Techniques

Spectroscopic reductions using RESPECT software

T. P. Prabhu and G. C. Anupama
Indian Institute of Astrophysics, Bangalore 560 034

Abstract. The RESPECT software has been developed locally at the Vainu Bappu Observatory, Kavalur for spectroscopic data reduction, and is being upgraded continuously. The software is described here in the general perspective of data reduction.

Key words : astronomical spectroscopy—reduction techniques—software

1. Introduction

The RESPECT software package was developed in 1985 at Vainu Bappu Observatory (VBO), Kavalur with the objective of extending the experience gained in spectroscopic data reduction with locally developed digitizers and software to the newly available PDS microdensitometer and VAX 11/780 computer. Its optimization to the local hardware and software environment, and ease of use, maintenance, and development have contributed to its survival and growth. An early description of the software was provided by Prabhu, Anupama & Giridhar (1987). New features incorporated since then are described here in the general perspective of spectroscopic data reduction. A total of nearly 100 commands are available to date.

RESPECT commands are activated by logging into the software. This may result in replacing some of the user definitions by the RESPECT definitions in the process table. The QUIT command reactivates the definitions from the user's 'login.com' file. Some of the RESPECT commands related to operations on the CCD image data form a subpackage, and are activated using the command CCD.

RESPECT commands make use of the VAX/VMS Command Definition Utility and hence have a syntax similar to the Digital Command Language (DCL):

$ COMMAND/QUALIFIERS [= value] parameters.

The internal data storage is unformatted, and recognizes linear and two-dimensional images. The linear images may either be (x, y) pairs of data points, or simply y values at equal intervals (Δx) beginning with an initial value x_1, in which case the initial value x_1 and its increment are noted in the header area. In the latter case, y can be a complex variable as well, with the real and imaginary points at each x being stored contiguously. The different data types are labelled paired (P), sequential real (R), sequential complex

(C), 16-bit integer image (I) and 32-bit real image (J). Arithmetic operations are generally possible only between similar data types excluding the paired data. Further restriction is that the interval Δx (as also Δy in the case of images) should match exactly between the two files.

2. Input, output, and the log

Conversion of data to the internal format of RESPECT is done through the REFORM command. The qualifiers /PDS, /TAB, /CCD and /CCDA convert data from PDS tapes, ASCII tables, Photometrics CCD tapes, and Astromed CCD tapes, respectively. FITIN command inputs the FITS format data, and BDF2RES command operating under STARLINK environment and available in the LOCAL subpackage at VBO converts BDF (STARLINK) images into RESPECT. The INPUT command enables entering data directly from the keyboard, and the INPUT/EDIT command enables editing data files. There is a small amount of on-line help available during editing.

The output is in the form of ASCII, graphic display, or image display. The OUTPUT command displays the data values on the terminal, or prints on the printer. TITLE command displays the header information of the file as also the data type, x_1, Δx and the number of points in the data; if a new header is provided on the command line, it replaces the older header by the new one. the entire data file may be converted to ASCII using the ASCII command. Sequential real data can be converted to paired data during ASCII conversion by using the /PAIR qualifier.

The graphic display is achieved through DISPLAY command on the Tektronix 4115 terminal, or on the VT 200 and 300 series terminals after setting them into Tektronix mode using the command TEK. It is possible to select a portion of the one-dimensional image to be displayed, mark lines and label them as desired. VT series terminals can be set to their default mode of operation by the VT command. One can also PLOT the data on the Printronix printer/plotter. However, the command is not as flexible as DISPLAY since the purpose has been only to obtain working plots. The image data can be displayed on the COMTAL Vision 1/20 image monitor using the CCD command COMTAL. The window to be displayed, and the scale factor for the data values are chosen interactively.

On entering the RESPECT environment, a log file is created in the working directory if one is not already present. This file maintains a record of all operations performed. A NOTE can be added by the user as and when desired. The log can be TYPEd on the screen or PRINTed. TAIL command displays the end portion of the log on the monitor.

A list of headers of files on tapes containing the PDS data and the Photometrics CCD data can be obtained using the PDSLIST and CCDLIST commands, respectively. The command FITSLIST makes a list of header records from a FITS format tape.

On entering the RESPECT environment, HELP refers only to the RESPECT commands. A shorter help library, which lists only the format (or syntax) of a command, is activated by the command FORMAT. Help on system commands can be obtained by the SYS command. The MANUAL command may be used for further details on the software.

3. Extraction of CCD spectra

A CCD image is directly proportional to the incident intensity. However, one needs to extract the one-dimensional spectrum from the two-dimensional image after correcting for the electronic bias, thermal background, pixel-to-pixel sensitivity difference, and the sky background. The spectrum usually extends to more than one pixel perpendicular to the direction of dispersion, and the spectrum counts may be represented as

$$D(x, y) = \frac{R(x, y) - B(x, y)}{F(x, y)} - S(x, y)$$

where $R(x, y)$ is the raw spectrum at position x along dispersion and y perpendicular to the dispersion, $B(x, y)$ the corresponding image of electronic bias and thermal background, and $F(x, y)$ the image of a flat field containing information on the sensitivity of the pixels. $S(x, y)$ is an estimate of counts due to sky at position (x, y), assumed to be corrected for electronic bias and flat-field variations. Horne (1986, 1988) has developed an algorithm to extract the spectrum $D(x)$ as the weighted average of $D(x, y)$ over the direction y. The weights are inversely proportional to the square of noise. The latter is a sum of the readout noise and the shot noise. An estimate of the noise is made based on the readout noise in electrons and the 'gain factor' of the CCD system in terms of electrons per count supplied to the program externally (see Prabhu, Mayya & Anupama 1991 for a determination of these values for the two CCD systems in operation at VBO). Horne's method differs from older methods of extraction also in the manner in which the profile of the spectrum is estimated in the y direction. It is model-independent, and can handle moderate amounts of tilt of the spectrum with respect to rows/columns of CCD. The spectrum extraction procedures in RESPECT are based on this optimal extraction algorithm. The relevant commands are part of the CCD sub-package, and are described below.

The command SPECTRUM extracts the one-dimensional spectra from the two-dimensional CCD image. If the input image is already bias subtracted and flat-fielded, the SPECTRUM command simply extracts the spectrum. On the other hand, the command can also help in the bias subtraction and flat-fielding. A bias frame can be provided for pixel-to-pixel subtraction, or simply a global mean value of bias can be subtracted from the entire spectrum. Yet another possibility is to subtract the mean background level in the raw image of the spectrum itself at each wavelength. This option allows subtraction of the thermal background and also the scattered light in the spectrograph. flat-fielding can be effected pixelwise by supplying a normalized flat field image. On the other hand, it is advantageous in the case of spectroscopic data to normalize the flat field $F(x)$ for each y. The normalization may be achieved by dividing the line by the maximum value along the line. a better alternative is to obtain a highly smoothed version of the line $F_s(x)$, and to derive the normalized flat field as $F(x)/F_s(x)$. All these options are available.

The algorithm finds automatically the position on the CCD where the spectrum is exposed. In the case of echelle spectra it finds all the orders, and one can interactively choose the orders to be extracted. Alternatively, one may explicitly specify the pixel limits of the orders to be extracted using the /LIMS qualifier. This is useful in the instances of poor S/N data when the automatic order-finding may fail. If the image

contains more than one order the order number is suffixed to the output file name, and each order extracted is stored as a different file.

The above method of extraction assumes that the spectrum is exposed either along the rows or along the columns of the CCD. In fact the SPECTRUM command requires this information to be provided using the /COL or the /ROW qualifier. The algorithm can accomodate small tilts in the spectum with respect to rows or columns. On the other hand, if the tilt is large, one may indicate it with the /TILT qualifer. In this case, the orders are traced fully and the spectrum is extracted by simply summing the data perpendicular to the direction of dispersion at each wavelength.

It is assumed that the slit of the spectrograph is exactly aligned with either rows or the columns of the CCD. This condition can be met with in the case of conventional grating spectrographs. On the other hand, echelle spectrographs distort the spectrum considerably. Aligning the slit along the row or column makes the order tilt to a large extent, whereas, aligning the spectrum along a row or column tilts the slit. In the former case, the technique employed at present does not help in achieving the best signal-to-noise ratio, since the optimal extraction technique is not used when /TILT qualifier is present. In the latter case it results in a slight loss of resolution.

The following commands are readily available in an optimized form for the universal astronomical grating spectrograph available at the Cassegrain focus of the 1-m reflector at VBO, using the Photometrics CCD system with default settings.

The USPEC command extracts the spectrum. If the sky spectrum is exposed on either side of the star spectrum, the program allows its subtraction. A smooth continuous sky spectrum is estimated first. Subsequently emission lines that stand out about this continuum are identified and added to the estimate. The resultant spectrum is scaled to account for the difference in the effective number of pixels of object and sky spectra, and subtracted out from the object spectrum. This method is particularly useful when the continuum spectrum of sky is not well-exposed. On the other hand, if the sky spectrum is well-exposed, as with faint object spectroscopy on moonlit nights, it is advisable to extract sky spectrum separately using /LIMS qualifier, scale it to the width of the star spectrum, and subtract from the total (star + sky) spectrum.

A distinct command UCOMP has been made available for the extraction of comparison spectrum since the spectrograph is a conventional one with the comparison spectrum being exposed on either side of the star spectrum. In practice, the comparison spectrum images are taken before and/or after the object spectrum in order to avoid contamination of the object spectrum by the scattered light from the comparison source. the comparison window number (1 or 2) is suffixed to the output filename and one file is created for each comparison spectrum.

Both the commands USPEC and UCOMP assume that the spectrum is recorded parallel to the columns. The bias value is subtracted as the mean background level at each wavelength. If the input frame is already bias subtracted, one may suppress further bias subtraction using the /NOBIAS qualifier. Flat-field correction assumes normalization by a highly smoothed version.

The CCD subpackage consists also of a few more useful commands. The commands COLSUM and ROWSUM compress the two-dimensional images into a linear image by summing along columns and rows, respectively. The result can be examined graphically, for example, to interactively measure pixel limits for different orders, sky spectrum, etc.

Arithmetic opertions can be performed between two image using the IMADD, IMSUB, IMULT, IMDIV. Operations involving an image and an arithmetic constant are performed using the qualifier /C with each of the above commands.

4. Reduction of photographic spectra

Photographic spectrum has a highly nonlinear response to light, particularly when the darkening is measured in

Density $= -$ log (fractional intensity transmitted).

There is a background chemical fog even when no light is incident, a toe in the response curve where the low intensity of light does not lead to appreciable densities, a linear region where the density is proportional to incident intensity, and a shoulder or saturation region where further increase in intensity increases the density only slightly. The microdensitometers used to measure the densities themselves may have a nonlinear response that makes the shoulder appear at even lower densities. The PDS microdensitometer is linear over a larger dynamic range compared to most other densitometers. Another effect common to most densitometers used in astronomy is that they measure specular densities which makes the shoulder appear at even lower densities.

The first step in reducing photographic data is to determine the characteristic curve from auxiliary calibration registrations. The chemical background fog is subtracted out in the density domain before any other reduction is carried out. In the case of a spectrum, however, it is advisable to subtract the 'clear' value after smoothing.

CALIB command enables the measurement of calibration steps or spots interactively. The output file contains mean densities as a function of logarithms of relative intensities. The latter values are stored in the software, and correspond to the calibration spectrograph at VBO. Since CALIB is a string of basic commands, it can be easily modified to suit any other calibration registration. The mean densities in the output file are the Baker-transformed densities

$$B = \log (10^D - 1),$$

since in this representation, the toe of the characteristic curve disappears, and the curvature of the saturated region is reduced. CALIB1 command is more suitable if one desires to obtain also the statistics of noise as a function of densities (D). A polynomial fit to relative intensities as a function of B can be obtained using POLFIT command. The LINT command, with calibration curve as input, converts the density spectrum to log (relative intensities).

In the specific instance of a calibration spectrograph or step wedge record, the procedure can be automated. The command CLSHIFT identifies the beginning of the darkest step. Further, if the plate has been obtained with the spectrograph in use at VBO since 1970s, the command CLSTEP automatically extracts the density values. Often one assumes that the relative exposure at each step is proportional to the angular opening of the rotating sector in front of the spectrograph. A correction due to departure from this assumption can be made using an exposure obtained without the sector in position. The command string CALCOR helps obtaining a corrected calibration curve automatically if the calibration records with and without the sector are input.

It is desirable to smooth the raw spectrum in density units. One may wish to see the power spectrum of data and decide on the cut-off frequency in Fourier space, or decide to use an 'optimal filter'. The command SMOOTH helps in the interactive smoothing of the spectrum. The noise in data depends on densities. A transformation of the observed densities to a new scale in which the noise is constant improves the resolution of the final spectra. The command MDENS helps in converting the ordinary densities to modified densities and vice versa once the noise characteristics are determined through CALIBI command. The smoothing of photographic spectra is discussed in detail by Anupama (1990).

5. Computation of final spectra

The CCD spectra at the end of section 3, and the photographic spectra at the end of section 4 are in the units of counts or relative intensities as a function of pixel or position on the detector. They need to be calibrated for wavelength, and at times, to flux density incident above earth's atmosphere. These reductions are described below.

5.1. *Wavelength calibration*

The comparison spectra are used to calibrate the object spectra for wavelength. Individual emission lines can be measured on the graphic terminal using the WLID command. This command requires an ASCII file containing wavelengths and their identifications in a specific format. The identifications are carried out in the same order, though it is possible to skip the listed lines that are not detectable in the spectrum at hand. The output file contains positions and wavelengths of identified lines. If more than one measurement of comparison spectra are available, the individual files can be merged by the JOIN command. In case the file names are identical except for the last character that indicates a serial number, the files can be concatanated using the CAT command. The output file is automatically named without the serial number; for example,

$ CAT file

concatanates all the available files

file1.dat, file2.dat, ..., file$n$.dat

to form a file 'file.dat'. A polynomial fit in the sense wavelength as a funciton of position is obtained through the POLFIT command. WSCALE then converts the position or pixel number in the spectra to wavelengths and spline interpolates the spectra to a uniform wavelength interval.

5.2. *Atmospheric extinction and absorption bands*

ATMEX computes the atmospheric extinction at each wavelength in magnitude units. Before activating this task one needs to define the following quantities: RA, DEC and EPOCH of these coordinates; DATE and UT of observations; LATitude of the observatory; DEXC or differential extinction coefficient defined such that

$$\text{extinction in magnitudes} = DEXC/[\text{wavelength } (\mu m)]^4.$$

In the absence of definition, EPOCH defaults to the date of observation, LAT to the latitude of CBO, and DEXC to 0.014, the mean value at VBO. The output file of

ATMEX can be transformed from the magnitude units to the units of the spectrum file (*e.g.* relative intensities or counts in linear or logarithmic scale) by simple arithmetic and the correction affected.

Correction for absorption in atmospheric bands requires observations of a hot comparison star. The bands in these spectra can be used to scale to unit continuum intensity, spectrum outside these bands masked by the MASK command, the resultant files scaled to the airmass of the object and the absorption features removed by division in flux or intensity units. Horne (1988) finds that the strengths of telluric absorption lines vary as $(\text{airmass})^{0.6}$. If desired, the masked telluric spectrum may be scaled with this law. On the other hand, one can also make separate masks for O_2 and H_2O band, and determine the scale factor for each one iteratively, until they are fully removed from the spectra.

5.3. *Flux calibration and correction for interstellar reddening*

The observed spectra are calibrated for fluxes using the instrumental chromatic response curve determined from a spectrophotometric standard star, or occasionally from a laboratory continuum source (*cf.* McIntyre, Gilmore & hearnshaw 1990). If a spectrophotometric standard star is used on a night of good photometric quality in conjunction with a photometric detector, one obtains absolute fluxes, and otherwise only the relative fluxes. Once the observed spectrum of the spectrophotometric standard is reduced to relative fluxes and corrected for earth's atmosphere, the INSTRES command computes the instrumental response using the standard wavelengths and magnitudes or fluxes stored in an input file. The output file contains response in the same units as the standard values and at the same wavelengths. One can spline interpolate the response at the wavelengths of the observed spectrum using the SPLINE command. The standard values stored in a paired data file in magnitude units, can be transformed to flux per unit frequency interval, or flux per unit wavelength interval in linear or logarithmic units using the MLAM command.

Narrow-slit spectrophotometry, and also spectrophotometry in poor weather, can yield only relative flux calibration. If the broadband magnitudes are available for the object of interest, one may compute the correction factor needed to bring the observations to the absolute flux scale. The MAG command estimates the UBVRI magnitudes based on the observed spectrum. If the accurate magnitudes are provided, it stores the difference in the output file, which can be input to the FLUX command to correct the observed relative fluxes and bring them to an absolute scale. It is also possible to apply a linear or quadratic correction to the flux spectrum such that it agrees with all the observed magnitudes. This is particularly useful when the absolute flux scale has wavelength-dependant errors.

One may often wish to correct the observed spectrum for interstellar extinction before affecting a comparison between the observed fluxes and a physical model. The command DRED does this if the colour excess $E(B - V)$ is supplied. The standard extinction curve of Savage & Mathis (1979) is used.

6. Measurement of spectra

Now that the spectra are calibrated, one may proceed to make measurements on them. The simplest measurement is to EXAMINE or measure wavelength and intensity at

different continuum or line positions. One can add a short identification of the point measured. The measurement and identification are written in the log file. The measurement of a set of identified lines can be done also by the WLID command in order to generate a file of standard wavelengths against measured wavelengths. These measurements will be useful, for example, in the determination of radial velocities.

Absorption line spectroscopy generally involves the measurement of equivalent widths. One does not need to reduce spectra to flux scale in this case, but it helps to divide the observed spectra by an estimated continuum. The estimation of continuum requires special attention and depends on the type of spectrum. The basic command that helps locating the continuum points is the CTMPT command. This command is an interactive one and stores in the output file the points located using the cursor. The continuum may be SPLINE interpolated between these points. Alternately, one may use POLFIT to determine a polynomial fit to the continuum points and construct the continuum using PLNM command. Command procedures are available to affect continuum reduction using these two methods: CTMR and CTMRP respectively.

LINES command measures the equivalent width, full width at half maximum, centroid and the wavelength and intensity at the maximum of an emission line or minimum of an absorption line. The qualifier /FLUX informs the program that one is interested in total fluxes (*e.g.* of emission lines) and not in the equivalent widths. If one desires to obtain these quantities by fitting a Gaussian profile, one can use the GAUSS command on individual lines. LINES command also clips individual lines of interest and this output can be fed to GAUSS. Otherwise, one needs to clip lines through the CLIP command. If an individual line has a complex profile either intrinsically, or due to line blending, MLTGAUSS does a multiple Gaussian fit. The number of components (a maximum of 5), and their approximate parameters are fed interactively, and the final fit is reached iteratively following Marquardt's algorithm. If one wishes to obtain the Gaussian fits or decompositions in the velocity domain instead of the wavelength domain, the line profile needs first to be converted to the velocity scale using the command VELCON.

The flux calibrated spectra can be matched visually with black-body spectra or the model atmosphere spectra. The command BB generates blackbody curves at a desired temperature in the units of surface emissivity.

The software can thus be used for obtaining most of the measurement normally needed in the interpretation of spectroscopic data.

Acknowledgements

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