A Pan-Spectral Method of Abundance Determination

A. Sapar, A. Aret, L. Sapar, and R. Poolamäe

Tartu Observatory, 61602 Tõravere, Estonia `sapar@aai.ee`

Summary. We propose a new method for determination of element abundances in stellar atmospheres aimed for the automatic processing of high-quality stellar spectra. The pan-spectral method is based on weighted cumulative line-widths $Q_\lambda = \int_{\lambda_0}^{\lambda} \left| \frac{dR_\lambda}{dZ} \right| (1 - R_\lambda) d\lambda$, where R_λ is residual flux and Z is abundance of studied element. Difference in quantities Q_λ found from synthetic and observed spectra gives a correction to the initial abundance. Final abundances are then found by rapidly converging iterations. Calculations can be made for many elements simultaneously and do not demand supercomputers.

1 Description of the method

Essential developments in observational high-precision and high-resolution spectroscopy, and fast-growing computing facilities stimulate to seek new automatic methods of analysis of stellar spectra. We recently started to develop a pan-spectral (or broad-band) method for determination of abundances of chemical elements and their isotopes in stellar atmospheres and to compose a software necessary for its application.

The method is based on weighted cumulative line-widths Q_λ defined as

$$Q_\lambda = \int_{\lambda_0}^{\lambda} \left| \frac{dR_\lambda}{dZ} \right| (1 - R_\lambda) d\lambda \; , \tag{1}$$

where R_λ is the residual flux (intensity) and $Z = \log(N_{elem}/N_{tot})$ is the abundance of studied element or isotope.

Integral (1) can be easily reduced to the equivalent width of a spectral line by omitting the derivative $|dR_\lambda/dZ|$ and integrating only over wavelengths of this line. We call the quantity Q_λ cumulative because integral is taken over all lines starting from some initial wavelength to the current wavelength. And we call it weighted because the derivative of residual flux R_λ with respect to abundance Z can be treated as a weight function. This derivative automatically excludes spectral regions insensitive to changes of the abundance of studied element and gives a large contribution in the most sensitive regions, i. e. in the centers of non-saturated lines and in the steep wings of strong lines of this element.

Weighted cumulative widths Q_λ for both observed and synthetic spectra are calculated using the derivative of R_λ found from the synthetic spectra. For small abundance changes the derivative can be replaced by differences, thus

$$\frac{dR_\lambda}{dZ} = \frac{R_\lambda^+ - R_\lambda^-}{Z^+ - Z^-} \ , \tag{2}$$

where flux R_λ^+ corresponds to abundance $Z^+ = Z + \delta Z$ and flux R_λ^- corresponds to abundance $Z^- = Z - \delta Z$. Correction to the abundance of studied element Z can then be found by formula

$$\Delta Z = \frac{(Z^+ - Z^-)(Q_\lambda^{obs} - Q_\lambda^{syn})}{Q_\lambda^+ - Q_\lambda^-} \ , \tag{3}$$

where Q_λ^{obs} is found from the observed spectrum and Q_λ^{syn} from the synthetic spectrum with initial (guessed) abundance Z. Quantities Q_λ^+ and Q_λ^- correspond to synthetic spectra with abundances Z^+ and Z^-, respectively.

Abundance of element can be found iteratively using the corrections ΔZ, the number of iterations needed depends on difference between initial and best-fit abundance values. Abundance determined by such a procedure is a best fit for all lines of the element, diminishing thus an influence of possible atomic data errors. We would like to point out that here the contribution of blended lines is duly taken into account. Abundances can be found simultaneously for many elements. Our calculations show that the method works well for line-rich elements, but for line-poor elements further refinements are necessary.

The method can be used also for determination of the effective temperature and gravity, using as the weight function the derivative of residual flux with respect to T_{eff} or $\log g$, respectively.

2 Testing the method

2.1 Observational Data

We applied the weighted cumulative width method to determine element abundances in the atmosphere of the chemically peculiar star HD 175640. High resolution spectral atlas of this star, covering the 3 040 – 10 000 Å region, was recently published by Castelli and Hubrig [1]. The spectrum with resolution 90 000 – 110 000 and signal-to-noise ratio 200 – 400 was obtained at ESO 8 m UT2 telescope with the UV-Visual Echelle Spectrograph (UVES). Castelli and Hubrig [1] also computed a synthetic spectrum for the whole observed interval with the SYNTHE code [4] and determined abundances for 48 ions of 39 elements by the visual best fit of synthetic and observational spectra of selected lines. The model atmosphere accepted was an ATLAS12 model [2]

with parameters $T_{eff} = 12\,000$ K, $\log g = 3.95$, $\xi = 0$ km s^{-1}. Improved and extended Kurucz atomic line list used in computations is available at F. Castelli website (`http://wwwuser.oat.ts.astro.it/castelli/stars.html`).

We had to ignore most of the IR spectrum due to telluric lines and also some spectral regions with weak overlap or gaps between adjoined echelle spectral orders.

2.2 Synthetic spectrum

In computations of synthetic spectra we based on the Kurucz ATLAS9 [3] model atmospheres and on the line lists and initial element abundances provided by Castelli and Hubrig [1]. Computations of the synthetic spectra were carried out with program SMART composed by our team during last decade [5]. SMART is a compact and simple software and does not demand large computer facilities. We used the same spectral resolution (500 000) as Castelli and Hubrig in computations with SYNTHE [4]. Gauss broadening and the noise cutoff parameters were found to achieve best fit of observed and synthetic spectra. Obtained synthetic spectrum agrees reasonably well with the observed one.

2.3 Application of the pan-spectral method

To estimate the domain of applicability of the method, we obtained abundances of 12 line-rich elements (Mn, Ti, Cr, Fe, Y, Mg, Si, Ca, O, S, Yb, Ni) in the atmosphere of HD 175640. Regions of Balmer and Paschen continua were studied separately because abundances of studied metals turned out to be larger in outer layers of atmosphere (UV region) than in inner layers (visual region).

We started with abundances derived by Castelli and Hubrig [1] and iteratively found corrections to these values. Abundances of Si, O and S from UV spectrum have not been found since there were only few weak lines of these elements in UV region. Final abundances were found with only two iterations since necessary corrections were small. Weighted cumulative widths Q_λ for chromium computed with initial abundance are presented in Fig. 1. Corresponding corrections to Cr abundance are +0.16 dex in UV and -0.14 dex in visual region.

Obtained abundances of the studied elements and comparison with results of Castelli and Hubrig [1] are presented in Table 1. Our results differ somewhat from the abundances obtained by Castelli and Hubrig. However, the differences in obtained element abundances may partly be caused by use of different spectral synthesis programs, not only by difference of used methods. This is particularly true for S and Si. Also the difference of used model atmospheres should be mentioned.

We conclude that the proposed method is promising for analysis of chemical composition and other main parameters of stellar atmospheres.
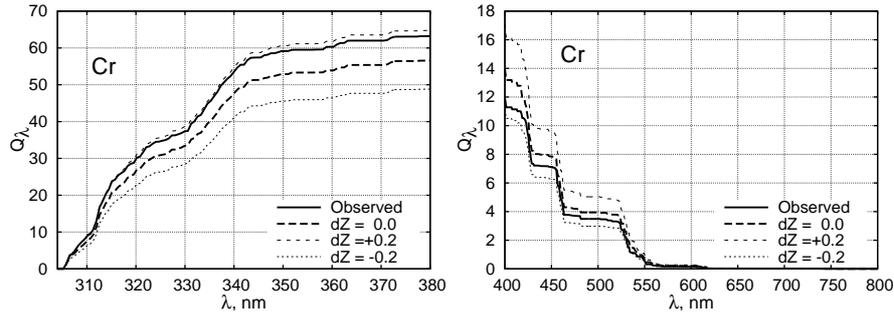
Fig. 1. Weighted cumulative width Q_λ for Cr.

Table 1. Element abundances $[N/N_\odot]$ for HD175640

| | Castelli & Hubrig (2004) | | | | | | Present study | |
| | UV | | | Vis | | | UV | Vis |
	ion I	ion II	ion III	ion I	ion II	ion III		
Mn	+2.47	+2.40	–	+2.46	–	–	+2.75	+2.57
Ti	–	+1.43	–	–	+1.30	–	+1.62	+1.31
Cr	+1.19	+1.03	–	+1.13	+0.96	–	+1.24	+0.96
Fe	-0.36	–	–	-0.21	-0.30	–	-0.23	-0.33
Y	–	+3.38	–	–	+3.01	–	+3.26	+3.04
Mg	–			+0.18	-0.25	–	-0.19	-0.09
Si	–			–	-0.23	-0.09	–	+0.21
Ca	–	-0.15	–	+0.42	+0.06	–	+0.10	+0.24
O	–			+0.03	–	–	–	+0.10
S	–			–	-0.41	–	–	+0.03
Yb	–	+3.14	+3.66	–	+2.76	–	+3.64	+2.79
Ni	–	-0.22	–	–	-0.35	–	-0.12	-0.43

References

1. F. Castelli, S. Hubrig: A& A **425**, 263 (2004)
2. R. Kurucz: Model Atmospheres for Individual Stars with Arbitrary Abundances. In: *The Third Conference on Faint Blue Stars*, ed by A. G. D. Philip, J. Liebert, R. A. Saffer (L. Davis Press, Schenectady 1997) p 33
3. R. Kurucz: CD-ROM, No. 13 (1993)
4. R. Kurucz: CD-ROM, No. 18 (1993)
5. A. Sapar, R. Poolamäe: "SMART": A Compact and Handy FORTRAN Code for the Physics of Stellar Atmospheres. In: *ASP Conf. Ser. 288: Stellar Atmosphere Modeling*, ed by I. Hubeny, D. Mihalas, K. Werner (Astronomical Society of the Pacific, San Francisco 2003) p 95