An Automated System to Classify Stellar Spectra I.

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ABSTRACT

Analyses of stellar spectra often begin with the determination of a number of parameters that define a model atmosphere. This work presents a prototype for an automated spectral classification system that uses a 150 Å-wide region around Hβ, and applies to stars of spectral types A to K with normal (scaled solar) chemical composition. The new tool exploits synthetic spectra based on plane-parallel flux-constant model atmospheres. The input data are high signal-to-noise spectra with a resolution greater than about 1 Å. The output parameters are forced to agree with an external scale of effective temperatures, based on the Infrared Flux Method. The system is fast – a spectrum is classified in a few seconds – and well-suited for implementation on a web server. We estimate upper limits to the 1σ random error in the retrieved effective temperatures, surface gravities, and metallicities as 100 K, 0.3 dex, and 0.1 dex, respectively.

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

1 INTRODUCTION

Mass, radius, and luminosity are some of the most interesting properties of a star. Unfortunately, it is non-linear combinations of them that produce quasi-linear changes on a stellar spectrum. Stellar fluxes are commonly interpreted in terms of atmospheric temperature, pressure, and chemical composition. In the context of classical flux-constant model atmospheres, these fields are simply specified with three scalars: the effective temperature, the surface gravity, and a solar-scaled metallicity. Nevertheless, extracting the three from an observed spectrum is rarely trivial.

A spectroscopic classification system has been developed independently of the physical parameters. The MK system (Morgan, Keenan & Kellman 1943) lays out a series of rules to assign spectral classes from medium-low resolution spectra. This method has the advantage of providing a standard reference independent of models. However, it is somewhat artificial, in the sense that the defined spectral classes are obviously correlated with the relevant atmospheric parameters. Moreover, the classical MK system does not provide for metal-poor stars. One may note, as an example, that the metal-poor giant HD 122563, which has an effective temperature around 4600 K, has been often classified as a late-F or early-G type star. On the other hand, classification methods based on physical parameters are more natural, but model-dependent.

Both the MK and the physical classification systems have their own advantages, and this may be the reason why they still coexist. But, the fact that it is the physical parameters what is ultimately demanded for astronomical applications is shifting most of the recent research toward the direct extraction of those quantities. As recognized by many specialists, repeatability and high speed in spectroscopic stellar classification can only be achieved by using automatic methods. A recent discussion of the most used methods can be found in Bailer-Jones (2001).

Derived stellar parameters may differ when determined from different wavelength ranges or spectral features. Among other reasons, this may be caused by using models that are too simplistic. As the parameters will be derived from their expected effect on the spectra, inaccurate predictions, or neglect of other relevant parameters, will bias the results. Details in the implementation of a classification procedure are also a reason to worry. The wide range of effective temperatures that have been assigned to the metal-poor subgiant HD 140283 in the recent literature serves as testimony of the respectable uncertainties still involved in the scale of effective temperatures (see, e.g., the discussion in Snider et al. 2001).

Discrepancies produced by interpreting stellar spectra with model atmospheres that are too simple will decrease as progress in theory takes place. For main-sequence stars, remarkable advances are happening as efforts focus on relaxing the assumptions of Local Thermodynamic Equilibrium (LTE) and hydrostatic equilibrium. Systematic differ-

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ences that arise in the implementation of different methods
for spectroscopic classification can be controlled by estab-
lishing standards. A reference implementation would be far
more powerful than a set of standard stars. Modern infor-
mation technologies have paved the way for implementing
a public automatic classification system accessible over the
Internet. Such open system, if reliable and fast, could serve
as a standard reference.

This paper discusses the first steps toward the imple-
mentation of a prototype for an open classification system.
This work will only deal with a section of the HR diagram;
stars with spectral types A to K and scaled solar metal abun-
dances. Section 2 describes the selected wavelength band,
§3 the working parameters space, and §4 provides details of
the implementation. Section 5 is devoted to connecting the
parameters derived from spectroscopy to a widely accepted
scale of effective temperatures based on the Infrared Flux
Method, and checking the performance of the method. Sec-
tion 6 concludes with a summary of present results and ideas
for subsequent work.

2 WAVELENGTH RANGE

When using equivalent widths and classical flux-constant
model atmospheres in abundance analyses, the relevant pa-
rameters can be usually reduced to four: the stellar effec-
tive temperature ($T_{\text{eff}}$), the surface gravity ($g$), the
microturbulence ($\xi$), and the metal abundances – commonly
considered proportional to the iron abundance. For stars with
spectral types A–K, the most useful and accessible observa-
tional probes for these parameters are the flux distribution
and the spectral lines: excitation and ionization equilibrium
of metals, the pressure-enhanced wings of strong metal lines,
and the hydrogen lines. Different procedures to derive stell ar
parameters rely on one or several of these indicators.

At this point we set aside potential difficulties to model
some of the spectral features mentioned above. We refer the
reader to the papers by Dragon & Mutschlecner (1980),
Castelli, Gratton & Kurucz (1997), or Bell, Balachandran
& Bautista (2001) regarding the modelling of the continu-
um flux; Thévenin & Idiart (1999) or Asplund et al. (2000)
on the calculation of Fe I line profiles; and Fuhrmann,
Axer & Gehren (1996), Gardiner, Kupka & Smalley (1999),
Barklem, Piskunov & O’Mara (2000), or Cowley & Castelli
(2002) on modelling Balmer lines. With the ultimate goal
of deriving chemical abundances, most spectroscopic observ-
ations aim at providing reliable line profiles or equivalent
widths for lines of weak-to-moderate strength. Ideally, one
would use the same type of spectra to determine the stellar
atmospheric parameters. In addition, accurate spectropho-
tometry is challenging and highly vulnerable to reddening.
Forcing the excitation and ionization equilibrium balance
for metal lines is, in most cases, insufficient to reliably de-
terminate the quartet ($T_{\text{eff}}$, log $g$, [Fe/H] and $\xi$). Therefore, we
resort to a second feature, the Balmer lines.

We selected a continuous spectral window around H$\beta$:
4810–4960 Å. This wavelength range represents a balance in
many aspects. It is red enough that the continuum opacity
is well described by H and H$^-$ for the stars under consid-
eration, avoiding the difficulties of dealing with much more
complicated (metal) opacities, and it is blue enough that
the presence of spectral lines makes possible a reliable de-
termination of the metal abundance – even in metal-poor
stars.

3 WORKING DOMAIN

Use of equivalent widths, quantifying the strength of a spec-
tral line by a single number, represents a loss of informa-
tion. Use of line profiles introduces more variables in the
analysis through the different line broadening mechanisms.
Accounting for the broadening involves a number of difficul-
ties in the practical implementation of a classification algo-
rithm, although it also comes with extra information, e.g.
projected rotational velocity, or instrument spectral resolu-
tion. At this point we wish to restrict the classification to
($T_{\text{eff}}$, log $g$, [Fe/H], $\xi$) and, therefore, we use a fixed resolving
power $R \equiv \lambda/\delta \lambda \simeq 5000$. We covered the selected spectral
range with 301 points, equally spaced in wavelength (every
0.5 Å). Our choice of resolution is a compromise: low enough
to make rotational and macro-turbulent broadening in late-
type stars negligible, and high enough to be able to recover
information on the stellar atmospheric parameters. Fig. 1
shows observations for the Sun (solid; Kurucz et al. 1984),
Procyn (dashed; Allende Prieto et al. 2002), and Arcturus
(dash-dotted; Hinkle et al. 2000). The most relevant features
have been identified in the figure.

The range for each of the atmospheric parameters was
selected to avoid some extreme conditions where classical
model atmospheres in general, or those used here in particu-
lar, are expected, or known, to fail: cool temperatures at
which the contribution of molecules to the equation of state
is incomplete in the models; hot temperatures at which de-
partures from LTE are important for the atmospheric struc-
ture; or too extended an atmosphere that the plane-parallel
approximation is inadequate. The selected domain is:

\[
\begin{align*}
4500 & \leq T_{\text{eff}} & \leq 8000 \quad \text{K} \\
2.0 & \leq \log g & \leq 5.0 \quad \text{dex} \\
-4.5 & \leq [\text{Fe/H}] & \leq +0.5 \quad \text{dex} \\
0 & \leq \xi & \leq 2 \quad \text{km s}^{-1}.
\end{align*}
\]

Arcturus is probably cooler than our lower limit for $T_{\text{eff}}$
[Griffin & Lynam-Gray (1999) assign 4290 ± 30 K to this
star], but it serves the purpose of showing an example of
the coolest spectra in our working sample. As will become
clear later, our raw $T_{\text{eff}}$ are systematically higher than other
scales and thus a star with this effective temperature is tech-
nically within the limits of our grid.

Extensive testing showed that the flux in the selected
spectral window satisfies a one-to-one relationship with most
of the parameters space. In other words, for a given combi-
nation of the four atmospheric parameters considered, the
resulting flux in this window is unique. Approaching the ex-
treme metal-poor limit, below [Fe/H] $\sim -3$, degeneracy is
unavoidable, as metal lines vanished, and so does the informa-
tion on metallicity, gravity and microturbulence. The flux
in the selected window is not equally sensitive to changes in

\[ [\text{Fe/H}] = \log \frac{N(\text{Fe})}{N(\odot)} - \log \frac{N(\text{H})}{N(\odot)} \]

1 [Fe/H] represents the number density of the element E.
Figure 1. Observed fluxes for Procyon, the Sun and Arcturus in the selected window. The original very high dispersion observations have been convolved with a Gaussian profile with a FWHM of 1.0 Å. The observations in the McDonald atlas of Procyon (Allende Prieto et al. 2002) have been continuum normalized by P. S. Barklem (see Barklem et al. 2002 for more details). A missing interval in the spectrum of Arcturus is severely affected by telluric lines.

the different stellar parameters. Changes in $T_{\text{eff}}$ affect the most the spectrum, followed by variations in the metal abundance. The effect of changes in the surface gravity is mainly felt through the different sensitivity of lines of neutral and ionized metals to pressure, and it is more subtle than the response to $T_{\text{eff}}$ or [$\text{Fe/H}$].

4 IMPLEMENTATION

To find the set of parameters that best reproduces an observed spectrum, we need to choose an algorithm. We want to minimize (or maximize) a function of the stellar parameters. This will require us to evaluate a function – thus compute synthetic spectra – a number of times. This number can be very large, and therefore a strategy to reduce computing time is needed. We have tackled this problem by computing a discrete grid and interpolating. We adopted the following increments for the four parameters involved: 500 K in $T_{\text{eff}}$, 1.0 dex in $\log g$, 1.0 dex in [Fe/H], and 1.0 km s$^{-1}$ in $\xi$. These were chosen to keep the changes in the spectrum small enough so that a fast multilinear interpolation would provide a reasonable approximation. Interpolation errors can reach up to 2 % for the warmer stars in the grid, but up to 7 % for the coolest metal-rich stars. These errors are smaller than the precision with which the real spectra can be reproduced, and it was later verified that use of a finer grid does not improve the performance of the classification method.

We used a genetic algorithm (GA) to solve our minimization problem. GAs are suitable for solving global optimization problems in complex landscapes where local extrema can confuse simpler algorithms (see Charbonneau 2002 for an informal introduction).

The grid of synthetic spectra was based on non-overshooting Kurucz (1993) model atmospheres. These models include mixing-length convection with $\alpha = 1.25$, and $\xi = 2.0$ km s$^{-1}$. The radiative transfer equation was solved with the code Synspec (Hubeny & Lanz 2000), using very simple continuous opacities: H, H$^-$, Rayleigh and electron scattering (as described in Hubeny 1988). An atomic line list was prepared with the data obtained from the Vienna Atomic Line Database (VALD; Kupka et al. 1999). This line list includes 7169 lines that are expected to contribute to the opacity in a solar-like atmosphere. The computed spectra were degraded to a resolving power of about 5000, sampled with a common wavelength vector, and normalized.

The presence of a very broad line in the spectral window ($H\beta$) makes normalization difficult. We have adopted a straightforward unsupervised polynomial normalization. Although the results of this scheme would visually displease most stellar spectroscopists (see Fig. 1), this simple procedure can be carried out quickly, and repeatability is easily achieved for a given set ($T_{\text{eff}}$, log $g$, [Fe/H], $\xi$). In addition, the fluxes were also divided by a constant, 1.8, to enforce flux values between 0 and 1 – a requirement of the GA software.

We implemented a FORTRAN routine to perform multilinear interpolation in the four parameters under consideration. This routine is the interface between the grid of synthetic spectra and the genetic algorithm. The function we chose to maximize is:

$$1 - \sum_i w_i (f_i - O_i)^2$$

where $\mathbf{f}$ is the vector of interpolated synthetic flux, $\mathbf{O}$ is the vector of observations, and the index $i$ indicates a particular wavelength bin. We adopted

$$w_i = (f_i^\odot - O_i^\odot)^{-2}/10^4,$$

as derived from the solar spectrum and a synthetic flux calculated with solar parameters, but reset to
Figure 2. Comparison between the observed (O) and (linearly interpolated) synthetic (f) corrected fluxes for the Procyon (F5 IV), the Sun (G2 V), Arcturus (K1.5 III), and the metal-poor HD 2665 (G5 III; [Fe/H] \(\simeq -1.9\)). The difference of the two vectors is also plotted.

\[
\begin{aligned}
&\left\{ \begin{array}{ll}
10 & \text{if } w_i > 10 \\
0 & \text{if } 1.0 > w_i.
\end{array} \right.
\end{aligned}
\] (4)

The many necessary multilinear interpolations are very fast, as the grid of previously computed synthetic spectra is kept in memory. In fact, a non-negligible fraction of the time is invested in loading those data. We adopted a publicly available GA software\(^2\) due to D. L. Carroll (see, e.g., Carroll 1996). The default parameters were kept, namely, a micro-GA with uniform crossover. The GA was run for 500 generations. This number was chosen from inspection of the convergency curve for a limited number of stars, but it was later verified that increasing this value to 2000 generations did not produce any improvement in the performance. Classification of a single spectrum takes about 3 seconds on a Sun Ultra5. Fig. 2 illustrates the agreement between the observed and the matched synthetic spectra for Procyon, the Sun, Arcturus, and the metal-poor star HD 2665 ([Fe/H] \(\simeq -1.9\)). The spectrum of HD 2665 was obtained from the Elodie library (Prugniel & Soubiran 2001).

5 CONNECTING OUR STELLAR PARAMETERS TO THE IRFM \(T_{\text{EFF}}\) SCALE

Detailed modelling of H\(\beta\) is an issue. Even though the wings of Balmer lines are considered to form very close to LTE conditions, that does not apply to their cores. A tougher complication is the fact that Balmer lines are commonly affected by the temperature distribution in the deepest atmospheric layers, which for late-type stars are significantly influenced by convection. Convection is typically treated using a mixing-length formalism which implies a choice for one or several parameters. This represents an important additional source of uncertainty in the derived parameters – very likely a systematic bias in the derived \(T_{\text{eff}}\). Such a bias in \(T_{\text{eff}}\) will, because of the tight coupling between \(T_{\text{eff}}\), \(g\), and [Fe/H], will also produce a bias in the other two parameters. In our view, the best possible option is to anchor our spectroscopic \(T_{\text{eff}}\) scale to a more reliable scale. The systematic effect in \(g\) and [Fe/H] implied by the necessary correction to our derived \(T_{\text{eff}}\) can be easily predicted. Empirical studies have shown that a shift in an adopted \(T_{\text{eff}}\) will, through the iron excitation-ionization balance, translate to a shift in \(\log g\):

\[
\Delta \log g \simeq \Delta T_{\text{eff}}/466.
\] (5)

\(^2\) Available from \url{http://cuaerospace.com/carroll/ga.html
\[ \Delta [\text{Fe/H}] \approx \frac{\Delta \log g}{3.0} \]  
(6)

(e.g. Gray 1992; Allende Prieto et al. 1999).

As we will be applying this correction to our \( T_{\text{eff}} \) scale, and the sensitivity to \( T_{\text{eff}} \) of the selected spectral region relies largely on the H\( \beta \) profile, there is no need to make a serious emphasis on the accuracy of the calculated absorption profile for H\( \beta \). We can make use of some approximations, and take advantage of a reduced computing time. In particular, we use an approximate broadening treatment described in the Appendix B of Hubeny, Hummer & Lanz (1994). As this approach underestimates the width of the solar H\( \beta \) profile, we apply a zeroth order correction, using twice the default value. This modification is not strictly necessary, as the correction to be applied later to the \( T_{\text{eff}} \) scale would be able to fix this zero point as well.

We decided to anchor our spectroscopic \( T_{\text{eff}} \) scale to that of Alonso, Arribas & Martínez-Roger (1996, 1999), which is based on the Infrared Flux Method, as modelled with fluxes from Kurucz (1993) model atmospheres. A library of high-resolution spectra recently published by Prugniel & Soubiran (2001) is used as testing field for our classification scheme. This library, hereafter the Elodie library, consists of more than 908 spectra from 709 stars spanning a large fraction of, and in some instances exceeding, our parameter space. We determine the \( T_{\text{eff}} \) for each star using the Alonso et al. calibrations for \( (B-V) \). These calibrations use \( (B-V) \) and [Fe/H], and both parameters were adopted from those given in the Elodie library. The division of the stars in IV-V or I-III classes, in order to select the appropriate IRFM calibration, is based on the gravities provided in the Elodie library, setting the division line at \( \log g = 3.8 \).

The spectra in the library with a resolution of \( R = 10,000 \) are convolved with a Gaussian profile with a FWHM of 1.0 Å, and then fed to our classification system to find a best-fitting vector \( (T_{\text{eff}}, g, \text{[Fe/H]}, \xi) \). Then, the values derived for \( T_{\text{raw}} \) are compared against those from the IRFM calibrations. The two scales are confronted in Fig. 3. A second-order least-squares polynomial fit is adopted to anchor the derived \( T_{\text{raw}} \) to the IRFM scale:

\[ T_{\text{raw}} = 5783 - 0.6686 \, T_{\text{IRFM}} + 0.0001159 \, (T_{\text{IRFM}})^2, \]  
(7)

and this correction is also translated to \( \log g \), and [Fe/H], based on the correlation expected for the excitation-ionization balance (see Eqs. 5 and 6). Fig. 3 reveals a tendency for some stars to clump at certain values of \( T_{\text{eff}} \), in particular at \( \approx 5375 \) K. Too aggressive a choice for the steps in the grid parameters (with the implied errors in the linear interpolation) is not to blame for this systematic effect, which is related to caveats involved in the implementation of GAs. Noticeably, the scatter is not symmetrically distributed about the adopted mean relationship, defined by the polynomial fit. This is actually what we expect when reddening is not negligible, introducing significant errors in the photometric \( T_{\text{eff}} \) which are based on unreddened values for \( (B-V) \). Addressing these and other issues exceeds the scope of this exploratory study.

The corrected \( T_{\text{eff}} \), \( \log g \), and [Fe/H] values can be directly compared to those given in the Elodie library. The mean difference and the \( \sigma_{\text{rms}} \) (607 spectra) are

\[ \begin{align*}
T_{\text{eff}}: & \quad 37 \pm 150 \text{ K} \\
\log g: & \quad 0.16 \pm 0.52 \text{ dex} \\
[\text{Fe/H}]: & \quad 0.02 \pm 0.18 \text{ dex}
\end{align*} \]  
(8)

and Fig. 4 compares the two sets of parameters.

A contribution to the error bars is connected with the parameters adopted for the Elodie library, mainly compiled from the literature. The library also provides estimates of the reliability of the adopted values. Restricting the comparison to the spectra with the most trusted parameters\(^3\) we find (71 spectra)

\[ \text{Using the library’s code: } q(T_{\text{eff}})=4, q(\log g)=1, q([\text{Fe/H}])=4 \]
Figure 4. Comparison between the stellar parameters selected (mainly from the literature) for the Elodie stars (Prugniel & Soubiran 1999 and references therein) with those from spectral fitting derived in this work.

The $\sigma_{rms}$ for the same stars between the IRFM $T_{eff}$, and those we derived is 80 K. The agreement for $T_{eff}$ and [Fe/H] is satisfying, but it is not so for log $g$. As explained in §4, the sensitivity of the spectrum to this parameter is not nearly as high as to the others. We find that 36 stars from the last set are included in the determination of stellar parameters by Allende Prieto & Lambert (1999) based on the comparison of observed colors and parallaxes with evolutionary models. The mean and median uncertainties for the reference gravities are both 0.08 dex. For these stars, we find a more satisfactory mean difference and $\sigma_{rms}$ in log $g$: 0.05 ± 0.28 dex, as shown in Fig. 3, which leads us to believe that 0.3 dex is a reasonable estimate for our random errors in gravity.

6 CONCLUSIONS AND FUTURE APPLICATIONS

We have implemented a spectroscopic classification algorithm that provides estimates for $T_{eff}$, log $g$, [Fe/H], and $\xi$ based on the observations with a resolving power $R \geq 5000$ in the spectral range 4810–4960 Å. The classification system is based on synthetic spectra calculated with classical flux-constant model atmospheres, and it is anchored to the photometric calibrations of effective temperature derived by Alonso and collaborators (Alonso et al. 1996, 1999) based on the Infrared Flux Method. By using the Elodie spectroscopic library (Prugniel & Soubiran 2001) and the gravities determined by Allende Prieto & Lambert (1999) for nearby Hipparcos stars, we derive upper limits to the uncertainties in the retrieved $T_{eff}$, log $g$, and [Fe/H], as 100 K, 0.3 dex, and 0.1 dex, respectively.

Our classification algorithm can be used on spectral types A to K, for main-sequence and evolved stars with gravities as low as log $g = 2$, and all metallicities. The system is able to classify a stellar spectrum in only 3 seconds.
on a modern workstation. Work is in progress to improve the accuracy of the synthetic spectra by using a more realistic line absorption profile for H$\beta$. We also plan on varying the parameters that affect the performance of the employed GA, and testing different optimization algorithms. An important question to answer is how the performance of our system improves or degrades with spectral resolution and signal-to-noise ratio. Different spectral ranges should be explored. Spectral bands with lines of metals whose abundances do not scale well with iron should be avoided, unless more parameters are included in the search, which is certainly feasible.

Different classification algorithms for stellar spectra have been tested in the literature. In particular, artificial neural networks hold the promise for the highest speeds, which may be critical for problems involving a large number of free parameters (see, e.g. Bailer-Jones 2001; Snider et al 2001). When the number of parameters is limited, like in the spectroscopic classification considered here, GAs have the advantage of not requiring training. This, in turn, allows us to explore different strategies, such as the selection of the spectral range or the resolving power, very quickly, while keeping the search global.

Our final goal is to provide a web interface and make this or a similar system publicly available. Future work will target hotter spectral types, using calculations based upon non-LTE model atmospheres. Extension to the bottom of the main-sequence and beyond could follow, although theoretical modelling of cool atmospheres has not yet reached the same level of maturity as for warmer stars. The adopted strategy can easily accommodate future improvements in model atmospheres and spectral synthesis.

### ACKNOWLEDGMENTS

Paul Barklem, Tim Beers, Norbert Christlieb, David Lambert, Chris Sneden, and Ted von Hippel are thanked for inspiring discussions. I am obliged to David Carroll for making his GA software publicly available, and to the Elodie team for sharing their database of stellar spectra. NSF support (grant AST 00-86321) is gratefully acknowledged.

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