ARES+MOOG - a practical overview of an EW method

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Abstract The goal of this document is to describe the important practical aspects in the use of an Equivalent Width (EW) method for the derivation of spectroscopic stellar parameters. A general description of the fundamental steps that compose any EW method is given here. In this description we point out possible differences that may be found in different methods used in the literature. This differences can significantly influence the final obtained results. The ARES+MOOG is then used as an example where each step of the method is described in detail. A special focus is given for the specific steps of this method, namely the use of a differential analysis to define the atomic data for the adopted line-list, the automatic EW determinations, and the way the best parameters are found at the end of the procedure. Finally a practical tutorial is given where we focus on simple exercises that are helpful to illustrain and explain the dependence of the abundances with the assumed stellar parameters. The interdependences are described and a clear procedure is given to find the "correct" stellar parameters.

1 Introduction

For the derivation of spectroscopic stellar parameters people normally have to choose between two possible methods. One normally referred as the synthetic method, the other referred as an Equivalent Width (EW) method. The synthetic method typically starts with the synthesis of theoretical spectra which are then compared to the observed spectrum. The "correct" parameters in this case are found when we are able to fit the correspondent synthetic spectrum to the observational spectrum. Alternatively, the EW method starts directly with the observational spec-

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trum, measuring the strength of selected and well visible absorption lines which are translated into individual line abundances, assuming a given atmospheric model. Only then the computed abundances are compared with the respective theoretical predictions to find the "correct" parameters.

It is clear that both approaches have their own advantages and disadvantages. From one side the EW method can be faster than the synthetic method since it is focus on only a specific bunch of lines, while the synthetic method need a more complete description of the spectrum. On the other hand, if the individual lines used by the EW method cannot be properly isolated then this may lead to inaccurate results. For these specific cases the synthetic method can be more powerful because is supposed to reproduce the full spectrum.

The goal of this document is to give a description of a specific EW method, the ARES+MOOG which is named after the two main codes used in this method for the spectroscopic analysis. ARES is the code for the automatic EW measurements of the observed spectrum, and MOOG here used to perform the individual abundance calculations. Both codes will be properly introduced in the next sections. The method ARES+MOOG, like other EW methods, allows the derivation the stellar atmospheric parameters: effective temperature - $T_{\rm eff}$, the surface gravity - log g, the microturbulence - ξ and the iron abundance [Fe/H]. The method makes use of the excitation and ionization balance from the iron lines where the [Fe/H] is used as a proxy for the metallicity. This method has been successfully applied to several large samples of FGK solar type stars (e.g. Sousa et al. , 2008, 2011). Since the theoretical approach is described in previous documents (REF), here we will focus on the practical details of an EW method where we will use the ARES+MOOG method as a specific example.

2 EW Method - a General Overview

A good way to describe an EW method is to present it in a diagram with the correspondent data flow and the respective important steps that are required for the method. Figure 1 is a detailed sketch for the ARES+MOOG method. An EW method can be generalized from this diagram, where we can easily identify the general steps for an EW method based on the excitation and ionization balance of iron lines:

- 1. A list of iron absorption lines with the correspondent atomic data is selected for the analysis;
- 2. The observational spectrum is analysed where the EWs are measured independently in a line-by-line analysis;
- 3. A stellar atmospheric model is adopted given the correspondent atmospheric parameters;
- The measured lines and the atmospheric models are used to compute the individual line abundances;



Fig. 1 The data flow diagram of the ARES+MOOG method. Here we can see the several important items of the method described in this document.

5. The "correct" spectroscopic parameters are found once the excitation and ionization balance is valid for all the individual lines analyzed, otherwise we go back to point 3 where different parameters must be adopted;

These are the basic steps required for the use of an EW method. The differences between the EW methods found in the literature are typically found on the use of different line-lists, models and codes used in each one of the steps.

2.1 Line-list

The selection of the lines for the analysis (first point) is crucial for the accuracy and precision of the spectroscopic analysis with this method. There are many linelists used by different EW methods, some with a large set of lines where it is taken the advantage to increase the statistical strength of the derived spectroscopic stellar parameters. Others only use a reduced and very well defined set of absorption lines that are considered to be very well known or at least very well adapted for a specific type of stars (e.g. giant stars).

Not only the selection of the lines is important, but also the adopted atomic data for each one of the lines. Although we can find very consistent sets in what regards the rest wavelengths and excitation potentials for each line, the oscillator strengths $(\log g f)$ are not so precisely known. These values can be derived in laboratory, how-

ever they also carry significant large uncertainties which can propagate and affect dramatically the precision and accuracy of the derived spectroscopic parameters.

2.2 Measuring EWs

Although the definition of the an EW is quite simple, its determination from an observed spectra can still be quite tricky (second point). The determination of the correct position of the continuum level continues to be an important source for the uncertainties in these measurements. Another important aspect here is to understand if a given line that needs to be measured is completely isolated (the ideal case) or if there are close-by lines that are blended together. In the latter case the correct identification of all the lines is fundamental for a good measurement.

Another important aspect for the measurements is the profile function that is used for the fit and correspondent strength calculation of each lines. The Gaussian profile is widely used and is considered to be an almost perfect approximation for weak absorption lines. However some caution should be taken when measuring stronger lines (typically EW > 150 mA). In this case the Gaussian profile cannot perfectly fit the wings of the line. For these cases several authors prefer to use the Lorentzian profile to fit the stronger lines and their respective wider wings.

Until very recently, these measurements were only feasible using interactive routines such as "splot" from IRAF¹, where people have to go through the spectrum line by line, selecting the continuum position by eye and marking as initial guess for every line needed to be fitted in case of blended lines. This is of course a quite boring and very time consuming task. Even worse, the subjectivity involved in such interactive routines may lead to inconsistency between the measurements of different line. To overcome this issues, several automatic codes are now on the market (e.g. ARES(Sousa et al. , 2007), DAOSPEC(Stetson et al. , 2008)) that measure the EWs in more efficient and consistent way.

2.3 Atmospheric Models

The choose of the atmospheric models in the third point can also vary for different EW methods. From the literature there are a significant variety from where we can choose. The models created by Kurucz (Kurucz et al., 1993), closely followed by the MARCS models (Gustafsson et al., 2008), clearly standout as the most used set of atmospheric models for the derivation of spectroscopic and chemical abundances.

The way the models are created and used in each method can also differ. Some prefer to create the models on the spot making use of the available codes. In alter-

¹ IRAF is distributed by National Optical Astronomy Observatories, operated by the Association of Universities for Research in Astronomy, Inc., under contract with the National Science Foundation, USA

native, and to increase the efficiency of each method, grids are created with precomputed atmospheric models which can be directly selected for each step of the iteration, or instead, the grid of models can be used for interpolation allowing this way a better refinement in the search of the stellar parameters.

As one could expect, for the creation of the models there are a series of important physical parameters and approximations that need to be defined and used for the correspondent computation. For FGK solar-type stars the plane-parallel approximation is proved to be a safe approach, but when dealing with different types of stars, "special" models may be necessary for such specific purposes (e.g. metal-poor stars, giant and evolved stars).

2.4 Computing Abundances

In point number four we have the computation of the iron abundance (or any other chemical element). This point clearly depends on the measured strength of the line as well as the selection of the atmospheric model. Here we also may discuss the typically assumed local thermodynamical equilibrium (LTE) that is also commonly used as a valid approximation for FGK solar-type stars. As for the atmospheric models, this approximation may not be completely valid for other types of stars. As an example, for very metal-poor stars it may be necessary to use NLTE corrections to derive accurate and reliable spectroscopic stellar parameters (Bergemannet al. , 2012).

2.5 Finding the correct parameters

Finally, we are left out with point number five. In this point we need to verify the excitation and ionization balance for the results. The verification for itself is simpler, where the correlation between the Excitation potential and the iron abundances strongly constrain the effective temperature, the correlation between the reduced equivalent width and the individual abundances constrain the microturbulence and the ionization balance observed from the difference between the FeI and FeII mean abundances serves to constrain the surface gravity. For the determination of the "correct" spectroscopic parameters we are actually looking for no correlations at all i.e. when we see all the lines given the same individual abundance we stop the process and keep the parameters from the adopted atmospheric model. The iron abundance comes as an additional result from this analysis and is just taken as the mean abundance from all the lines.

The main difference between the EW methods here may be related with the way that the parameters are found and constrained. There are different minimization algorithms that may be used to explored the parameter space and the respective interdependences. Finally the constraints used to stop the method and check for the correct convergence of the parameters (i.e. where is the definition of no correlation from the data, e.g. does a slope with a value of 0.01 represents already no correlation?) is a crucial final decision for each method that may change the final parameters.

3 ARES+MOOG

In the last section it was described a general overview of an EW method. Here we will go through the points once again and describe the specific choices made in the ARES+MOOG. The data flow of this method is fully described in Fig. 1.

3.1 Line-list

Since this method was designed to be completely automatic, for the compilation of the line-list we have selected as many lines as possible. This allow us to increase the statistical strength of the derived parameters. However each line was carefully selected in order to be considered "stable" for this method (for further details on the stability of the lines see Sousa et al. (2008)).

In what regards the atomic data, in order to overcome the uncertainties for the $\log gf$ described before, we made use of a differential analysis technique. This technique consists in selecting a benchmark star (typically the Sun) with very well constrained parameters. The goal of this analysis is to recompute the $\log gf$ using an inverse analysis. We first measure the EWs for our selected lines in the solar spectrum. Then assuming the solar known parameters (Teff = 5777K, log g = 4.44 dex, $\xi_t = 1.00 \text{ kms}^{-1}$, and log(Fe) = 7.47), the values for each log gf are then changed until we derive the "correct" individual abundance for each line.

Using this differential analysis it is possible to reduce both the errors on the atomic parameters as well as part of the measurement errors on the equivalent widths that are still present. When measuring the lines in a benchmark star we are also including errors given by the spectrum itself. An example being the existence of small undetected blended lines, or the bad position of the continuum in that region of the spectrum. When computing the $\log gf$ for these lines we are including all these errors, and this way we are partially compensating for the errors assuming a systematic measurement of the EW for the same lines of the stars being analyzed. An obvious draw back from this analysis is that the results strongly deteriorate as we use the log gf in stars that are become more and more different that the benchmark star.

3.2 Measuring EWs

The Equivalent Width of the lines are automatically determined using ARES² code (Sousa et al. , 2007) following the approach of Sousa et al. (2008) and Sousa et al. (2011) to adjust the *re jt* parameter of ARES according to the S/N of each spectrum. In the next section it will be described in detail the input parameters for ARES and some advices are given in order to select the best input parameters.

3.3 Atmospheric Models and Abundance Determination

We use MOOG³ (Sneden , 1973) to compute the line by line abundance for each star assuming LTE. In our standard method we use a grid of Kurucz Atlas 9 planeparallel model atmospheres (Kurucz et al. , 1993) which is used for interpolation to generate the stellar atmosphere model. This model is then feed as an input into MOOG to compute the abundances through the driver *abfind*.

3.4 Finding the correct parameters

Although we don't describe in this document the full automatization of the method, in the original ARES+MOOG we use a minimization algorithm, the Downhill Simplex Method (Press et al., 1992) which is used to find the best parameters. Moreover in order to identify outliers caused by incorrect EW values, we perform a $3-\sigma$ clipping for the FeI and FeII lines after a first preliminary determination of the stellar parameters. After this the procedure is done once again without the rejected lines.

4 ARES+MOOG - Quick Tutorial

The tutorial presented here follow the procedures and codes that were made available at the "Spring School of Spectroscopic Data Analyses". The codes are available either at the respective web-pages or are still accessible from the school web-page: http://spectra.astro.uni.wroc.pl/

As described before, the first step for ARES+MOOG is the definition of the linelist. We will use the very well defined line-list composed of nearly 300 iron lines. The line-list and respective details are presented in Sousa et al. (2008). If the reader is interested in a recent update of the line-list see the work of Tsantaki et al. (2013).

² The ARES code can be downloaded at http://www.astro.up.pt/

³ http://www.as.utexas.edu/~chris/moog.html



4.1 Using ARES

You can find a complete description of ARES in Sousa et al. (2007). In this document we will only point out the essential points that are required to properly run the code.

A sketch of the ARES procedure can be seen in Fig. 2. The basic steps of ARES are: the reading of both the spectrum and the line-list; the local normalization of the spectrum which is performed for each line in each iteration; the detection of the local lines that are needed to be fitted (blended lines); the fit itself and the respective calculation of the EW; All the EWs are then stored in an output file.

4.1.1 Preparing the spectrum

The first step for this method is the preparation of the observed spectra. The available version of ARES only works with an one dimensional FITS spectrum. The requirement is that in the respective FITS header the CDELT1 and CRVAL1 keywords need to be defined.

Another fundamental condition is that the spectrum should be corrected in radial velocity so that the absorption lines are found at the rest frame, otherwise ARES will not be able to find the correct line for the analysis.

4.1.2 The line-list

The only requirement for the line-list to be feed in to ARES is to provide the correct wavelength. The file with the list of lines should be consisted of a column with the wavelength. ARES will read this file line by line for the respective EW measurement. It may be useful to keep in this file the atomic data for each line that will be required later on.

4.1.3 ARES input parameters

The input parameters for ARES are the following:

- *specfits*: The name of the 1D fits file with the spectrum corrected in RV (e.g. HD1234_rv.fits).
- *readlinedat*: The name of the file with the list of lines to be measured (e.g. line-list.dat).
- *fileout*: The name of the file that will contain the output of the results (e.g. HD1234.ares).
- *lambdai*: Initial wavelength to search the lines (e.g. 3000 Å).
- *lambdaf*: Final wavelength to search the lines (e.g. 7000 Å).
- *smoothder*: Smooth value for the derivatives that are used for the line detection procedure (e.g. 4 recommended value for high resolution spectra and good S/N).
- space: Size of the local spectrum interval in Angstroms around each line. Only
 this interval is used for the individual computations for each line (e.g. 3 Å- recommended value).
- *rejt*: Parameter for the calibration of the continuum position. This value strongly depends on the S/N of the spectrum. A good reference for the values to be used here can be found in Sousa et al. (2008, 2011) (e.g. 0.996 for a spectra with S/N \sim 400).
- *lineresol*: This parameter sets the line resolution of the input spectra; This parameter is helpful to distinguish real lines from noise (e.g. 0.1 Å- recommended value for high resolution spectra).
- *miniline*: Lines with strength weaker that this value are not printed in the output file (e.g. 2 mÅ).
- *plots_flag*: Flag for the plots (0-runs in batch, 1-shows the plots and stops for each line calculation).

There are specific input parameters that are very important to obtain correct EWs. A proper selection of the *rejt* parameter is fundamental in order to track the correct continuum position. Wrong values of this parameter may systematically give larger (or smaller) EWs. Although there are a clear dependence on this parameter with the S/N we choose to leave this as a free parameter given the high degree of subjectivity when defining the continuum position. If you want to define your own S/N dependence we advice you to select only a few isolated lines for a bunch of spectra with different S/N and make use of the plots to select the best values for each S/N. For more details on such exercise see the work of Mortier et al. (2013).

For the other parameters, the recommended values should be kept fixed. We may only consider tweaking the *smoothder* parameter for higher values in case of very low S/N spectra. This may help for the correct identification of real lines in noisy spectra.

4.2 Generating an atmospheric model

The creation of the atmospheric models in ARES+MOOG is done by an interpolation code which in turn uses a grid of pre-computed KURUCZ models. The interpolation of models was choose here for efficiency purposes. The interpolation code provided consists actually in two separated Fortran codes, the first for the interpolation itself. The second to accommodate the model in a file with a specific format ready to be read by MOOG. A script named "make_model.bash" is provided in order to run both codes directly. In order to run the script you will simply have to give as input the parameters (T_{eff} , $\log g$, ξ , and [Fe/H]) to generate the model which will be stored in a file named "out.atm".

4.3 Using MOOG

MOOG is a code that performs a variety of LTE line analysis and spectrum synthesis tasks. The typical use of MOOG is to assist in the determination of the chemical composition of a star. In our case we want to measure individual iron line abundances to derive the stellar parameters.

There are several drivers available to run MOOG for several different purposes. The MOOG user's manual have a complete description of the several drivers. For ARES+MOOG we just make use of the *abfind* driver.

One of the chief assets of MOOG is its ability to do on-line graphics. However in ARES+MOOG the graphics are not used at all. The visualization of different plots are quite useful to see the dependences of the different parameters with the individual abundance determination. Together with a modified MOOG version (where the internal plots were ignored since it requires a propriety library) it was provided a simple Python code to perform the plots (named read_moog_plot.py). This code is used to illustrate the parameters dependences and respective correlations in the next sections.

Another important point for MOOG is that it needs to read the atomic data for each line in order to perform the individual abundance calculations. For this purpose an additional script was provided (make_linelist_local.bash) that reads the output of ARES and the initial line-list to create the required formated file for MOOG's input.

4.4 Search for the correct model

For this tutorial we will make use of the solar type star HD1461 for which a HARPS spectra was taken with high resolution and high s/n. The parameters for this star was derived automatically by ARES+MOOG in Sousa et al. (2008). The parameters derived for this star are: $T_{\text{eff}} = 5765$ K, $\log g = 4.38$ dex, a $\xi = 0.97$ m/s and [Fe/H] = 0.19 dex. Going through the method, i.e. computing the EWs for the



Fig. 3 Abundance of FeI as a function of excitation potential(E.P.) and reduced wavelength (R.W.). The top panel shows the result for the "correct" stellar parameters while in the bottom panels the temperature was change to a lower value (5600 K) - left panel, and an upper value (5900 K) - right panel.

line-list, creating a atmospheric model with these values, and running MOOG, we will get to the result that is presented in the top panel of Fig. 3. This figure shows the correlations between the iron abundance (Ab(FeI)) and the excitation potential (E.P.) and the reduced equivalent width (R.W.). In the same figure it is also indicated together with the respective slopes of the correlations the difference between the average abundances of FeI and FeII (<Ab(FeI)> - <Ab(FeII>>). From the values indicated in the figure we can see that the slopes of the correlation are nearly zero, as well as the difference between FeI and FeII is close to null.

In these series of exercises our goal is to present the dependence of each correlation with the spectroscopic parameters. From the theoretical studies one can easily understand that the $T_{\rm eff}$ has a strong influence in the correlation Ab(FeI) vs. E.P.. The same happens for the microturbulence for the correlation of Ab(FeI) vs. R.W.. As described before the surface gravity is connected directly with \langle Ab(FeI) \rangle – \langle Ab(FeII) \rangle . In this tutorial we show these dependences in a practical way making use of the codes provided for the ARES+MOOG method.



Fig. 4 Same as Fig. 3 but instead of changing the temperature, here we change the surface gravity to a lower value (4.10 dex) - left panel, and an upper value (4.50 dex) - right panel.

4.4.1 Teff dependence

The lower panels of Fig. 3 shows the computed abundances for a model with exactly the same parameters with exception of the temperature. It is clear that the slopes of the correlations change dramatically. Not only the Ab(FeI) vs. E.P. changes but also the same happens for Ab(FeI) vs. R.W. showing that the stellar parameters are strongly inter-dependent. This inter-dependence makes the job of finding the correct parameters harder.

From the practical point of view, an important message from these plots can be withdrawn. We can check how Ab(FeI) vs. E.P. varies to the changes in temperature so we can react accordingly to find the correct temperature. We can see a clear difference between the slopes in the two cases with different temperature. When we underestimate the temperature the slope is positive, while when we overestimate the real temperature, the slope becomes negative. Therefore in the cases when we don't know the correct temperature, after a first guess, we may look to the slope of Ab(FeI) vs. E.P. where its signal let us know in which direction is the correct temperature.

4.4.2 Surface Gravity dependence

A similar exercise can be done for the surface gravity. Here the temperature was set back to its "correct" value and we want to change only the gravity and check how $\langle Ab(FeI) \rangle - \langle Ab(FeII) \rangle$ changes accordingly. Figure 4 shows the calculated abundances for this exercise. Again we see a clear difference in the two cases. When we underestimate the surface gravity $\langle Ab(FeI) \rangle - \langle Ab(FeII) \rangle$ is positive. In this case we underestimate the abundances of the ionized iron. Note that the atomic iron is nearly unaffected by the changes of the surface gravity while the ionized iron changes significantly. This is the reason why the ionization balance can be used to constrain the surface gravity. For the case where we overestimate the surface gravity



Fig. 5 Same as Fig. 3 but instead of changing temperature, here we change the microturbulence to a lower value (0.5 m/s) - left panel, and an upper value (1.5 m/s) - right panel.

we see an opposite effect where the difference becomes negative. In this case the abundances of the ionized iron are seriously overestimated.

One interesting fact is that the changes on the surface gravity nearly does not affect Ab(FeI) vs. E.P.. This is clearly observed in the figure and is clearly reported in the values of the slopes for both cases. This means that the log g derived from this method is nearly independent of the temperature, and vice-versa. This is certainly an advantage for this method showing that the temperature and the iron abundance are independently well constrained. This is an outcome of the reduced number of ionized iron lines that are available for such an analysis (~ 15 FeII lines when compared to ~ 300 FeI lines). The disadvantage here is that the log g is also not very well constrained. From one side we can be safe in deriving the temperatures and iron abundances, but an extra caution should be considered for the derived values of the surface gravity which relies on few ionized lines. For more details on this issue see the work of Torres et al. (2012).

4.4.3 Microturbulance dependence

A final exercise can be made for the microturbulence. Again all parameters are set to the "correct" ones with exception of the adopted microturbulence. This parameter is connected with the saturation of the stronger iron lines. A good value for the microturbulence will allow us to derive the same abundances for weak and strong iron lines.

The left panel of Fig. 5 shows the result of the abundances when the microturbulence is underestimated. The slope of Ab(FeI) vs. R.W. is positive in this case. So imagine that we already found a good excitation and ionization balance and we derive a slope for Ab(FeI) vs. R.W. which is positive. This means that the "correct" value for the microturbulence should be higher. The opposite happens when you overestimate the microturbulence as can be seen from the right panel of Fig. 5.

5 Summary

In this document we have described in practical terms the use of the EW method to derive spectroscopic stellar parameters. We have made a general overview of the several steps that are required to use this method. We have described several options that are used by different authors, namely the use of different line-lists, and the use of different atmospheric models.

The ARES+MOOG method is described here in some detail where we try to give the best advices for a proper use of it, namely in what regards the use of the ARES code to automatically compute the equivalent widths.

The details on how the method finds the "correct" set of stellar parameters are clearly exposed here. From the practical point of view, the essential steps of the method are described and can be used as a guideline for future works. Some additional points to fully complete the description of ARES+MOOG were left a side. These include the minimization algorithm which allows a proper automatization of the full process. For more information related with the minimization process we point the reader to Press et al. (1992); Saffe (2011).

The other additional important point that was not discussed here is related with the estimation of the errors of the parameters. These are directly connected with the dispersion of the abundance points presented in the correlations. The dispersion comes from several sources, namely the spectra quality, the atomic data, and the errors on the equivalent widths. For a proper description on the estimation of the errors for the ARES+MOOG method we point the reader to Sousa et al. (2011).

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