

DATA ANALYSIS

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ABSTRACT

The relationship between the r.m.s. photometric accuracy on the data points of a stellar spectrum and the final accuracy on abundances and physical parameters derived from these data is discussed.

1. INTRODUCTION

Modern detectors allow to achieve nominal signal/noise ratio of several hundreds in stellar spectroscopy. However, the final accuracy on the physical parameters in which we are interested does depend not only upon the photometric accuracy of the spectra, but of what is happening during several steps of reduction, involving most of the time substantial losses in accuracy. This makes, in practice, the accuracy on abundances, for example, only 15% good, even if one starts with spectra obtained with a signal to noise ratio of 200.

It is not our intention to treat the whole subject in a few pages, so we shall focus on just a few critical points. The first one has to do with the accuracy reachable on the equivalent width of weak lines with a given signal/noise ratio in the continuum. The second point is the accuracy obtainable from the analysis of Balmer lines on temperature differences between two stars. Because the equivalent width of weak neutral lines are very insensitive to gravity, for F, G and K stars, the accuracy on equivalent widths, plus the accuracy on temperature determination largely control the accuracy obtainable on abundance ratios between two stars belonging to these spectral classes.

2. FROM THE FLUX DATA POINTS TO THE LINE PARAMETERS

Assuming that instrumental effects have been properly corrected for, by dark exposures subtraction and flat-fielding (not forgetting that these operations degrade the row signal/noise ratio by an appreciable amount) the data consist of a set of ordinates s_i running from one to the number of pixels of the detector, $n= 1872$ for most reticons in use). We assume that we know the statistical mean error on each s_i and, for simplicity, we consider first the academic case where we can find a spectrum subinterval in which the spectrum can be described by a continuum of constant level and a single absorption line of gaussian profile :

$$(1) \quad S(x) = S_c - S_c u \cdot \exp \left\{ - \frac{1}{2} \left(\frac{x - v}{w} \right)^2 \right\}$$

We also assume, which is even more academic, that S_c is known, from unperturbed regions of the spectrum.

Then the characteristics (v wave-length of the line center, w standard width, u central depth of the line) of the line must be derived from the usually over-determined system (solved by least square)

$$(2) \quad r_i = 1.0 - \frac{S_i}{S_c} = u \cdot \exp \left\{ - \frac{1}{2} \left(\frac{x_i - v}{w} \right)^2 \right\}$$

$$i = i_{min} , i_{max}$$

Where i_{min} is the data point of smallest wave-length and i_{max} the data point of the largest wave-length used in the least-square procedure. Of course $(i_{max} - i_{min})$ must be at least equal to 2 (three points) and preferably larger. This immediately poses the problem of the pixel size :

$$(3) \quad \delta x = x_{i+1} - x_i$$

with respect to w . The common sense requests that the data point must be influenced by the presence of the line at a level larger than the noise. So if ϵ is the r.m.s. relative photometric accuracy on the flux :

$$(3) \epsilon = \frac{1}{S_c} < \delta s^2 >^{\frac{1}{2}} = < \delta x^2 >^{\frac{1}{2}}$$

one should have :

$$u \exp\left\{-\frac{1}{2} \left(\frac{1.5 \delta x}{w}\right)^2\right\} > \epsilon$$

The factor 1.5 holds because the most central data point is, at the most, at a distance of half a pixel to the real center of the line.

This gives for $u = 0.1$ and $\epsilon = 0.01$

$$\delta x < 1.43w$$

or :

$$\delta x < 0.6 \times FWHM$$

as a function of the full width at half maximum, FWHM

However this condition, which is necessary to find the center and the width of the line is not necessary if one is only interested in its equivalent width, as we shall see later.

Landman, Roussel-Dupré and Tanigawa (1982) have solved the problem of finding the accuracy on u , v and w for a given photometric accuracy ϵ . The result is :

$$(3) \quad < \delta u^2 >^{\frac{1}{2}} = \left(\frac{3}{2}\right)^{\frac{1}{2}} \left(\frac{1}{\pi}\right)^{1/4} \left(\frac{\delta x}{w}\right)^{\frac{1}{2}} \epsilon$$

$$(4) \quad < \delta v^2 >^{\frac{1}{2}} = \frac{\sqrt{2}}{\pi^{1/4}} (w \cdot \delta x)^{1/2} \frac{\epsilon}{u}$$

$$(5) \quad < \delta w >^{\frac{1}{2}} = < \delta v^2 >^{\frac{1}{2}} = \frac{\sqrt{2}}{\pi^{1/4}} (w \cdot \delta x)^{\frac{1}{2}} \frac{\epsilon}{u}$$

provided $\delta x \ll FWHM$. (In practice is it enough that $\delta x \leq w$).

An interesting consequence stems from these formulae : if the observation is photon noise limited, $\epsilon \sim \delta x^{-\frac{1}{2}}$ and the errors are all independent of the pixel size.

Landmann and al. (1982) have not given the error on the equivalent width. As δu and δw are correlated it is not possible to compute the error on the product uw using the above formulae. The exact computation gives :

$$(6) \quad \langle \delta W^2 \rangle^{1/2} = \frac{\sqrt{3\pi}}{\pi^{1/4}} (w\delta x)^{1/2} \epsilon$$

or :

$$(6') \quad \langle \delta W^2 \rangle^{1/2} \simeq 2.3 (w\delta x)^{1/2} \epsilon \simeq 1.5 (FWHM \cdot \delta x)^{1/2} \epsilon$$

A similar formula can be obtained in a much simpler way. The equivalent width is by definition :

$$W = \int_{-\infty}^{+\infty} r(x) dx = \sum_{i=i_1}^{i_2} r_i \delta x = \delta x \sum_{i=i_1}^{i_2} r_i$$

the sum Σ being extended to all pixels potentially affected by the line. For a gaussian profile it is fairly safe to sum over a width equal to 6 times the standard deviation, and the error on w comes as :

$$(7) \quad \langle \delta W^2 \rangle^{1/2} = \delta x \cdot \epsilon \sqrt{\frac{6w}{\delta x}} = 2.45 (w\delta x)^{1/2} \epsilon$$

$$\simeq 1.6 (w\delta x)^{1/2} \epsilon$$

So whatever is the method for getting the equivalent width, the root mean square error on it is the product a numerical factor close to 1.5, by the geometrical mean between the pixel size and the FWHM, and by the relative r.m.s. the photometric accuracy in the continuum.

If one applies this formule to conditions frequently met at the CAT reticon spectrograph at ESO one gets :

$$FWHM = 0.1 \text{ \AA} \quad \delta x = 0.035 \text{ \AA}$$

and with :

$$\epsilon = 1/200$$

$$\langle \delta W^2 \rangle^{1/2} = 0.4 \text{ m \AA}$$

3. FURTHER PHYSICAL LIMITATIONS ON THE ACCURACY OF SMALL EQUIVALENT WIDTHS.

Repeated measurements of equivalent widths on several spectra of the same star show that formulae (6) or (7) are too optimistic. The scatter on such measurements is more frequently of the order of 1 to 2 mÅ rather than 0.4 mÅ. The principal source of additional error is the fact that the continuum is not known exactly, and worse, not even definable with an accuracy of 0.5 %. One is easily convinced of that by taking a look at a segment of the "Solar flux Atlas from 296 to 1300 nm by Kurucz et al. 1984 (see fig.1). In the numerical example at the end of section 2, if we assume an error of 0.5 % in the location at the continuum this induces an error of $6w \times .005$ in the equivalent width (no more square root cancellation !) or :1.3 mÅ on W , three times larger than the statistical photometric error.

In order to minimize this error we found that is better to requestion in the least square fit the exact position of the continuum i.e. to have S_c as unknown as will as a , w and v . We also found that v is usually not to be taken as unknown for weak lines, the wave-lengths differences being known with high accuracy from tables and not "negotiable".

In practical cases it is found that the line under scrutiny is always more of least "blend" with other lines. It is easy to generalize the least square fit to n lines :

$$S(x) - S_c \left\{ 1 - \sum_{i=1}^n u_i \cdot \exp \left(- \frac{1}{2} \left(\frac{x - v_i}{w} \right)^2 \right) \right\}$$

$$W_i = \sqrt{2\pi} \cdot u_i w$$

Then the value of w become much more critical : if two consecutive lines are too close in wave-length, the least-square procedure collapse, or, if well handled allow only to determine the sum of the equivalent widths of the two nearby lines but not how much is ascribable to each of them.

So it may be necessary to increase the resolution mainly for separating the line from its nearest neighbours.

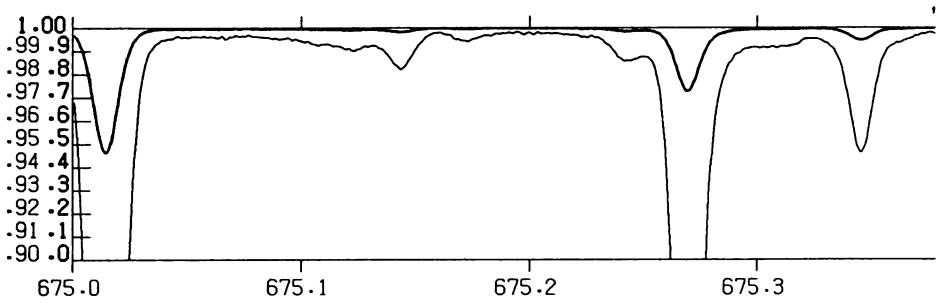


Fig.1- Structure of the "continuum" in the solar spectrum, from Kurucz et al. 1984. The wave-length scale is in nanometers. The thin line has an ordinate scale enlarged by a factor of 10 (left scale). One clearly sees that there is no well defined continuum at the 1% level.

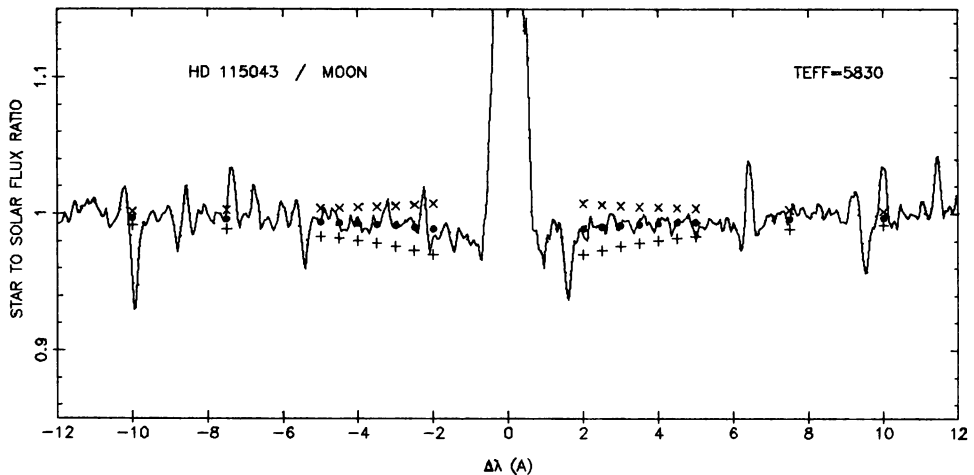


Fig.2-Ratio of stellar (HD 115043) to moon spectra in the $H\alpha$ region. Comparison with theoretical ratios for effective temperatures 5830 K and 5830 ± 100 K. The precision of the determination is clearly better than 50K. The central (-2,+2 Å) portion is strongly affected by chromospheric activity in HD 115043 (UMA stream) and of no use for temperature determination.

4. TRADE-OFF BETWEEN NOISE LEVEL AND SATURATION EFFECTS.

Taking now $1.5 \text{ m}\text{\AA}$ as a reasonable r.m.s. error on equivalent widths (independent of W) what equivalent widths are most useful for abundance work ?

The relative error decreases when W increases, but soon saturation effects become dominant and the error due to the uncertainty on the "microturbulence" takes over. A $15 \text{ m}\text{\AA}$ equivalent width suffers a 10 % uncertainty and at this point an error by 0.1 dex on the Doppler width contributes by only 3 %. The balance between the two sources of error occurs at about $20 \text{ m}\text{\AA}$ and we consider that this is a kind of optimal compromise between the need of keeping the saturation effects small and having good relative accuracy on the W s. The relative accuracy is then only of the order of 10 % even if we started from a nominal S/N ratio 200 in the continuum. This example shows how difficult it is to take full advantage of very high S/N ratio of 500 or more. My conclusion is indeed very close to the one given by D. Gray : before making meaningful use of high photometric S/N noise one hits difficulties as undefinable physical continuum, slight residual instrumental effects due to a different collimation of stellar and flat-field or calibration beams in the spectrograph, etc ... The effort should then go as well towards mastering these effects (as exemplified by the HF cell for accurate wave length measurements) as to still improve the purely photometric accuracy, any-how unimprovable above the limit set by the granular nature of light.

5. EFFECTIVE TEMPERATURE DETERMINATION FROM BALMER LINE WINGS.

For abundance work it is as important, to derive an accurate effective temperature as to have accurate equivalent widths of weak lines. High-signal to noise spectra have allowed to use the wings of the Balmer lines, and more specifically of $H\alpha$ which is located in a region where the spectrum is clean and the efficiency of reticons high. Fig.2 show the comparison between the ratio of a stellar spectrum to moon light in the $H\alpha$ region, compared to the predicted ratio computed from Gustafsson's models.

The theoretical ratios are computed with $T_{\text{eff}}=5770 \text{ K}$ for the solar (full disk) spectrum.

One sees from the figure that a temperature difference is easily detectable, even if as small as 50 K. This is just about what is needed if the error on the Boltzmann population factor for a neutral lines lying 5 eV below the ionization level is to be kept below 10 % at 6000K. Recent work on the broadening theory of Balmer lines (Stehlé et al. 1983) shows that the Vidal, Cooper and Smith (1973) prescription is valid at a few angströms from line center for $H\alpha$. Because the population of H^0 and of neutral lines are both proportional to the electronic pressure, the equivalent width ratio of a weak neutral line in a star and in the sun does depend only on the abundance ratio and on the temperature difference. The abundance ratio may in principle be determined from one line with 0.1 dex accuracy, and if more lines of the

same element are available, some \sqrt{n} gain may be achieved, this is particularly true for iron.

6. CONCLUSION

- Simple formulae are given to obtain the rms errors on line position, line width, line depth, and line equivalent width for a given r.m.s. noise at continuum level.

One conclusion is that 1) the pixel size is not at all a critical parameter. 2) increasing the spectral resolution decreases the r.m.s. error on equivalent widths (as the square root of the line width) as long as the line width follows the spectral resolution. Once the intrinsic width of the line is reached no more gain is obtainable by further increasing the spectral resolution.

- At signal/noise ratio above 200 the final accuracy obtainable on equivalent widths of weak lines is more set by the difficulty of defining a continuum than by the photometric error on the signal. It is recommendable to use a very local determination of the continuum by including the continuum position in the least-square fitting.

- Differences in effective temperatures as small as 50K can easily be detected from the strength of the wings of H α in late F to mid-G dwarf star with high S/N ratio spectra.

- Abundance ratios between stars of similar spectral types can be determined with an accuracy of 0.1 dex, from a single line, from spectra with a S/N ratio of 200.

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DISCUSSION

SODERBLOM I would like to ask Ingemar Furenlid to remind us how the continuum level was established for the solar flux atlas, since Dr. Cayrel pointed out the lack of true continuum windows.

FURENLID The continuum of the Solar Flux Atlas (Kurucz et al., 1984) is determined by a global fit to high points over wavelength ranges of a couple of thousand angstroms. It should thus be emphasized that it is strictly speaking a pseudo-continuum.

WALKER How do you correct for scattered light ? What kind of error does it introduce ?

R. CAYREL The correction is simple : if there is 5% straylight the equivalent widths are decreased by this amount.

G. CAYREL We have not applied the correction because our analyses were differential : the corrections cancel out.