A FORTRAN 77 PROGRAM

HEC 35D

USER'S MANUAL

PREPARING DATA FOR DISENTANGLING: PRINCIPLES AND SOME PRACTICAL ADVICE

Release 1.2 of the manual: March 20, 2008

Written by Petr Harmanec

Astronomical Institute of the Charles University, V Holešovičkách 2, 180 00 Praha, Czech Republic

FAX (420) 283 072 577 Telephone: (420) 283 072 573

e-mail: hec@sirrah.troja.mff.cuni.cz

Contents

1 BASIC PRINCIPLES

Digitalized, fully reduced and rectified spectra can usually be recorded as pairs

wavelength λ *relative flux* $I(\lambda)$

sorted in an ascending order in wavelength. The optimal storage of such digitized spectra is that the stored wavelengths and fluxes correspond to the original pixels of the detector. It happens, however, that spectra stored in some archives are already rebinned, most frequently to a constant step in wavelength. Unless needed for further scientific analysis, any rebinning of the original spectra is not desirable since one looses a part of information content due to the fact that the dispersion of the spectrograph is not a linear function of wavelength. This can be illustrated on the specific case of the spectrograph installed in the coudé focus of the Ondřejov 2.0-m reflector. Since 1992 until July 2000, a Reticon 1872RF detector was used in the medium camera of the spectrograph with the focal length 702 mm. Altogether, 1696 pixels of the detector (separated by 0.015 mm) were used to record the stellar spectra. At present, there is a CCD detector SITe-005 with 2030×800 pixels. Along the spectral dispersion, 1997 elements, also separated by 0.015 mm, are used. In the most often used red region of the spectrum, from 6255 to 6767 Å, the difference between the two neighbouring pixels amounts to about 0.25 Å and the difference in radial velocity decreases from shorter to longer wavelenghts from about 12.3 do 11.35 km s^{-1}. Since the geometry of the spectrograph was not changed, this is true for both, the Reticon and CCD detectors. There is a difference, however. While the Reticon data are stored in original pixels, the CCD spectra in the Ondřejov archive are already rebinned to a uniform step in wavelength. At the same time, the rebinned spetrum contains again only 1997 pixels. This seems a bit unfortunate since it means that the resolution of the spectrum at the longward end is slightly degraded. If such a rebinning is required, one should adopt the smaller difference in wavelength corresponding to the longward edge of the spectrum, which would lead to a larger than original number of pixels.

Modern methods of radial-velocity determination (cross-correlation, disentangling, broadening functions) all require spectra rebinned into uniform step in radial velocity to allow linear mutual shifts of the spectra. Some authors like Simkin (1974) (who was the first to pioneer the use of cross-correlation technique in astronomy) recommend to this purpose to replace the scale of wavelengths λ by that linear in the natural logarithm of wavelength $\ln\lambda$, for the following reason. Since the stellar radial velocities (RVs hereafter) are usually much smaller that the speed of light in vacuum, it is legitimate to use the classical Doppler formula in the well-known form

$$\lambda = \lambda_0 \left(1 + \frac{RV}{c}\right). \tag{1}$$

Logarithm of this formula gives

$$\ln\lambda = \ln\lambda_0 + \ln\left(1 + \frac{RV}{c}\right). \tag{2}$$

For $RV \ll c$, one can replace the second term on the right side of eq. (2) by a Taylor series and neglect all higher terms to get

$$\ln\left(1 + \frac{RV}{c}\right) \doteq \frac{RV}{c}. \tag{3}$$

One can then rewrite Eq. (2) into differential form

$$c \cdot \triangle \ln\lambda \doteq \triangle RV, \tag{4}$$

from which it follows that a shift in $c \cdot \ln\lambda$ represents directly the difference in RV between two spectra.

Let us investigate how justified the neglection of higher terms of the Taylor series is for practical applications. The wavelength given by the approximate relation (3), $\lambda_{\rm approx.}$, inserted into Eq. (2), is

$$\lambda_{\rm approx.} = \lambda_0 {\rm e}^{\frac{RV}{c}}, \tag{5}$$

so that the corresponding difference in RV will be

$$RV - RV_{\rm approx.} = RV - c\left(\frac{\lambda_{\rm approx.} - \lambda_0}{\lambda_0}\right) = RV - c\left({\rm e}^{\frac{RV}{c}} - 1\right). \tag{6}$$

Note that the error in RV caused by the use of the approximate relation does not depend on wavelength. For example, for $RV = 400$ km s^{-1} the error amounts to 0.267 km s^{-1} while for $RV = 1000$ km s^{-1}it is already 1.67 km s^{-1} . For truly accurate RV measurements, these are not negligible errors.

One could consider a Taylor series with more terms, but there is a better solution. It is important to realize that the original spectrum was recorded with a detector having a constant separation s between the centres of two neighbouring pixels. The dispersion element (grating or prism) changes this linear scale into a non-linear one. The latter, however, can be converted into a scale having a constant *resolving power* R given by

$$R = \frac{\lambda}{\triangle\lambda} = \frac{\lambda}{W \cdot s}, \tag{7}$$

where W is the linear reciprocal dispersion and s the distance between the centres of two adjacent pixels along the dispersion axis. This way, the rebinned spectrum will be perfectly linear in RV, without any approximation.

The practical realization of this procedure is that one starts with the wavelength corresponding to the first pixel, λ_1, and chooses a constant step in radial velocity, $\triangle RV$. From the relation (1) the wavelength of the n-th rebinned element $\lambda_{\rm n}$ then follows as

$$\lambda_{\rm n} = \lambda_1 \left(1 + \frac{\triangle RV}{c}\right)^{\rm n-1} . \tag{8}$$

It is important to pay attention to the proper choice of the RV step. It must not too large since it would degrade the resolving power of the original spectrum. On the other hand, the usage of too fine RV step would not provide new pieces of information and the only result would be a longer time needed on processing of larger data files. The optimal step should be equal, or a bit smaller than the minimum RV difference between two adjacent pixels over the considered interval of wavelengths.

For our purpose it is important to note that the rebinning carried out with the help of formula (8) will work properly for the spectra having wavelengths corresponding to original pixels but also for spectra with a constant step in wavelength.

For completeness, it is useful to remark that it follows from Eq. (2) that constructing the logarithmic wavelength scale with a *constant shift* in $\ln(1 + RV/c)$ would also ensure uniform spacing in radial velocity.

-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-o-

2 AVAILABLE PROGRAMS FOR DISENTANGLING

The technique which allows determination of orbital elements of a binary and determination of the spectra of individual components was first suggested by Simon and Sturm (1994) and called spectra disentangling. Hadrava (1995, 1997) showed that solving the task in the space of Fourier images of the spectra is much faster. He developed his own Fortran program KOREL which is able to disentagle even a hierarchical system of five stars. This program, a few auxiliary programs and a User Guide are publicly available – see Hadrava (2004).

Later, Ilijić a kol. (2001,2004) developed another program for disentangling based on the same principles. This program, called FDBINARY, currently allows to disentangle binary and triple systems only. It automatically calculates a large number of solutions with different initial values of orbital elements and prints several of them with the best sums of residuals. This approach is very convenient given the fact that disentangling does not always converge to the optimal solution – see, e.g., the comments on this issue by Hadrava (2004) or a detailed discussion in Southworth and Clausen (2007). The program FDBINARY with detailed instrutions how to use it is available at

http://sail.zpf.fer.hr/fdbinary .

3 MY SIMPLE PROGRAMS TO PREPARE SUITABLE INPUT DATA FOR DISENTANGLING

The following programs are designed to prepare suitable data for the program KOREL but only a change of output format would make them usable also for other programs for disentangling.

An example of the input file PREKOR.LST required by Dr. Hadrava's program PREKOR, in the form suitable for the program HEC35D. The columns (in fixed format) are: name of the ASCII file with rectified spectrum in the DOS convention, time (HJD-240000), weight, zero specifying that ASCII files are used, and possible additional RV correction (currently not used in HEC35D).

Fixed (A12,1X,F10.4,F8.3,I2,F8.3) format

```
--------------------------------------------------------------------------------
         10        20        30        40        50        60        70        80
....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|

v3c00001.asc 53335.4496   1.214 0     .0
v3c00002.asc 53579.4961   1.077 0     .0
v3c00003.asc 53594.4558    .994 0     .0
v3c00004.asc 53611.6085   1.497 0     .0
v3c00005.asc 53613.3252    .825 0     .0
v3c00006.asc 53613.3438    .964 0     .0
v3c00007.asc 53623.3667   1.375 0     .0
v3c00008.asc 53650.3219   1.241 0     .0
v3c00009.asc 53653.2570   2.268 0     .0
v3c00010.asc 53655.3108   1.430 0     .0
v3c00011.asc 53659.3305   1.039 0     .0
v3c00013.asc 53745.2911   1.159 0     .0
v3c00014.asc 53791.5672   2.206 0     .0
v3c00015.asc 53832.5222   1.214 0     .0
v3c00016.asc 53846.4514   1.342 0     .0
v3c00017.asc 53847.5795   1.737 0     .0
v3c00018.asc 53920.3771   1.120 0     .0

....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|
         10        20        30        40        50        60        70        80
--------------------------------------------------------------------------------
```

According to my experience the solution with KOREL is much more stable when individual spectra are given weights proportional to the square of their S/N ratios. I therefore prepared two simple programs: program SN2.FOR to estimate the S/N ratios, and program SNVAHY which uses output from SN2 to derive relative weights of spectra and produce an output file identical to PREKOR.LST but containing these weights.

3.1 Program SN2

The user has to inspect the spectra and decide which spectral interval is featureless and therefore suitable to the estimate of the S/N ratio.

Program SN2 first asks the user to specify the file with the list of spectra. It is optimal to use the file 'PREKOR.LST' in its standard format required also by Hadrava's preparatory program PREKOR which creates input data for KOREL. See the example of PREKOR.LST file above.

Then the program asks the user to specify the minimum and maximum wavelength defining the region of continuum without lines. It than calculates the estimate of the S/N ratio simply as the ratio of an average signal (a value close to 1.0 in the rectified spectra) and the rms error of that average, i.e.

$$S/N = \left(\frac{\sum S}{m} / \sqrt{\frac{(\sum S^2 - (\sum S)^2/m)}{m-1}} \right), \tag{9}$$

where m is the number of pixels within the specified interval of wavelengths.

The output contains the times of spectra (HJD-240000), S/N, mean value of the signal, its rms error, and filenames of the spectra. An example of such output file is shown in the next Table.

An example of the output file from the program SN2 using the file PREKOR.LST shown above.

```
--------------------------------------------------------------------------------
        10        20        30        40        50        60        70        80
....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|

Range of continuum:   6620.0 -   6635.0 A
    HJD       S/N     mean     rms       filename

53335.4496  273.0  .99590  .00365  v3c00001.asc
53579.4961  257.1  .99202  .00386  v3c00002.asc
53594.4558  247.0  .99984  .00405  v3c00003.asc
53611.6085  303.1  .99419  .00328  v3c00004.asc
53613.3252  225.1  .99773  .00443  v3c00005.asc
53613.3438  243.3  .99360  .00408  v3c00006.asc
53623.3667  290.5  .99575  .00343  v3c00007.asc
53650.3219  276.0  .99713  .00361  v3c00008.asc
53653.2570  373.1  .99781  .00267  v3c00009.asc
53655.3108  296.3  .99850  .00337  v3c00010.asc
53659.3305  252.5  .99914  .00396  v3c00011.asc
53726.1885   38.5  .95639  .02481  v3c00012.asc
53745.2911  266.7  .99654  .00374  v3c00013.asc
53791.5672  368.0  .99870  .00271  v3c00014.asc
53832.5222  273.0  .99832  .00366  v3c00015.asc
53846.4514  287.0  .98975  .00345  v3c00016.asc
53847.5795  326.5  .99759  .00306  v3c00017.asc
53920.3771  262.2  .99344  .00379  v3c00018.asc

....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|....|
        10        20        30        40        50        60        70        80
--------------------------------------------------------------------------------
```

3.2 Program SNVAHY

This program only reads the output from the program SN2 and creates an output file, identical in structure to file PREKOR.LST, where the weights from the original file PREKOR.LST are replaced by weights proportional to the square of S/N and normalized in such a way that the weight 1.0 corresponds to the mean S/N of all files. After checking the result, the user can rename the output file from SNVAHY for PREKOR.LST.

3.3 Program HEC35D

It is first necessary to explain why a new program for the preparation of data for KOREL if there is the program PREKOR provided together with KOREL by Dr. Hadrava. There are a few limitations in the current version of PREKOR:

1. In PREKOR, the user can only specify the initial wavelength and a step in RV which gives little flexibity as far as the interval of wavelengths to be used is concerned since the optimal RV step is given by the properties of the spectrograph and detector used as explained in sect. 1.

2. Only linear interpolation of fluxes into the scale linear in RV is used in PREKOR.

3. The current maximum of pixels to be generated in PREKOR is 4096 although KOREL itself is prepared to accept data of arbitrary length, with the only condition that the number of pixels will be an integer multiple of 512.

4. PREKOR does not provide tapering at the edges (although there is another program in the KOREL package which can do that task).

5. There is no direct possibility to block some wavelength intervals containing either flaws or, for instance, interstellar lines.

Program HEC35D was therefore designed in such a way as to avoid the above mentioned limitations.

The user is asked to specify both, the initial and last wavelength, and the step in RV. The program adds a number of pixels with the flux set to 1.0 at the beginning of each file and also at the end in such a way as to preserve the total number of the output data pixels equal to some integer multiple of 512. The interpolation of the fluxes to the wavelength points, calculated for the linear RV scale according to formula (8), is carried out with the help of Hermite interpolation formula adopted after Hill (1982). This interpolation also ensures a smooth transition between the artificial continuum at both edges and the first pixels of actual values of the relative flux.

Besides, the user can specify up to ten wavelength intervals which should be ignored in the spectra. The program again sets all fluxes in these intervals equal to one.

The resulting output file is always called KOREL.DAT, has the format identical to such a file created by PREKOR and can immediately be used as the input file by KOREL.

If required by the user, the program also creates another output file called KOREL.ASC which contains the pairs of wavelenghts and fluxes on the scale linear in RV. Such a file can be used to some graphical plots and tests.

The obvious advantage of using HEC35D is that one can create KOREL.DAT file of arbitrary length, in simple cases the whole spectra. It is only necessary to compile KOREL with large enough arrays specified in the file KORELPAR.F.

My first practical experience with this approach seems quite encouraging.

Yet, a word of warning is appropriate. Both, the tapering and 'erasing' of some parts of the spectra should be used with some caution. The user must be sure that no spectral line will move to these parts of the spectra during orbital motion. The elimination of some parts of the spectra, for instance interstellar lines, can only be successfully carried out for lines which start from the stellar continuum and are not blended with some stellar lines like Ca II K line with the H7 Balmer line. In the latter case, such lines have to be edited out from the spectra if necessary in some other way.

Any questions and/or criticism concerning the programs as well as reports of their possible malfunctions should be addressed to the author and are welcome.

Any suggestions how to improve this manual will also be appreciated.

Acknowledgements

Over the time, I profitted from the discussions on the various aspects of the subject with Drs. Petr Hadrava, Herman Hensberge, David Holmgren, Saša Ilijić, Krešimir Pavlovski, Andrej Prša, and Slavek Rucinski. The responsibility for the content of this text is, of course, only mine.

References

[1] Hadrava P. 1995 A&AS 114, 393

[2] Hadrava P. 1997 A&AS 122, 581

[3] Hadrava P. 2004 Publ. Astron. Inst. Acad. Sci. Czech Rep. No. 92, 15

[4] Ilijić, S., Hensberge, H., Pavlovski, K. 2001, Lectures Notes in Physics, 573, 269

[5] Ilijić S., Hensberge H., Pavlovski K., Freyhammer L. M., 2004, ASP Conf Ser 318, 111

[6] Hill G. 1982 Publ. Dominion Astrophys. Obs. 16, 67

[7] Simkin S.M. 1974 A&A 31, 129

[8] Simon K.P., Sturm E. 1994 A&A 281, 286

[9] Southworth J., Clausen J.V. 2007 A&A 461, 1077