Stellar Atmospheric Parameters: The Four-Step Program and Gaia’s Radial Velocity Spectrometer

Carlos Allende Prieto

Mullard Space Science Laboratory, University College London, Holmbury St. Mary, Surrey RH5 6NT, United Kingdom

Abstract.
The determination of atmospheric parameters is the first and most fundamental step in the analysis of a stellar spectrum. Current and forthcoming surveys involve samples of up to several million stars, and therefore fully automated approaches are required to handle not just data reduction but also the analysis, and in particular the determination of atmospheric parameters. We propose that a successful methodology needs, at the very least, to pass a series of consistency tests that we dub the ‘four-step program’. This and related issues are discussed in some detail in the context of the massive data set to be obtained with the Radial Velocity Spectrometer onboard Gaia.

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INTRODUCTION

Modern spectroscopic surveys reach data acquisition rates far superior to those possible with conventional astronomical facilities. Fast speed is achieved by multiplexing on dedicated instruments, which demands sophisticated data reduction pipelines. The most basic and general parts of the data analysis must also be streamlined for a rich science return. In the case of stellar spectroscopy, such basic analysis covers the determination of atmospheric parameters: surface temperature and gravity, and overall metallicity. Secondary parameters that may be involved are the projected rotational velocity and the atmospheric micro- and macro-turbulence velocities. The determination of detailed chemical compositions is also amenable to automation.

The development of automated methods for deriving atmospheric parameters for all types of stars is a major undertaking. The set of parameters that can be recovered is highly dependent on the class of stars under consideration, and the characteristics of the data. Therefore, a modular approach is necessary, with different branches devoted to different classes of stars, aimed at extracting the most relevant parameters in each case.

Regardless of the target classes of stars and the type of spectra and supplementary data available, it is possible to list a number of general requirements that must be always met. A suitable analysis protocol must be able to extract the sought-after information in the spectra, and do so in a reasonable time. The derived quantities need to be free of significant systematic errors, i.e. a calibration to track such systematics must be in place. The analysis must also provide realistic error bars, as expected from the uncertainties in the input data, which combined with the systematic errors will give an adequate description of the uncertainty in the final results.
These requirements can be translated into a series of tests involving both simulated data and real spectra. In this contribution, I propose a recipe for such a validation scheme (the four-step program) and provide examples relevant to the European mission Gaia, and in particular to the analysis of spectra of AFGK stars from the Gaia Radial Velocity Spectrometer (RVS).

**THE FOUR-STEP PROGRAM**

The four-step program sketched below attempts to address the most fundamental requirements that should be asked from an automated spectral analysis tool. A successful protocol needs to answer affirmatively to the following questions:

1. Information content: Is the information we seek contained in the data?
2. Robustness: Can one recover the information with meaningful uncertainties in the presence of realistic noise?
3. Accuracy: Do our models resemble nature?
4. Implementation practicalities: speed, memory, etc.: Are these constraints satisfied? Are error estimates adequate?

The design of an analysis tool will also involve an additional step, previous to those above: the selection of the target stellar type(s), the relevant parameters for them, and which parts of the available data set will be used. The design process will require some form of iteration in which after part or all of the suggested checks are performed, the target parameters and data selection are modified, and the tests performed again.

Most of the discussion below is generally applicable to any method for parameter determination. It is assumed that models are used to compute spectra for different parameters, and one can use them to assign most probable values for the parameters to any given observed spectrum. There is some times a distinction in the literature between analyses based on models or empirical data, but such a separation is usually artificial: the parameters assigned to a library of templates used for training or calibration will be ultimately linked to model atmospheres employed in earlier analyses.

With the purpose of illustrating our discussion, we will be using simulated data that resemble those to be obtained by the Gaia RVS. The basic characteristics are a FWHM resolving power $R \equiv \lambda / \delta \lambda \simeq 11,500$ for bright targets and roughly half that value for $V > 10$, a spectral coverage between 847 and 874 nm, and a signal-to-noise ratio per pixel that will range from a few hundred at $V \sim 6$ to 6 at $V \sim 14$. The RVS spectral window is dominated by the Ca II infrared triplet lines, and therefore Ca/H, more even so than Fe/H, is a key parameter.

For our examples, we will deal with the 4-dimensional problem of finding surface temperatures, gravities, iron and calcium abundances from RVS spectra. We will search for the optimal solutions using a minimum distance method based on the Nelder-Mead algorithm (Nelder & Mead 1965) and interpolation on a grid of synthetic spectra covering the spectral types A-K computed with Kurucz model atmospheres (Kurucz 1997). The search algorithm has been coded in FORTRAN90 and described in previous reports (Allende Prieto 2004; Allende Prieto et al. 2006, 2008; Kilic et al. 2007).
We will consider two cases, using either absolute or normalized fluxes. The first one corresponds to the situation when the angular diameter of a star is known — model atmospheres predict the flux at the stellar surface, while observations measure it at the Earth. Alternatively, one can also use absolute fluxes when stellar radii are adopted from stellar evolution models and the parallaxes are known. For a given chemical composition, the parameters that define a model atmosphere (surface gravity and effective temperature) can be mapped into a stellar mass and radius. We will also test the analysis of RVS spectra normalized to the continuum.

**INFORMATION CONTENT**

The most fundamental requirement we should ask from a protocol for automated determination of stellar atmospheric parameters, is that the input data contain enough information to constrain the sought-after parameters. The two obstacles to overcome are called (lack of) sensitivity and degeneracy. If the data have very low or zero sensitivity to the parameters of interest, the design needs to be reconsidered. The same is true if the response of the spectra to changes in different parameters are very similar.

One can directly test for the presence of these two pathologies using model spectra. The analysis protocol should return consistent and unique solutions for the very same models used for training/calibration. For some algorithms, e.g. neural networks, a successful training process will already address this matter.

To illustrate this phase we use the aforementioned library of Gaia RVS synthetic spectra. We feed the same spectra to the optimization code and compare the results with the true values used in the calculations. The model fluxes at the edges of the grid are excluded, given that the algorithm has special difficulties in those areas; there are 1875 spectra. The mean difference (and the root-mean-squared scatter) between output and input iron and calcium abundances, temperatures, and gravities were, respectively 0.0005 dex, 0.13 K, and 0.001 dex. Very similar results are obtained for the analysis of normalized spectra. It is interesting to note that the widths of the distributions for the Fe and Ca abundances, as well as for the surface gravities, are dominated by truncation errors. In spite of this issue, the output matches the input parameters so tightly that we can consider that our analysis design has succeeded in this test.

**ROBUSTNESS**

Real spectra will be subject to noise of multiple origins. We will divide the sources of noise into *systematic* and *random*. It is usually the case that there are several random components, following different distributions.

The systematic errors can also include multiple components or sources. For example, some manifest themselves as time-independent deviations between observations and models. Another kind of systematic errors, those that can offset as a whole a model spectrum from an observed one, can be considered as random variables. This is the case, for example, when an angular diameter is used to scale model fluxes computed at the stellar surface to observations: a random uncertainty in the angular diameter causes a
FIGURE 1. 1σ uncertainties in the derived parameters after adding noise to the model spectra. The solid lines correspond to Gaussian noise added at the pixel level. The dashed lines correspond to the same noise at the pixel level and an additional noise that systematically shifts any given spectrum by a random factor from a Gaussian distribution with a $\sigma = 1/20$ ($S/N_{\text{sys}} = 20$). The dash-dotted lines correspond to the case of continuum-corrected spectra.

systematic offset of the entire spectrum.

To evaluate robustness, one can use the same model spectra produced for the analysis, add random noise, and perform a new analysis. However, one needs to go one step further, producing new models with different parameters. This is particularly critical for testing the performance of different interpolation schemes, as the results are fairly immune to interpolation errors when searching for solutions located at the grid nodes.

To exemplify this phase, we go back to our Gaia RVS models and introduce random Gaussian noise. Firstly, the spectra are degraded to a signal-to-noise ratio per pixel of 100, 50, 20 and 10. The results are summarized in Fig. 1. We also consider the case when there are additional systematic offsets that affect each spectrum’s flux level (we arbitrarily chose $S/N_{\text{sys}} = 20$), and this corresponds to the dashed lines in Fig. 1. The absolute flux level is key to constrain the effective temperatures, and as such the uncertainties for the cases when a systematic offset is present are much larger and independent of the signal-to-noise ratio. On the other hand, the continuum shape has little information about abundances and surface gravities, which makes them fairly insensitive to systematic errors.

Finally, we analyze the case in which the spectra are normalized to the continuum. The results are also included in Fig. 1 using dash-dotted lines. Quantities that have a very
limited effect on the continuum shape exhibit very similar error bars as for the previous two cases, but surface temperatures are more poorly recovered and their uncertainties increase faster as the signal-to-noise degrades.

**ACCURACY**

Even if our system works *in theory*, as demonstrated after it has successfully passed the tests described in the previous sections, subtle differences between the model spectra and the real stellar spectra can ruin our prospects of performing a serious scientific analysis.

The ultimate challenge consists in using a set of well-studied objects with trustworthy parameters. A number of libraries from the literature can be used (e.g. Le Borgne et al. 2003, Valdes et al. 2004, Mouttaka et al. 2004, Bagnulo et al. 2003, Allende Prieto et al. 2004, Sánchez-Blázquez et al. 2006), but it is often the case that high quality data are only available for a few stars with a limited range of atmospheric parameters. In this situation, a convincing demonstration requires using several data sets. This step usually involves substantial data processing, in order to transform existing data to resemble our working setup. Typical data transformations include adding noise and reducing the spectral resolution.

In the case of Gaia, the use of the Near-IR spectral window restricts the applicability of most of the existing libraries, as they tend to focus on optical wavelengths. Among the obvious choices, there are only two possibilities: the UVES Paranal Observatory Project (Bagnulo et al. 2003) and the S$^4$N survey (Allende Prieto et al. 2004). Unfortunately, the former library does not include a catalog of atmospheric parameters and abundances. To make use of it for calibration purposes it is necessary first to undertake a detailed analysis of the library spectra. S$^4$N includes such a catalog, but it is affected by severe incompleteness: it only covers about 100 stars and the Southern targets were observed with a single spectral setup that left inter-order gaps affecting the RVS window. This leaves us with just 64 stars.

Fig. 2 illustrates the results of the analysis of the S$^4$N spectra. This library does not include absolute fluxes, and therefore we only experimented with continuum-normalized data. There is a reasonable correlation between the catalog parameters and those we derive from the Gaia window, but the rms scatter is disappointingly large: 217 K, 0.44 dex, 0.11 dex, and 0.13 dex for $T_{\text{eff}}$, $\log g$, [Fe/H], and [Ca/Fe], respectively. These figures compare poorly with other results from similar or even lower resolution analysis (e.g. Allende Prieto et al. 2006, 2008). Note, however, that all these studies handle only three parameters, assuming a coupling between $\alpha$ and Fe.

The synthetic spectra give a fair match to the observed ones, albeit the agreement becomes less satisfactory for warm F-type stars. The limited spectral range and lines it contains does not leave much room for error. The sensitivity of the wings of the strong Ca II triplet lines to both the calcium abundance and the stellar surface gravity ties the uncertainties in these two parameters. For cool stars, where the electron pressure is much smaller than the gas pressure and the continuum is dominated by the H$^-$, the gas pressure at a constant temperature is approximately proportional to $g^{2/3}$ (see Gray 1992). The wings of the Ca II lines grow proportionally to the calcium abundance and to $g^{1/3}$, and thus the uncertainties in the derived surface gravities are expected to be three
times larger than those in the calcium abundance, as confirmed by the numbers above.

The comparison between the uncertainties in the analysis of the S$^4$N spectra and the theoretical expectations described earlier suggests that the synthetic spectra must become more realistic to allow us to cleanly disentangle the effect of the different atmospheric parameters, in particular gravity and chemical abundances, from Gaia spectra of bright sources. Accounting for departures from LTE and/or empirically correcting the atomic parameters to match one or several well-observed reference spectra will likely help. The availability of absolute fluxes and parallaxes, will surely provide a much tighter constraint on the surface gravities that must be taken advantage of.

**IMPLEMENTATION**

Speed and other practicalities may get in our way. In the case of Gaia, the large number of sources places stringent constraints in the type of analysis that is possible within reasonable time scales. Other issues must also be considered, such as the required memory. For the Gaia tests described above, linear interpolation in the 4D parameter space appears accurate enough. Our tests, which involved 1122 frequencies per spectrum, used up about 50 Mbytes of memory, mostly to hold the model grid, and took about $10^{-2}$ seconds per spectrum on a modern processor. If suitable RVS observations have a mini-
mum signal-to-noise ratio per pixel of about 10, we are left with a sample of $2 - 4 \times 10^7$ stars down to $V < 13 - 14$, which could be processed in just a few days.

Our procedure must be able to evaluate, realistically, the uncertainties in the estimated parameters. This can be achieved in multiple ways, but the most popular methods involve calculating the covariance matrix or running Monte Carlo simulations. Tests with both procedures are underway for the Gaia case and will be described elsewhere.

CONCLUSIONS

In this contribution I highlight the need for accurate atmospheric parameters determined without human supervision in modern stellar spectroscopic surveys. Successful programs must pass a series of rigorous consistency and performance checks. A proposal for such a set of tests is presented – which we dub the four-step program– based on Monte Carlo simulations and libraries of real observed spectra. The program will need to be customized for each particular data set and analysis algorithm, but the basics are likely of general application.

We illustrate the different phases of the four-step program with simulated data for the Gaia RVS. It is pointed out that there is no existing spectral library of observations that is up to the task of calibrating the tools for deriving atmospheric parameters for this particular data set. An appropriate catalog of high-resolution spectra should be assembled. A consistent spectral analysis of the targets included in such library should be carried afresh, taking advantage of a wider spectral range (including the visible), in order to avoid inheriting systematic errors introduced by combining results from multiple sources in the literature.

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