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PEEC: Spectroscopy of planet-host stars

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ABSTRACT

Aims. The accurate derivation of the stellar atmospheric parameters is important for stellar and exoplanet characterization. In this work, we present the foundation of an expansion of the ODUSSEAS tool to derive T_{eff} and [Fe/H] values for K stars.
Methods. We implement a new reference dataset that consists of values of T_{eff} and [Fe/H] for K stars, taken from the SWEET-Cat database. The stellar parameters are determined using the machine learning Python "scikit-learn" package by studying the correlation between the reference parameters and the pseudo-equivalent widths (EWs) of absorption lines in the spectra.
Results. We show that the new model can derive accurately and with precisions of $\sim$ 60 K for T_{eff} and $\sim$ 0.053 dex for [Fe/H] for K stars, although it could be improved with the use of a proper line list. We also test models using combinations of the new K stars reference dataset and the previous photometry and interferometry datasets for M dwarfs. The K stars + M dwarfs (photometry) model achieves high machine learning scores and has mean absolute errors of 49 K for T_{eff} and 0.047 dex for [Fe/H], although it underestimates the values of T_{eff}. The K stars + M dwarfs (photometry) model achieves high machine learning scores and has mean absolute errors of 63 K for T_{eff} and 0.053 dex for [Fe/H], which is less accurate, but more precise than the previous model at determining T_{eff}, but slightly worse for [Fe/H].

Key words. methods: data analysis— techniques: spectroscopic – stars: atmospheres – stars: fundamental parameters

1. Introduction

The determination of the effective temperature, T_{eff}, and metallicity, [Fe/H], of exoplanet host stars are crucial in exoplanet characterization, since the host stars' physical properties influence those of the transiting exoplanets (Loaiza-Tacuri et al. (2023)). For fainter stars, such as in the case of M dwarfs, these parameters are difficult to determine. The spectroscopic analysis of M dwarfs is more complicated compared to that of FGK stars because molecules are the dominant sources of opacity. The molecules create thousands of spectral lines with poorly known molecular line strengths. This makes it difficult to determine the position of the continuum in the spectra of M dwarfs.

A general approach to the determination of the effective temperature, T_{eff} and [Fe/H] in FGK stars is by measuring the equivalent width (EW) of many metal lines of the spectrum. However, for M dwarfs, this technique is adapted and the pseudo-EWs are measured by setting a pseudo continuum for each line (Neves et al. (2014)). In Antoniadis-Karnavas et al. (2020), the authors present ODUSSEAS [1](Observing Dwarfs Using Stellar Spectroscopic Energy-Absorption Shapes), a machine learning tool that quickly determines T_{eff} and [Fe/H] for M dwarfs using the stars' 1D spectra and resolutions as input. This tool, which makes use of the machine learning "scikit learn" package of Python, is based on a supervised machine learning algorithm, meaning that it is provided with both input and expected output and uses these to create a model. The input of the machine learning function is the values of precomputed pseudo-EWs for a set of HARPS spectra, depending on the reference selected, and the expected output is the values of their reference Teff and [Fe/H] from chosen literature studies.

In the latest version of the tool (Antoniadis-Karnavas et al. (2024)), there are two reference datasets for M dwarfs: "photometry" and "interferometry". In "photometry", the reference values of T_{eff} were taken from Casagrande et al. (2008), following the IRFM method modified for M dwarfs, and the reference values of [Fe/H] came from Neves et al. (2012), for a dataset of 65 stars. The "interferometry" reference uses a dataset of 47 stars with interferometry-based T_{eff} from Khata et al. (2021) and Rabus et al. (2019) and [Fe/H] derived with the method from Neves et al. (2012) using the updated parallaxes from GAIA RD3 (Collaboration et al. (2020)).

The machine learning code starts by training with part of the HARPS dataset selected, and then produces a model to test it on the rest of the data. It predicts the values of the stellar atmospheric parameters and compares them with the expected reference values, and so examines the accuracy and precision of the model. The model is then utilized to determine the stellar parameters of unknown spectra.

The tool of ODUSSEAS focuses only on extracting the stellar atmospheric parameters of M dwarfs. The purpose of this work is to extend this tool so that it is also able to determine T_{eff} and [Fe/H] of K stars [2]. This article is organized as follows: in Sect.2 we describe how ODUSSEAS measures the pseudo-EWs. In Sect.3, we describe the new reference dataset. In Sect. 4 we regard the machine learning efficiency for models with references from only the K stars dataset and combinations of the

[1] https://github.com/AlexandrosAntoniadis/ODUSSEAS.git

[2] This new version can be found on: https://github.com/ZMiguel2/ODUSSEAS_PEEC.git

K stars and M dwarfs datasets. Finally, Sect.5 summarizes the work done in this project.

2. Pseudo-EW measurement

The measurement of pseudo-EWs is done by setting a pseudo-continuum in each absorption line, since for M dwarfs it is very hard to determine the continuum of the spectrum, since many lines meld with each other. This is done by using the list of 4104 features from Neves et al. (2014), with left and right boundaries of where the absorption lines are created. In this line list, it was not included the parts where the activity-sensitive Na doublet and Hα lines and strong telluric lines reside (Antoniadis-Karnavas et al. (2020)). The code "HARPS_dataset.py" computes the pseudo-EWs of the stars present in the file "RefHARPSfilelist.dat". The outcome is a file with the values of the pseudo-EWs for each central wavelength where the absorption occurs and the reference values of T_{eff} and [Fe/H], for each star. This code was modified to make it all more organized and user-friendly; all of the changes in the code are included in the appendix section of this work Appendix B. The code starts by reading the line list and the 1D fits files of the spectra. In a certain interval where the absorption line is supposed to be, it is identified the position of the minimum of the flux, that is, the central absorption wavelength. After this, the code identifies the maximum on each side and traces the pseudo-continuum with a straight line, connecting these two points. The pseudo-EWs are obtained by calculating the area between the pseudo-continuum and the spectrum's flux:

$$pseudo - EWs = \sum \frac{(F_{pp} - F_{\lambda})}{F_{pp}} \Delta\lambda \qquad (1)$$

where F_{pp} is the value of the pseudo-continuum and F_{λ} is the flux of the line at each integration step. Figure 1 is a visual representation of this code.

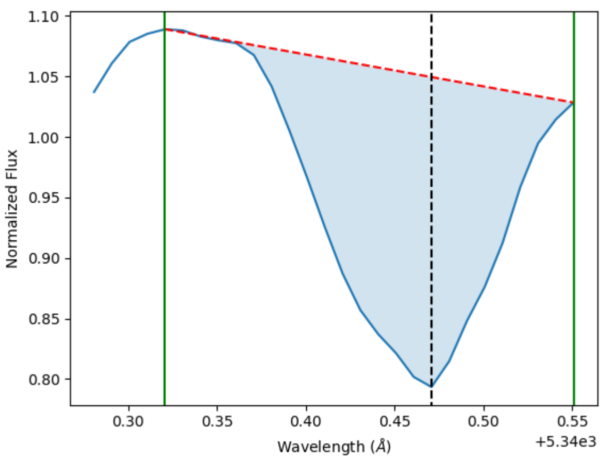

Fig. 1. Measurement of the pseudo-EW for a line with central λ = 5340.47Å of the star 75 Ceti. The green lines represent the interval given by the list of spectral lines from Neves et al. (2014). The pseudo-EW is equal to 24.18mÅ.

3. New reference scale

The goal of this project is to extend the ODUSSEAS tool to analyze the spectra of K stars and compute their stellar atmospheric parameters. For this, we need a new reference scale to train the machine learning code with the values of pseudo-EWs for each central wavelength and the expected values of T_{eff} and [Fe/H], for K stars. The reference values for T_{eff} and [Fe/H] were taken from the SWEET-Cat database (Santos et al. (2013)). We obtain a new K-stars reference scale using the HARPS-S spectra from 75 stars in the "HARPS_dataset.py" code. A few of those stars are M dwarfs, which will help us bridge the gap between M dwarfs and K stars. The new reference dataset is presented in the table A.1. The range of the reference stellar atmospheric parameters is presented in Fig. 2.

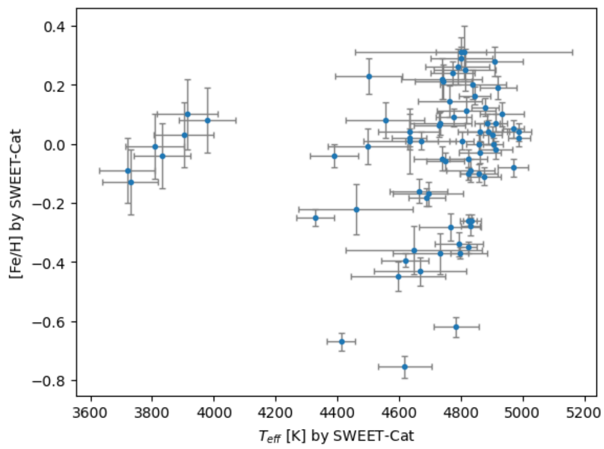

Fig. 2. Distribution of reference T_{eff} and [Fe/H] from the 75 K stars from SWEET-Cat.

This new reference ranges from 3720 to 4989 K for T_{eff} and from -0.755 to 0.31 dex for [Fe/H]. Users can select this new reference in the options by choosing the "kstar" reference.

4. Machine Learning efficiency

In order to study the machine learning efficiency, accuracy, and precision of this new reference dataset, we followed the steps of Antoniadis-Karnavas et al. (2020). This new dataset has 75 stars, so we changed the percentage of stars in the training group back to 70%, after it was changed to 80% in Antoniadis-Karnavas et al. (2024), to accommodate a study with fewer stars. In this work, we studied variations of the new reference dataset to make a more complete and precise tool that can account for K stars and M dwarfs.

The machine learning process aims to provide an output value, or prediction, by fitting a linear regression to the input variables. In our case, the predicted value is one of the stellar parameters, y, and the input variables are the values of the pseudo-EWs for each central wavelength, x. The relation is given as

$$y(w, x) = w_0 + w_1 x_1 + ... + w_p x_p \qquad (2)$$

where $w = \{w0, w1, ..., w_p\}$ are coefficients, determined differently depending on the regression model selected. Variables with higher coefficients will have more weight in the determination of the predicted parameter.

For this project, we worked with the "ridge" regression model, from the machine learning Python "scikit-learn" package, since it provided better results for M dwarfs (Antoniadis-Karnavas et al. (2020)). The "ridge" model improves the ordinary least squares (OLS) method. The OLS fits a model that minimizes the residual sum of squares between the reference values and the predictions:

$$w = \arg\min_{w} \sum_{i=1}^{N} (y_i - x_i w)^2 \tag{3}$$

The problem with this model is that it doesn't account for multicollinearity. In the case of two or more variables with a high linear correlation, the OLS method returns high coefficients. If one or more coefficients are too high, the model's prediction becomes too sensitive to minor differences in the input data, making the model unstable.

The ridge model penalizes the size of the coefficients:

$$w = \arg\min_{\omega} \sum_{i=1}^{N} (y_i - x_i w)^2 + \alpha \sum_{k=1}^{K} w_k^2 \tag{4}$$

for $a \geq 1$. This way, higher coefficients are more penalized than smaller ones, and the model prevents overfitting. An example of the fitting of the model is presented in Fig.3. For $\lambda = 5339.6$ Å, where there is a clearer correlation, the absolute value of w is higher than the one for $\lambda = 5340.2$ Å, where a correlation is not so evident.

4.1. K stars reference dataset only

First, we test to see if the new reference scale works, that is, if we were able to adapt ODUSSEAS for K stars. We calculated the machine-learning regression metrics of "explained variance" (E.V.) and "r2" scores, as well as the mean absolute errors of the models, for our new reference dataset. We test using a different set of stars on spectra from HARPS-N with known stellar parameters from SWEET-Cat. A plot with the reference and the predicted parameters of the model testing, as well as their differences, to represent the model's accuracy, is presented in Fig.4.

For this model, the E.V. score varies between 0.8552 and 0.894, with an average of 0.876, while the r2 score is between 0.842 and 0.888, and an average value of 0.867. These values are very similar to the "interferometry" model presented in Antoniadis-Karnavas et al. (2024), although that model has fewer stars. Still, these scores were deemed high enough to predict with sufficient precision and accuracy the stellar parameters of M dwarfs, so we use the same criteria for K stars.

The average of the mean absolute errors is around 60 K for T_{eff} and 0.053 dex for [Fe/H], and their dispersion values are 32 K and 0.042, compared to the average errors for the T_{eff} and [Fe/H] of the reference dataset, 65 K and 0.05 dex. The model is a bit more accurate at determining T_{eff}.

As presented in Fig. 4, the model underestimates temperatures below 4000 K, that is, for M dwarfs, since not many M dwarfs were used in the reference. To solve this, we will next add the previous references for M dwarfs to this new one.

Before that, we have to address a caveat of this model. While using the line list from Neves et al. (2014), we noticed that values of pseudo-EWs for some wavelengths and spectra had low values, close to zero. We made visual representations of the calculation of the pseudo-EWs, like how we did in Fig. 1, and saw that some of the lines weren't well defined for K stars. An example of this problem is presented in Fig.5.

Given that the line list was derived from the analysis of M dwarfs' spectra, it was bound to happen that some of the lines wouldn't exist or not be well defined for K stars. However, given

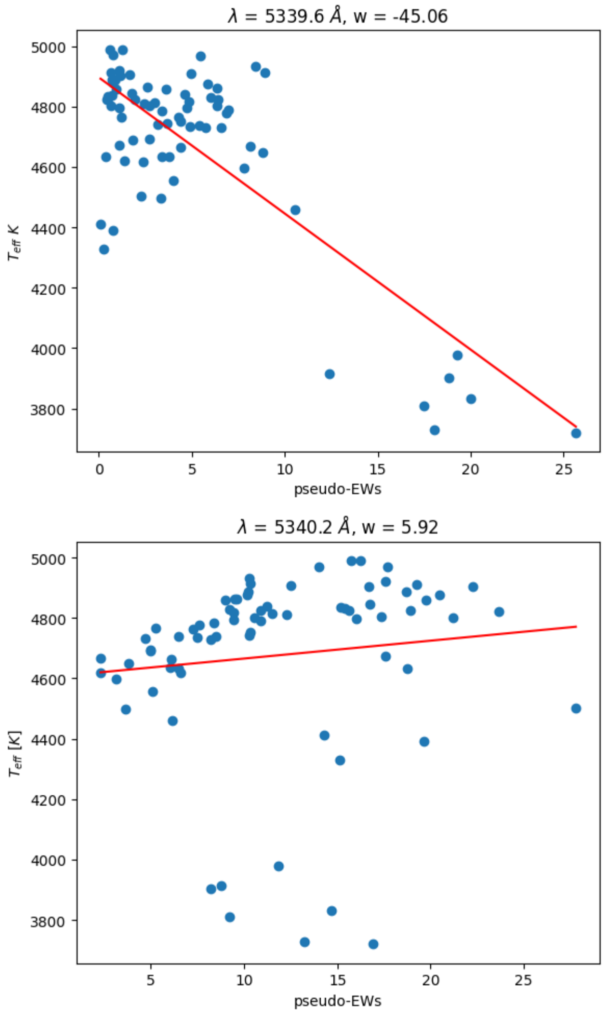

Fig. 3. Fitting done by ridge regression model between the values of pseudo-EWs and T_{eff}, for two different wavelengths. The parameter w represents the regression coefficient.

the results of this model, this doesn't seem to affect its prediction capability, given the high values of the E.V. score and r2 score. Still, two different analyses were done as an effort to improve the model and only work with well-defined lines.

First, looking at the values of the pseudo-EWs of the hottest K star, HD148427, we selected only the lines for which this star's pseudo-EWs > 5 mÅ. The thought was, if for the hottest star the following line is well-defined, then in principle it must be well-defined for all the other stars. Working with this reference of 881 lines, the new model has an E.V. score of 0.865 and an r2 score of 0.855, a bit lower than before.

The second approach was to look at the stars with [Fe/H] > 0. For each central wavelength, if around 10% of stars had a pseudo-EWs value inferior 5 mÅ, the line would be removed from the list. In the end, 954 lines from the original 4104 lasted. This model doesn't work well, as it has an E.V. score of 0.581 and an r2 score of 0.524.

These two approaches don't improve the model's efficiency. Despite being poorly defined, these lines contribute to the model's efficiency. Since we are working with a list of lines for M dwarfs, the intervals where some of the lines may change for K stars, or some lines may not exist at all. In future work, one should create a new list for existing lines of K stars.

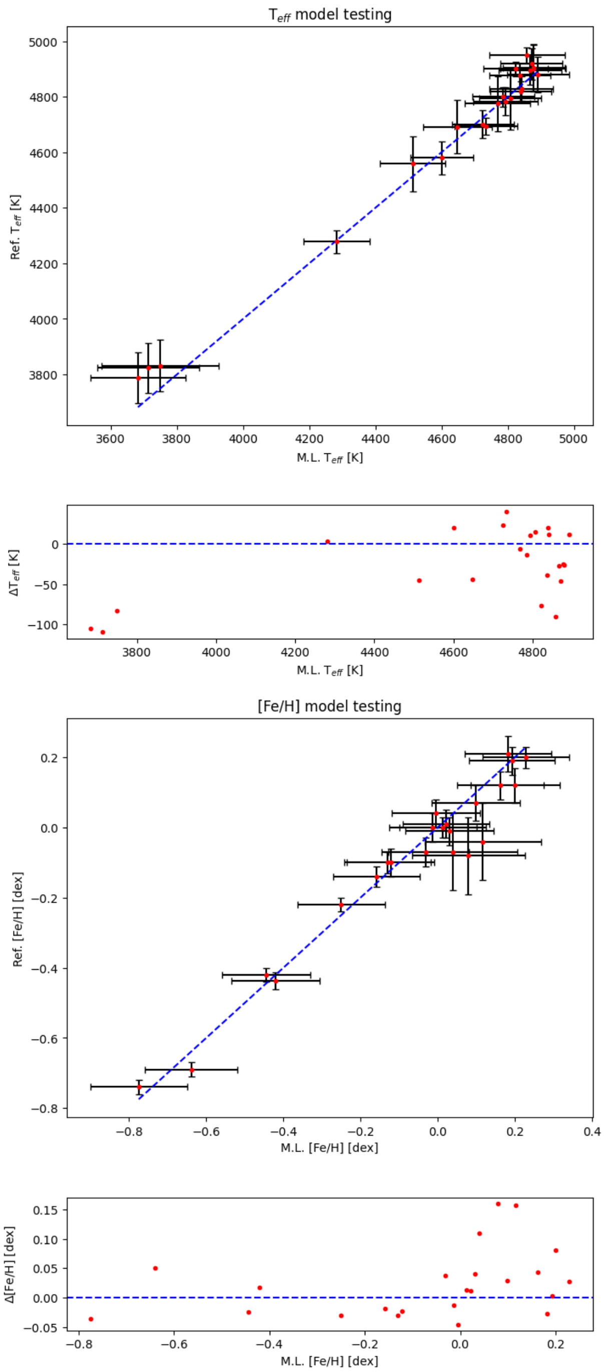

Fig. 4. Predictions of the machine learning code, using the K stars reference dataset, of the stellar atmospheric parameters of the stars on the HARPSN spectra. *Upper panel*: T_{eff} values expected (Ref.) and predicted (M.L.), with the residuals below. *Lower panel*: [Fe/H] values expected (Ref.) and predicted (M.L.), with the residuals below. The y-error bars are from the reference's errors, while the x-error values depend on the maximum between the standard deviation, wide error, and mean absolute error of the parameter at each point.

4.2. K stars + M dwarfs reference datasets

Given that HARPS spectra have a resolution of 115000, we joined the K stars reference dataset to the ones previously available for M dwarfs. First, we used the reference where the results come from spectra obtained with photometry (Antoniadis-Karnavas et al. (2020)). The results from this new dataset are presented in Fig. 6.

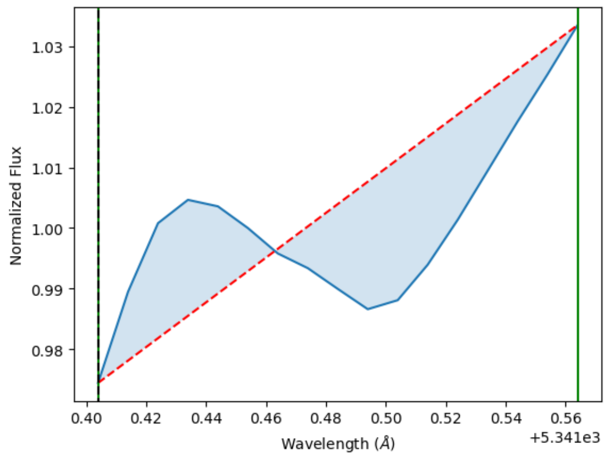

Fig. 5. Representation of the measurement of the pseudo-EW for a line with central λ = 5341.40Å of the star HD148427. The pseudo-EW is equal to 2.01mÅ.

This model has an average E.V. score of 0.941 and an average "r.2" score of 0.939, better than the previous model, as expected, since this model fits better for the M dwarfs present in the HARPS-N spectra. The average uncertainties of T_{eff} and [Fe/H] are 49 K and 0.047 dex, with dispersions of 38 K and 0.019 dex, respectively. While the [Fe/H] is slightly better predicted, these errors and looking at Fig. 6, the overall values of T_{eff} are underestimated, not only for M dwarfs, comparatively with the results from the K stars only model (Fig.4). This problem has been mentioned before in Passegger et al. (2022), that the photometry reference dataset underestimates the values of T_{eff} of M dwarfs. This seems to spread out to the K stars. The "interferometry" reference dataset was created in Antoniadis-Karnavas et al. (2024) in response to this problem for M dwarfs.

The "interferometry" dataset has fewer stars than the "photometry" reference (65 compared to 47, respectively), but the "interferometry" model obtains more accurate predictions (Antoniadis-Karnavas et al. (2024)). The predictions using the combination of the K stars and "interferometry" reference datasets are presented in Fig.7.

This model's average E.V. score is 0.934, and its average r2 score is 0.931, which are very similar to the previous model's. The average uncertainties of T_{eff} and [Fe/H] are 63 K and 0.053 dex, and dispersions of 23 K and 0.020 dex, respectively. These values and the results from Fig.7 show that this model is less precise, but is more accurate in determining T_{eff}, but slightly worse at determining [Fe/H] accurately.

A summary of all the results can be found in table 1.

5. Summary

In this work, we upgrade the tool ODUSSEAS for the derivation of T_{eff} and [Fe/H] in K stars. We provide an explanation on how ODUSSEAS calculates the pseudo-EWs values for each spectral line in the star's spectra. We present the range of T_{eff} and [Fe/H] in the new reference dataset, with reference values taken from SWEET-Cat database. We explain how the machine learning process works and measure different models' efficiency. The new dataset with reference parameters and pseudo-EWs measurements of K stars achieved high machine learning scores of around 0.87 and achieves predictions with mean absolute errors

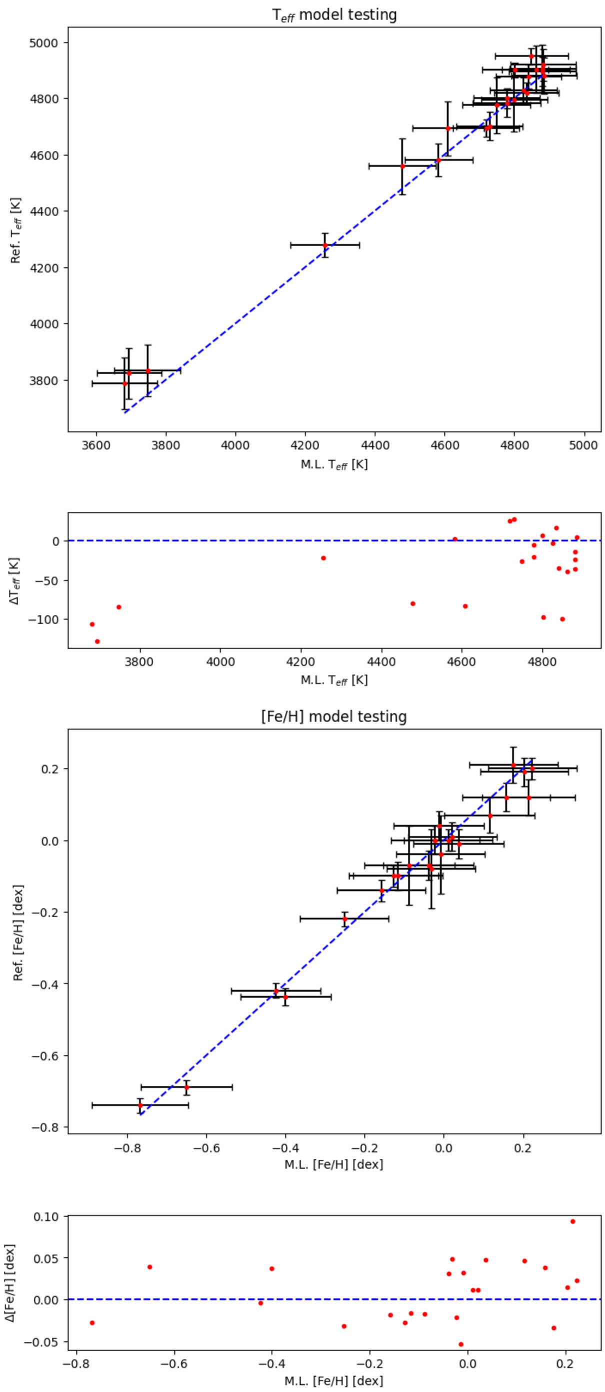

Fig. 6. Same plot as in Fig. 4, but using the K stars + Photometry reference scale.

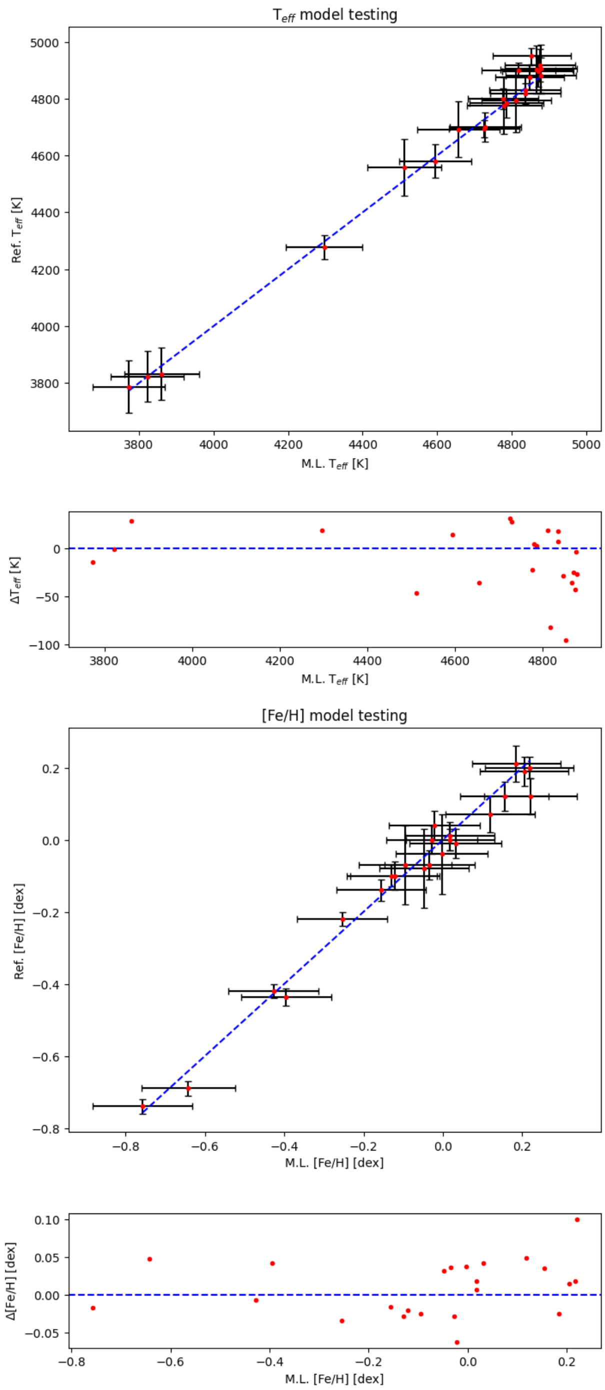

Fig. 7. Same plot as in Fig. 4, but using the K stars + Interferometry reference scale.

of ~ 60 K for T_{eff} and ~ 0.05 dex for [Fe/H]. Given that some lines are poorly-defined for some stars, in future work, we re-run ODUSSEAS with a new line list for K stars, as an effort to improve this model.

We test the models that use combinations of the K stars reference dataset and the available photometry and interferometry datasets, from previous works by Antoniadis-Karnavas et al. (2020) and Antoniadis-Karnavas et al. (2024), respectively. The K stars + photometry model has an average E.V. score of 0.941 and an r2 score of 0.939, and mean absolute errors of 49 K for T_{eff} and 0.047 dex for [Fe/H]. Despite this, this model underestimates the values for T_{eff}, which is a recognized problem for the photometry dataset. The K stars + interferometry model has an average E.V. score of 0.934 and an r2 score of 0.931, and mean absolute errors of 63 K for T_{eff} and 0.053 dex for [Fe/H]. This model is less precise than the previous one mentioned, but is more accurate at determining T_{eff}, but very slightly worse at determining [Fe/H]. We have established the basis for an expansion of the ODUSSEAS tool to determine the stellar atmospheric parameters of K stars. In a future work, besides creating the aforementioned new line list, we can use the results from this work and derive the stellar parameters from spectra of K stars with unknown parameters. Additionally, we can use this upgraded tool

Table 1. Average values of the scores, mean absolute errors (M.A.E) and range of errors of T_{eff} and [Fe/H], for each reference dataset model.

Ref. dataset	E.V. score	r2 score	M.A.E T_{eff} (K)	M.A.E [Fe/H] (dex)	Disp. T_{eff} (K)	Disp. [Fe/H] (dex)
K stars only	0.876	0.867	60	0.053	32	0.042
K stars + M dwarfs (photometry)	0.941	0.939	49	0.047	38	0.019
K stars + M dwarfs (interferometry)	0.934	0.931	63	0.053	23	0.020

to study the correlation between the planetary mass and stellar metallicity of K stars systems.

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Appendix A: New reference dataset for K stars

Table A.1. Reference values of the HARPSS spectra used in the reference dataset "kstar".

Star	[Fe/H] (dex)	T_{eff} (K)
11Com	-0.26	4824
7CMA	0.24	4773
75Cet	0.03	4903
81Cet	0.0	4859
91Aqr	0.01	4673
BD-082823	0.01	4635
BD-114672	-0.36	4648
BD-1763	0.08	4555
epsTau	0.19	4921
GJ3998	-0.13	3729
GJ649	-0.09	3720
GJ676A	0.08	3978
HD100655	0.07	4887
HD102272	-0.35	4823
HD103720	-0.02	4914
HD104067	-0.05	4824
HD110014	0.23	4502
HD114386	-0.1	4859
HD125595	0.04	4633
HD128356	0.26	4789
HD148427	0.04	4989
HD162020	-0.06	4751
HD1690	-0.25	4328
HD181433	0.31	4810
HD189733	-0.08	4969
HD192263	-0.11	4876
HD20868	0.07	4734
HD215152	-0.09	4830
HD215497	0.28	4908
HD218566	0.21	4744
HD27442	0.31	4801
HD27894	0.25	4813
HD330075	0.04	4888
HD33142	0.02	4989
HD40307	-0.34	4795
HD4313	0.05	4971
HD47366	0.0	4905
HD47536	-0.67	4412
HD5319	0.07	4912
HD5891	-0.37	4796
HD63454	0.09	4777
HD93083	0.1	4933
HD99492	0.2	4839
HIP5158	0.22	4738
HIP63242	-0.28	4832
HIP67851	0.01	4803
NGC24233	0.02	4633
SAND364	-0.04	4390
WASP-69	0.29	4802
GJ9827	-0.45	4597
epsIndA	-0.17	4694
gammaLib	-0.26	4836
GJ143	-0.01	4497
HD23472	-0.16	4664

Table A.2. Table A.1 cont.

Star	[Fe/H] (dex)	T_{eff} (K)
HD103949	-0.05	4739
HD8326	0.04	4863
HIP36985	-0.01	3809
HIP38594	0.03	3903
HIP4845	0.1	3915
GJ740	-0.04	3832
HD22496	-0.223	4460
HD29399	0.163	4845
HD360	-0.1	4826
TOI-431	0.063	4730
TOI-2194	-0.394	4620
GJ9714	-0.432	4668
HD125271	-0.181	4690
HD168863	0.113	4817
HD16905	0.144	4764
HD29985	-0.372	4732
HD86065	-0.031	4862
HIP35965	-0.62	4785
HIP948	-0.755	4618
nuOctA	0.124	4878
HIP54597	-0.283	4765

Appendix B: Changes in ODUSSEAS code

Appendix B.1: HARPS_dataset.py

- Line 11: "convolve_now = False" (or True) instead of "convolve_now = "yes"".
- Line 18: Included "if convolve_now == True:" to prevent unnecessary convolution.
- Line 55: Changed the index from 1 to 4, due to changes in the paths.
- Line 116: Changed to "if convolve_now == True:" because of the change to boolean values.
- Line 122: "name_of_input = "Files/RefHARPSfilelist.dat"" because the file it is now in the path "Files".
- Line 132: Same change as in Line 122.
- Line 136: Same change as in Line 122, this time for the "lines.rdb" file.
- Lines 140-141: Included an intermediary results folder to save the datasets used along the code, to organize everything more neatly.
- Line 167: Minor change from "spectra" to "Spectra" in the path.
- Line 173: Include the intermediary results path, since the dataset is there now.
- Lines 183-184: Same change as in Line 122, this time for the "centrallines.dat" file.
- Lines 193,198,205: Same change as in Line 173.
- Removed line 210 of the original code.
- Line 210: Same change as in Line 122, this time for the "Refparameters.dat" file.
- Line 212: The "Refparameters.dat" file used already has a "starname" column, making this line useless.
- Line 215: Same change as in Line 173.
- Line 222: Changed merging from "outer" to "inner", because otherwise the final dataset would come be deorganized.
- Line 223: There isn't a "Star" column no more.
- Lines 225-228: Included a final results folder/path.

Appendix B.2: machinelearning.py

- Line 61: Changed test_size=30 .

Appendix B.3: main.py

- Line 17: " help = "... or 'kstar' for K stars only reference." "

Appendix B.4: utils.py

- Line 30-32: Included provisional errors for the "kstar" reference. This in the future will be updated with realistic values.
- Line 83: Included "kstar" reference.