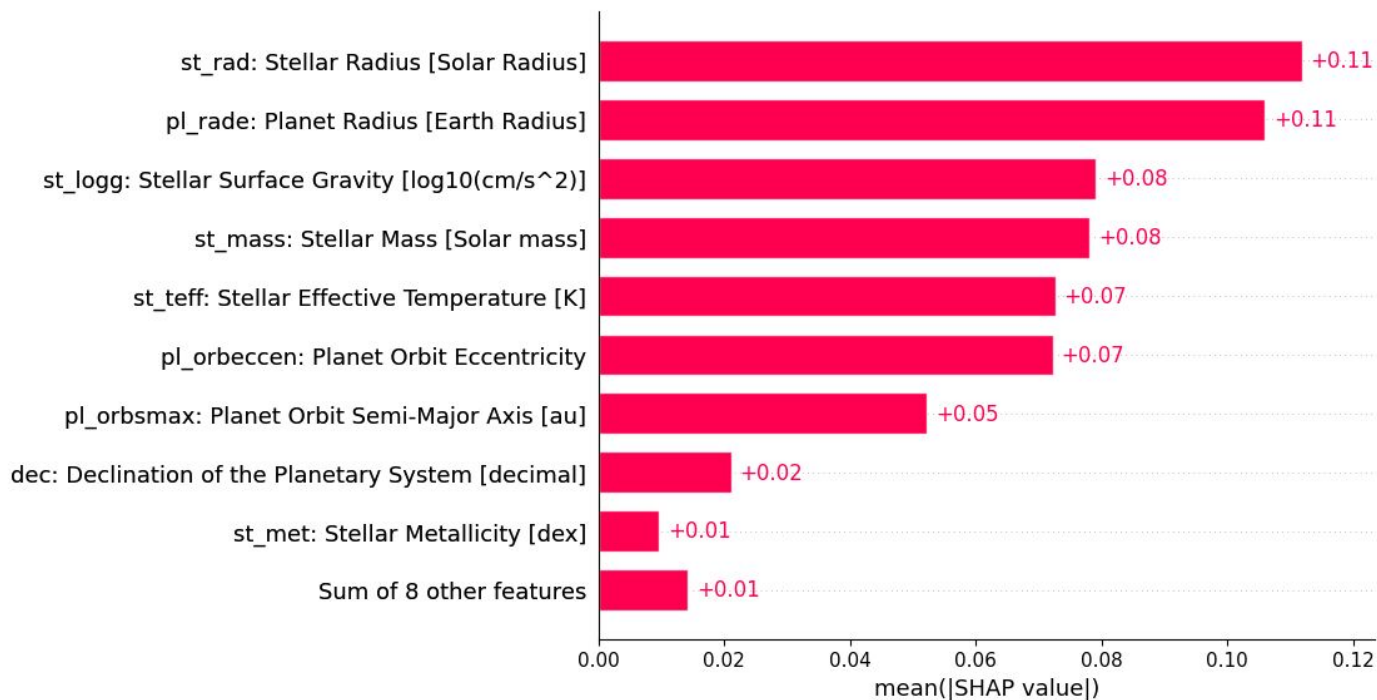
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- ◆ Also, **ADDITIVE**.

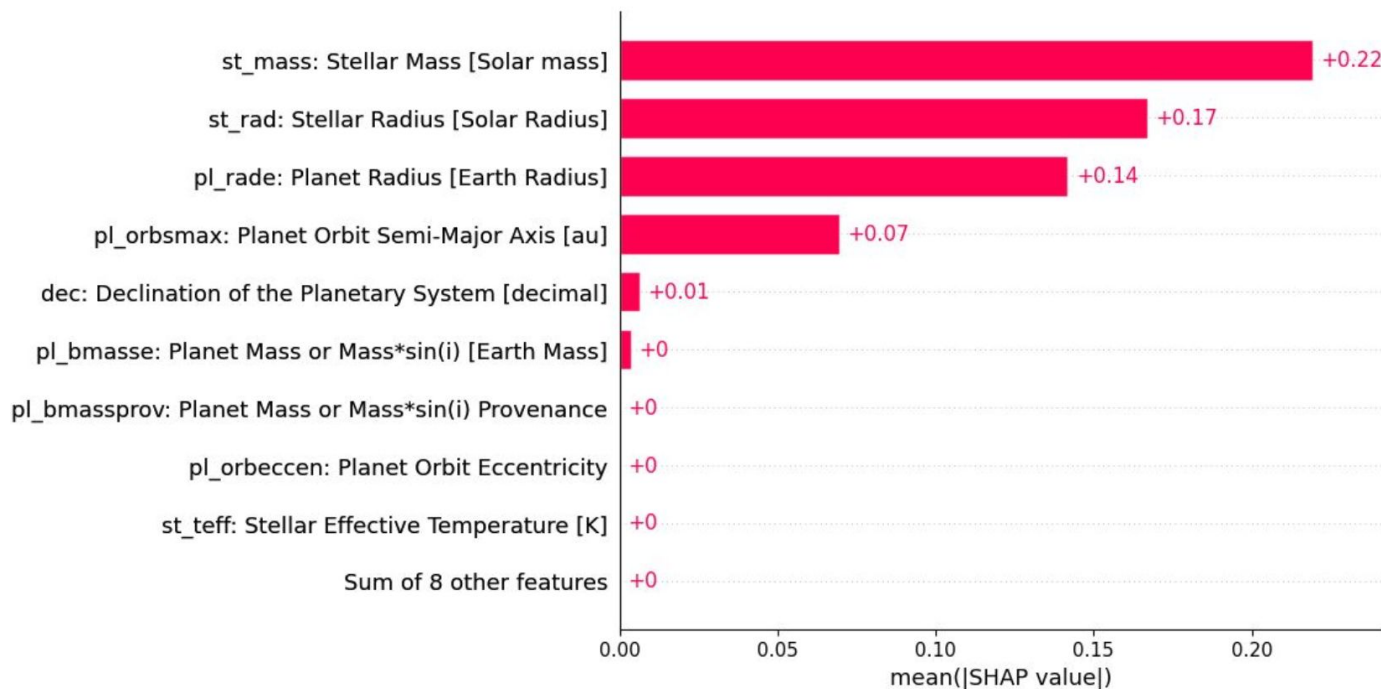
Exoplanet Habitability

Overall Analysis – Random Forest



Exoplanet Habitability

Overall Analysis – XGBoost



| Exoplanet Habitability

You can go further with SHAP!!

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You can go further with SHAP!!

- ◆ Can analyze whether a feature pushes the exoplanet **towards** habitability or **away**.

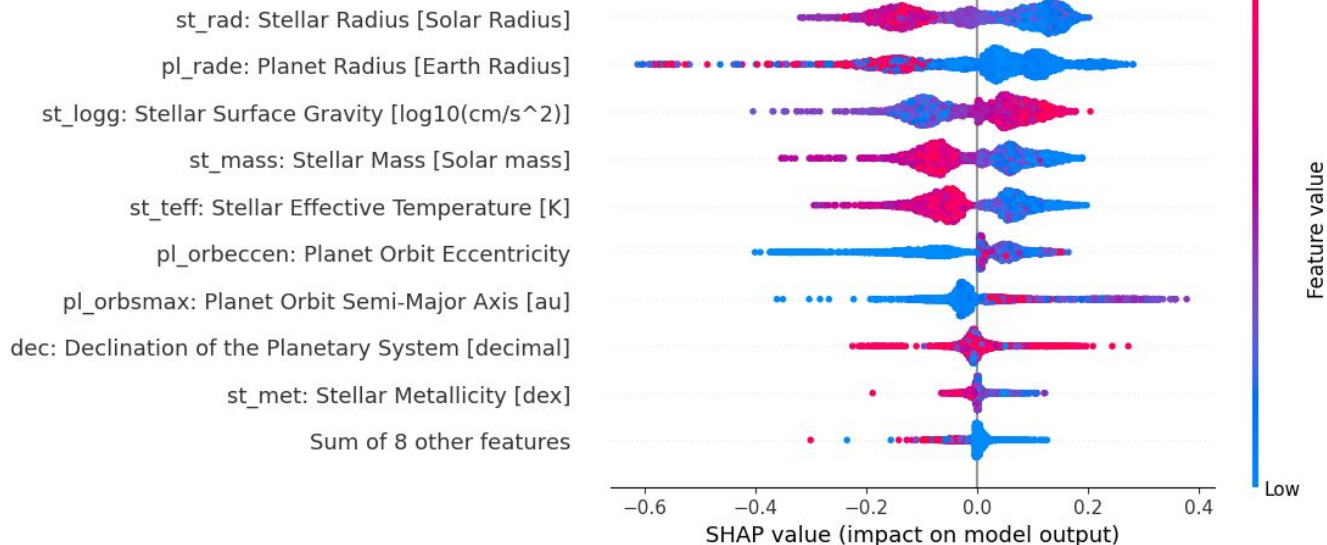
| Exoplanet Habitability

You can go further with SHAP!!

- ◆ Can analyze whether a feature pushes the exoplanet **towards** habitability or **away** from it.
 - ◆ Positive SHAP value → towards.
 - ◆ Negative SHAP value → away.

Exoplanet Habitability

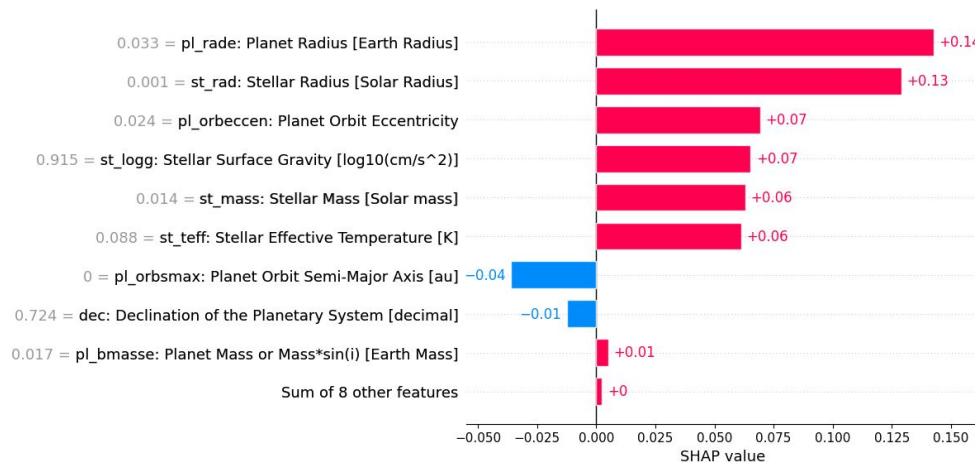
Beeswarm Plot – Random Forest



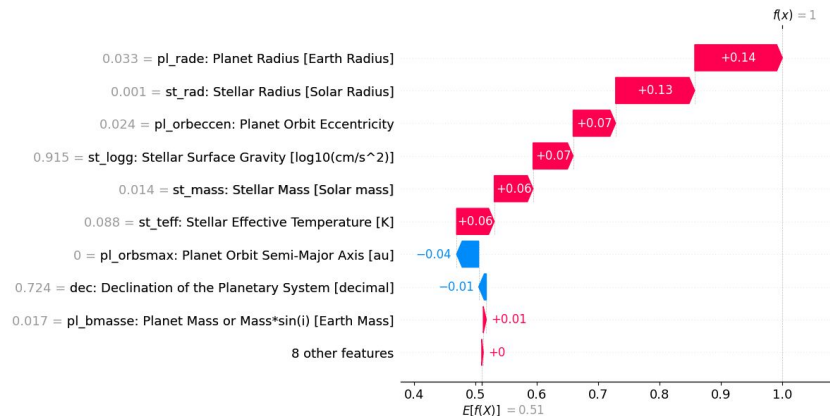
- ◆ Higher values (relative to other samples in dataset) of stellar radius, planet radius, stellar mass, and stellar effective temperature lead towards negative predictions, while lower values lead towards positive outcomes.
- ◆ Planet orbit semi-major axis, on the other hand, has the opposite impact on prediction outcomes, with higher values leading toward positive predictions while lower values leading towards negative outcomes.

Exoplanet Habitability

Local Plots – Random Forest



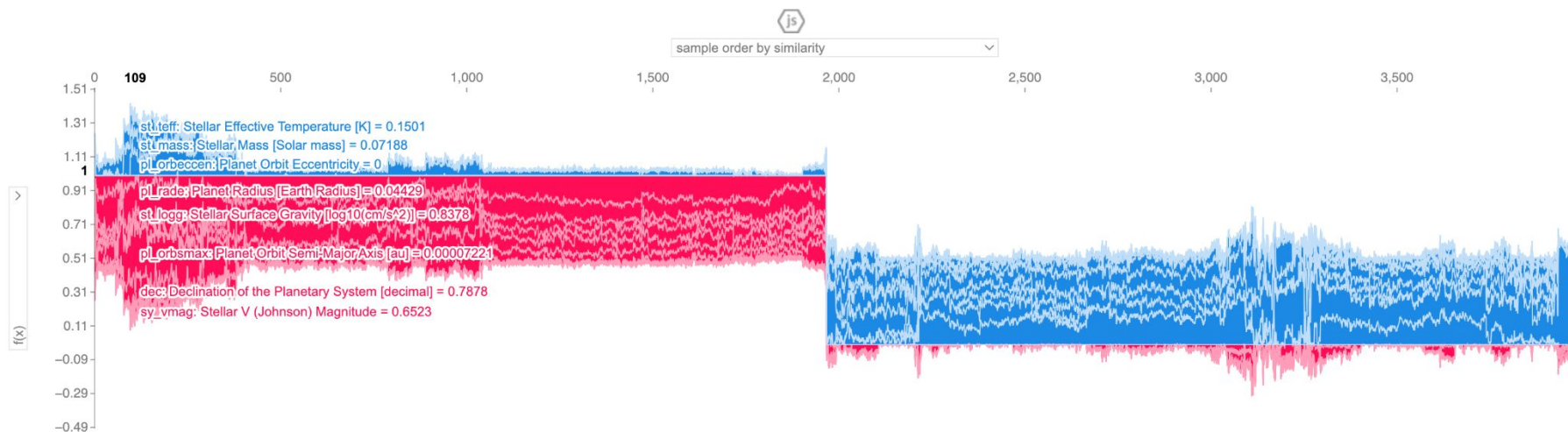
SHAP local bar plot for one sample in the dataset



SHAP waterfall plot for one sample in the dataset

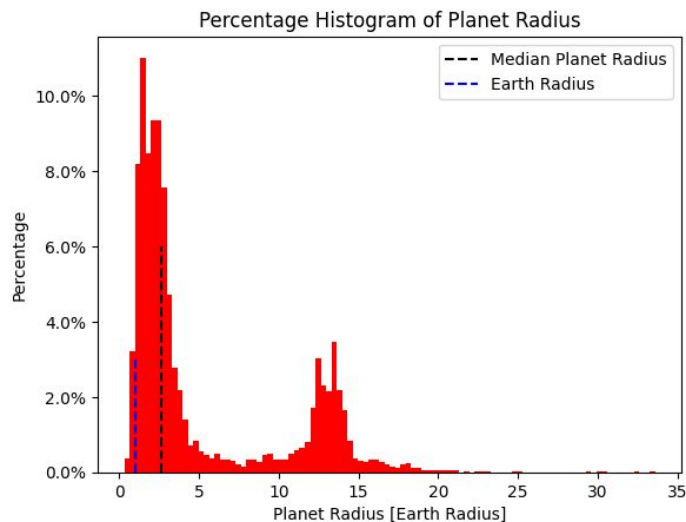
Exoplanet Habitability

Force Plots – Random Forest

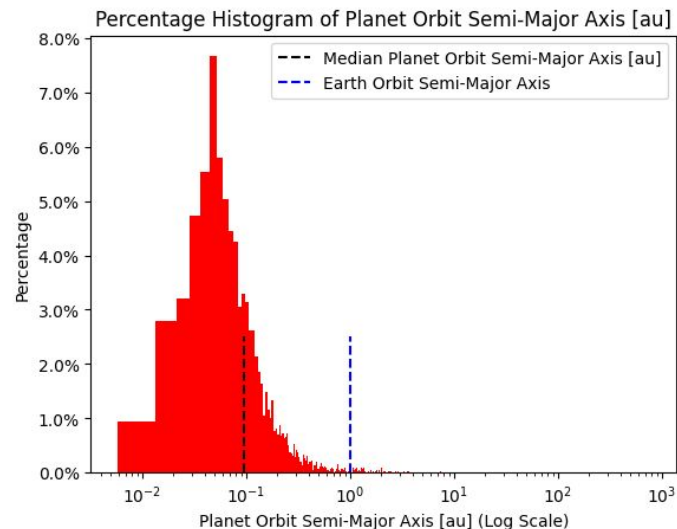


Exoplanet Habitability

Sanity check: does all this align with reality?



SHAP analysis indicates a higher planet radius leads towards negative predictions, while lower value leads towards positive predictions.



SHAP analysis indicates a higher planet orbit semi-major axis leads towards positive predictions, while lower value leads towards negative predictions.

Exoplanet Classification

New Paper

Prof. Seager's 2013 Paper

SPECIAL SECTION

REVIEW

Exoplanet Habitability

Sara Seager

The search for exoplanets includes the promise to eventually find and identify habitable worlds. The thousands of known exoplanets and planet candidates are extremely diverse in terms of their masses or sizes, orbits, and host star type. The diversity extends to new kinds of planets, which are very common yet have no solar system counterparts. Even with the requirement that a planet's surface temperature must be compatible with liquid water (because all life on Earth requires liquid water), a new emerging view is that planets very different from Earth may have the right conditions for life. The broadened possibilities will increase the future chances of discovering an inhabited world.

For thousands of years people have wondered, "Are we alone?" Now, for the first time in human history, the answer to this and other long-standing questions in the search for life beyond our solar system may finally be in reach through the observation and study of exoplanets—planets orbiting stars other than the Sun.

The recent field of exoplanets has grown dramatically since the first planet orbiting a Sun-like star was discovered nearly 20 years ago (1). Nearly 1000 exoplanets are known to orbit nearby stars, a few thousand more planet "candidates" have been identified, and planets are so common that on average every star in the Milky Way should have at least one planet (2, 3). The numbers of exoplanet candidates found by NASA's Kepler space telescope are high enough that robust statements of the frequency of their occurrence is possible, including the astonishing finding that small planets by far outnumber large planets in our galaxy (4, 5), and the first statement about how common Earth-size planets are in the habitable zones of small stars (5).

The habitable zone is a region around a star where a planet can have surface temperatures consistent with the presence of liquid water. All life on Earth requires liquid water, so the planetary surface-temperature requirement appears to be a natural one. The climates of planets with thin atmospheres are dominated by external energy input from the host star, so

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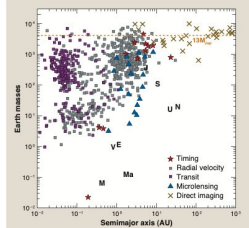


Fig. 1. Known exoplanets as of March 2013. Exoplanets are found at a nearly continuous range of masses and semimajor axes. Many different techniques are successful at discovering exoplanets, as indicated by the different symbols. The solar system planets are denoted by the first one or two letters of their name. The horizontal line is the conventional upper limit to a planet mass, 13 Jupiter masses. The sloped, lower boundary to the collection of gray squares is due to a selection effect in the radial velocity technique. Small planets are beneath the threshold for the current state of almost all exoplanet detection techniques. Data are from <http://exoplanet.eu>.

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The habitable zone for exoplanets was first presented and modeled in detail by (9), who also suggested an empirical version based on the concept that both Venus (0.7 astronomical units (AU) from the Sun, where an AU is the Earth-Sun distance) and Mars (1.5 AU) may have had liquid surface water at some point in the past. Most exoplanet habitable-zone research that followed continued to focus on terrestrial-like planet atmospheres orbiting main-sequence stars (see (10) and references therein). This article reviews updates to the habitable zone and their rationale.

A planet in the habitable zone has no guarantee of actually being habitable. Venus and Earth may both be argued as being in the Sun's habitable zone and would appear from exoplanet discovery techniques to be the same size and mass. Yet, Venus is completely hostile to life owing to a strong greenhouse effect and resulting high surface temperatures (>700 K), whereas Earth has the right surface temperature for liquid water oceans and is teeming with life.

If there is one important lesson from exoplanets, it is that anything is possible within the laws of physics and chemistry. Planets of almost all masses, sizes, and orbits have been detected (Fig. 1), illustrating not only the stochastic nature of planet formation but also a subsequent migration through the planetary disk from the planet's place of origin (e.g., (11)). The huge diversity of exoplanets and the related anticipated variation in their atmospheres, in terms of mass and composition, have motivated a strong desire to revise the view of planetary habitability. In parallel, there is a growing acceptance that even in the future, the number of suitable planets accessible to detailed follow-up observations may be very small. To maximize our chances of identifying a habitable world, a broader understanding of which planets are habitable is a necessity.

Habitable Planets, Conventionally Defined
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SPECIAL SECTION

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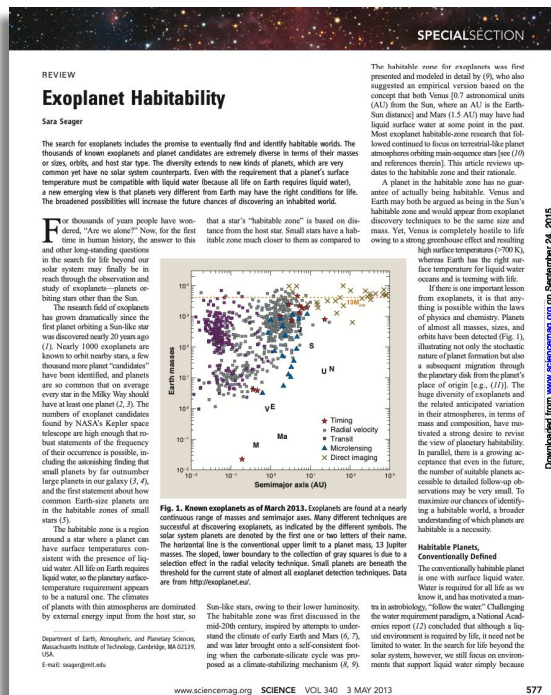
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Prof. Seager's 2013 Paper



- ◆ Emphasizes wide diversity of exoplanets (mass, size, orbital configurations)
- ◆ Discusses difficulties in defining habitability

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REVIEW

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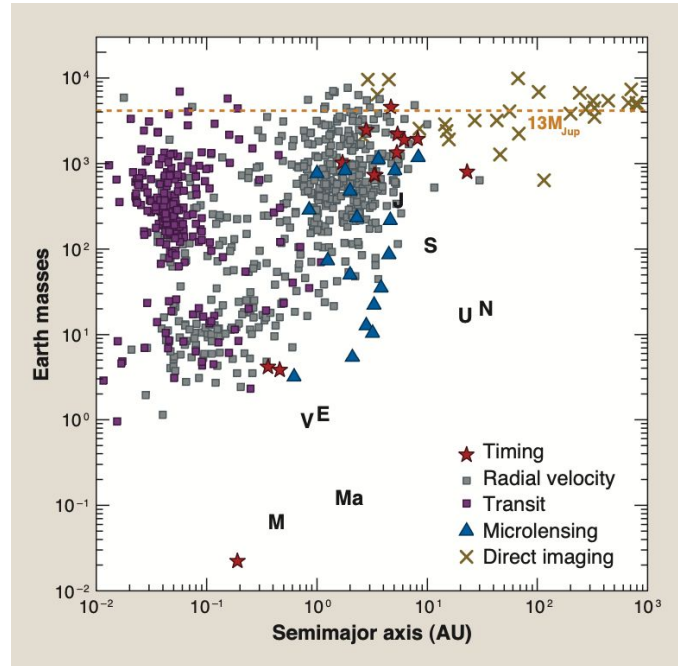
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- ◆ Emphasizes wide diversity of exoplanets (mass, size, orbital configurations)
- ◆ Discusses difficulties in defining habitability
- ◆ At time of publication, only 1000 exoplanets had been discovered.

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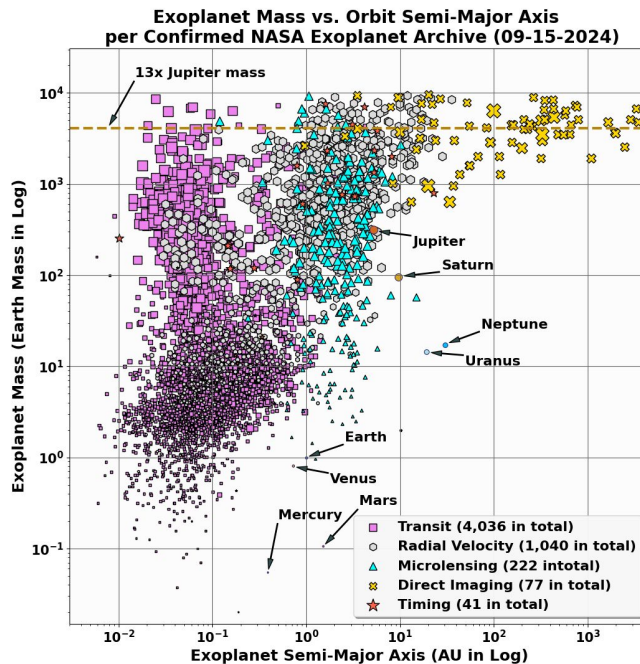
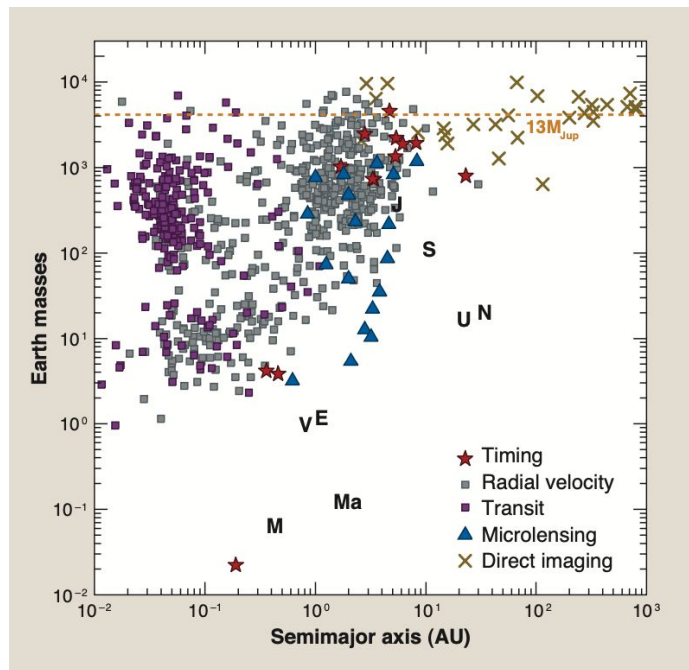
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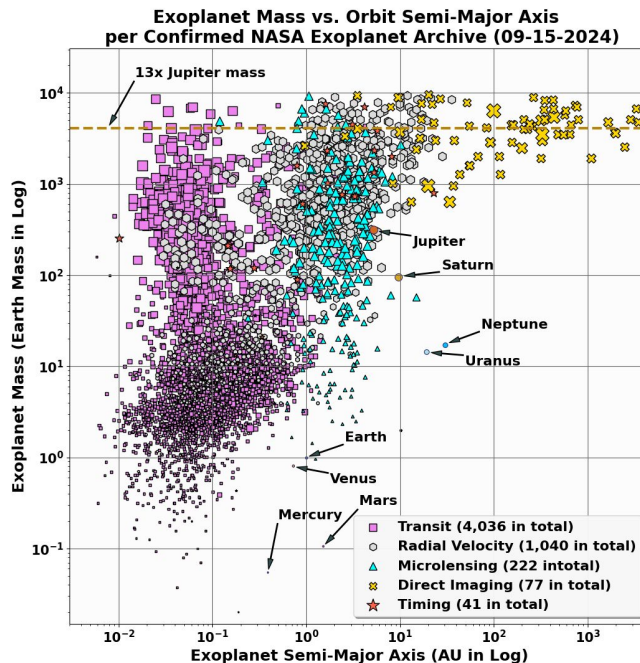
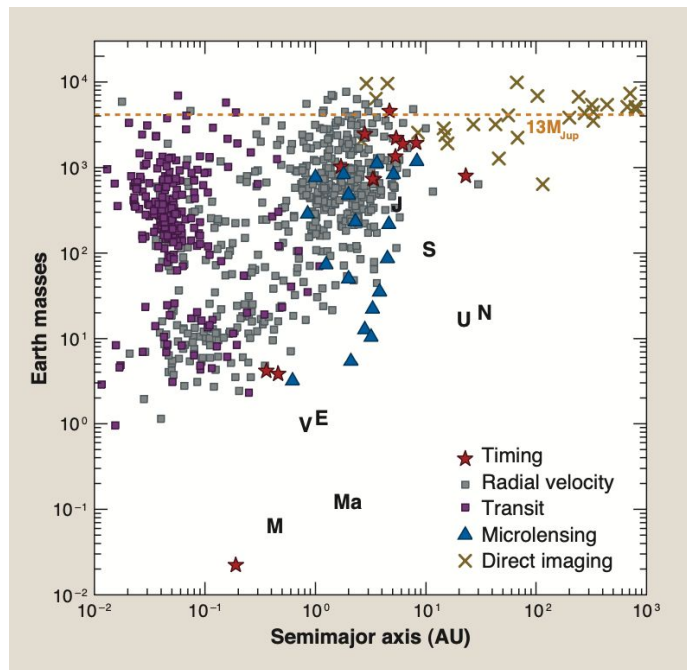
Prof. Seager's 2013 Paper



◆ Included solar system figures

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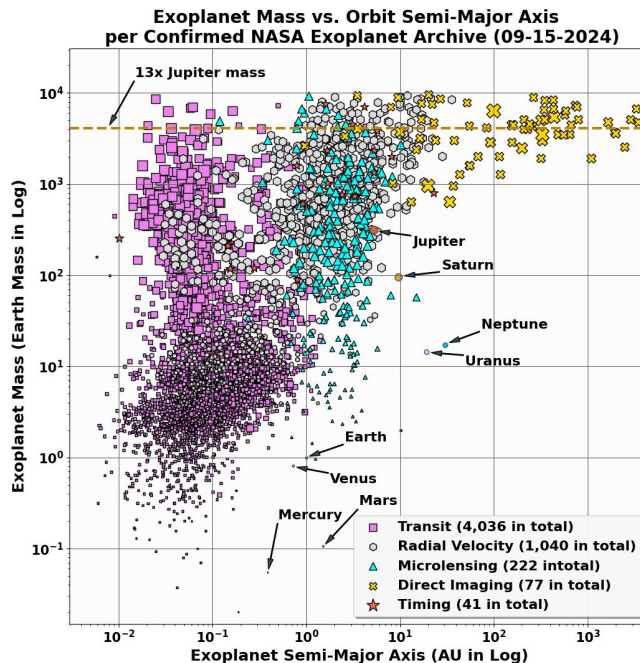
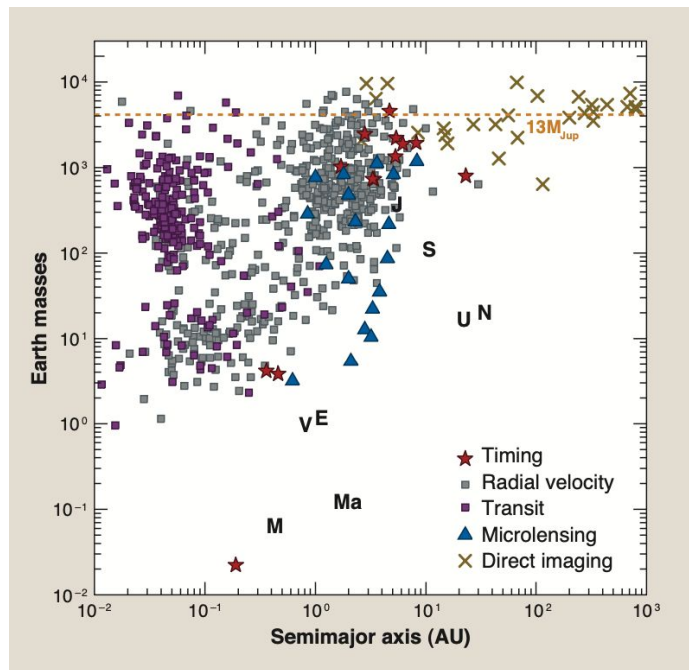
Prof. Seager's 2013 Paper



- ◆ Included solar system figures
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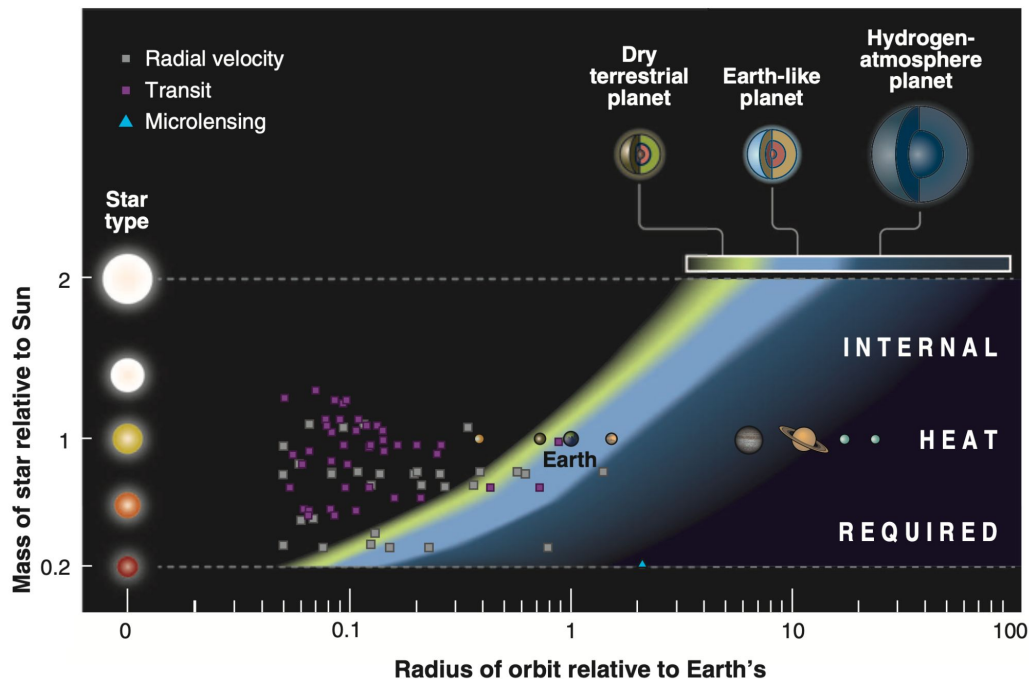
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- ◆ Solar system planets further than standard for their masses

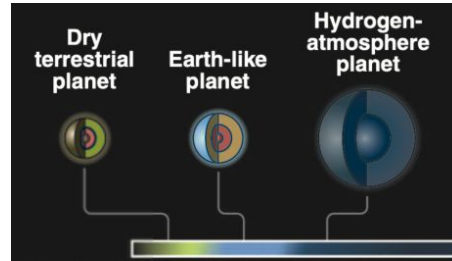
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Prof. Seager's 2013 Paper: Star Mass v. Exoplanet Orbital Relationship



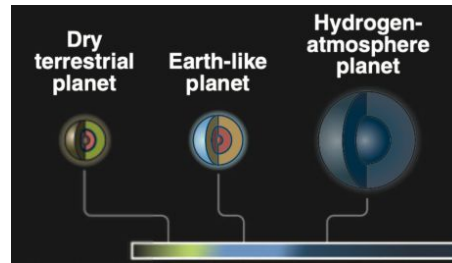
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Prof. Seager's 2013 Paper introduces 3 types of exoplanets:



| New Paper

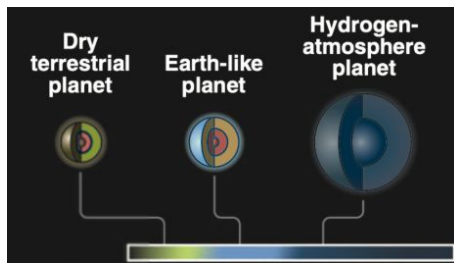
Prof. Seager's 2013 Paper introduces 3 types of exoplanets:



My new revision includes **4 types of exoplanets:**

New Paper

Prof. Seager's 2013 Paper introduces 3 types of exoplanets:



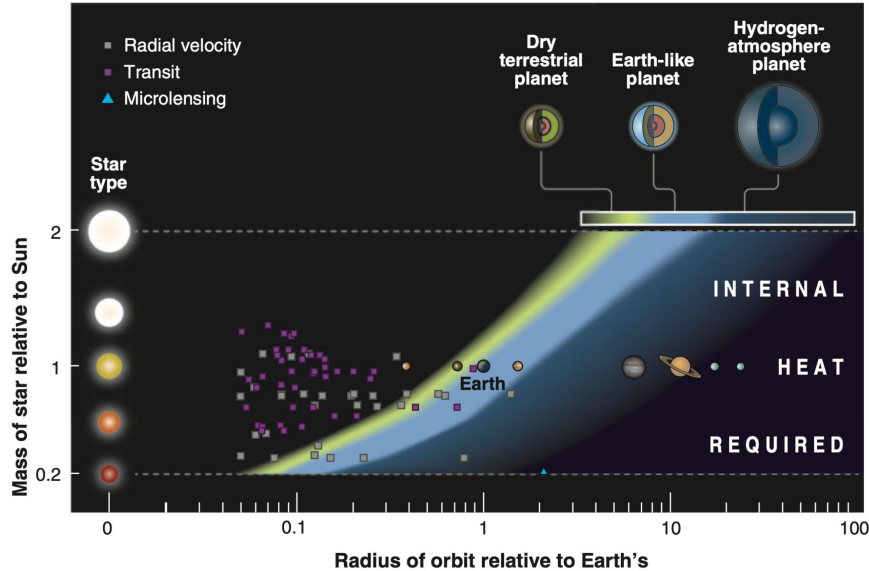
My new revision includes **4 types of exoplanets:**

- ♦ **Terrestrial:** planetary radius ≤ 1 Earth radius
- ♦ **Super-Earth:** $1 \text{ Earth radius} < \text{planetary radius} \leq 3.86 \text{ Earth radius}$
- ♦ **Neptune-Like:** $3.86 \text{ Earth radius} < \text{planetary radius} \leq 9.14 \text{ Earth radius}$
- ♦ **Gas-Giant:** $9.14 \text{ Earth radius} < \text{planetary radius}$

(based on NASA classifications)

New Paper

Prof. Seager's 2013 Paper: Star Mass v. Exoplanet Orbital Relationship



<https://doi.org/10.3847/2515-5172/add46f>

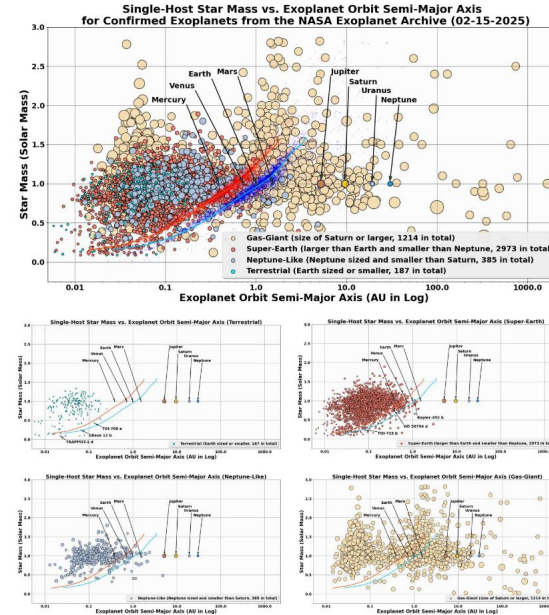


Figure 1. Top: single-host star mass vs. exoplanet orbital semi-major axis diagram. Exoplanets are colored by type and scaled by radius. Each pair of red and blue markers show the computed inner and outer HZ boundaries respectively for each host star, with the 5th-degree polynomial fits (from the least squares regression) indicated by the red and blue solid curves. Graphs on the mid-left, mid-right, bottom-left, and bottom-right are the breakdown diagrams for Terrestrial, Super-Earth, Neptune-Like, and Gas-Giant exoplanets respectively.

Future Work

| Future Work

- ◆ Continuing research in exoplanet classification.
 - ✧ More work in stellar system classification and developing good categorizations for exoplanets.
- ◆ Working on applying my research to newer ML models.
 - ✧ Potentially looking at synthetic data? (ex. Gen 3 Bern Model)

Thank you!!