Jet Propulsion Laboratory
California Institute of Technology

Automating Verification and Validation in the EXCALIBUR Pipeline for the Atmospheric Analysis of Exoplanets

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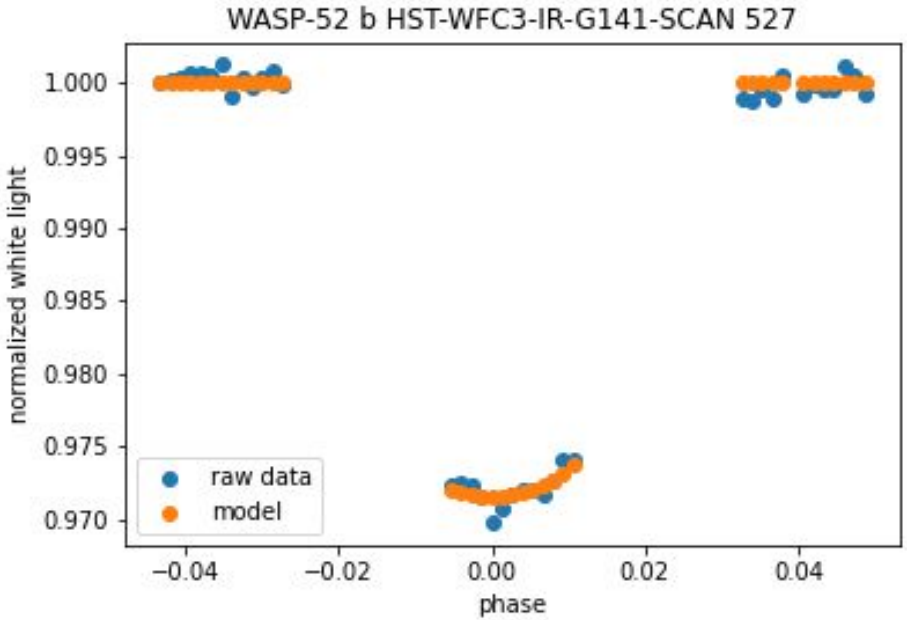
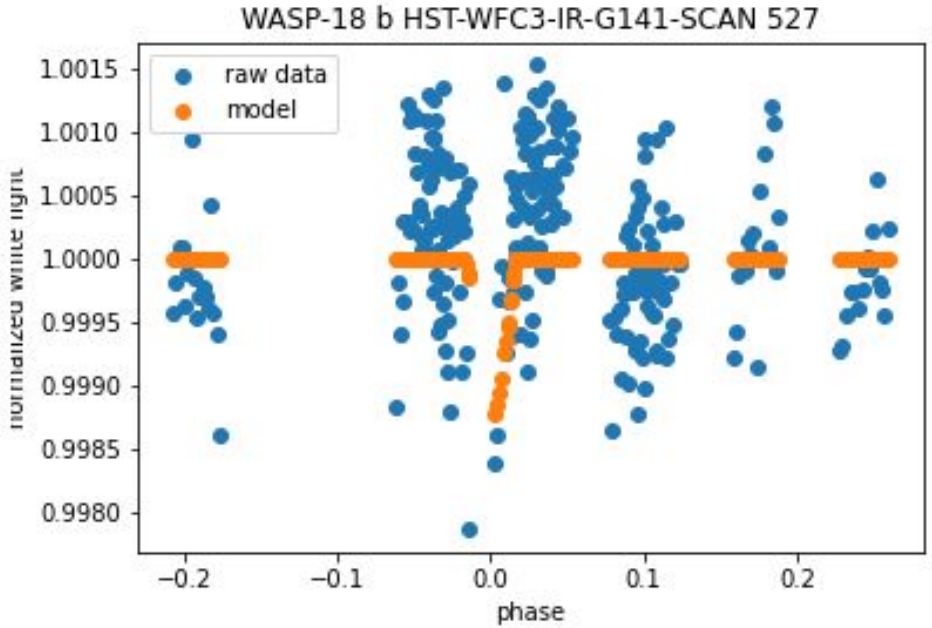
EXCALIBUR Pipeline

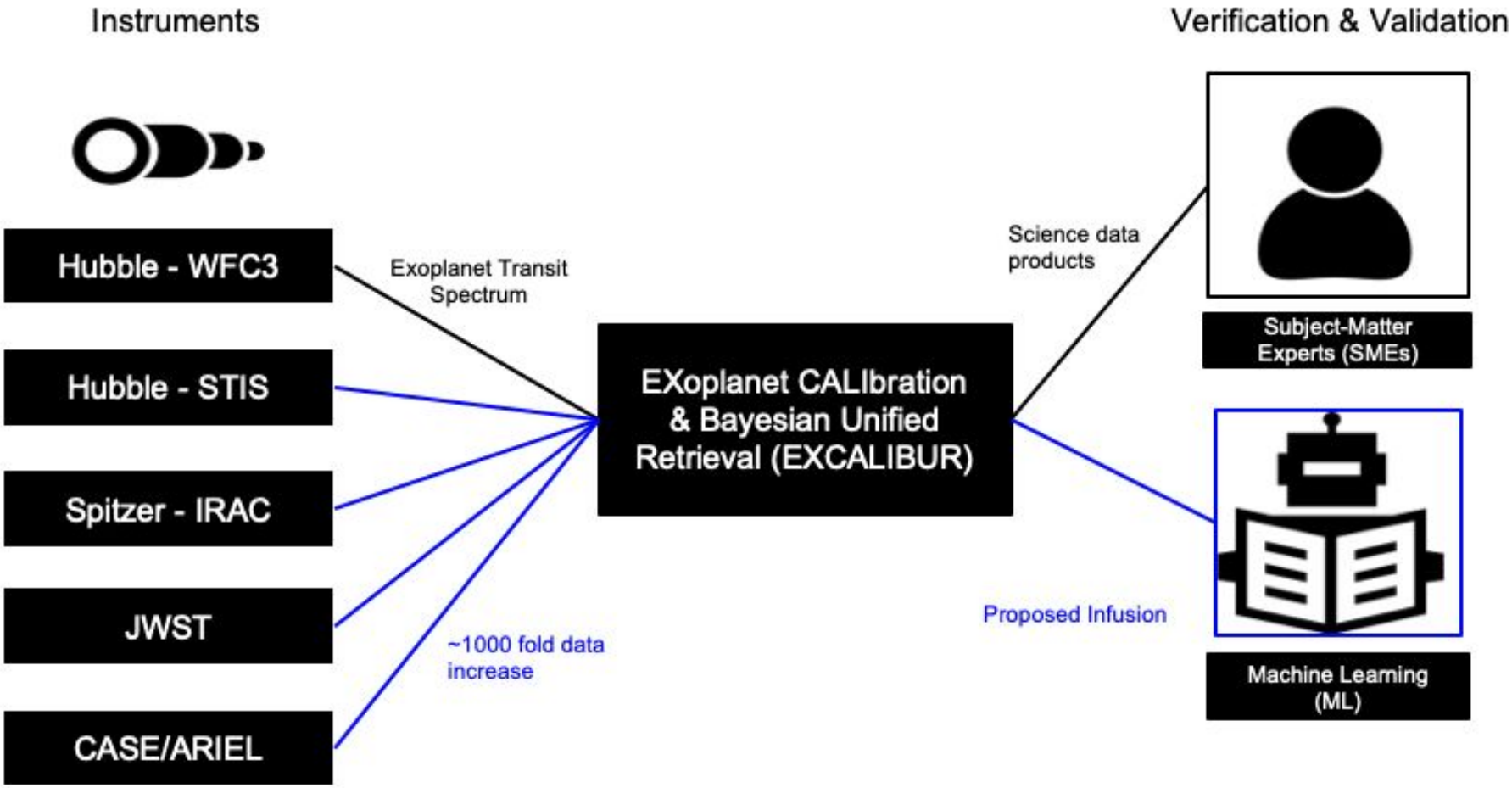
- Scrapes telescopic data on exoplanets from archival sources
  - HST-WFC3-IR-G141-SCAN, HST-STIS-CCD-G430L-STARE, HST-STIS-CCD-G750L-STARE
  - Ex. HAT-P-11b, 55 Cnc e, WASP-17b
- Applies algorithms to scraped data to model it
- Performs atmospheric analysis based on the model/raw data qualities

Transit Whitelight Curve Ex.



Bad Transit Whitelight Curve Ex.




Instruments
Verification & Validation
Hubble - WFC3
Hubble - STIS
Spitzer - IRAC
JWST
CASE/ARIEL
Exoplanet Transit Spectrum
~1000 fold data increase
EXoplanet CALIbration & Bayesian Unified Retrieval (EXCALIBUR)
Science data products
Proposed Infusion
Subject-Matter Experts (SMEs)
Machine Learning (ML)

Project Goal

Improving automatic Verification and Validation of targets in EXCALIBUR

Two sided improvements

- Generate more training data for the ML model to learn better
- Develop features rigorously for the ML model to use data better

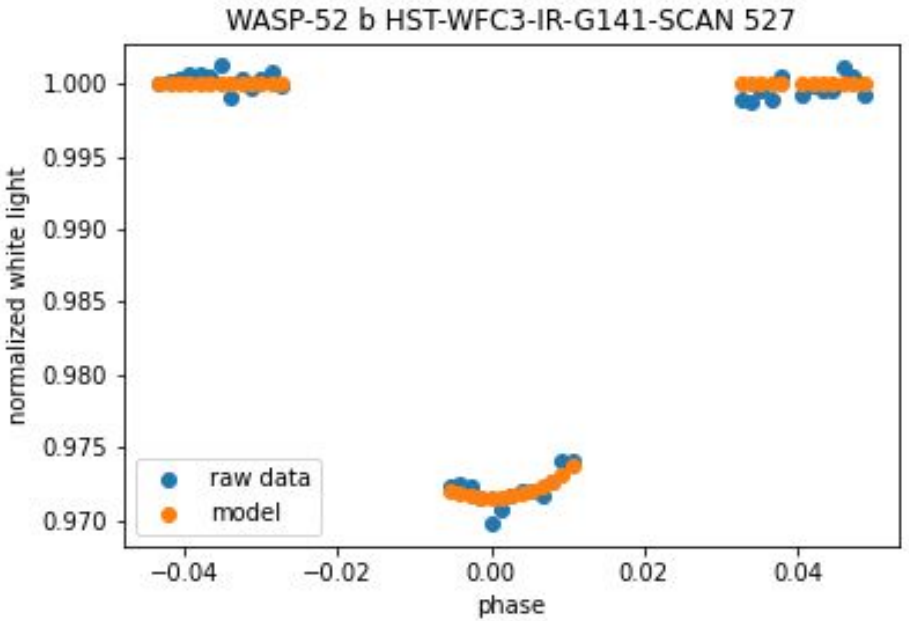
Steps

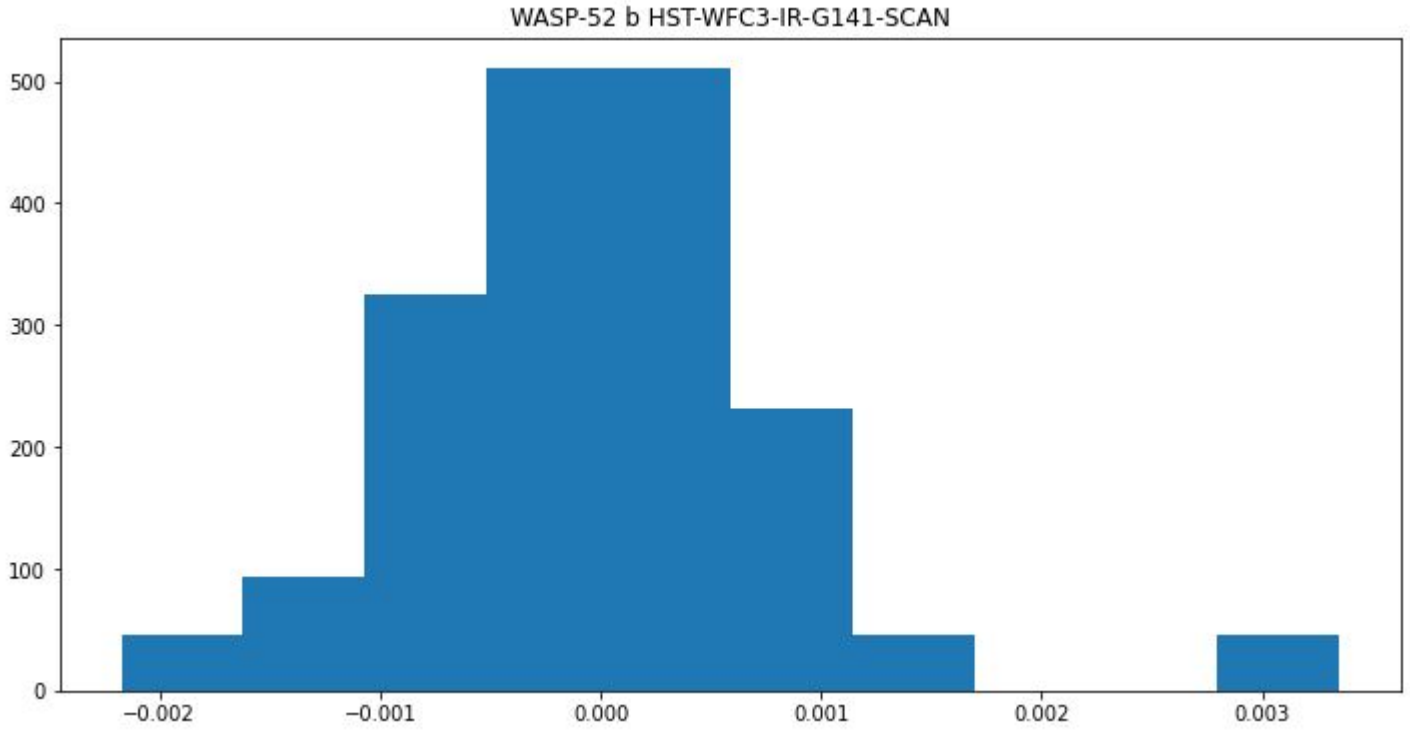
- Data simulation
- Feature development
- ML model exploration
- Feature selection
- Model selection

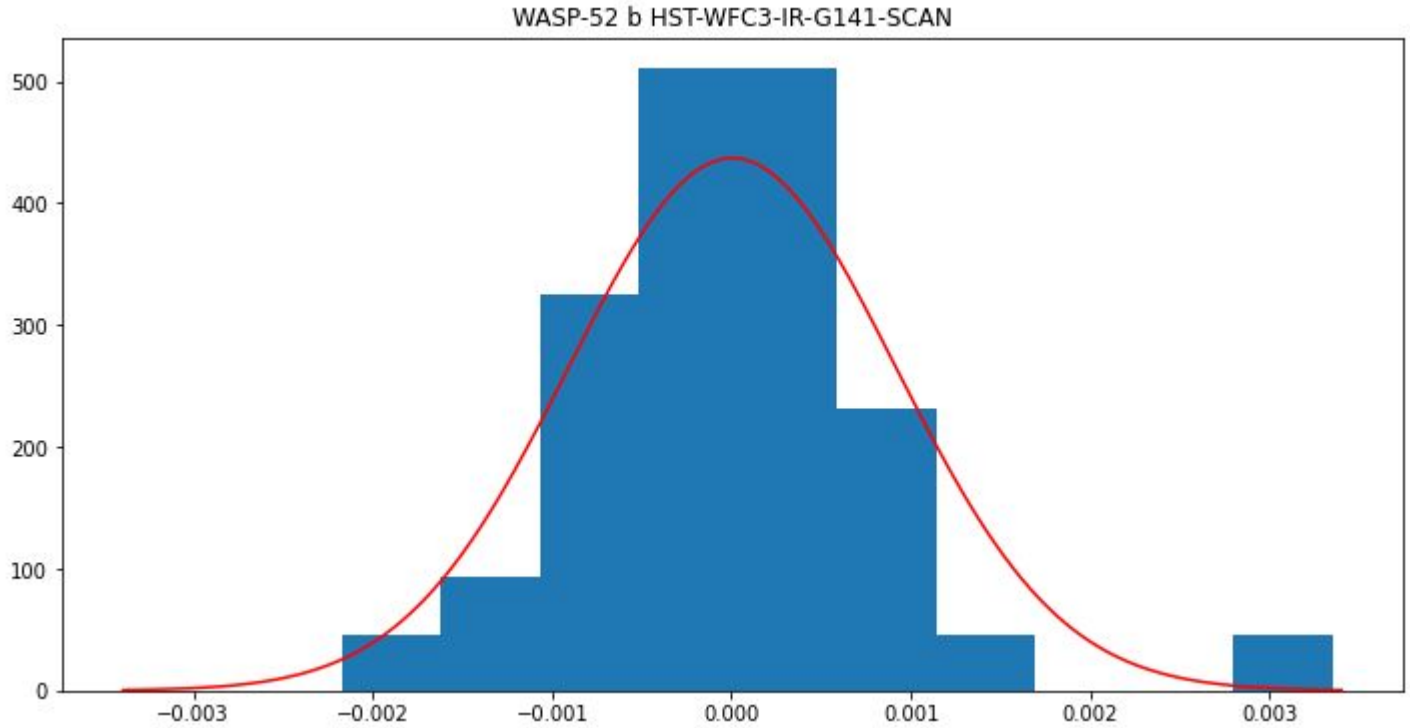
Data Simulation

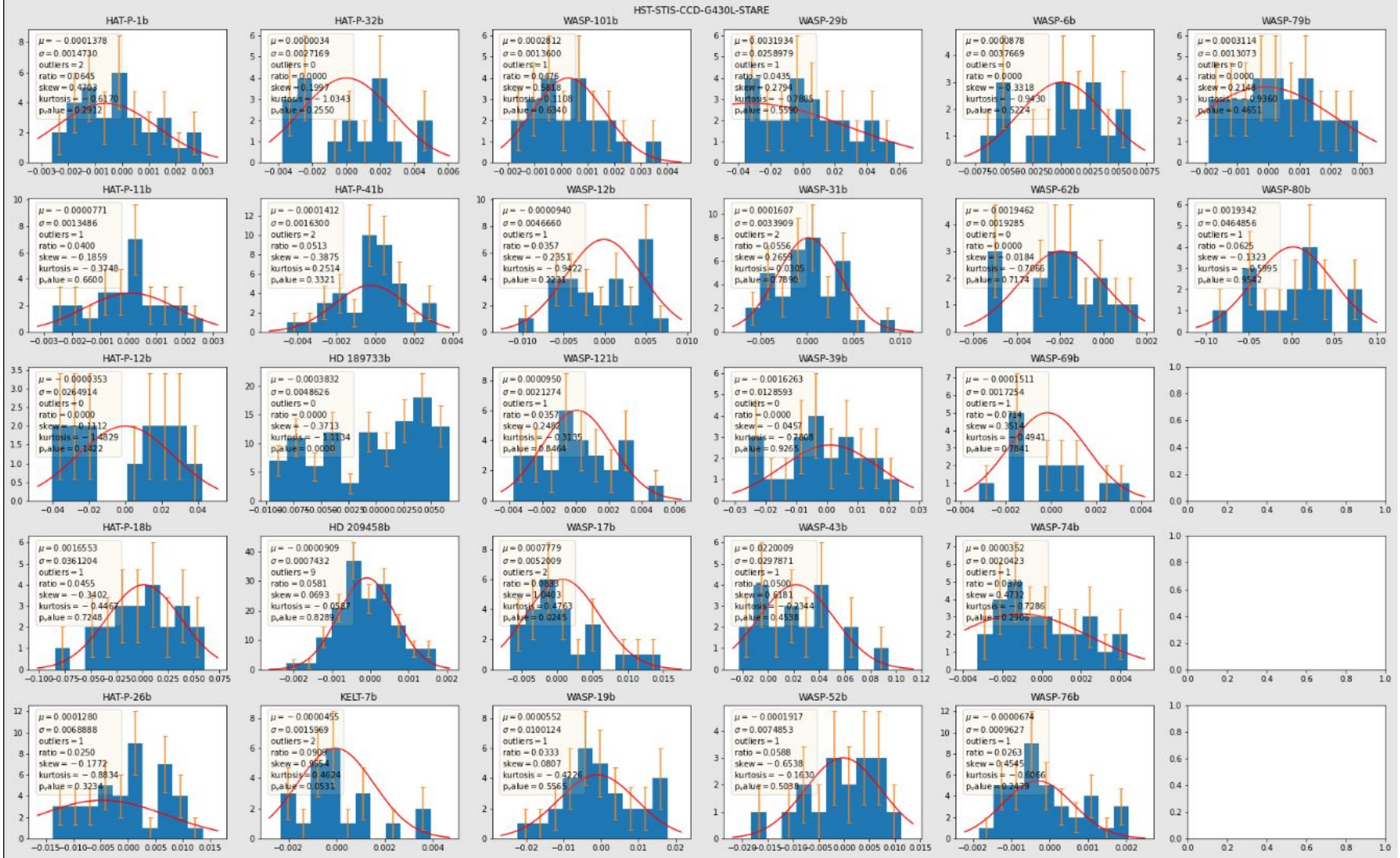
Approach to data simulation

1. Simulate residuals for each target
2. Add simulated residuals to model data points to create synthetic raw data
3. Repeat n times for each target

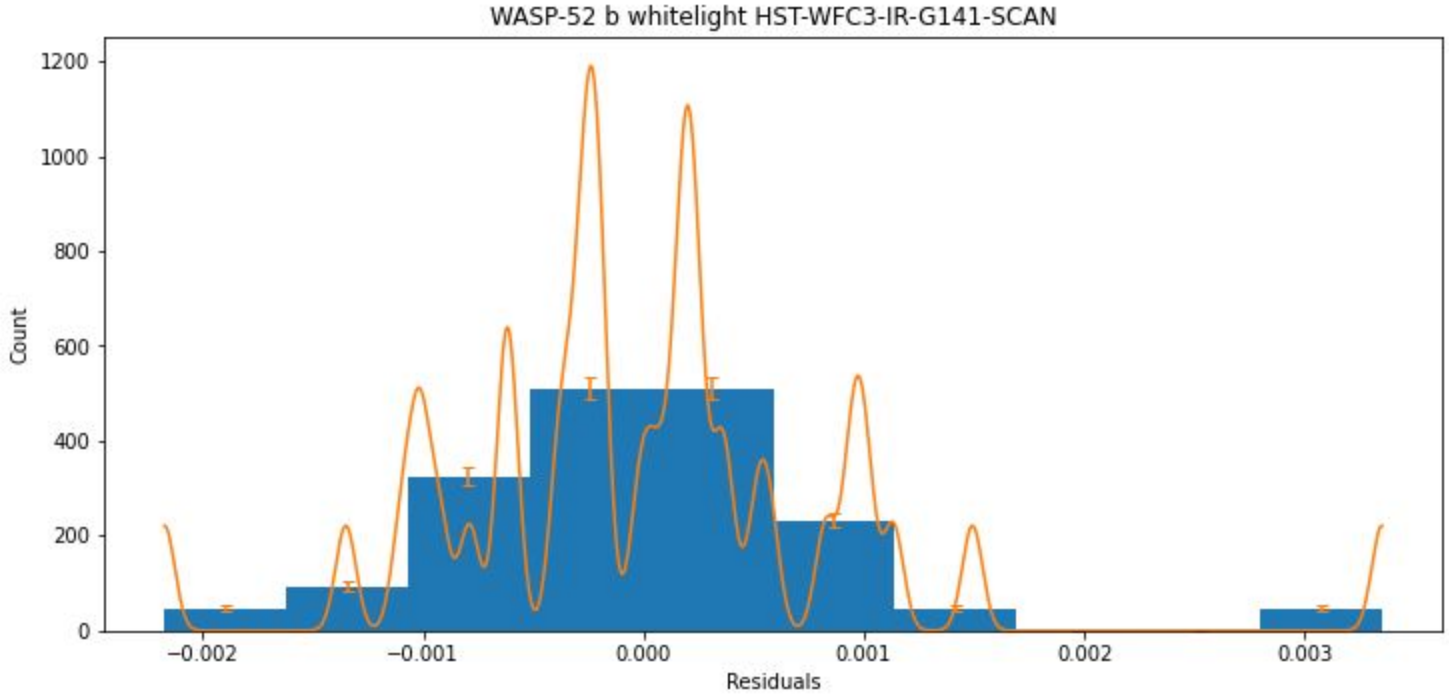


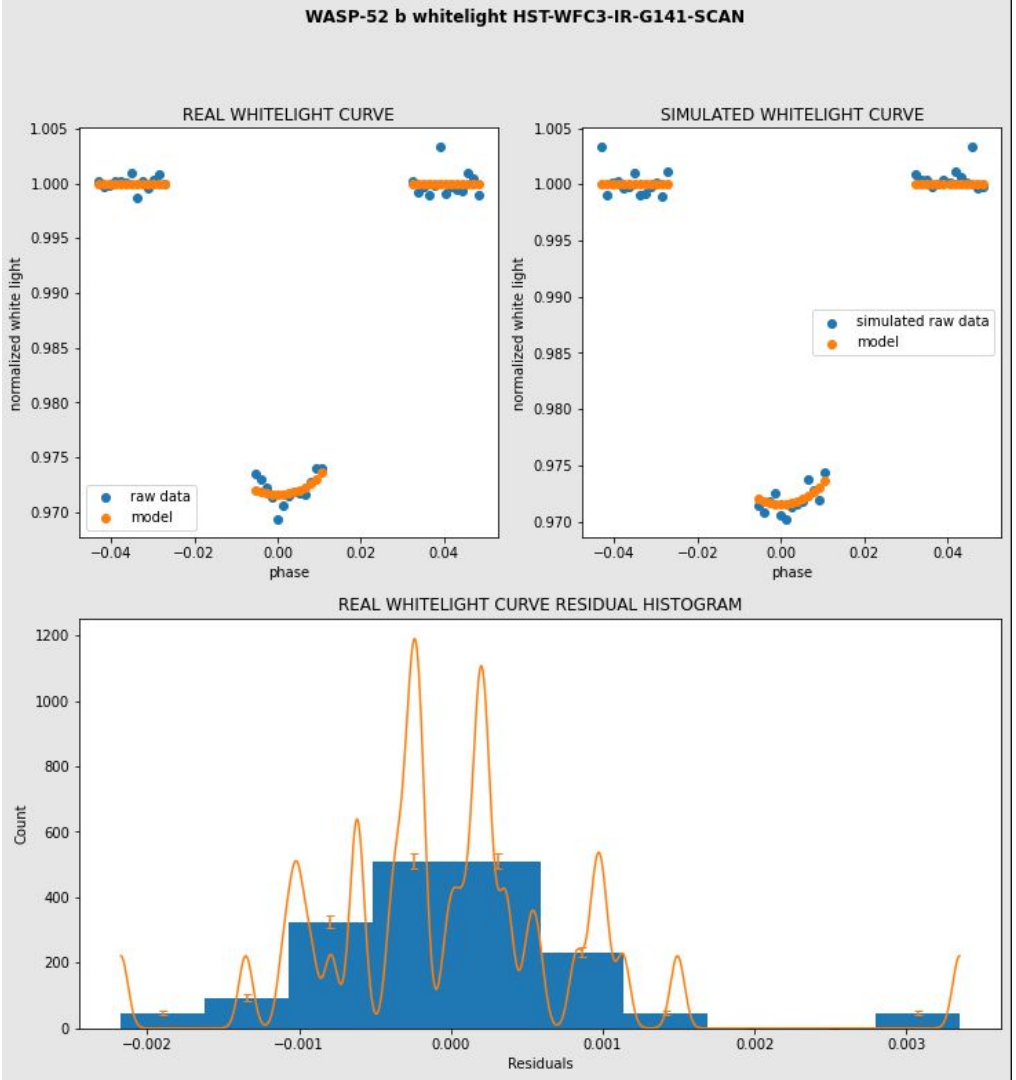

WASP-52 b HST-WFC3-IR-G141-SCAN
500
400
300
200
100
0
−0.002
−0.001
0.000
0.001
0.002
0.003


WASP-52 b HST-WFC3-IR-G141-SCAN
500
400
300
200
100
0
−0.003
−0.002
−0.001
0.000
0.001
0.002
0.003


HST-STIS-CCD-G430L-STARE
HAT-P-1b
μ = −0.0001378
σ = 0.0014730
outliers = 2
ratio = 0.0645
skew = 0.4703
kurtosis = −0.6170
p-value = 0.2912
HAT-P-32b
μ = 0.0000034
σ = 0.0027169
outliers = 0
ratio = 0.0000
skew = −0.1997
kurtosis = −1.0343
p-value = 0.2550
WASP-101b
μ = 0.0002812
σ = 0.0013600
outliers = 1
ratio = 0.0476
skew = 0.5818
kurtosis = 0.1108
p-value = 0.6340
WASP-29b
μ = 0.0031934
σ = 0.0258979
outliers = 1
ratio = 0.0435
skew = 0.2794
kurtosis = −0.7885
p-value = 0.5590
WASP-6b
μ = 0.0000878
σ = 0.0037669
outliers = 0
ratio = 0.0000
skew = −0.3318
kurtosis = −0.9430
p-value = 0.5224
WASP-79b
μ = 0.0003114
σ = 0.0013073
outliers = 0
ratio = 0.0000
skew = 0.2148
kurtosis = −0.9360
p-value = 0.4651
HAT-P-11b
μ = −0.0000771
σ = 0.0013486
outliers = 1
ratio = 0.0400
skew = −0.1859
kurtosis = −0.3748
p-value = 0.6600
HAT-P-41b
μ = −0.0001412
σ = 0.0016300
outliers = 2
ratio = 0.0513
skew = −0.3875
kurtosis = 0.2514
p-value = 0.3321
WASP-12b
μ = −0.0000940
σ = 0.0046660
outliers = 1
ratio = 0.0357
skew = −0.2351
kurtosis = −0.9422
p-value = 0.2231
WASP-31b
μ = 0.0001607
σ = 0.0033909
outliers = 2
ratio = 0.0556
skew = 0.2659
kurtosis = 0.0305
p-value = 0.7890
WASP-62b
μ = −0.0019462
σ = 0.0019285
outliers = 0
ratio = 0.0000
skew = −0.0184
kurtosis = −0.7866
p-value = 0.7174
WASP-80b
μ = 0.0019342
σ = 0.0464856
outliers = 1
ratio = 0.0625
skew = −0.1323
kurtosis = −0.5995
p-value = 0.9542
HAT-P-12b
μ = −0.0000353
σ = 0.0264914
outliers = 0
ratio = 0.0000
skew = −0.1112
kurtosis = −1.4829
p-value = 0.1422
HD 189733b
μ = −0.0003832
σ = 0.0048626
outliers = 0
ratio = 0.0000
skew = −0.3713
kurtosis = −1.1134
p-value = 0.0000
WASP-121b
μ = 0.0000950
σ = 0.0021274
outliers = 1
ratio = 0.0357
skew = 0.2492
kurtosis = −0.3135
p-value = 0.8464
WASP-39b
μ = −0.0016263
σ = 0.0128593
outliers = 0
ratio = 0.0000
skew = −0.0457
kurtosis = −0.7808
p-value = 0.9265
WASP-69b
μ = −0.0001511
σ = 0.0017254
outliers = 1
ratio = 0.0714
skew = 0.3514
kurtosis = −0.4941
p-value = 0.7841
HAT-P-18b
μ = 0.0016553
σ = 0.0361204
outliers = 1
ratio = 0.0455
skew = −0.3402
kurtosis = −0.4467
p-value = 0.7248
HD 209458b
μ = −0.0000909
σ = 0.0007432
outliers = 9
ratio = 0.0581
skew = 0.0693
kurtosis = −0.0587
p-value = 0.8289
WASP-17b
μ = 0.0007779
σ = 0.0052009
outliers = 2
ratio = 0.0833
skew = 1.0403
kurtosis = 0.4763
p-value = 0.0245
WASP-43b
μ = 0.0220009
σ = 0.0297871
outliers = 1
ratio = 0.0500
skew = 0.6181
kurtosis = −0.2344
p-value = 0.4538
WASP-74b
μ = 0.0000352
σ = 0.0020423
outliers = 1
ratio = 0.0370
skew = 0.4732
kurtosis = −0.7286
p-value = 0.2905
HAT-P-26b
μ = 0.0001280
σ = 0.0068888
outliers = 1
ratio = 0.0250
skew = −0.1772
kurtosis = −0.8834
p-value = 0.3234
KELT-7b
μ = −0.0000455
σ = 0.0015969
outliers = 2
ratio = 0.0909
skew = 0.9564
kurtosis = 0.4674
p-value = 0.0531
WASP-19b
μ = 0.0000552
σ = 0.0100124
outliers = 1
ratio = 0.0333
skew = 0.0807
kurtosis = −0.4726
p-value = 0.5565
WASP-52b
μ = −0.0001917
σ = 0.0074853
outliers = 1
ratio = 0.0588
skew = −0.6538
kurtosis = −0.1630
p-value = 0.5038
WASP-76b
μ = −0.0000674
σ = 0.0009627
outliers = 1
ratio = 0.0263
skew = 0.4545
kurtosis = −0.5066
p-value = 0.2479

Gaussian Kernel Density Estimate (KDE)



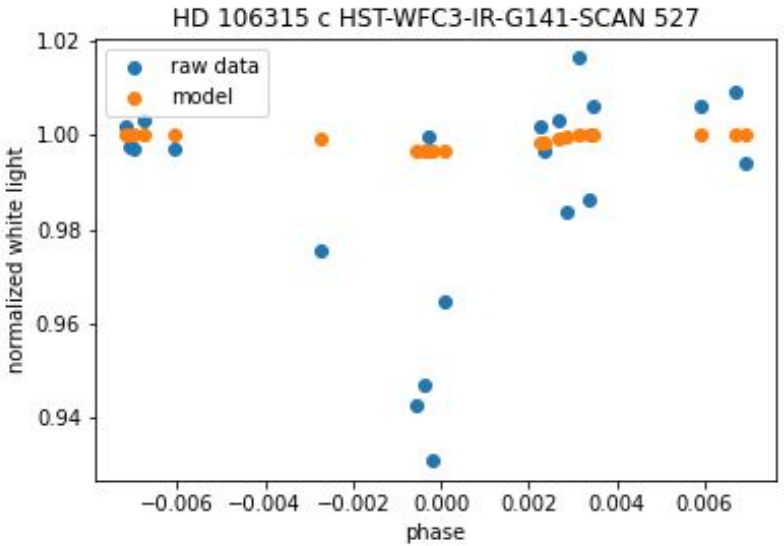

WASP-52 b whitelight HST-WFC3-IR-G141-SCAN
REAL WHITELIGHT CURVE
SIMULATED WHITELIGHT CURVE
normalized white light
phase
raw data
model
simulated raw data
model
REAL WHITELIGHT CURVE RESIDUAL HISTOGRAM
Count
Residuals

Feature Extraction

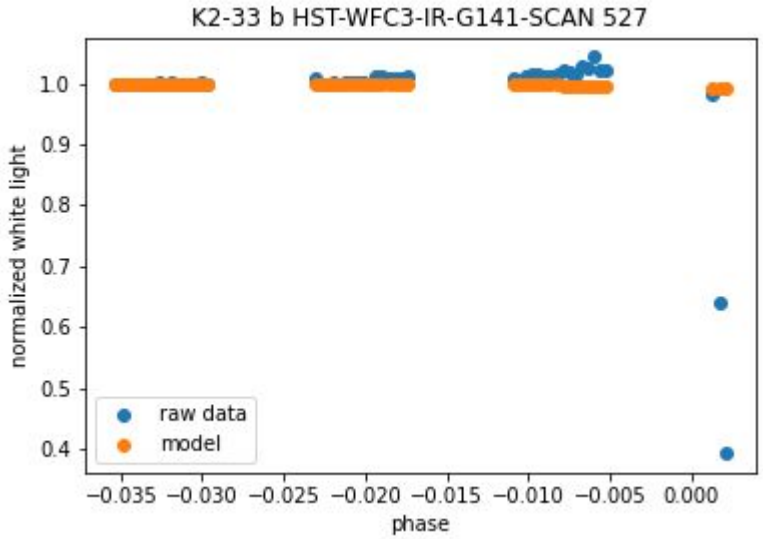
Qualities of a poorly modeled lightcurve

- Incorrect estimation of
  - Transit depth
  - Transit duration (Spitzer)
  - Transit time (Spitzer)
- Not enough points in transit
- Spectrum is too high variance

Transit Depth



Number of in-transit points



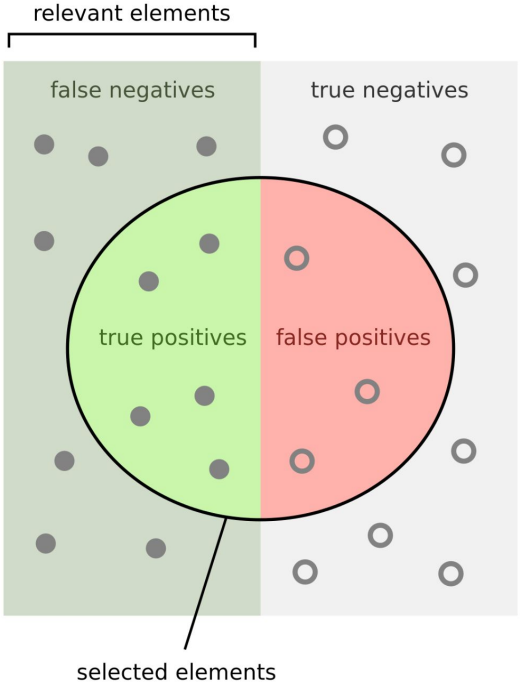
ML Model Development

ML Model Development

Imbalanced Classes (80% of examples are plausible)

- Random Forest Classifier
- Support Vector Machine
- Logistic Regression

How do you decide which model works best?



How many selected items are relevant?

$$\text{Precision} = \frac{\text{true positives}}{\text{selected elements}}$$

How many relevant items are selected?

$$\text{Recall} = \frac{\text{true positives}}{\text{relevant elements}}$$

https://en.wikipedia.org/wiki/Precision_and_recall

Model should maximize F1 Score

Occurs when precision = recall = 1

$$\text{F1 Score} = \frac{2 \times (\text{Precision} \times \text{Recall})}{\text{Precision} + \text{Recall}}$$

Feature Selection

Feature Selection

Narrows down the 30+ features created. Also selects the best model

2 Step Selection Process

- Iterative feature removal
- Subset feature selection

Features Chosen

Random Forest Model was chosen

Scale Height

- Standard Deviation vs Scale Height: Ratio of the standard deviation of a target's spectrum to its scale height

Raw Residuals

- Average Absolute Residual: The average value of the absolute value of the residuals for a target

Residual Z-Scores

- Absolute median residual z-score: The absolute value of the median of the z-scores for the residuals
- Median absolute residual z-score
- Median residual z-score

Model Performance

Model Performance on Simulated Training Data

F1 Score = 0.76

	Predicted Plausible	Predicted Implausible
Actually Plausible	1497	223
Actually Implausible	129	571

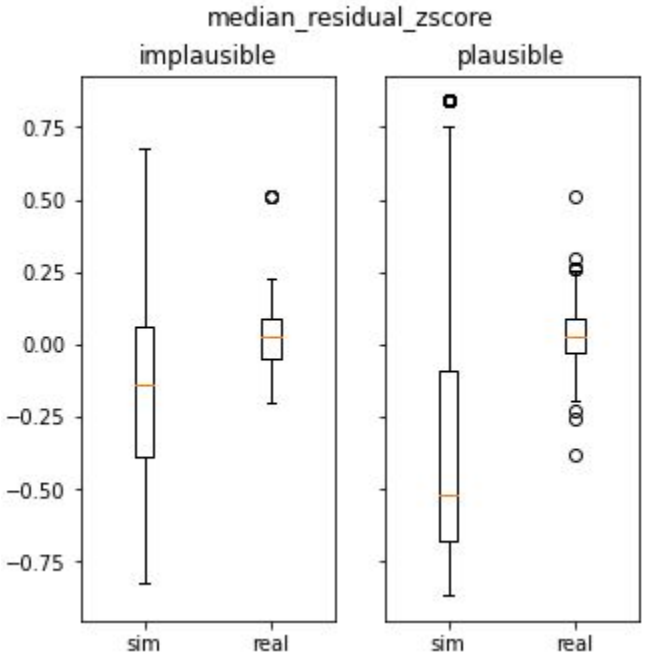
Model Performance on Real Test Data

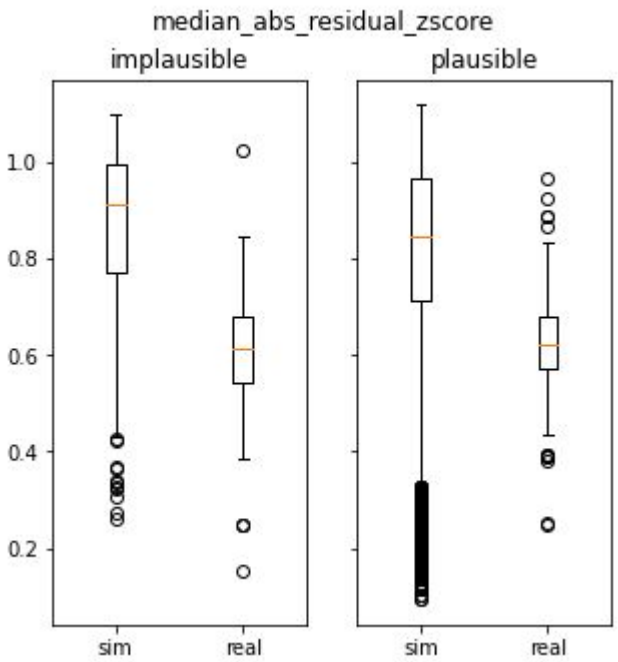
F1 Score = 0.38

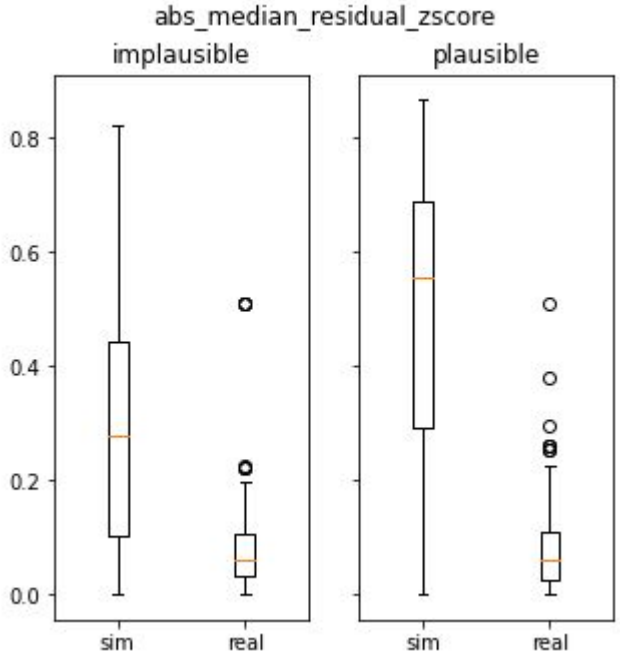
	Predicted Plausible	Predicted Implausible
Actually Plausible	118	161
Actually Implausible	45	64

Error Analysis

Feature Analysis

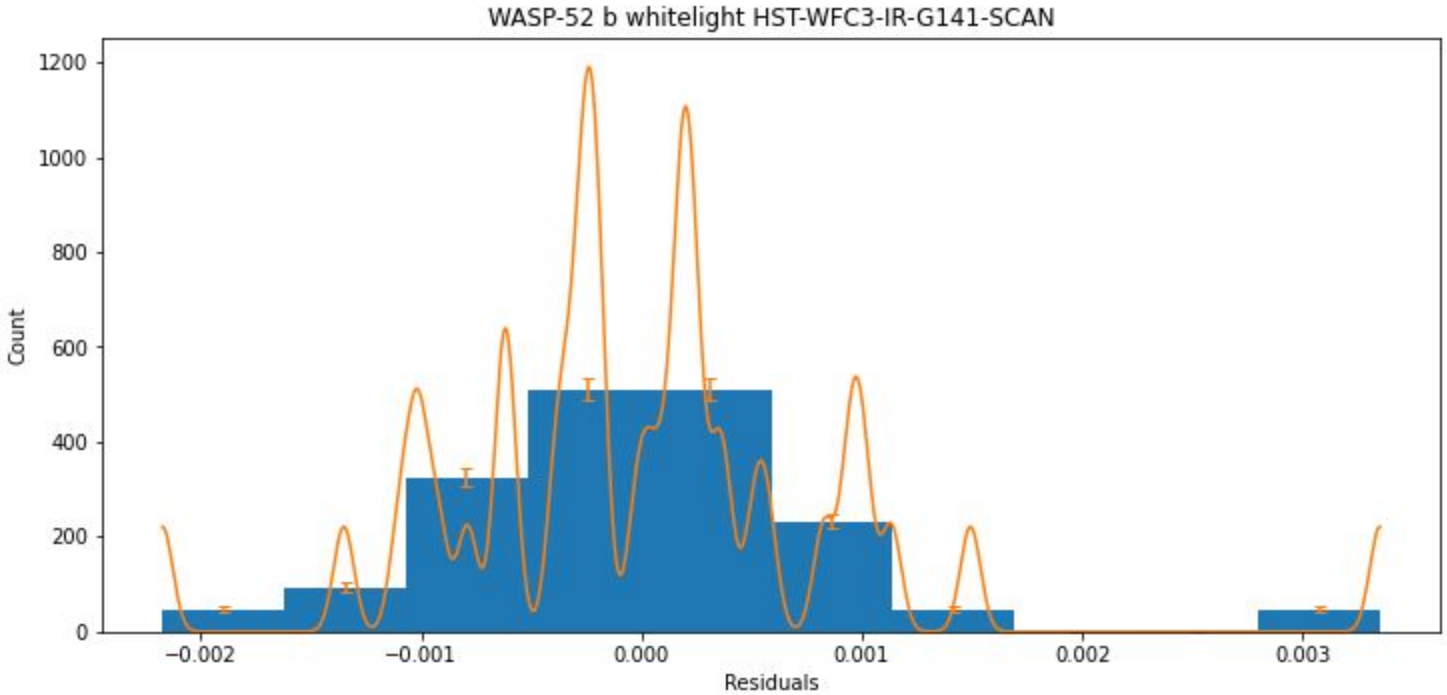



median_abs_residual_zscore
implausible
plausible
1.0
0.8
0.6
0.4
0.2
sim
real
sim
real

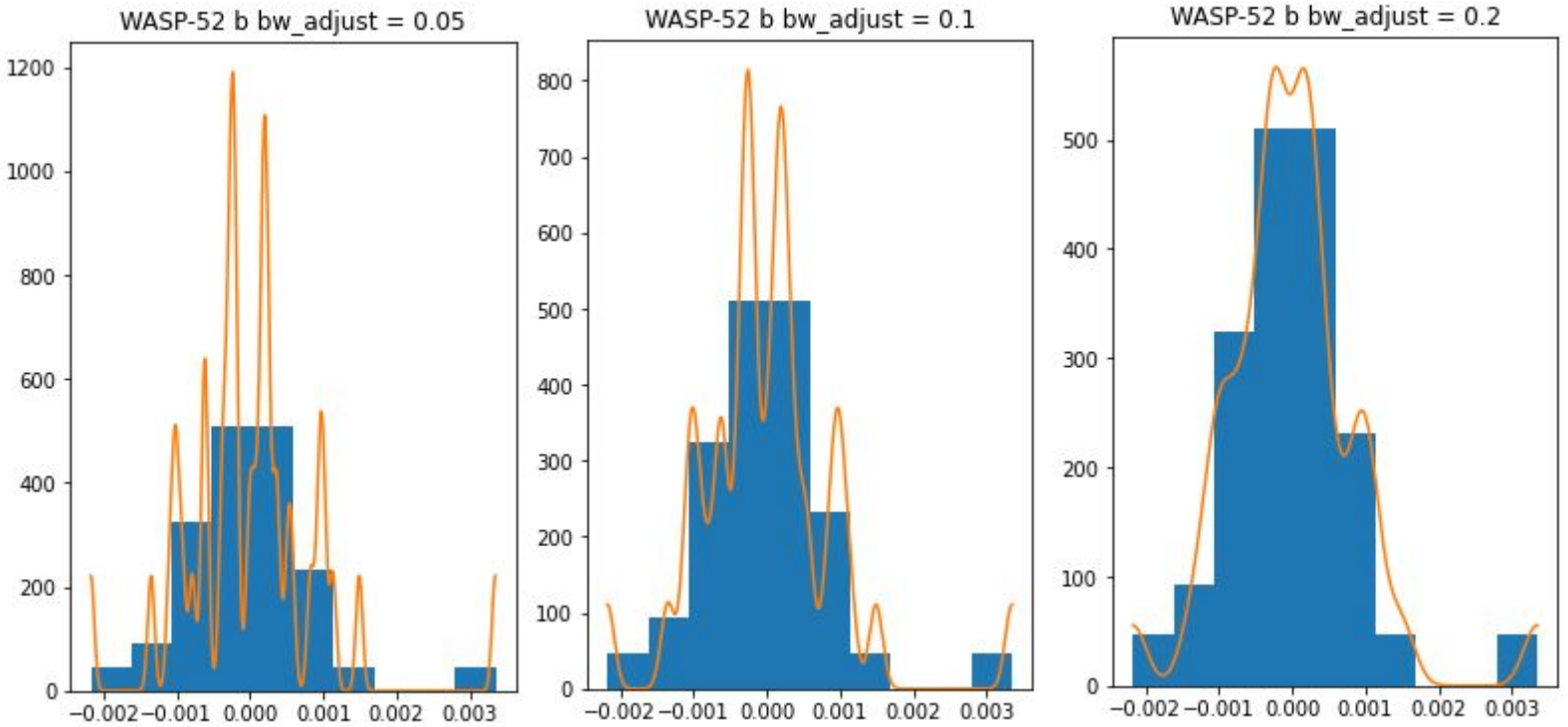

abs_median_residual_zscore
implausible
plausible
0.8
0.6
0.4
0.2
0.0
sim
real
sim
real

Future Steps

Improving the quality of data simulation



Varying bw_adjust



Project Accomplishments

Principal Achievements

- Laid the groundwork for future data simulation efforts
- Developed a larger set of potential features
- Created a robust and hands-off method for feature selection
- Maintained a modular codebase that can be easily altered/updated

Acknowledgements

- Virisha Timmaraju
- Dr. Mark Swain
- Dr. Gael Roudier
- JPL's Exoplanet Discovery Research Group
- JPL and Caltech's Summer Intern Program

Jet Propulsion Laboratory
California Institute of Technology

Subhash Kantamneni

A little about me

- Freshman at MIT studying Physics and Computer Science
- Originally from Jupiter, Florida
- Hobbies include reading, whistling, hiking, ultimate frisbee, and basketball
- Member of JPL's Exoplanet Discovery Research Group this summer