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Spectroscopic reduction and analysis programs at the DAO

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Abstract. In this paper I outline the FORTRAN programs available at the DAO to process and synthesize spectra, loosely described under the generic name `REDUCE`. The viewpoint is that of a research scientist who develops and uses his own software, and who writes collaboratively for colleagues. Much of the software has been available on the DAO's VAX machines since the early 80s and is slowly being converted to SUNs, although recent developments involve the use of DEC Alphas. The rationale behind the various reduction and analytic software is outlined, as well as the way the programs are controlled, e.g., menu, questions and answers, keywords and values, or the cursor. Some particularly useful tools are mentioned, such as, interpolation, optimization, and error analysis.

1. Introduction

Since the mid-70s, I have been developing software for the reduction of digital spectra. Initially, the software was developed to process digitized scans of photographic spectra to measure radial velocities (RV) using techniques akin to those employed by Grant measuring engines, or the DAO equivalent: ARCTURUS. This involved line-by-line measurements (`VELMEAS`, Hill et al. 1982a), which was inadequate when blended profiles were encountered. Considering that binary stars were the major source of data, this was not much of an advance, but it did serve to give me experience with digital data and interactive graphics. When the *IUE* satellite flew, I spent a lot of time writing software to plot the data, and, later, to measure the lines by fitting Gaussian, Lorentzian, or rotational profiles to the data—*sans* reseau marks. This software, now called `VLINE` (Hill et al. 1982b), was combined with `REDUCE` (Hill et al. 1982c) to provide the basis for the next development. The need to measure blended line strengths spurred me (reluctantly) to modify `REDUCE` to include scans of the calibration wedges, in order to convert density to intensity. This led to the re-discovery of the "Baker density" (Baker 1925; de Vaucouleurs 1968), which provides a reliable way to generate intensity from the characteristic curve.

Early in the 80s, McLean (1981a,b) wrote a cross-correlation package for the velocity analysis of binary stars, and used data from the DAO to demonstrate the method. He applied it to the most difficult of systems—the W UMa stars—and showed that good velocities could result from the method. This was a breakthrough, and really marked the advent of "modern" binary-star velocity measurements. In 1981 I wrote software (VCROSS) (Hill 1982a) that also used the technique, following a visit from McLean's advisor, Ron Hilditch. It is now the heart of most of the velocity measures that I make.

As the software began to be developed I started exporting it, and continue to do so. Its use was originally on a collaborative basis but I have now abandoned that. But initial development of any new software is still on a collaborative basis. In this paper I outline the software I have been responsible for developing at the DAO. A previous summary is given by Hill & Fisher (1986a). Note that throughout the paper, program names are given in bold face.

2. Spectroscopic Data

2.1. Observing Context

In this section it is worth describing the data. The software was originally written for high dispersion spectroscopy, i.e., plates that were 8 in long taken, at 2.5–6.5 Å mm^{-1}, and (under-)sampled every 7–8 μm. Later, the software was modified to handle low dispersion spectra—(80 Å mm^{-1}). Both of these extremes produced problems: the former because the size of the data sets (typically 25,000 by 4) was too small by a factor of 3–4. and the latter because of the difficulty in automatically predicting the position of an arc line in a crowded spectrum accurately enough for it to be measured automatically. The latter problem was harder to solve. The storage problem required the switch to the VAX. In the mid-1980s, when the Reticon became available, it was easy to convert the software to deal with it, particularly when the detector was linear.

The thrust of the observing programs has been twofold: (1) to measure velocities of stars, and (2) to measure the line strengths, or equivalent widths (EW) of spectral lines. In the former case the measurements are quite routine for single stars or galaxies, since there are rarely any complications. A simple fit to the peak of the cross-correlation-function (CCF) will generally suffice, though a red-shifted emission-line galaxy spectrum might pose problems of interpretation. For binary stars the spectra are more complex, and a successful measurement demands a composite CCF or a series of spectral lines, depending on what you are doing. It is an exacting task to extract this information, even with a high signal-to-noise (S/N) CCF or line profile. The critical problem is matching line-shapes to the fitted function. When I first began the measurement of highly blended profiles, typified by W UMa systems, I fitted Gaussian profiles to the CCFs. They gave good mass ratios, but the systemic velocities from the two orbits taken independently almost always differed. Once realistic shapes were used to measure the CCFs, however, the systemic velocities became consistent and the precision of the velocity measures improved. It then became possible to measure masses to the 1–3% accuracy that one desires for the study of stellar evolution (Andersen 1991). I refer the reader to some recent papers on V566 Oph (Hill et al. 1989b) and V599 Aql (Hill & Khalesseh 1991).

These developments drove me toward more realistic fitting functions, mostly defined by the data themselves and not, as before, simply chosen by virtue of being analytic. This approach parallels the point-spread-function (PSF) concept used in direct imaging. The same problem is encountered in measuring line profiles. Here the observations have not been smoothed and added, like that of a CCF, and S/N is usually a problem. Again, without a realistic profile shape, an EW measurement may not be very good. The ability to measure EWs with excellent precision for blended spectra has been enhanced by the work of Bagnuolo & Geis (1991), who developed a useful algorithm to separate out the component spectra. The tomographic method they employ derives from medicine, and has proven most useful, as shown by Hill & Khalesseh (1993) for V1425 Cyg, Hill & Holmgren (1994) for Y Cyg, and Hill et al. (1994) for CC Cas. Another method, developed by Simon & Sturm (1994), promises to be even better.

Another spur to software development was the availability of data with high S/N (~2000:1). Naturally, EW measurements are easier, but such high quality data need to be matched to stellar atmosphere models to derive directly the effective temperature (T_e), surface gravity (log g), rotational velocity $V \sin i$, abundance (log Fe/H), and microturbulence (ξ). To do, this the Model atmospheres of Kurucz, calculated over a suitable grid (every 500 K from 7500–11,500 K, 0.5 dex steps in log g from 3.0–4.5, unequal steps of 0.3–0.5 dex in log Fe/H from -1 to +1, and at 0, 1, 2, and 4 km^{-1} for ξ) are required. The size of this grid, when coupled with a requirement for spectral coverage of at least 500 Å (sampled at 0.01 Å), produces some difficulties in memory size. At high dispersion with the Reticon, we typically sample 1870 points and cover only 70 Å. Any analysis would require something larger than that to enable Hγ to be examined. (Note that in an A-star the hydrogen lines might extend over 100 Å and still not reach the continuum). From these figures, we need about 260 MB of memory to handle just 20 Å of spectrum. We are not there yet; our current need, without including log Fe/H as an unknown, is 50 MB.

2.2. Type of Observation

While the CCD and Reticon have simplified spectroscopy, they have also produced the potential for inaccuracy, since wavelength calibrations are made at different times. Unlike a photographic plate, where all the information needed to analyze it is carried on it (arcs, star, clear plate and calibration data), the digital detectors generate sequential files which must be tracked. It is, of course, a problem for the observer and not one intrinsic to the detector. With non-coudé systems, arcs should be taken before and after each stellar exposure. For coudé systems, where the system is stable, it is not necessary to get arcs with the In addition we need bias frames (CCD), darks perhaps, and certainly flat-fields. An echelle observation creates a particular difficulty, as well as an opportunity, but we do not have such a spectrograph at the DAO (thank God!). Shortridge's FIGARO software, however, is particularly effective in processing echelle spectra.

3. Comments on Software

My philosophy has largely been defined by my experience. As someone who started programming in FORTRAN in the early 1960s I have had many years to develop bad habits as well as to gain a good knowledge of the language. This, coupled with a structured approach and excellent software editors, has meant that a new program can be developed remarkably quickly for each new application. With the simplifications that came to us from the VAXs acquired throughout the early 1980s, I discovered that monolithic programs were far too inefficient. Generalizing problems seemed to get me into more trouble than it was worth. For that reason I have adopted the philosophy of writing independent programs to do different tasks. This philosophy covers graphics, as well as the application itself. Initially I wrote a "catch-all" plotting package, where one or two calls would define the whole graph, but I quickly abandoned it as being awkward and unwieldy. Now each application has its own graphics. This has simplified program development a great deal, since one does not need a manual to revise the graphics. Smaller programs are easier to understand and modify.

I have concluded that the software must be interactive, driven by the cursor and keywords—questions and answers must be minimized. It took a while before I realized that a system of keywords and associated values, tasks, etc., would be very useful. I developed my own decoding software to enable the strings to be interpreted (see Hill & Fisher 1986a,b). It really made program operation much easier. One could measure a velocity in about 15 minutes using ARCTURUS, so the computer had to give answers quickly. The programs must be easy to use, i.e., they all must have the same "look" or "feel." With the system of keywords and graphics, with mostly identical cursor commands, I have largely achieved this goal. All the software has manuals. But converting from printed (dedicated word-processor) to on-line manuals has been particularly burdensome.

Many of the repetitive tasks (measuring arcs, linearization, measuring velocities of single stars) are organized to work from a file of file names which can be processed in sequence, either automatically or manually. My favorite automatic feature is the playback mode, which stems from the robot welding on the Japanese assembly lines. Hard copy is a factor here since I have always felt it necessary to be able to retrace the reduction steps, particularly during the analysis process. For the automatic processing hard copy is therefore integral to the process.

Graphics have always been a problem. Initially the software was developed for a Tektronix 4012 terminal (768 by 1024) and its hard-copy unit. From Tektronix's `PLOT 10`, higher level graphics routines were written to facilitate program development (`TGRAPHLIB`, Hill 1986). With the growth of laser printers and PostScript, this software became inadequate, so I converted to `Lick Mongo` (Allen & Pogge 1991). This, too, created difficulties in exporting my software because `Lick Mongo` is not widely available. I am currently converting to `PGPLOT` (Pearson 1989), which is simpler to implement off-site.

The hardware platform also has an effect on things. The swing from VAXs to SUNs leaves software developers caught between two stools since one's clients are not all shifting at once. Thus I have been stuck with trying to maintain two systems (even the switch from VAXes to Alphas is not routine). Fortunately some simplifications have occurred along the way: the general adoption of a single hardware platform, FITS (Wells et al. 1981), and later, the large software packages IRAF and FIGARO (Shortridge 1987). But for reductions as specialized and as difficult as found in the binary star arena, "canned," generalized software cannot do the job.

4. Reduction of Spectra

In this section I deal with all the steps leading up to measuring a digital spectrum; analysis will be covered in the next section. Prior to that, the way that I do book-keeping is noted.

4.1. File Naming

Typically, a datafile name is based on the detector, telescope, year, and sequence number of the observation. A CCD image (number 1780) taken with the 1.22 m telescope in 1994 would have a file name C122941780. In addition to this, I follow the convention defined by Gulliver (1976) and Irwin (1978); this simple scheme facilitates record-keeping since each type of file or each reduction process simply alters the prefix. The arcs, clear plates, etc., are therefore uniquely identified with the stellar observations. The exact processing path depends on whether one has photographic or CCD (or Reticon) data. For photographic spectroscopy, the data are produced by a PDS machine which scans both arcs, the stellar spectrum, and a predetermined stretch of clear plate. The calibration is also scanned at this time. Such a series of scans yields the files listed in Table 1. As noted in the table, some of these steps are omitted for the digital detector.

Table 1. File-naming convention for plate or file 122941780

Raw spectroscopic data		Processed data	
Calibration	T122941780*	Linearized in λ	W122941780
Clear plate	L122941780	Converted to intensity	I122941780*
Arc	F122941780	Normalize to continuum	R122941780
Stellar	S122941780	Converted to log λ	U122941780†

*Necessary only for photographic spectroscopy

†Generally unnecessary

4.2. FITS Files

The original DAO disk FITS file system was written by Poeckert in 1981, and has seen many incarnations since then. Each processing step that a spectrum undergoes is logged in the header to show what has happened to the data. This, along with the above file-naming sequence, allows the user to know the status of their reductions in an instant.

4.3. Photographic Reductions

These are routine since the scans all have related names.

4.4. Reticon Observations

In dealing with Reticon data, we try to emulate the photographic procedure. Given a long string of observations, the program `RET72` allows one to produce a similar set of files. The data are plotted and examined, the flats are identified for a given night, and an average defined. Given the starting and ending file numbers, the data are normalized by the flats. `RET72` automatically identifies arcs straddling stellar spectra and renames them, prefixing them with an "F" under the name of each stellar spectrum. The result for each stellar file is an "F-file" comprising the straddling files abutted end to end (2 dimensions). Incidentally, the arcs are automatically identified by a skewness value $\gg 1000$, but the algorithm will fail for emission-line spectra. The whole process can be done manually.

A similar scheme is planned to convert the CCD data that I am now acquiring at the DAO to one-dimensional (1-D) form. When using data from the AAT or WHT, I use the FIGARO software to produce the 1-D files that feed the reduction software. The arcs are measured by `REDUCE` (Hill et al. 1982a), an interactive program based on the method uses to measure arcs with ARCTURUS. The heart of the scheme is a standard plate—the prediction of a position x in μm—for a given λ, based on the spectrograph parameters. In essence, it is a differential method for finding the correction of each line from a predicted position. One must first identify one line with a given pixel (hardly an onerous task); that value is contained in the F-file which `RET72` produces. Once a spectrum has been measured, the keystrokes are recorded and later measures are done in a playback mode. The same arcs, which might also straddle other stellar observations, are not re-measured but are updated according to the velocity correction to the sun.

Once the arcs are measured, the spectra are linearized in λ. The conversion is based on an interpolation using `INTEP` (Hill 1982b), which uses cubic splines to interpolate a reasonable curve *through* the data. It is an extraordinarily effective workhorse in all the reduction and analysis programs.

5. Required Measurements

As noted in Section 2.1 the types of measures we need to make are:

RV: Done either line-by-line, or all together. With binary stars, the measures may be very difficult;

λ: These are also very difficult, and are generally only made for single stars;

EW and $V \sin i$: The measures of line strengths and rotational velocities are also line-by-line and very difficult. The spectra often have low S/N;

High dispersion, high S/N: For high dispersion work we are looking at the physical parameters of single stars, which is a much easier, but CPU-intensive task. To date we have only worked on high S/N data ($\sim$2500:1) and small 20 Å stretches of spectrum. The software is ready to deal with spectra of B–A stars to measure T_e, $\log g$, $V \sin i$, log Fe/H and ξ.

6. Summary of Analysis Software

6.1. Prerequisites

All of these applications require wavelength linearized spectra, normalized to the continuum. The format of choice is FITS, although I occasionally write conversion software to provide the desired FITS format (the conversion from ASCII already exists). In this section I outline the programs in regular use at the DAO.

6.2. Reduction and Measurement of Spectra

Processing of Reticon observations. `RET72` allows the user to plot raw data, average the flat field observations, normalize and assemble files in the desired forms of arc (F-files, 2-D) and stellar (S) files. It produces FITS files that can be measured for arc, linearized, and then rectified to the continuum by `REDUCE`. FIGARO performs the same function when we are dealing with CCD results from the WHT or AAT. `RET72` is routinely used at the telescope, where it enables the observer to monitor the night's work very closely. Monitoring has been done off-site from Manitoba.

Radial velocity. `VLINE` measures up to 12 lines simultaneously. It requires a file of line identifications, and will fit either Gaussian, Lorentzian, rotational, or digital (PSF) profiles to selected non-contiguous pieces of the data.

`VCROSS` measures RV by cross-correlating selected pieces of spectrum with a reference spectrum or template. The reference spectrum may be real or synthetic (see Hill et al. 1993). It can fit analytic or digital profiles to the CCF, produce PSF digital profiles for use, create artificial binaries for testing, and combine inhomogeneous (data sampled at different wavelength intervals) FITS files. The $\ln \lambda$ conversion is done automatically. The last two features are transparent to the user. It can run from a list of file names interactively or automatically (only recommended for single stars).

`VLINESUM` measures RV by summing lines identified from a line list. It simulates an RV scanner, and is useful for working on visual binaries where the separations are small, and where the blended profiles will be further masked by the smoothing effect of a cross-correlation.

Wavelength, EW. `VLINE` measures up to 12 lines simultaneously, and will fit either Gaussian, Lorentzian, rotational, or digital (PSF) profiles to selected non-contiguous pieces of the data yielding EW, FWHM, and $V \sin i$. `LINEMEAS` is a less sophisticated version of `VLINE`, and only measures single (unblended) lines. It fits various profiles and is fast to use.

6.3. Analysis and Modeling

Binary stars. `TOMOGRAPHY` separates a series of composite spectra into two components. Given a series of spectra measured for RV (both components), it will deconvolve them into separate components. When cross-correlated with a reference spectrum, the resultant CCF provides the CCF PSF-profiles with which to re-measure the material, and hence to repeat the process.

Given files of RV and $JD_\odot$, RVORBIT calculates the spectroscopic orbit for any combination of parameters. It handles either single or double-lined spectroscopic binaries using either Sterne's (1941) method or the method of Lehmann-Filhés (1894). Errors are calculated by the usual error-matrix analysis and by Monte-Carlo or bootstrap statistics.

Spectral synthesis. ROTATION generates spectra from large files of synthetic intensity spectra derived from Kurucz's atmosphere models. The assembly of these spectra into a data-base is ongoing. Models are based on Roche geometry and Collin's (1963) formulation. Integration is based on the Gauss-Legendre scheme used by Collins and by Hill (1979) in LIGHT2 . The synthesized spectra are compared to the observations and then automatically solved for T_e, $\log g$, $V \sin i$, log Fe/H and ξ. In certain cases (stars rotating at $\geq 50\%$ of breakup speed, with $i \ll 10°$), the inclination can be determined. It will be become extraordinarily useful for deriving physical parameters of "normal" stars, since it will happily interpolate automatically in four unknowns.

VSUN calculates the velocity correction to the sun ($RV_\odot$), as well as the heliocentric correction and Julian date. I usually use it to log the observations as I make them, and certainly use it at the end of the observing run. The file it produces, when combined with those generated from earlier observing, provides the data-base for PHASES (see below).

EPHEMERIS provides planning software for binary star observing. Given the site, date, UT range needed, and the ephemerides for the binary stars, the program outputs a table of phases for each night. It is possible to limit the phases (e.g., ranges around quadrature or eclipse), and to restrict observations above a given airmass (χ). It is also possible to pre-select a list of stars with varying phase constraints. This requires a constraint file of hour angle (HA) as a function of declination (not the same for all telescopes, even at the same latitude). The tables can be listed star-by-star over the nights desired or all stars on each night. Auxiliary tables giving HA, χ, and $RV_\odot$ may also be printed.

PHASES calculates the phases from the spectroscopic data-base produced by VSUN, and sorts and summarizes the data. Histograms of acquired phase data for each star help in the planning of an observing run.

Related tools and useful aids. Given a file of light-curve data (magnitude vs. phase or JD) LIGHT2 will solve for any combination of parameters, e.g., relative radii and polar temperatures of either or both stars, and i. It can also provide line profiles for W UMa systems for use with VCROSS. It uses modified black-body intensities and linear limb darkening derived from theoretical models. It can be modified to use the intensity data ROTATION uses, once all the atmospheres have been calculated. It is described by Hill (1979, 1985) and by Hill & Rucinski (1993).

CURFIT is Bevington's (1969) venerable optimizing program—still remarkably potent. The algorithm has proven to be wonderfully flexible, and I use it throughout the software described above. It has been modified to enable the user to freely vary the parameters. All non-linear optimizing schemes have their warts when it comes to local or global minima, but, if used judiciously CURFIT does the job for these applications. In ROTATION we buttress the method by doing an extensive search through parameter space to verify the derived minima.

In `LIGHT2` I use differing starting points. `CURFIT` is used to measure the arc lines in `REDUCE` and to perform all of the fitting in `VLINE` and `VCROSS`.

`INTEP` is an interpolation program based on cubic splines (Tsipouras & Cormier 1973) which has proven to be remarkably useful. It is stable, and fits a "reasonable" curve *through* data without the enhanced wiggles one sees in high order polynomials. The software for this, with some examples, is given by Hill (1982b). It has proven to be very reliable for the fitting of continua, unlike least-squares spline fits which do not go through the data. It is used for the re-binning of data, e.g., in the linearizing process, and within `VCROSS` when it is used to homogenize data prior to calculating the CCF.

7. Error Analysis

The calculation of errors is often the bane of any analysis, particularly when the parameters are correlated. In spectroscopic orbits, the classic problem involves the derivation of the longitude of periastron and the time of periastron passage. In addition `CURFIT`, as described by Bevington, has a bug in its error matrix analysis. I find that fits to CCFs often produce unrealistically low errors, even though the *relative* values derived from a list of measures are likely to be accurate. To get alternative estimates of the errors I have used Monte-Carlo and bootstrap statistics (e.g., Hill et al. 1989b).

Monte-Carlo methods. These are easy to implement—simply take the derived parameters, generate data for each time or phase, add the observational noise, and solve again. Make 100–1000 solutions, and then calculate the errors in each parameter.

Bootstrap statistics. These are equally easy to use, although it becomes impractical for CPU-bound analyses, such as solving a light curve or using `ROTATION` to calculate i for Vega (Gulliver et al. 1994). It would be interesting to see whether the DEC Alphas could do the job. The algorithm is straightforward: if you have n data points, take a random selection of n points from your data and analyze them. Repeat 100–1000 times, and sort the parameters in order. The values at the 16-th and 84-th percentile give twice the error.

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