

Physical parameter estimates of M-type stars: a machine learning perspective.

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ABSTRACT

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Modelling – Learning from BT-Settl spectra library

TODO: Luis, cambiar spectral libraries por stellar atmosphere models o synthetic spectral libraries.

1. Introduction

2. Methodology.

The objective addressed in this Section is to develop an automated procedure to identify spectral bands that yield good atmospheric temperature, gravity and metallicity (hereafter physical parameters) diagnostics for M type stars. Given the lack of a calibration set of benchmark stars with observed spectra and homogeneous coverage of the space of physical parameters, we must turn to synthetic libraries of spectra. Furthermore, only temperatures and gravities can be calibrated independently of the spectra (for example as in Ségransan et al. 2003, using interferometry): all metallicity estimates in the literature are based on collections of synthetic spectra, and therefore spectral synthesis codes are the only resource to construct regression models. Even in the case of interferometry, the estimates of radii (and therefore gravity) depend on stellar models (although less strongly) via the limb darkening corrections.

As an alternative to the methods based on genetic algorithms used in this work, the atomic or molecular line/band parameters can be used in principle to select the spectral features that are more sensitive to changes in the physical parameters as in Passegger et al. (2016). However, the suitability of spectral features as diagnostics of the stellar atmospheric properties depends not only on the individual behaviour of each line/band, but also on the relative properties of neighbouring features in the same spectral region, that may overlap depending on the spectral resolution. Furthermore, good spectral diagnostics at a given signal-to-noise ratio (SNR) may show a severely degraded predictive power in the low SNR regime. Therefore, we propose an alternative selection approach that takes the resolution and SNR ratio

into account, to assess the utility of spectral features for the task of inferring physical atmospheric parameters.

In the following, we adopt the BT-Settl library of synthetic spectra (Allard et al. (2013)) as the framework where spectral diagnostics will be searched for. These synthetic spectra were pre-processed in several steps as described below.

2.1. Spectral preprocessing

First, and in order to define good temperature diagnostics, spectra between 2000 and 4200K in steps of 100 K were selected, with $\log(g)$ in the range between 4 and 6 dex (when g is expressed in cm/s^{-2}), in steps of 0.5 dex. The metallicity of the representative spectra was restricted to the set 0, 0.5 and -1 dex. This yields a total set size of 535 available spectra.

A series of preprocessing steps were then carried out in order to match the spectral resolution and wavelength coverage and sampling of the synthetic library to that of the collection of observed spectra (IPAC or IRTF, see below). This required the definition of a common wavelength range present in all available observed spectra, and the subsequent trimming to match that range. A unique wavelength sampling was also defined and all spectra (synthetic and observed) interpolated to match the sampling. Finally, all spectra, both synthetic and observed were divided by the integrated flux in order to factor out the stellar distance.

In order to avoid selecting spectral features that are good predictors only in the unrealistic $\text{SNR}=\infty$ regime, the search for optimal diagnostics of the atmospheric parameters of M stars was carried out for three SNR values (10, 50 and ∞) by degrading the synthetic spectra with Gaussian noise of zero mean. These values were found to be sufficient in a wide range of experiments carried out in parallel and described in . The special $\text{SNR}=\infty$ case has been retained for the sake of completeness although show that training sets derived from noiseless spectra are, at best, unnecessary, and at worst damage performance severely.

2.2. Feature definition and selection

As mentioned in Sect. 1, defining good spectral diagnostics for the prediction of atmospheric physical parameters of M stars is an extremely difficult task.

The work in Cesetti et al. (2013) defined wavelength regions in the I and K bands optimal for the diagnostic of physical parameters based on the sensitivity exhibited by the flux emitted in these segments to changes of the physical parameters. The sensitivity was measured in terms of the derivative of the flux with respect to the physical parameter. The approach adopted here is to select spectral features that yield the best accuracy when used as predictive variables in a regression model that estimates the stellar atmospheric physical parameters (T_{eff} , $\log(g)$ and metallicity). The evaluation of the accuracy of the estimates produced from a subset of features is described further below. We consider the effective temperature as the dominant parameter influencing changes in the stellar spectra (a strong feature) and thus, it was estimated first, and then used as input in the regression models for the gravity and metallicity.

Here, a feature F is defined as

$$F = \int_{\lambda_1}^{\lambda_2} \left(1 - \frac{f(\lambda)}{F_{cont}}\right) \cdot d\lambda \quad (1)$$

where $f(\lambda)$ denotes the normalized flux from the star at wavelength λ , and where F_{cont} is the average flux in a spectral band between $\lambda_{cont;1}$ and $\lambda_{cont;2}$. We explain below how we search for the band definitions that produce physical parameter predictions with the smallest errors.

Another type of features defined as

$$F' = \frac{\int_{\lambda_1}^{\lambda_2} f(\lambda) \cdot d\lambda}{\int_{\lambda_3}^{\lambda_4} f(\lambda) \cdot d\lambda} \quad (2)$$

were considered, where $\lambda_1, \lambda_2, \lambda_3$, and λ_4 delimit two spectral bands such that the ratio of the integrated fluxes in the two bands is hoped to be a good predictor (alone or in combination with other features) of the star atmospheric physical parameters. The results obtained with this alternative feature definition did not differ significantly on average from the ones observed with the one adopted in Eq. 1, and including them here would result in an excessively lengthy paper. In view of the equivalent global performances, we preferred the former because it allows direct comparison with the features proposed by Cesetti et al. (2013).

We used Genetic Algorithms (hereafter GAs) to solve the optimization problem described above, that is, the problem of finding the features (band boundaries) that minimize the prediction error of a regression estimate of the physical parameters. We used the implementation of genetic algorithms publicly available as the R (R Core Team 2013) GA package. The concept of using in-silico evolution for the solution of optimization problems was introduced by Holland (1975). Although its application is now reasonably widespread (Goldberg et al. 1989, see e.g.), they became very popular only when sufficiently powerful computers became available. GAs were presented to the astronomical community in Charbonneau (1995), and have been used extensively in the past (see , for the last application of GAs in astronomy at the time of writing).

For the sake of simplicity let us define Genetic Algorithms (GAs) as search algorithms that are based on the principle of evolution by natural selection. The procedure works by evolving in the sense explained below, chromosomes (in our case, sets

of spectral features as defined by Eq. 1) from an initial random population. Evolution proceeds via cycles of differential replication, recombination and mutation of the fittest chromosomes. The concept of fittest is context dependent, but in our case fitness is defined in relation with the accuracy with which a given chromosome (a set $\{F_i\}$ of spectral features) predicts the physical parameters.

The data set used to search for the optimal set of spectral features will be, as mentioned before, the BT Settl collection of synthetic spectra, where each spectrum is tagged with the effective temperature, gravity and metallicity of the model atmosphere from which the spectrum emerged.

The implementation of the GA comprises the following steps:

- **Stage 1:** Definition of the population of potential features (chromosomes).
- **Stage 2:** Each chromosome in the population is evaluated by its ability to predict the physical parameters of each star in the dataset (fitness function).
- **Stage 3:** Chromosome selection. The new generation of individuals is initialised by transferring a number of the most fitted ones in the previous generation. The percentage of individuals transferred is known as the degree of elitism.
- **Stage 4:** The population of chromosomes is replicated. Chromosomes with higher fitness scores will generate more numerous offspring.
- **Stage 5:** The genetic information contained in the replicated parent chromosomes is combined through genetic crossover. Two randomly selected parent chromosomes are used to create two new chromosomes.
- **Stage 6:** Mutations are then introduced in the chromosome randomly. These mutations produce new genes used in chromosomes. Steps 5 and 6 are applied over the chromosomes established at Step 4.
- **Stage 7:** This process is repeated from Stage 2 until a target accuracy is achieved or the maximum number of iterations is attained.

We test features defined by bands (the numerator and denominator of Eq. 1) that comprise ten consecutive bins (fluxes) of a spectrum. The bands tested in different features may overlap by as much as 5 consecutive bins (which in practice implies that we define the first feature as the spectral chunk between wavelength bins $i = 1$ and $i = 10$, the second feature between bins $i = 6$ and $i = 15$, the third feature between bins $i = 11$ and $i = 20$, etc). The spectral bands in the numerator and denominator of a test feature cannot overlap.

It would be possible to evaluate the predictive performance of individual features defined with Eq. 1. An obvious conceptual limitation of this univariate approach (considering chromosomes that code a single predictive feature) would be the lack of consideration that features work in the context of interconnected pathways and, therefore, it is their behavior as a group that has to be evaluated in terms of the predictive accuracy. In other words, a single feature can yield a poor predictive performance alone, but improve very significantly the prediction accuracy when used in combination with other features. Multivariate selection methods thus seem more suitable for the analysis of the regressors since variables are tested in combination to identify interactions between features. In this work we define a chromosome as a set of ten individual genes, and each gene codes a pair of non-overlapping spectral bands, the ratio of which is used as predictor of the physical parameters according to (1).

The population size was set to 8000 individuals and the maximum number of accepted iterations set to 4000. We produced three randomly started populations so as to provide enough initial variety. The crossover and mutation probabilities were set to 0.85 and 0.35 respectively. Elitism was fixed to 0.15. We used a binary codification of the chromosomes and a parallel implementation of the GA in a farm of fifteen computers per physical parameter¹

Feature fitness was defined in terms of the Akaike Information Criterion (AIC) for linearity between the potential feature against the physical parameter. **TODO: RMSE? Why AIC?**

It is important to stress that the regression model used to evaluate the fitness of the feature sets (chromosomes) is not the same model that will be used in practice to predict physical parameters for observed spectra as described in Section 2.3 below. For fitness evaluation in the GA we used a simple multilinear model for the sake of speed, given the extreme size of the search space of all possible combinations of 10 spectral features. In the IRTF context, these 10 features in each chromosome are selected amongst the roughly 6000 potential features. This is $\binom{6000}{10}$ which has an order of magnitude of 10^{24} .

The GA procedure provides us with a large collection of chromosomes, each one of them consisting of ten spectral features. Although these are all potential solutions of the problem, it is not immediately clear which one should be selected for the final regression model. In this work we have selected the most frequent features amongst the fittest chromosomes as predictive variables of the physical parameters in regression models. Features appearing in less than five chromosomes were initially discarded as they can not be relevant by themselves and just arise randomly by combination with other stronger chromosomes.

TODO: Rewrite It is relevant to say that when genes of a chromosome induced as ratio of two gaussian variables have extremely wide wings if any of the features is centered around zero, the fitness criteria removes it as a candidate feature as it is not able to explain the physical parameter. Therefore, the single regression model should, to some extent, be descriptive of the population. The simpler strategy would be to use the frequency of the chromosome in the population as criterion for inclusion in a forward selection strategy. However we preferred to select the features based on their highest fitness as it enhances the value of the direct contribution to explain the physical parameter. As we have accepted that complex interactions between individual features are possible, it was selected a fixed number of features allowing both, enough room for developing those complex dependency relationships but to keep the complexity of the coming regression models under control. Therefore, it was selected ten as the suitable number of features being considered per physical parameter.

Once the GA has generated a proposal set of features for predicting each of the physical parameters, the next step consists in training the regression model based on these features. This is described in the next Section.

2.3. Models considered.

Once a feature set (the predictor variables) was selected from the output of the GA, we construct regression models to predict the physical parameters (response or predicted variables) from

it. In the context of Machine Learning, constructing a regression model consists in using a training set (a set of cases defined by the predictor variables for which the predicted variables are available) to infer the parameters of an (often analytical) mapping between predictor and predicted variables. The regression model parameters should not be confused with the physical parameters of the atmosphere we aim at inferring. **TODO: Check if every occurrence of parameter is clear**

In this case, our training set is again the BT Settl collection of synthetic spectra, for which we already computed the predictor variables (the features) as part of the GA selection procedure. And, of course, for each spectrum we also have available the effective temperature, the gravity and the metallicity. Once the model is trained, we will apply it to observed spectra as described in Sections 3 and 4.

Several regression models are trained for the prediction of each physical parameter in order to evaluate their performance:

- Bagging with Multiadaptive Spline Regression Models (*hereafter MARS*).
- Random Forest Regression Models (*RF*).
- *k*-Nearest Neighbours (*KNN*).
- Generalized Boosted Regression Models (*GBM*).
- Support Vector Regression with Gaussian Kernel (*SVR*).
- Multi-layer Perceptron Neural Networks (*NNET*).
- Kernel Partial Least Squares Regression (*KPLS*).
- Rule Regression Models (*RR*).

In order to assess the validity of our feature sets we also compare the predictions based on them with other input spaces. In particular, we also compute physical parameters that yield the the minimum χ^2 , and train a Projection Pursuit regression models with the Independent Components derived from each spectrum. **TODO: add reference for ICA.**

Including here a sufficient description of each and every regression model that we trained would render the manuscript excessively lengthy but interested readers can find additional information in Baraud (2002); Geman et al. (1992); Elith et al. (2008); Meyer et al. (2003); Svetnik et al. (2003). Suffice it to say that each one of them can be thought of as a parametric model that predicts one physical parameter from an input vector. The input vector can be the full normalised spectrum, the ICA lower-dimensional representation of the full spectrum, the spectral features selected by Cesetti et al. (2013) or those selected by the GA. The regression model parameters are inferred (using strategies that differ from one regression model to the other) from a set of examples. As explained above, this set of examples (spectra of stars for which we know the physical parameters) is called the training set, and the process by which the model parameters are determined from the training set, is called training of the model. In the next paragraph we give minimal details of each regression model trained, and references for the interested reader.

In order to avoid the well known problem of overfitting (see e.g. Dietterich 1995), we use five-fold cross-validation to estimate the prediction errors. *n*-fold cross validation consists in dividing the trainings set into *n* disjoint subsets and training ten different regression models, each one of them with (*n*-1) of the *n* subsets. The *n*-th subset not used for training is used to estimate the errors.

As every type of model has its own set of tunable parameters as well as its own training procedure, the authors have selected a common R R Core Team (2016) wrapper for all models named caret (short for Classification And REgression Training) from Jed Wing et al. (2016). This wrapper enables a common

¹ All computations needed for this work were carried out in the CeSViMa (<http://www.cesvima.upm.es/>) power7 HPC which involves processors with 8 cores and four threads per core, running at 3,3 GHz and with 32Gb of RAM each.

interface, as well as the use of the same set of training/set samples for the adopted five-fold cross-validation error estimation. As explained above, each regression model has its own set of model parameters. For each model we have searched for the parameter set that minimized the Root Mean Square Error (RMSE) in a grid of values defined *ad hoc* for each technique.

The adopted procedure for learning the models can then be summarized as the pseudocode 2.1.

TODO [Joaquín]: define each element in the pseudocode

Algorithm 2.1: MODEL LEARNING(*DataSet*, *ParRanges*)

```

 $S_{ModelParameters} \leftarrow ParRanges$ 
 $S_{DataFolders} \leftarrow Preprocess(DataSet)$ 
for each  $x \in S_{ModelParameters}$ 
  for each  $z \in S_{DataFolders}$ 
    do {
       $HDS(z) \leftarrow \text{Hold-out specific samples}$ 
       $Model(z) \leftarrow Fits(S_{DataFolders} \setminus HDS(z))$ 
       $Perf(z) \leftarrow Predicts(Model(z), HDS(z))$ 
       $Perf(x) \leftarrow Average(Perf(z)) \quad \forall z \in S_{DataFolders}$ 
    }
   $OPS \leftarrow argmax(Perf(y)) \quad \forall y \in S_{ModelParameters}$ 
   $Model \leftarrow Fits(DataSet, OPS)$ 

```

As mentioned above, the training set was constructed from the BT Settl library of stellar spectra. The interested reader may find different approaches in the literature to the problem of finding an optimal set of training examples. Ness et al. (2015) for example prefer to use real observed spectra rather than synthetic libraries to create a generative model in which the individual spectral fluxes are modelled as second degree polynomials with the physical parameters as arguments. The real observed spectra have physical parameters taken from the literature, which in turn are almost always inferred using synthetic spectral libraries. In our opinion, this approach does not solve the dependence of the predicted parameters on the necessarily imperfect synthetic libraries, but has the advantage that the relative frequencies of examples in the training set represents better the biases naturally encountered in surveys than the uniform sampling of parameter space found in synthetic libraries. Recently, Heiter et al. (2015) have started a program to compile a set of stars with accurate physical parameter determinations inferred independently of spectroscopic measurements and atmospheric models (as much as possible). Unfortunately, this ambitious program only contains 34 stars of spectral types F, G, and K. In the M regime we find similar approaches in Boyajian et al. (2014) and references therein, where the atmospheric parameters are derived using interferometric measurements of stellar radii. Again, this only amounts to a very small number (21 K and M stars) of examples and a very sparse sampling of the parameters space.

All efforts to compile training sets of stars with accurate, homogeneous, and reliable physical parameters derived independently of spectroscopic measurements are valuable not only because they allow for the improvement of the stellar atmospheric models but also because they help increase the reliability of the regression models by making them independent of these atmospheric models. But until these training sets with sufficient and homogeneous sampling of the parameter space are available, we must turn to the use of synthetic libraries.

3. Physical parameters of the IRTF collection of spectra.

3.1. Spectral bands selected

During the preprocessing stage (described in Sect. 2) the spectral resolution of the BT-Settl library was degraded to the IRTF resolution ($R \approx 2000$) by convolving with a Gaussian. Then, the spectra were trimmed to produce valid segments between 8145.92 and 24106.85 Å, which is the spectral range common to all M stars in the IRTF library. Finally, all spectra were divided by the total integrated flux in this range in order to factor out the stellar distance.

3.1.1. Spectral features for the estimation of effective temperatures.

The application of the GAs to the selection of features for the prediction of effective temperature from noiseless spectra with the IRTF wavelength range and resolution results in the features included in Table A.1. Features are ordered by the fitness value (the AIC) and we only consider features that are present in at least 5 sets.

TBD by Luis: interpret the features.

When noise is added to the BT-Settl spectra, we obtain the features included in Table A.2.

Tables A.1 and A.2 show a very wide variety of features with very few repetitions. Only spectral features 4, 5, 6, and 9 in the SNR=50 experiment are found too in the SNR=∞ and SNR=10 feature sets (albeit with different continuum definitions). This reinforces the impression that the information useful for the estimation of the effective temperatures is spread over the entire IRTF spectrum.

A closer look at features 4, 5, 6, and 9

As a reference, Table A.3 lists the features found by Cesetti et al. (2013) using sensitivity maps.

3.1.2. Spectral features for surface gravity estimation.

For gravity estimation (on a logarithmic scale), the GA search procedure produces the features presented in Tables A.4 and A.5 for the noiseless signal and signal-to-noise ratios of 10 and 50, respectively.

3.1.3. Spectral features for metallicity estimation.

Finally, the best features found by the GA for metallicity estimation are listed in Table A.6 for the noiseless BT-Settl spectra, and in Table A.7 for signal-to-noise ratios equal to 10 and 50.

3.2. Regression models

In the following, we will summarise the results obtained for the IRTF data set. We deal with the different physical parameters in separate Sections. We start by reporting the Root Mean/Median Square Errors (RMSE/RMDSE) with respect to the parameters gathered from the literature by Cesetti et al. (2013) and included in their Table 3.

3.2.1. Effective temperature models

Table A.1 summarises the RMSE/RMDSE for the complete set of models: the minimum χ^2 estimate based on the full spectrum

(χ^2), the projection pursuit regression based on the ICA components (PPR-ICA) and models trained on the spectral features proposed by the GA (GA-RF, GA-GBM, GA-SVR, GA-NNET, GA-MARS, GA-KPLS, GA-RR). For each model, we report the RMSE/RMDSE obtained for several noise levels of the training sets. SNR= ∞ corresponds to noiseless spectra. In the GA-cases, the model is trained with the spectral features found by the Genetic Algorithms when applied to BT-Settl spectra of the corresponding SNR.

Make sure we always have Rule-Regression models everywhere or discuss why not.

Table A.1 shows that the performance of classifiers based on the full spectrum (or in a compressed version in the form of ICA components) and the best classifier based on features derived from limited spectral bands is equivalent. The Bartlett test shows that the variances are homogeneous with a Bartlett's K-squared of 8.5 with 2 degrees of freedom and a p-value of 0.01426. The Flinger-Killen test shows that homokedascity is verified at the $p=0.005886$ level. Finally, the F-ANOVA test clearly shows that there is no significant difference between models. Thus, we conclude that the quality of features from the two approaches are equivalent in predictive performance. The difference between the performances of the best classifier (GA – KNN; best on average over SNR), the minimum χ^2 classifier, and the PPR – ICA classifiers are not statistically significant. The Bartlett test shows that the variances are homogeneous with a Bartlett's K-squared of 8.5 with 2 degrees of freedom and a p-value of 0.01426. The Flinger-Killen test shows that homokedascity is verified at the $p=0.005886$ level. Finally, the F-ANOVA test clearly shows that there is no significant difference between models. Thus, we conclude that the quality of features from the two approaches are equivalent in predictive performance. In any case, it is evident that the RMSE is significantly above the grid spacing in temperature. We interpret the small differences as an indication that there is as much information spread over the entire spectrum shape as can be distilled from a few spectral bands.

The comparison with the effective temperatures compiled by Cesetti et al. (2013) shows however some significant differences across models when evaluated not by the RMSE/RMDSE, but by the average bias (see Table A.2).

In general, all classifiers tend to predict lower effective temperatures than those in the literature except in the noiseless scenario. The models trained with noiseless spectra tend to overestimate T_{eff} , suggesting that the optimal SNR is between SNR=50 and ∞ . The minimum- χ^2 approach and the GA-KNN model systematically underestimate T_{eff} for all SNR regimes. This shared behaviour is not surprising since minimum χ^2 is a single nearest neighbour method applied in the space of the entire spectrum as opposed to the space selected features.

We have found in previous studies that, at least for input spaces constructed from ICA compressions of the spectra, it is not necessary to adapt the training set SNR to match exactly that of the prediction set. On the contrary, we find that two regimes are sufficient to obtain acceptable results. The two regimes are separated at SNR=10. The model trained with SNR=50 spectra gives close to optimal results for spectra with SNRs above 10, while below that limit the same situation holds for the model trained with SNR=10 spectra. **Cite paper by Ana.**

Figure ?? shows the correlation between the T_{eff} estimates of the best (in the RMDSE sense) regression models and the effective temperatures in Table 3 of Cesetti et al. (2013).

TODO: make and include figure

We then compare the predicted effective temperatures with the spectral types listed in the IRTF spectral library in order to

increase the size of the validation sample beyond the 57 cases with estimated temperatures in Table 3 of Cesetti et al. (2013). We converted the spectral types into effective temperatures using the calibration of Stephens et al. (2009). Both the RMSE and RMDSE were used to evaluate the prediction accuracy (see Table ??).

TODO: Make table

Faltan las tablas y figuras.

We have trained the same non linear regression models discussed above using the features suggested by Cesetti et al. (2013). The performance of the models based on these features are included in Table A.3.

How do you explain that the best SNR=10 model has the poorest performances for SNR=50 or ∞ ?

From the comparison of Tables A.1 and A.3 we can draw the following conclusions:

- the RMSE for SNR=10 and 50 is equivalent for the regression models trained on GA features and those recommended in Cesetti et al. (2013);
- however, the RMDSE is significantly higher in the case of the latter features for all SNR values.
- in the unrealistic case of noiseless spectra, the features proposed by Cesetti et al. (2013) produce RMSE and RMDSE significantly worse than the GA features.

As a summary, we believe that the features found by the GA are to be preferred to the ones proposed by Cesetti et al. (2013).

3.2.2. Surface gravity models

For the validation of our models, we only have 10 literature values of the surface gravity available in Table 3 of Cesetti et al. (2013). Unfortunately, this is too small a number to draw significant conclusions on the comparison of methodologies from external data. Hence, we are left only with plausibility arguments for the selection of models. In this Section we will use $\log(T_{\text{eff}}) - \log(g)$ diagram comparisons to select the most plausible model results. An important difference with respect to the models discussed above is that we use the T_{eff} estimated in the previous stage as input of our models. **do we have some hint whether this was beneficial, neutral or detrimental?**

Table A.4 shows the RMSE and RMDSE of the $\log(g)$ regression models for the same SNR regimes discussed for the estimation of T_{eff} .

Again, as in the case of the effective temperatures, the differences between the various models as measured by the RMSE or RMDSE are not statistically significant. This is not surprising given the extraordinarily small sample of gravity measurements gathered from the literature and used as reference for the computation of errors. However, we can evaluate the models according to plausibility arguments relative to the distribution of the model predictions in $T_{\text{eff}} - \log(g)$ diagrams. Figure 1 shows this distribution for four models selected based on these plausibility criteria: GA-RR, GA-PLS, GA-KNN (the three of them for SNR=50), and PPR-ICA (clockwise, starting at the top left corner).

Is χ^2 much worse now for the weak parameter $\log g$? I guess no. This needs to be discussed

Discuss these plots in the case of Cesetti features.

3.2.3. Metallicity models

Finally, the same machine learning models are trained to infer the metallicity, again considering the effective temperature as an

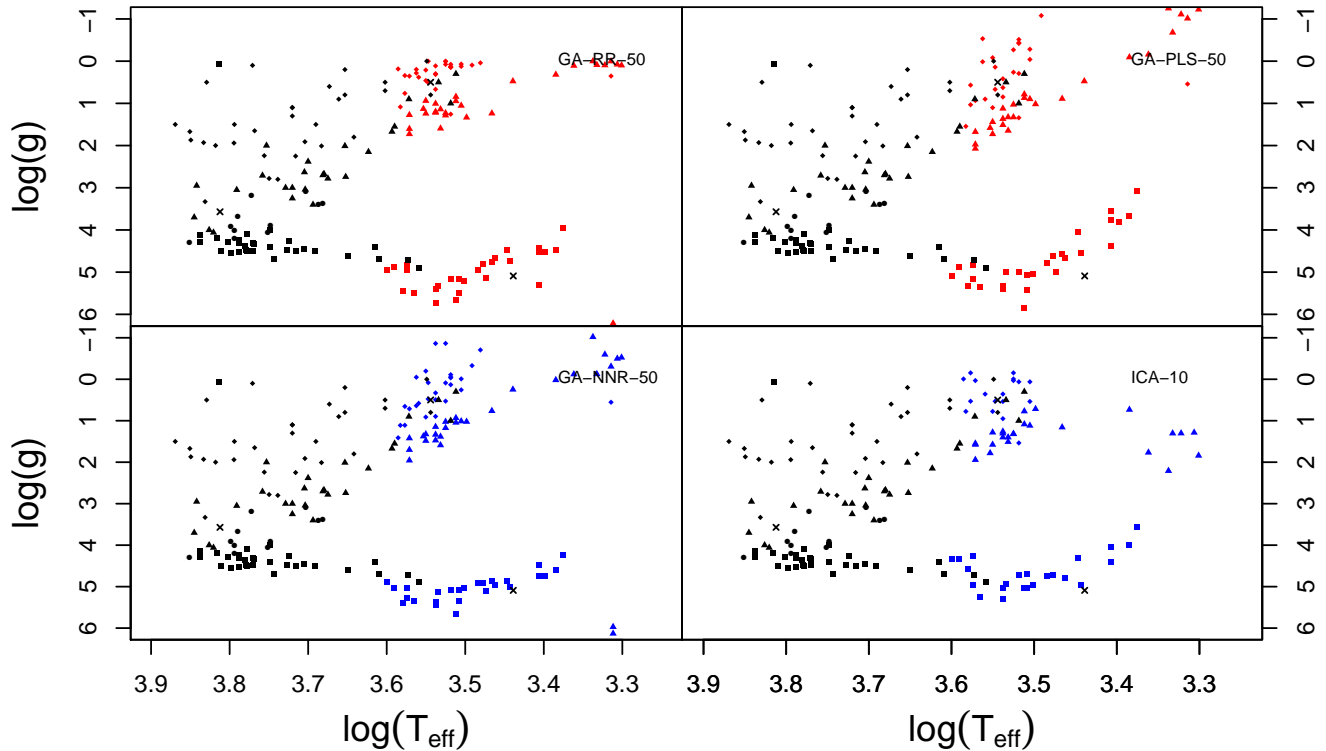


Fig. 1: $\log(T_{\text{eff}})$ – $\log(g)$ diagrams produced by the GA-KNN (SNR= ∞) effective temperatures and gravities derived with the GA-RR (SNR=50), GA-PLS (SNR=50), GA-NNR (SNR=50), and χ^2 models (clockwise, starting from the top left plot).

input feature as in the $\log(g)$ regression models. Table A.5 shows the RMSE and RMDSE obtained for each regression model for the only seven M-type stars in Table 3 of Cesetti et al. (2013). The minimum values are consistently obtained with the minimum χ^2 , $PPR - ICA$ and $GA - KNN$. The differences are only marginal, but we see that even at these intermediate resolutions the reduction of dimensionality (either with ICA or GA) produces an improvement in the predictions. This is even more evident if we compare our predictions with more recent metallicity estimates not included in Cesetti et al. (2013). We have gathered estimates for stars in both the IRTF collection and a series of recent metallicity catalogs by Rojas-Ayala et al. (2012), Neves et al. (2013), Newton et al. (2014), Gaidos et al. (2015), and Mann et al. (2015). All of the aforementioned references provide us with estimates of the iron abundance ratio $[\text{Fe}/\text{H}]$ except Rojas-Ayala et al. (2012) that provides both the overall metallicity $[\text{M}/\text{H}]$ and the $[\text{Fe}/\text{H}]$ ratio. Our estimates, coming from the BT-Settl library, are for the $[\text{M}/\text{H}]$ ratios, so some offset could be expected from the different nature of the quantities compared. Hence, when comparing our estimates with those from the literature, we compute the RMSE or RMDSE after subtracting any difference in the mean. It turns out that, after correcting for biases, $PPR - ICA$ trained with SNR=10 examples yields the lowest RMSE/RMDSE. Figure 2 represents the estimates of $[\text{M}/\text{H}]$ obtained from the $PPR - ICA$ based regressor, as a function of the values taken from these references for the sources in common. The black empty circles represent values from Cesetti et al. (2013); orange filled circles, values from Neves et al.

(2013); green filled squares, values that the Vizier catalog entry for Table 8 of Neves et al. (2013) links to Jao et al. (2005), although we find no evidence that Jao et al. (2005) contains estimates of metallicities; cyan and blue filled squares, the values of $[\text{M}/\text{H}]$ and $[\text{Fe}/\text{H}]$ respectively in Rojas-Ayala et al. (2012); red filled squares, values from Mann et al. (2015); yellow filled squares, values from Newton et al. (2014); and, finally, black filled squares, values from Gaidos et al. (2015).

Compare the 7 or 6 values available. Discuss. χ^2 is the most popular method by far. We compare predictions of machine learning methods with minimum chi-squared. We first do histogram plots. Then, the same $\log T_{\text{eff}}$ – $\log g$ plots as above but with metallicity coded in colour.

Include table as annex with metallicities from the literature?

3.3. Comparison with previous feature sets

For metallicities, we again find that the only feature space that results in reasonable results is based on ICA projections and SNR=10. Comparison of the correlation coefficients of the various regression results with the literature values shows no significant difference between the GA-based features and those taken from Cesetti et al. (2013). Therefore, neither set is competitive with the ICA projections. In Fig. 4 we show the results of the regression technique that results in the highest correlation with the literature values (RF-50).

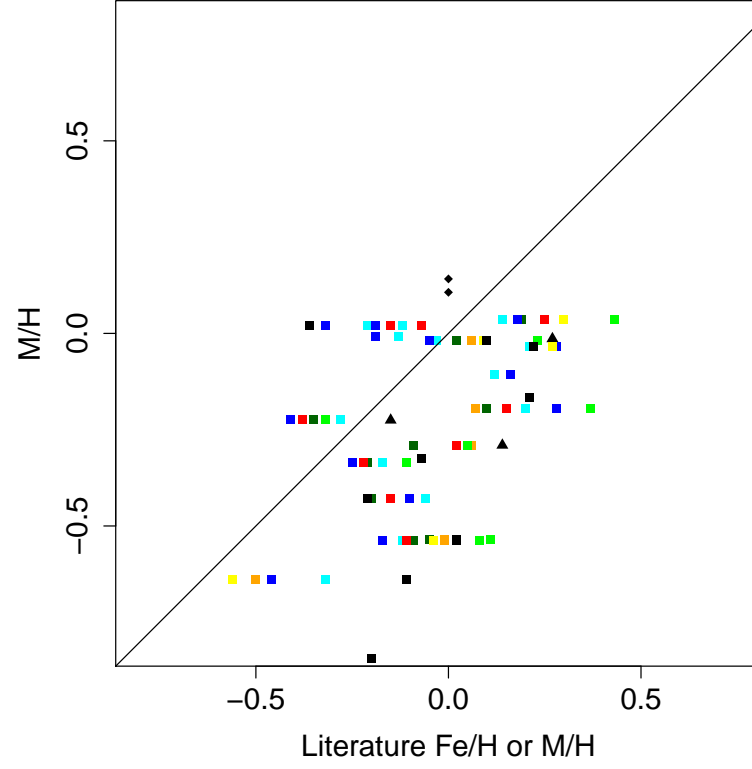
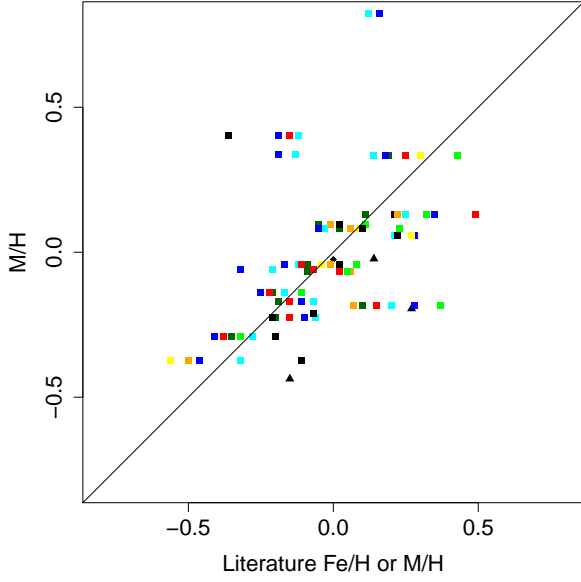


Fig. 2: Comparison between metallicity estimates from the literature and predictions from the PPR-ICA (SNR=10) model. Black empty circles represent values from Cesetti et al. (2013); orange filled circles, values from Neves et al. (2013); green filled squares, values that the Vizier catalog entry for Table 8 of Neves et al. (2013) links to Jao et al. (2005), although we find no evidence that Jao et al. (2005) contains estimates of metallicities; cyan and blue filled squares, the values of $[M/H]$ and $[Fe/H]$ respectively in Rojas-Ayala et al. (2012); red filled squares, values from Mann et al. (2015); yellow filled squares, values from Newton et al. (2014); and, finally, black filled squares, values from Gaidos et al. (2015).

Fig. 4

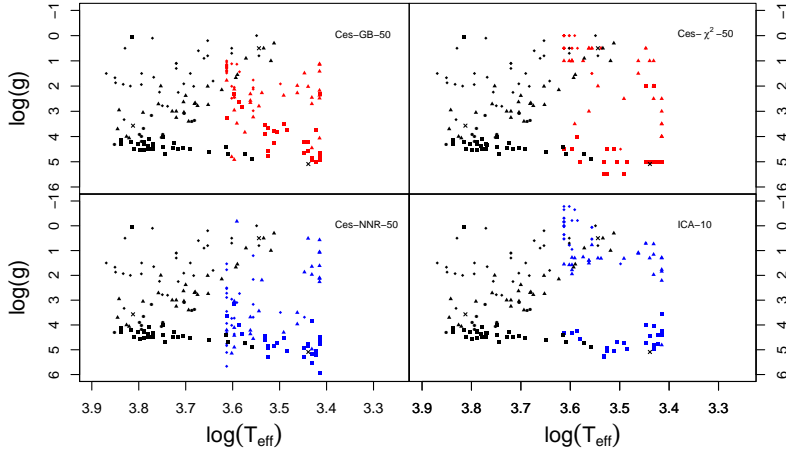


Fig. 3

4. Physical parameters of the IPAC collection of spectra.

4.1. Spectral bands selected

As for the IRTF spectra, the spectral resolution of the BT-Settl library was degraded to match the average resolution of IPAC spectra in the Dwarf Archives². **What is the average resolution?** Then, the spectra were trimmed to produce valid segments between *** and *** Å, which is the spectral range common to all M stars in the archive. Finally, all spectra were divided by the total integrated flux in this range in order to factor out the stellar distance.

There is little hope *a priori* for reasonable accuracies with regression models that predict the surface gravity and metallicity from such wavelength-limited, low/intermediate resolution spectra. Anyhow, we provide the results obtained applying the same methodology as in Section 3 (and described in Section 2) to show the limitations.

4.1.1. Spectral features for the estimation of effective temperatures.

The application of the GA to the selection of features for the prediction of effective temperature from noiseless spectra within the IPAC wavelength range and resolution, results in the features included in Table B.1. Features are ordered by the fitness value (the AIC) **and we only consider features that are present in at least 5 sets**. For the noisy spectra of SNR=10 and 50 we select the spectral features listed in Table B.2.

TBD by Luis: interpret the features.

Tables B.3 and B.4 show the spectral features selected by the GA for noiseless BT-Settl spectra and the same spectra with SNR=10 and 50, respectively.

Finally, the best features found by the GA for the estimation of the metallicity are listed in Table B.5 for the noiseless BT-Settl spectra, and in Table B.6 for signal-to-noise ratios equal to 10 and 50.

4.2. Regression models

In the following, we will summarise the results obtained for the IPAC data set. We deal with the different physical parameters in separate Sections. We start by reporting the cross validation Root Mean Square Errors (RMSE) and Root Median Square Error (RMDSE) for the five-fold cross-validation strategy, and we subsequently discuss the accuracy of the predictions with respect to literature values where available.

4.2.1. Effective temperature models

Table B.1 summarises the RMSE/RMDSE for the complete set of models: the minimum χ^2 estimate based on the full spectrum (χ^2), the projection pursuit regression based on the ICA components (PPR-ICA) and some models trained on the spectral features proposed by the GA (GA-RF, GA-GBM, GA-SVR, GA-NNET, GA-MARS, GA-KPLS). For each model, we report the RMSE/RMDSE obtained for several noise levels of the training sets.

Again, as in the IRTF case, we see that the compression of the spectra results in a performance degradation. Figure ??

Explain the spt-teff calibration used.

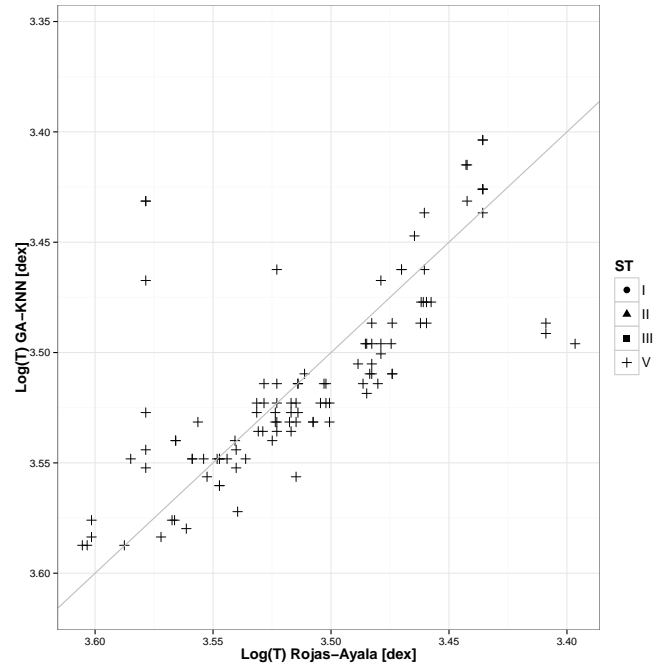


Fig. 6: Relationship between $\log(T)$ from Rojas – Ayala in the x axis and $\log(T)$ as predicted by KNN with SNR=10

Biases?

We do have problems with the prediction at low temperatures when trained with SNR= 10 or 50.

Include plot with 4 models

Having shown that the feature selection with GAs degrades the performance of regression models, one can wonder whether a different feature selection procedure would produce better results. In particular, we investigate the possibility that the features proposed by Cesetti et al. (2013) result in a performance equal to or even better than the one achieved with χ^2 .

We train the same regression models applied to the GA selected features, to the features selected in Cesetti et al. (2013), again learning from BT-Settl spectra of various SNRs and predicting over the IPAC set. A summary of the results can be found in Table B.2, where we use CS- to indicate that the model was trained using the features by Cesetti et al. (2013).

For SNR=10, the GA best models (GA-KPLS in RMDSE or GA-RF in RMSE) outperform the best CS model (GA-GBM). For SNR=50 the situation depends on the figure-of-merit used to compare the classifiers: in RMSE the best model is CS-GBM while in RMDSE GA-GBM outperforms all CS-models. Finally, for the unrealistic case of noiseless spectra, Table B.2 shows an overwhelming degradation of the prediction accuracy from CS-features. **Overfitting?** But even in the only case where the CS features outperform those selected by the GA, the performance is below the one achieved by the minimum- χ^2 approach.

The relationship between the GA predicted Temperature and the one measured by Rojas-Ayala can be found in the Figure 6

4.2.2. Surface gravity models

As in the IRTF exercise, we attempt to select features for surface gravity estimation from BT-Settl spectra using GAs despite the much lower spectral resolution and smaller wavelength coverage of the IPAC spectra. Since there is no substantive compilation

² <http://spider.ipac.caltech.edu/staff/davy/ARCHIVE/index.shtml>

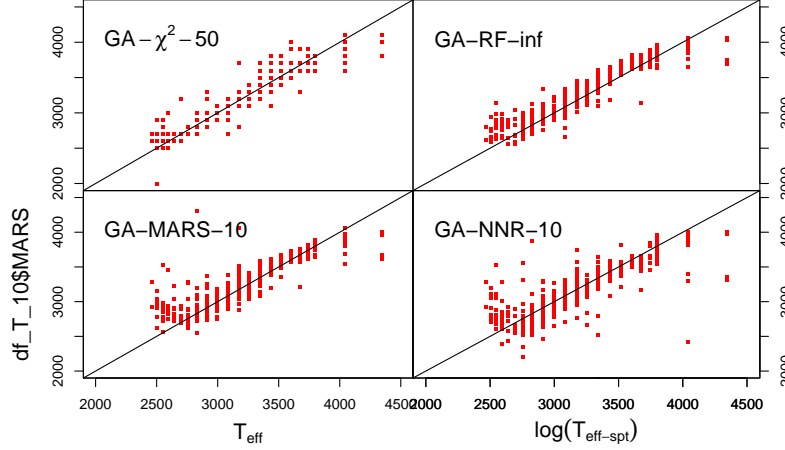


Fig. 5: Comparison between Temperature estimations from Theoretical Temperature in x axis and the modeled ICA based estimation at SNR=∞ on y-axis

of surface gravities that we could cross match with the IPAC list of M stars in the Dwarf Archive, we are left with the same plausibility arguments used in the IRTF study which are based on the $\log(T_{\text{eff}})$ – $\log(g)$ diagram.

We again use the effective temperatures as input of the regression models. Table B.3 shows the cross-validation RMSE and RMDSE for the same set of regression models used throughout this article. It shows that the GA-RF model outperforms all other in all SNR regimes, giving a consistent RMDSE of 1.0 dex. Obviously, this is barely enough for classification in luminosity classes.

Figure 7 shows the $\log(T_{\text{eff}})$ – $\log(g)$ diagram for the GA-RF and GA-NNET models. The latter is, in our opinion, the one that shows the diagram that is most with Fig. ?? in this work, and Fig. 1 in Cesetti et al. (2013). All GA- models predict decreasing surface gravities for main sequence stars below $\log(T_{\text{eff}}) = 3.6$. GA-NNET predicts main sequence values between $4 \leq \log(g) \leq 6$, while luminosity classes III-I appear clearly separated from the main sequence with values concentrated in the 4-6 range except for the hottest cases with $\log(T_{\text{rmeff}}) > 3.55$. The GA-RF results, despite showing the best cross-validation errors (RMSE/RMDSE), result in unrealistic main sequence gravities. We interpret this as the result of overfitting to the training examples.

Right now, it appears that feature selected models are worse than χ^2 , judging only from the 10 available estimates (mail sent to jbmere). If so, the conclusion is clear: we should not do feature selection at these resolutions. This is useful as Cesetti et al do not question the utility of feature selection. For the IRTF (which is the dataset used by Cesetti et al), we should check this: are the models with feature selection better than χ^2 ?

4.2.3. Metallicity models

Finally, the same analysis is performed for metallicities, again using the previously inferred temperature as a fixed input feature. Table B.4 shows a summary of the cross-validation performance of the different models.

In general, models trained with SNR=∞ show much poorer performance except for the GA-RF and GA-GBM cases. The best

| Identifier | classification | Reference | GA-RF-∞ |
|------------|----------------|---------------------------|---------|
| LHS 3768 | usdM3 | Kirkpatrick et al. (1995) | -2.1 |
| LHS 2352 | esd | Kirkpatrick et al. (1995) | -2.0 |
| LHS 1691 | usdM2 | Lépine et al. (2007) | -1.95 |
| LHS 2023 | esdM6 | Riaz et al. (2008) | -1.95 |
| LHS 515 | esdM5 | Reid & Gizis (2005) | -1.8 |
| LP471-17 | sdM | Kirkpatrick et al. (1995) | -1.7 |

Table 1: TMP TBC

χ^2 model produces errors almost a factor two larger than the $GA - RF - \infty$ model (although it has to be borne in mind that, while our regressors are capable of predicting metallicities that are intermediate in the grid, the minimum χ^2 can only yield values in the grid, which has a step size of 0.5 dex). Models trained with SNR=10 and 50, on the contrary, show a more consistent behaviour for the entire set of regressors, with poorer performances than the apparently optimal $GA - RF - \infty$, but also smaller differences between models.

In order to select the best model, we again compare our model predictions with the reference catalogs used in Sect. 3.2.3. We select, as best model the Random Forest trained with noiseless synthetic spectra, which renders the minimum RMSE (0.3 dex). Figure 8 shows the comparison of our estimates with the reference catalogs, using the same symbols and colours as in Fig. 2.

Our value of the RMSE contrasts with the differences between estimates for the same star in the literature. We obtain a mean difference of 0.1 dex **TO BE COMPLETED ALSO FOR IRTF**

It is interesting to note that our predictions extend to metallicities as low as -2.1. Figure 9 shows a histogram of the metallicities predicted by the GA-RF-∞ model for the IPAC set of spectra. We find predictions below -1.5 for eleven sources, 6 of which have been previously identified as subdwarfs of different categories (see Table 1).

The remaining 5 stars with metallicities below -1.5 are 2MASS J17275631-3240430 (-2.0 dex); LHS 1625 (-1.97 dex); 2MASS J19215188+2802275 (-1.9 dex); 2MASS J19004675+2806462 (-1.7 dex), classified as K7III by Kirk-

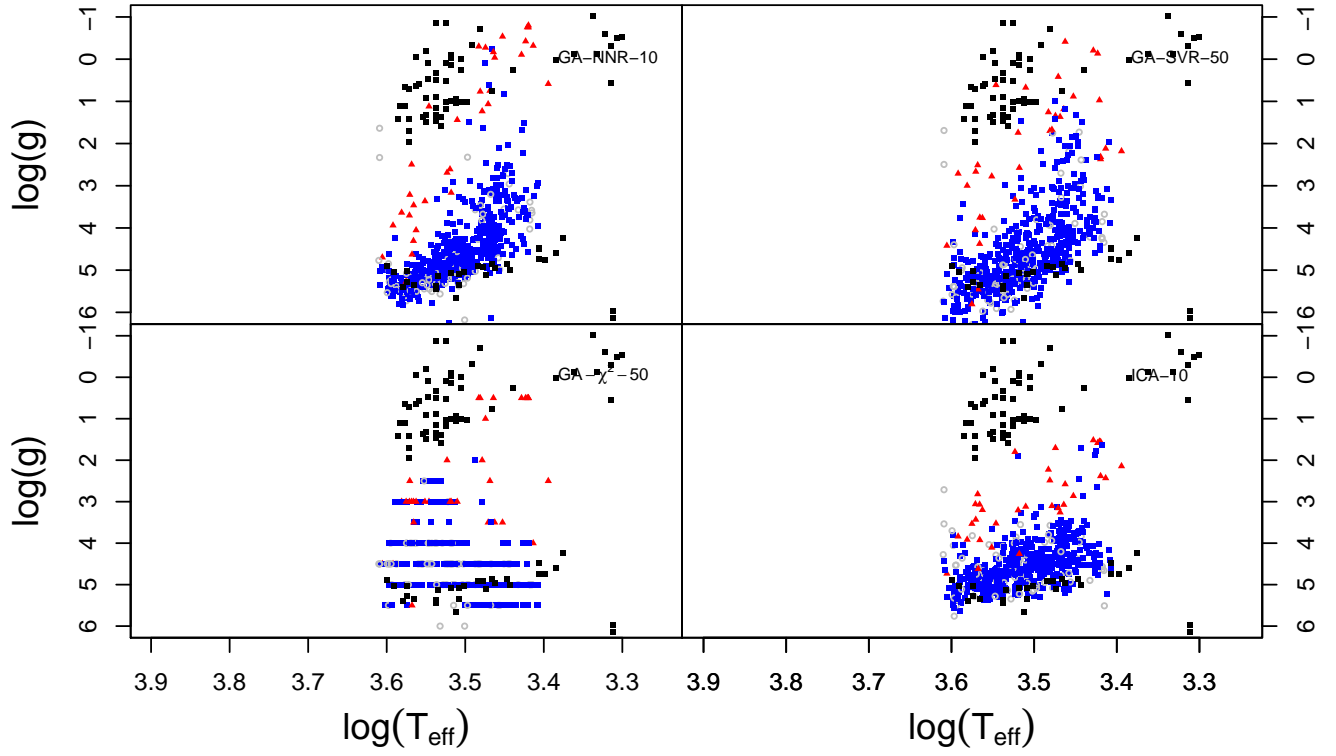


Fig. 7: Relationship between $\log(T)$ (x axis) and $\log(g)$ (y axis) for several regression models.

patrick et al. (1994)); and 2MASS J14465233-5320580 (-1.7 dex).

4.3. Comparison with previous feature sets

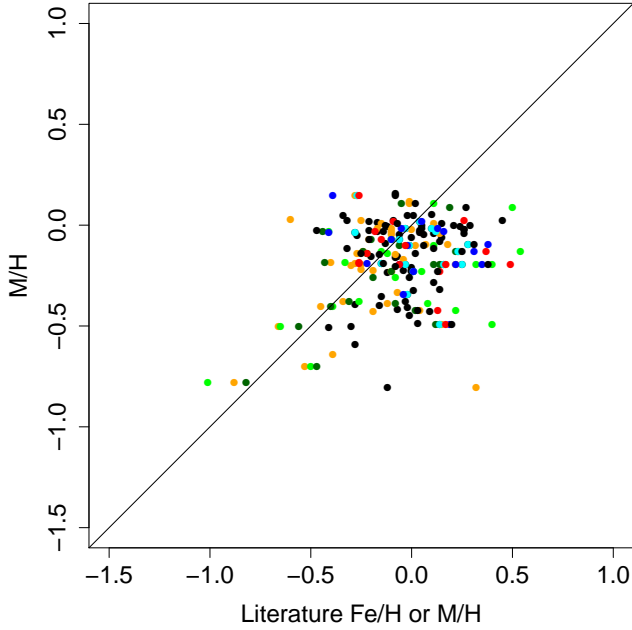


Fig. 8: Relationship between the $RF-\infty$ predictions for metallicity and values from the literature. Black empty circles represent values from Cesetti et al. (2013); orange filled circles, values from Neves et al. (2013); green filled squares, values that the Vizier catalog entry for Table 8 of Neves et al. (2013) links to Jao et al. (2005), although we find no evidence that Jao et al. (2005) contains estimates of metallicities; cyan and blue filled squares, the values of $[M/H]$ and $[Fe/H]$ respectively in Rojas-Ayala et al. (2012); red filled squares, values from Mann et al. (2015); yellow filled squares, values from Newton et al. (2014); and, finally, black filled squares, values from Gaidos et al. (2015).

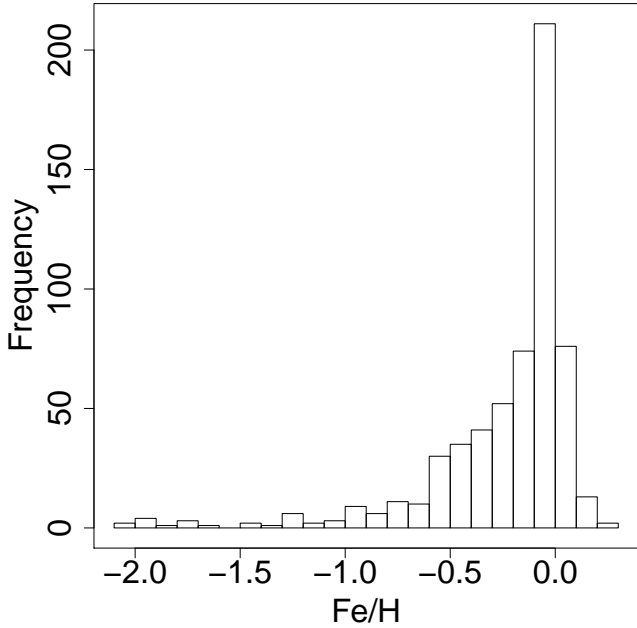


Fig. 9

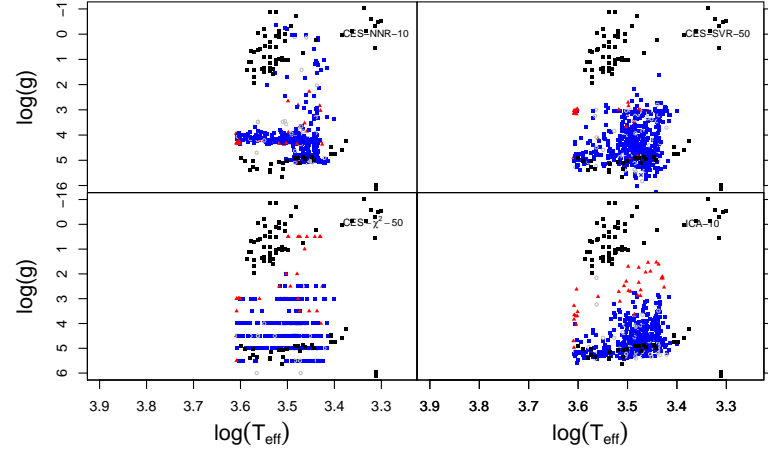


Fig. 10

5. Conclusions

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Appendix A: IRTF features

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 10245.88 | 10304.02 | 11241.29 | 11328.54 |
| 8415.91 | 8473.96 | 11511.51 | 11598.51 |
| 12906.56 | 12993.61 | 13041.48 | 13133.82 |
| 8716.00 | 8773.99 | 10425.90 | 10484.13 |
| 8805.93 | 8863.97 | 12816.72 | 12903.73 |
| 10126.02 | 10183.93 | 13086.46 | 13194.09 |
| 8176.03 | 8234.13 | 10971.57 | 11058.46 |
| 8626.02 | 8683.99 | 10746.43 | 10833.57 |
| 8536.03 | 8594.06 | 10215.95 | 10274.10 |
| 12951.62 | 13038.62 | 11196.56 | 11283.24 |

Table A.4: Recommended features and continuum bandpasses for predicting $\log(g)$ obtained using noiseless BT_Settl spectra.

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 12096.68 | 12183.66 | 12051.50 | 12096.68 |
| 9525.89 | 9584.05 | 12321.33 | 12408.32 |
| 8205.98 | 8263.96 | 10126.02 | 10183.93 |
| 8566.08 | 8624.07 | 12276.52 | 12363.34 |
| 11196.56 | 11283.24 | 11151.63 | 11196.56 |
| 11151.639 | 11238.46 | 11466.35 | 11553.33 |
| 9555.93 | 9614.06 | 8205.98 | 8263.96 |
| 11016.62 | 11103.37 | 10791.44 | 10878.40 |
| 9766.16 | 9823.94 | 12681.62 | 12768.68 |
| 9942.14 | 9999.92 | 9555.93 | 9614.06 |

Table A.6: Feature and Continuum bandpasses selected for predicting metallicity using noiseless BT_Settl spectra.

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 9225.86 | 9283.94 | 9736.02 | 9793.96 |
| 11106.48 | 11193.56 | 13497.81 | 13613.95 |
| 13438.08 | 13554.08 | 12006.54 | 12093.56 |
| 9135.89 | 9193.91 | 10002.04 | 9999.92 |
| 9555.93 | 9614.06 | 12951.62 | 13038.62 |
| 9466.08 | 9523.82 | 13137.94 | 13253.96 |
| 11196.56 | 11283.24 | 12546.46 | 12633.49 |
| 8566.08 | 8624.07 | 13258.32 | 13374.32 |
| 8266.11 | 8324.03 | 9856.06 | 9913.91 |
| 8235.96 | 8294.04 | 12366.32 | 12453.33 |

Table A.1: Features selected by the GA for predicting T_{eff} using BT_Settl noiseless synthetic spectra in the IRTF wavelength range and resolution.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 8235.96 | 8294.04 | 12681.62 | 12768.68 | 8145.92 | 8204.03 | 12636.48 | 12723.57 |
| 8505.89 | 8563.93 | 13378.12 | 13494.13 | 8895.95 | 8953.95 | 11331.57 | 11418.65 |
| 9376.07 | 9433.92 | 12951.62 | 13038.62 | 8176.03 | 8234.13 | 10611.36 | 10698.46 |
| 8145.92 | 8204.03 | 12366.32 | 12453.33 | 13438.08 | 13554.08 | 12546.46 | 12633.49 |
| 9195.86 | 9253.93 | 9135.89 | 9193.92 | 8235.96 | 8294.04 | 11961.44 | 12048.54 |
| 9585.95 | 9644.12 | 10002.04 | 9999.92 | 9376.07 | 9433.92 | 10002.04 | 9999.92 |
| 8385.99 | 8443.94 | 11826.48 | 11913.28 | 9406.09 | 9463.96 | 13258.32 | 13374.32 |
| 9135.89 | 9193.92 | 9225.86 | 9283.94 | 9346.13 | 9403.92 | 13086.46 | 13194.09 |
| 13618.20 | 13734.15 | 11376.63 | 11463.51 | 11106.48 | 11193.56 | 13438.08 | 13554.08 |
| 9105.87 | 9163.91 | 8865.98 | 8923.94 | 9255.86 | 9314.01 | 8865.98 | 8923.94 |

Table A.2: Recommended features and continuum bandpasses for predicting T_{eff} using BT_Settl with SNR= 10 and 50 and the IRTF wavelength range and resolution.

| Index | Element | Signal_from | Signal_To | Cont1_From | Cont1_To | Cont2_From | Cont2_To |
|------------------|-----------------------|-------------|-----------|------------|----------|------------|----------|
| Pa1 | H I | 8461 | 8474 | 8474 | 8484 | 8563 | 8577 |
| Ca1 | Ca II | 8484 | 8513 | 8474 | 8484 | 8563 | 8577 |
| Ca2 | Ca II | 8522 | 8562 | 8474 | 8484 | 8563 | 8577 |
| Pa2 | H I | 8577 | 8619 | 8563 | 8577 | 8619 | 8642 |
| Ca3 | Ca II | 8642 | 8682 | 8619 | 8642 | 8700 | 8725 |
| Pa3 | H I | 8730 | 8772 | 8700 | 8725 | 8776 | 8792 |
| Mg | Mg I | 8802 | 8811 | 8776 | 8792 | 8815 | 8850 |
| Pa4 | H I | 8850 | 8890 | 8815 | 8850 | 8890 | 8900 |
| Pa5 | H I | 9000 | 9030 | 8983 | 8998 | 9040 | 9050 |
| FeClTi | Fe I, Cl I, Ti I | 9080 | 9100 | 9040 | 9050 | 9125 | 9135 |
| Pa6 | H I | 9217 | 9255 | 9152 | 9165 | 9265 | 9275 |
| Fe1 | Fe I | 1.9297 | 1.9327 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Br δ | H I (n=4) | 1.9425 | 1.9470 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Ca1 | Ca I | 1.9500 | 1.9526 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Fe23 | Fe I | 1.9583 | 1.9656 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Si | Si I | 1.9708 | 1.9748 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Ca2 | Ca I | 1.9769 | 1.9795 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Ca3 | Ca I | 1.9847 | 1.9881 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Ca4 | Ca I | 1.9917 | 1.9943 | 1.9220 | 1.9260 | 2.0030 | 2.0100 |
| Mg1 | Mg I | 2.1040 | 2.1110 | 2.1000 | 2.1040 | 2.1110 | 2.1150 |
| Bry | H I (n=4) | 2.1639 | 2.1686 | 2.0907 | 2.0951 | 2.2873 | 2.2900 |
| Na _d | Na I | 2.2000 | 2.2140 | 2.1934 | 2.1996 | 2.2150 | 2.2190 |
| FeA | Fe I | 2.2250 | 2.2299 | 2.2133 | 2.2176 | 2.2437 | 2.2479 |
| FeB | Fe I | 2.2368 | 2.2414 | 2.2133 | 2.2176 | 2.2437 | 2.2479 |
| Ca _d | Ca I | 2.2594 | 2.2700 | 2.2516 | 2.2590 | 2.2716 | 2.2888 |
| Mg2 | Mg I | 2.2795 | 2.2845 | 2.2700 | 2.2720 | 2.2850 | 2.2874 |
| ¹² CO | ¹² CO(2,0) | 2.2910 | 2.3070 | 2.2516 | 2.2590 | 2.2716 | 2.2888 |

Table A.3: Features and continuum bandpasses defined in Cesetti et al. (2013) as relevant for the estimation of the effective temperature in bands I and K.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 8176.03 | 8234.13 | 9165.87 | 9223.91 | 11151.63 | 11238.46 | 13086.46 | 13194.09 |
| 10485.99 | 10563.41 | 10002.04 | 9999.92 | 8385.99 | 8443.94 | 13618.20 | 13734.14 |
| 8656.09 | 8714.047 | 10926.46 | 11013.60 | 8176.03 | 8234.13 | 11241.29 | 11328.54 |
| 9525.89 | 9584.059 | 10002.04 | 9999.92 | 8536.03 | 8594.06 | 13041.48 | 13133.82 |
| 8205.98 | 8263.967 | 13041.48 | 13133.82 | 12771.70 | 12858.73 | 10306.03 | 10363.88 |
| 10275.97 | 10333.96 | 11376.63 | 11463.51 | 13378.12 | 13494.13 | 10002.04 | 9999.92 |
| 10306.03 | 10363.88 | 11151.63 | 11238.46 | 8626.02 | 8683.99 | 10926.46 | 11013.60 |
| 9165.87 | 9223.91 | 8385.99 | 8443.94 | 9826.05 | 9883.91 | 10006.07 | 10064.01 |
| 9645.82 | 9704.16 | 13137.94 | 13253.96 | 10521.56 | 10608.46 | 11736.71 | 11823.49 |
| 8326.00 | 8383.94 | 12726.69 | 12813.71 | 8205.98 | 8263.96 | 9796.09 | 9853.94 |

Table A.5: Recommended features and continuum bandpasses for predicting $\log(g)$ obtained using BT_Settl with SNR= 10 and 50.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 8235.96 | 8294.04 | 11331.57 | 11418.65 | 9255.86 | 9314.01 | 13197.94 | 13313.92 |
| 9376.07 | 9433.92 | 10566.33 | 10653.62 | 8385.99 | 8443.94 | 9376.07 | 9433.92 |
| 10306.03 | 10363.88 | 9942.14 | 9999.92 | 8716.00 | 8773.99 | 9585.95 | 9644.12 |
| 11286.42 | 11373.45 | 11241.29 | 11286.42 | 8235.96 | 8294.04 | 13086.46 | 13194.09 |
| 9676.00 | 9734.02 | 13086.46 | 13194.09 | 9676.00 | 9734.02 | 10791.44 | 10878.40 |
| 8775.95 | 8833.94 | 8415.91 | 8473.96 | 8415.91 | 8473.96 | 12411.34 | 12498.41 |
| 12411.34 | 12498.41 | 10245.88 | 10304.02 | 8446.03 | 8503.94 | 9406.09 | 9463.96 |
| 8476.01 | 8534.03 | 12276.52 | 12363.34 | 8205.98 | 8263.96 | 8955.88 | 9013.95 |
| 12636.48 | 12723.57 | 12051.50 | 12138.72 | 8985.93 | 9043.98 | 12186.62 | 12273.48 |
| 8415.91 | 8473.96 | 13618.20 | 13734.14 | 9015.98 | 9073.98 | 11241.29 | 11328.54 |

Table A.7: Feature and Continuum bandpasses selected for predicting metallicity using noisy BT_Settl spectra with signal-to-noise ratios equal to 10 and 50.

Appendix B: IPAC features

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 7062 | 7094.4 | 7314 | 7346.4 |
| 7116 | 7148.4 | 7782 | 7814.4 |
| 7134 | 7166.4 | 7872 | 7904.4 |
| 6900 | 6932.4 | 7764 | 7796.4 |
| 7170 | 7202.4 | 7890 | 7922.4 |
| 7080 | 7112.4 | 7926 | 7958.4 |
| 7188 | 7220.4 | 7548 | 7580.4 |
| 7800 | 7832.4 | 7962 | 7994.4 |
| 6990 | 7022.4 | 7008 | 7040.4 |
| 7026 | 7058.4 | 6990 | 7022.4 |

Table B.1: Spectral features and continuum bandpasses selected by the GA for predicting T_{eff} using noiseless BT_Settl spectra in the IPAC wavelength range and resolution.

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 7134 | 7166.4 | 7044 | 7076.4 |
| 6954 | 6986.4 | 7152 | 7184.4 |
| 7512 | 7544.4 | 7890 | 7922.4 |
| 7062 | 7094.4 | 7224 | 7256.4 |
| 6936 | 6968.4 | 7854 | 7886.4 |
| 6900 | 6932.4 | 7746 | 7778.4 |
| 6918 | 6950.4 | 7800 | 7832.4 |
| 7008 | 7040.4 | 7134 | 7166.4 |
| 7872 | 7904.4 | 7008 | 7040.4 |
| 7962 | 7994.4 | 7980 | 8012.4 |

Table B.3: Spectral features and continuum bandpasses selected by the GA for predicting $\log(g)$ using noiseless BT_Settl spectra in the IPAC wavelength range and resolution..

| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
|-------------|-------------|--------------------|--------------------|
| 7188 | 7220.4 | 7854 | 7886.4 |
| 7080 | 7112.4 | 7926 | 7958.4 |
| 7116 | 7148.4 | 7098 | 7130.4 |
| 7422 | 7454.4 | 7836 | 7868.4 |
| 7350 | 7382.4 | 7998 | 8030.4 |
| 7224 | 7256.4 | 7818 | 7850.4 |
| 7710 | 7742.4 | 7062 | 7094.4 |
| 7476 | 7508.4 | 7944 | 7976.4 |
| 7134 | 7166.4 | 7584 | 7616.4 |
| 7836 | 7868.4 | 7278 | 7310.4 |

Table B.5: Spectral features and continuum bandpasses selected by the GA for predicting metallicity using noiseless BT_Settl spectra in the IPAC wavelength range and resolution.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 7692 | 7724.4 | 6936 | 6968.4 | 7062 | 7094.4 | 7296 | 7328.4 |
| 6990 | 7022.4 | 7998 | 8030.4 | 7026 | 7058.4 | 7044 | 7076.4 |
| 6900 | 6932.4 | 7548 | 7580.4 | 7080 | 7112.4 | 7926 | 7958.4 |
| 7854 | 7886.4 | 7710 | 7742.4 | 6900 | 6932.4 | 7548 | 7580.4 |
| 7116 | 7148.4 | 7908 | 7940.4 | 7134 | 7166.4 | 7836 | 7868.4 |
| 7278 | 7310.4 | 7926 | 7958.4 | 7296 | 7328.4 | 7962 | 7994.4 |
| 7152 | 7184.4 | 7746 | 7778.4 | 6936 | 6968.4 | 7728 | 7760.4 |
| 7134 | 7166.4 | 7764 | 7796.4 | 6972 | 7004.4 | 6900 | 6932.4 |
| 6918 | 6950.4 | 6900 | 6932.4 | 6990 | 7022.4 | 7944 | 7976.4 |
| 7224 | 7256.4 | 7962 | 7994.4 | 6918 | 6950.4 | 7782 | 7814.4 |

Table B.2: Spectral features and continuum bandpasses selected by the GA for predicting T_{eff} using BT_Settl spectra with SNR=10 and 50 in the IPAC wavelength range and resolution.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 6990 | 7022.4 | 6918 | 6950.4 | 6918 | 6950.4 | 6936 | 6968.4 |
| 6900 | 6932.4 | 7278 | 7310.4 | 6936 | 6968.4 | 7836 | 7868.4 |
| 7062 | 7094.4 | 7242 | 7274.4 | 7656 | 7688.4 | 7890 | 7922.4 |
| 7692 | 7724.4 | 7008 | 7040.4 | 6900 | 6932.4 | 7872 | 7904.4 |
| 7656 | 7688.4 | 7998 | 8030.4 | 7008 | 7040.4 | 7044 | 7076.4 |
| 6936 | 6968.4 | 7836 | 7868.4 | 7512 | 7544.4 | 7656 | 7688.4 |
| 7206 | 7238.4 | 7062 | 7094.4 | 7440 | 7472.4 | 7332 | 7364.4 |
| 7512 | 7544.4 | 7926 | 7958.4 | 7800 | 7832.4 | 7692 | 7724.4 |
| 7764 | 7796.4 | 7710 | 7742.4 | 7404 | 7436.4 | 7548 | 7580.4 |
| 7404 | 7436.4 | 7548 | 7580.4 | 7080 | 7112.4 | 7152 | 7184.4 |

Table B.4: Spectral features and continuum bandpasses selected by the GA for predicting $\log(g)$ using BT_Settl spectra of SNR=10 and 50 in the IPAC wavelength range and resolution.

| SNR = 10 | | | | SNR=50 | | | |
|-------------|-------------|--------------------|--------------------|-------------|-------------|--------------------|--------------------|
| λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ | λ_1 | λ_2 | $\lambda_{cont;1}$ | $\lambda_{cont;2}$ |
| 7692 | 7724.4 | 7026 | 7058.4 | 7098 | 7130.4 | 7926 | 7958.4 |
| 6900 | 6932.4 | 7008 | 7040.4 | 7188 | 7220.4 | 7962 | 7994.4 |
| 7350 | 7382.4 | 7908 | 7940.4 | 7368 | 7400.4 | 7980 | 8012.4 |
| 6918 | 6950.4 | 6900 | 6932.4 | 7116 | 7148.4 | 7872 | 7904.4 |
| 7098 | 7130.4 | 7314 | 7346.4 | 7062 | 7094.4 | 7206 | 7238.4 |
| 7440 | 7472.4 | 7872 | 7904.4 | 7584 | 7616.4 | 7170 | 7202.4 |
| 7134 | 7166.4 | 7962 | 7994.4 | 6936 | 6968.4 | 6918 | 6950.4 |
| 7368 | 7400.4 | 7926 | 7958.4 | 7692 | 7724.4 | 7890 | 7922.4 |
| 7080 | 7112.4 | 7044 | 7076.4 | 7134 | 7166.4 | 7548 | 7580.4 |
| 7044 | 7076.4 | 7980 | 8012.4 | 7494 | 7526.4 | 7998 | 8030.4 |

Table B.6: Spectral features and continuum bandpasses selected by the GA for predicting metallicities using BT_Settl spectra of SNR=10 and 50 in the IPAC wavelength range and resolution.

Appendix A: IRTF RMSE regression models

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 232 | 100 | 235 | 120 | 232 | 100 |
| PPR-ICA | 242 | 128 | 242 | 99 | 280 | 162 |
| GA-RF | 308 | 183 | 248 | 136 | 167 | 135 |
| GA-GBM | 287 | 160 | 248 | 149 | 233 | 113 |
| GA-SVR | 221 | 122 | 281 | 151 | 299 | 160 |
| GA-NNET | 283 | 192 | 264 | 114 | 326 | 212 |
| GA-KNN | 238 | 120 | 232 | 137 | 219 | 100 |
| GA-MARS | 253 | 113 | 254 | 95 | 226 | 133 |
| GA-KPLS | 275 | 120 | 300 | 119 | 387 | 218 |

Table A.1: Cross-validation RMSE and RMDSE for the various regression models that predict T_{eff} (K) in the IRTF wavelength range and resolution.

| | <i>SNR</i> = 10 | <i>SNR</i> = 50 | <i>SNR</i> = ∞ |
|------------------|-----------------|-----------------|-----------------------|
| χ^2 | -77 | -87 | -85 |
| <i>ICA + ppr</i> | -104 | -55 | -130 |
| GA-RR | -102 | -39 | 170 |
| GA-RF | -173 | -127 | -5 |
| GA-GBM | -141 | -109 | 32 |
| GA-SVR | -58 | -3 | 92 |
| GA-NNET | -147 | -36 | 39 |
| GA-KNN | -76 | -110 | -67 |
| GA-MARS | -57 | -88 | 98 |
| GA-KPLS | -120 | -4 | 214 |

Table A.2: Average bias in the T_{eff} (K) estimates computed (IRTF wavelength range and resolution) with respect to the reference values in Table 3 of Cesetti et al. (2013).

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| CS-RF | 234 | 180 | 264 | 218 | 321 | 265 |
| CS-GBM | 232 | 195 | 268 | 254 | 325 | 246 |
| CS-SVR | 268 | 227 | 293 | 257 | 432 | 364 |
| CS-NNET | 357 | 255 | 357 | 204 | 552 | 435 |
| CS-KNN | 249 | 172 | 293 | 256 | 327 | 230 |
| CS-KPLS | 351 | 162 | 856 | 456 | 1086 | 535 |

Table A.3: Regression model performance based on the features proposed by Cesetti et al. (2013)

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 0.82 | 0.45 | 0.93 | 0.61 | 3.5 | 3.48 |
| <i>PPR</i> – <i>ICA</i> | 0.54 | 0.48 | 0.3 | 0.17 | 0.72 | 0.57 |
| <i>GA</i> - <i>RF</i> | 0.64 | 0.38 | 0.77 | 0.72 | 0.53 | 0.39 |
| <i>GA</i> - <i>GBM</i> | 0.48 | 0.45 | 0.61 | 0.47 | 0.49 | 0.41 |
| <i>GA</i> - <i>SVR</i> | 0.66 | 0.40 | 0.63 | 0.58 | 0.46 | 0.21 |
| <i>GA</i> - <i>NNET</i> | 0.78 | 0.61 | 0.47 | 0.44 | 1.2 | 0.97 |
| <i>GA</i> - <i>MARS</i> | 0.84 | 0.57 | 0.54 | 0.37 | 0.99 | 0.76 |
| <i>GA</i> - <i>KNN</i> | 1.23 | 0.83 | 1.39 | 1.44 | 1.60 | 1.32 |
| <i>GA</i> - <i>KPLS</i> | 0.99 | 0.99 | 0.51 | 0.49 | 0.96 | 0.77 |
| <i>GA</i> - <i>RR</i> | 0.74 | 0.57 | 0.50 | 0.47 | 0.57 | 0.41 |

Table A.4: RMSE and RMDSE for the various log(*g*) regression models [dex] in the IRTF wavelength range and resolution.

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 0.76 | 0.22 | 0.36 | 0.18 | 0.36 | 0.18 |
| <i>PPR</i> – <i>ICA</i> | 0.24 | 0.13 | 0.31 | 0.22 | 0.43 | 0.27 |
| <i>GA</i> – <i>RF</i> | 0.33 | 0.25 | 0.73 | 0.41 | 0.61 | 0.36 |
| <i>GA</i> – <i>GBM</i> | 0.27 | 0.19 | 0.70 | 0.52 | 0.63 | 0.35 |
| <i>GA</i> – <i>SVR</i> | 0.33 | 0.22 | 0.45 | 0.32 | 0.92 | 0.89 |
| <i>GA</i> – <i>NNET</i> | 0.37 | 0.30 | 0.33 | 0.37 | 0.95 | 0.81 |
| <i>GA</i> – <i>KNN</i> | 0.69 | 0.55 | 0.23 | 0.15 | 0.21 | 0.15 |
| <i>GA</i> – <i>MARS</i> | 0.36 | 0.16 | 0.49 | 0.41 | 0.83 | 0.85 |
| <i>GA</i> – <i>RR</i> | 0.31 | 0.17 | 0.30 | 0.24 | 0.78 | 0.23 |

Table A.5: RMSE and RMDSE for the various regression models (IRTF wavelength range and resolution) predicting metallicity [dex].

Appendix B: IPAC RMSE regression models

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 147 | 79 | 121 | 56 | 126 | 57 |
| PPR – ICA | 188 | 126 | 164 | 95 | 191 | 130 |
| GA-RF | 160 | 97 | 196 | 103 | 145 | 94 |
| GA-GBM | 175 | 105 | 225 | 99 | 185 | 94 |
| GA-SVR | 203 | 112 | 285 | 106 | 368 | 154 |
| GA-NNET | 221 | 84 | 313 | 111 | 395 | 202 |
| GA-KNN | 183 | 119 | 193 | 109 | 224 | 110 |
| GA-MARS | 222 | 76 | 361 | 103 | 374 | 157 |
| GA-KPLS | 227 | 72 | 331 | 123 | 409 | 208 |

Table B.1: RMSE and RMDSE for the various regression models that predict T_{eff} (K) in the IPAC wavelength range and resolution.

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| CS-RF | 203 | 140 | 243 | 121 | 306 | 172 |
| CS-GBM | 188 | 120 | 161 | 138 | 337 | 222 |
| CS-SVR | 197 | 135 | 379 | 194 | 840 | 688 |
| CS-NNET | 207 | 135 | 514 | 296 | 719 | 489 |
| CS-MARS | 252 | 124 | 789 | 186 | 3464 | 784 |
| CS-KNN | 235 | 158 | 246 | 137 | 314 | 175 |
| CS-KPLS | 250 | 201 | 741 | 361 | 2247 | 1424 |
| CS-RR | 211 | 128 | 400 | 239 | 828 | 774 |

Table B.2: Performances of regression models trained on the features selected by Cesetti et al. (2013) and applied to BT-Settl spectra in the IPAC wavelength range and resolution.

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 2.2 | 1.6 | 2.2 | 1.4 | 2.2 | 1.6 |
| PPR-ICA | 2.1 | 1.8 | 1.8 | 1.4 | 4.3 | 4.2 |
| GA-RF | 1.3 | 1.0 | 1.6 | 1.1 | 1.4 | 0.9 |
| GA-GBM | 1.6 | 1.1 | 1.7 | 1.4 | 1.7 | 1.2 |
| GA-SVR | 2.0 | 1.8 | 2.1 | 1.9 | 2.3 | 1.6 |
| GA-NNET | 2.0 | 1.8 | 2.2 | 1.9 | 3.2 | 2.8 |
| GA-MARS | 1.8 | 1.5 | 2.0 | 1.7 | 2.0 | 1.5 |
| GA-KNN | 2.0 | 1.5 | 2.2 | 1.7 | 1.7 | 1.2 |
| GA-KPLS | 1.8 | 1.4 | 2.0 | 1.7 | 2.7 | 2.3 |
| GA-RR | 2.0 | 1.8 | 2.1 | 1.8 | 3.7 | 3.2 |

Table B.3: RMSE and RMDSE for the various regression models predicting $\text{Log}(G)$ [dex] in the IPAC wavelength range and resolution.

| <i>RegressionModels</i> | <i>SNR</i> = 10 | | <i>SNR</i> = 50 | | <i>SNR</i> = ∞ | |
|-------------------------|-----------------|--------------|-----------------|--------------|-----------------------|--------------|
| | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> | <i>RMSE</i> | <i>RMDSE</i> |
| χ^2 | 0.55 | 0.27 | 0.51 | 0.29 | 0.43 | 0.29 |
| <i>PPR</i> – <i>ICA</i> | 0.48 | 0.27 | 0.70 | 0.39 | 0.85 | 0.71 |
| <i>GA</i> – <i>RF</i> | 0.55 | 0.38 | 0.71 | 0.61 | 0.23 | 0.16 |
| <i>GA</i> – <i>GBM</i> | 0.64 | 0.43 | 0.87 | 0.84 | 0.31 | 0.23 |
| <i>GA</i> – <i>SVR</i> | 0.46 | 0.26 | 0.57 | 0.44 | 3.38 | 2.33 |
| <i>GA</i> – <i>NNET</i> | 0.52 | 0.45 | 0.66 | 0.54 | 2.03 | 1.88 |
| <i>GA</i> – <i>KNN</i> | 0.37 | 0.28 | 0.99 | 0.78 | 0.56 | 0.32 |
| <i>GA</i> – <i>MARS</i> | 0.71 | 0.47 | 0.80 | 0.69 | 1.15 | 0.68 |
| <i>GA</i> – <i>RR</i> | 0.47 | 0.29 | 0.50 | 0.36 | 1.18 | 1.18 |

Table B.4: RMSE and RMDSE for the various regression models predicting *Met* [dex] in the IPAC wavelength range and resolution.