Acquisition, Archiving, and Analysis (3A) Software Package

Reference Guide

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Chapter 1

General usage facilities

1.1 The menu bar and menus

The software described below is controlled from a menu environment. The menu environment consists of three parts visible on the screen: the menu bar at the top, the window area in the middle, and the status bar at the bottom.

The menu bar is the primary access to all the menu commands. The menu commands can be chosen in the following way:

Main menu selection: Press `F10` to activate the menu bar and the highlighted menu title appears. Use the arrow keys `Left` and `Right` to select the menu to be displayed. Then press `Enter`. To cancel an action press `Esc`. As a shortcut for this step, just press the highlighted letter of the menu title. For example, from the main menu, press `F` to quickly display the `File` menu. From anywhere, press and hold `Alt`, and the highlighted letter of the menu title to display it.

Menu selection: Use the arrow keys `Up` and `Down` to select the command. The currently *selected* menu command is highlighted. Then press `Enter`. Again, as a shortcut, just press the highlighted letter of a command to choose it once the menu is displayed.

At this point, the software program either carries out the command or displays another menu. If a menu command is followed by a colon (:), choosing the command displays a dialogue box. If the command is followed by a triangle (▷), the command leads to another submenu. A command without either a text string or a triangle indicates that once it was chosen, that it is immediately executed. Some of menu commands are unavailable when it would make no sense to choose them and these are displayed without a letter highlighted.

Many menu items have corresponding hot keys, one- or two-key shortcuts that immediately activate that command or dialogue box. The `Esc` key is used to exit from the menu window.

Figure 1.1: The menu environment with main menu bar, table window, and the menu status bar is shown. The table window has the header bar atop and the message bar at the bottom. The dialogue box is open to edit a record of the table.

The status bar of the menu environment appears at the bottom line of the screen. The status bar includes the following functions:

- Reminds of basic shortcuts or hot keys applicable at that moment in the active window.
- Tells what the program is doing and how the process can be stopped.
- Offers one-line short description of any selected menu command.

The contents of the status bar changes as windows or processes are switched.

1.2 Tables

A number of applications (database facilities, pickup lists and others) are using the table object to display various textual and numerical fields and are providing browsing and selection commands. Basically, the table window consists of three parts visible on the screen: the header bar at the top of the window, the records field in the middle, and the message bar at the bottom. A table record contains a number of fields. The beginning and end of a field are indicated by vertical delimiters in the header bar. The horizontally highlighted bar is used to indicate the position of the selected record.

For each application, there is a number of special commands operating with the records:

`Up/Down` Moves the bar one line up or down.

As a shortcut for the commands which move the cursor, just type the first few letters of the *first* field of the record to be selected. The program will search for the combination of the letters typed through the following records and the cursor will move to the first matching record.

`PgUp/PgDn` Moves the bar to the previous or following page.

`Home/End` Moves the bar to the first/last record of the table.

`Ctrl-Home/End` Moves the bar to the first/last line of the records area displayed in the window. Press and hold `Ctrl` when operating with the keys.

`Left/Right` Moves the bar one field of the record to the left or right scrolling the table horizontally if the record length is larger than the size of the window.

`Ctrl-Left/Right` Moves the bar one character of the record to the left or right. Press and hold `Ctrl` when operating with the arrow keys.

`Tab/Shift-Tab` Moves the bar to the next or previous column, if the application program supplies a multi-column table. Otherwise, moves the bar to the next or previous record.

`Ins` Marks, or highlights, a record. Press this key when the bar is on marked record to unmark the record.

`Enter` Selects the record at the bar position and exits the application.

`Alt-X` Closes the menu and exits from the application with no record selected. No subsequent action is taken by the calling program.

`Esc` Closes the program window and exits with no record selected.

1.3 Dialogue boxes

If a menu command is followed by a colon (:), the command opens a dialogue box. A table also allows to open a dialogue box to edit a record or create a new one. A dialogue box consists of a number of input boxes, which allow text to be entered. Any alphanumeric characters can be typed as text. Initially, the mode is set to *replace*, so any new character overwrites the old one. If there is more text than shown in the box, arrowheads appear at the ends (◁ and ▷) indicating the scrolling direction. The following text-editing commands work in the text box:

`Left/Right` Moves the cursor one character to the left or right.

`Ctrl-Left/Right` Moves the cursor one word to the left or right.

`Home/End` Moves the cursor to the beginning or end of a line.

`Ins` Toggles between *replace* (seen as the underlined text cursor) and *insert* (filled text cursor box) modes.

`Del` Deletes the character at the cursor.

`Backspace` Deletes the character to the left of the cursor.

`Ctrl-Del` Deletes the word at the cursor.

`Ctrl-Backspace` Deletes the word to the left of the cursor.

`Tab/Shift-Tab` Moves the cursor to the next or previous input box.

`Down/Up` Moves the cursor to the next or previous input box.

`Enter` Accepts the input and exits from the dialogue box.

`Esc` Discards the input and exits from the dialogue box.

The input text will be typed in the menu command line followed by the colon. If the text string does not fit to the output field of the menu line, the displayed text is truncated and the last three characters are replaced by dots (...). The record of the table will be typed again once it was modified using the dialogue box.

Many programs are using another kind of dialogue boxes to change keywords: press `Enter` to alter the parameter to one from a list of alternatives (for instance, `Yes/No` or `Ratio/Difference/None` are the lists of alternatives).

Some of the programs might open the list of these alternatives by displaying a vertical menu of keywords with a highlighted bar for choosing. The bar can be moved by the `Right/Left` arrow keys or by `Tab/Shift-Tab`. Press `Enter` to select a keyword and close the menu window.

1.4 Graphical marker

To indicate relevant parts of the graphical image on the screen, a special graphical marker is used in the graphical window area. The marker is the highlighted rectangle that can be moved by the arrow keys of the keyboard. The size of the rectangular box is not fixed and can be altered by using the keys. One stroke of the key moves the marker by one pixel of the display. Hold the key pressed to move the marker continuously.

A number of keys are used to manipulate the graphical marker as follows:

`Left/Up/Right/Down` Moves the marker in the direction indicated.

`Shift-Left/Right/Up/Down` Changes the size of the marker box. The upper left corner of the box remains fixed and only the right/bottom corner is moved in the direction indicated. Press and hold `Shift` when operating with the arrow keys.

`Alt-Left/Right/Up/Down` Changes the size of the marker box. The centre of the marker remains fixed and the width or height of the box is altered (contraction or expansion). Press and hold `Alt` when operating with the arrow keys.

`Ctrl-Left/Right` Changes the size of the marker box. The centre of the marker remains fixed and the area of the rectangular box is altered (contraction or expansion). Press and hold `Ctrl` when operating with the arrow keys.

`Ctrl-Up/Down` Changes the size of the marker box. It works in the same way as the previous case, but if either of the two keys is pressed, the box is transformed to a square. Press and hold `Ctrl` when operating with the keys.

`Alt-C` Toggles the marker box size between three states:

- Expands the marker box up to the axes of the graph.
- Displays it as a horizontal line at the centre of the graph.
- Displays it as a vertical line at the centre of the graph.

`F2/Ctrl-F2` Changes the colour of the marker box. Use the first key to increase the colour index, and the second to decrease.

When a control key (`Alt, Ctrl` and `Shift`) is pressed, the status line at the bottom of the screen informs of the keystrokes available.

Always use `Alt-C` and possibly `F2` to find the marker if it is not visible on the screen. The marker position is stored in physical coordinates, so with a new image displayed it can be just outside the screen.

The physical coordinates of the marker corners are displayed in the message bar at the bottom line of the graphical window. Usually, the length (the difference) of the marker box sides in physical coordinates are displayed in the brackets. Some programs allow to switch the positions into index scale (pixels instead of physical coordinates).

1.5 File name conventions

The following principles of the file naming are essential for 3A:

- The name of a file has always a sequential number. The FITS files are managed under the control of the database facility which displays the contents of their headers. Therefore, there is no need for constructing an 11-characters long file name which includes the date, object's name, observer's initials and/or some other identifiers to separate one file from the other.
- A three-character prefix is always preceding the sequential number. The prefix space is used e.g. for the numbering of the spectral orders extracted from the échelle image.
- The extension of a file indicates the most recent operation done with the file.

The name of a file is formed according to the template name. The zeroes are used as a format for the sequential number. The table gives an idea how it works:

Number	Template	File name
123	ccd00000.fit	ccd00123.fit
123	ccd.fit	ccd123.fit
123	0.fit	123.fit

The following table shows some possible extensions of the FITS files which might appear in the current working directory and database during data processing:

`*.fit`	The original FITS image
`*.avr`	Average of some files
`*.sum`	Sum of some files
`*.sub`	Difference of two files
`*.dvd`	Ratio of two files
`*.mul`	Product of some files
`*.med`	Median filtered data
`*.tmf`	Trimmed mean filtered data
`*.avf`	Average filtered data
`*.wmf`	Weighted median filtered data
`*.hpf`	Highpass filter
`*.gss`	Gaussian filtered data
`*.pol`	Polynomial curve
`*.sin`	Sine function
`*.ccf`	Cross-correlation function
`*.ns`	File with noise added to the data
`*.nor`	Normalized data
`*.col`	Image with the bias column subtracted
`*.row`	Image with the bias row subtracted
`*.cr`	Cosmic rays mask
`*.clr`	Image with the cosmic spikes removed
`*.dat`	Extracted spectral order
`*.wl`	Spectrum rebinned into wavelength scale
`*.hwl`	Spectrum in heliocentric wavelengths
`*.swl`	Spectrum in stellar rest wavelengths
`*.rv`	Spectrum in radial velocity units
`*.spn`	Spun up spectrum

The files with the extensions shown below are non-FITS files, so they do not appear in the database, and are used for the storage of information relevant to the data processing; they are stored in the current working directory:

`*.hst`	Histogram file
`*.zon`	File of marked zones of data
`*.spp`	Polynomials of the spectral orders
`*.pix`	File of the fine wavelength offsets
`*.txt`	Plain textual contents of a table
`*.ps`	PostScript file
`*.cbp`	Polynomial coefficients of the dispersion curve
`*.slp`	Table of the spectral line parameters
`*.sld`	Table of the spectral line displacements
`*.sol`	Table of the wavelength combinations
`*.sls`	Setup file of the spectral line parameters program

1.6 File pickup facility

The program is commonly used by a number of applications to select one or several files from the directory displayed in the table (Sec. 1.2, p. 8). Each record of the table consists of the fields listed in the header bar: file name, extension, size in bytes, date and time of the last modification.

The subdirectory names are added into the table and useful to change the directory levels. These names are printed in capital with `SUB-DIR` in the field of size. The parent directory name is marked as `(..)` with `UP-DIR` in the field of size. Move the table bar onto the directory name and press `Enter` to enter and display its contents. The current directory path is printed at the top border of the table window.

The message bar of the table shows the sequential number of the file currently selected and the number of marked files among the total amount of files in the directory. The program is called either in the full screen size and consists of two table columns or in the half screen with only one column.

The `File` menu contains the commands as follows:

`Viewer:` *name* `(F3)` Calls an external viewer program specified by its name to inspect the contents of the selected file.

`Editor:` *name* `(F4)` Calls an external text editor specified with the name to modify the contents of the selected file.

`Mark (Ins)` Marks, or highlights a record of the table of files. The command is relevant for those specific applications which require a multiple file selection.

`Toggle group (Grey±)` Changes the status of all records downwards starting from the table bar position. Use `Grey+` to mark the records and `Grey-` to unmark. The command is used for multiple file selection applications.

`Delete (Ctrl-Del)` Allows to delete a file pointed to by the table bar. Only one file can be deleted at a time. A warning message window appears asking to confirm the operation by using `Enter` or to disregard by `Esc`.

`Sort (F2)` Allows to sort the directory. The sorting order of the files can be selected from the menu:

- `Name` sorts by the name, and extension.
- `Extension` sorts by the extension, and name.
- `Date/Time` sorts by the date, time, name, and extension.
- `Size` sorts by size, extension, and name.

`Path/filter (F5)` Allows to change the disk drive, path to the directory, and the files to be displayed. If this does not exist, an error message appears and asks for the correct drive or path. The wildcard in the file name works as everywhere, and here are some possible combinations:

`*.*` All files in the directory.

`*.`*ext* All files in the directory with extension *ext*.

`*.` All files in the directory with no extension.

`.*` Directory names only.

`Select (Enter)` The command does one of the following:

- Changes from one directory to another if the file selected was the directory.
- Transfers a single file name selected with the table bar into the calling application program.
- Transfers a list of marked (highlighted) files (the table bar position is irrelevant) into the calling application which requested a multiple file selection.

The exit from the program follows.

The exit menu command `Alt-X` discards file selection(s) and exits with no subsequent action in the application program.

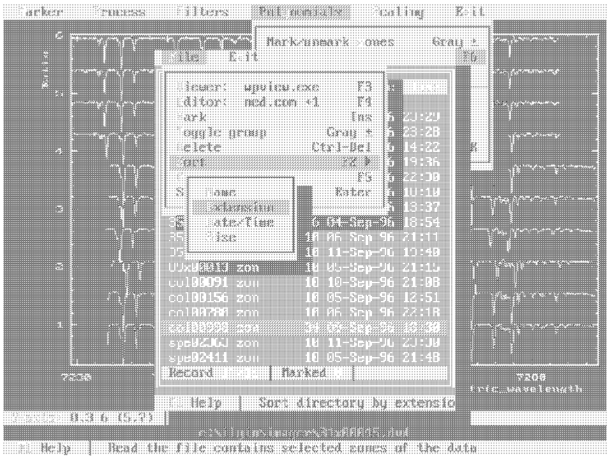

Figure 1.2: The file pickup window appeared in the spectrum program to select a file of zones. The submenu of the sort command is open.

1.7 Memory service

When some application wants to get access to the data of a FITS file, the program first loads the data into the expanded memory (a memory above 1MB, specific for DOS). When the application has finished to use the data, the file remains in the memory. If the application has changed the contents of a file allocated in the memory, it asks for confirmation to save the file into the hard disk. A file allocated once in the memory can be used or shared by a number of subsequent applications, so the number of time consuming operations to download a file from the disk is minimized. The program allocates a new memory area for a file which has to be loaded and which is not yet in the memory. One or few files, which are first in the list of files allocated in the memory, are released in one of two cases:

- If the file size to be loaded is larger than the amount of memory available.
- If the number of files allocated in the memory is large than the maximal number of the expanded memory entries. The number is set by the expanded memory driver with the default value being 64, and the maximal being 255 (Sec. ??, p. ??).

A special program was designed to check the contents of the expanded memory. The program window displays a table which shows the memory entries. The table can be browsed (Sec. 1.2, p. 8) with the table bar. Each record of the table displays the expanded memory entry number (EMM handle), the amount of memory allocated in 16KB

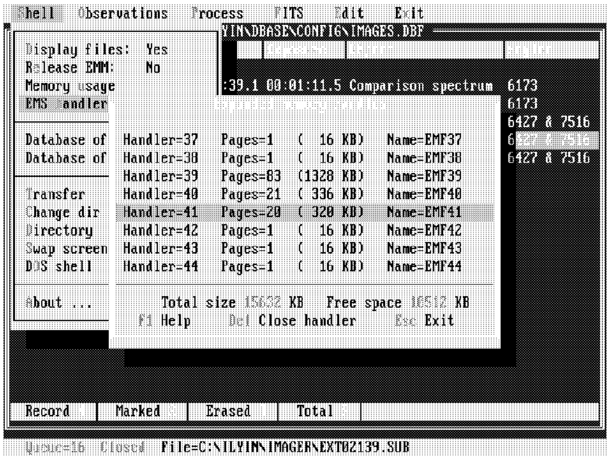

Figure 1.3: The table of data files allocated in the expanded memory is shown.

pages, and the name of the entry. The memory entry names created with 3A have `EMF` prefix for the files and `WIN` for the graphical screen swap. The program message bar displays the queue number of the file, which is used to release the old files, the status of the file (open, closed, or shared), and the full path name of the file loaded. Finally, the amount of memory available is shown.

Any of the memory entries can be deleted by `Alt-Del`. The program is asking for confirmation to delete if the memory area name is different from the two created by 3A and might belong to DOS or to some other program. *Never ever delete the DOS EMM handles which might crash the hard disk file system.* Exit from the table by simply pressing `Esc`.

1.8 Palette editor

The palette editor is useful when colours, contrast or brightness of the screen should be changed. In the present version of the program, the standard VGA mode is used, so only 16 different colours or grey levels are available. Once the program is activated, it displays the default grey levels palette or the palette used previously.

The graph displayed consists of 16 different vertical bars and each of them contains three RGB-registers (red, green and blue basic colours). Mixture of these three registers at different intensities are forming the colour or grey level of the given palette bar. The resulting colour is displayed atop of the window as a horizontal bar. Intensity of each RGB-register among 16 palette colours can be changed by using the arrow keys. Colours can be changed individually for the selected bin of the palette or for all of them at the same time by using an adjustable polynomial curve. Three RGB-registers of different intensities are forming the coloured bin, but equal intensities are forming the grey scale bin, so that the zero level is black and the maximal level is white.

The background colour of the screen is formed at the first, leftmost palette bin and the foreground is at the last, rightmost bin. The contrast of the screen is defined by the slope of the curve approximating the colours. The brightness depends on the height of that curve.

A number of arrow key combinations, as it is written in the menu status bar of the program window, allows to manipulate the colours:

`Left/Right` Moves the small triangle-like pointer in the direction indicated to select either of three RGB-colours of the palette bin.

`Ctrl-Right/Left` Moves the pointer from the colour register of one palette bar to the same register of the next/previous palette bar.

`Up/Down` Changes the intensity of the selected colour register, therefore the colour of the palette bin is altered.

`Shift-Up/Down` Changes the intensity of the colour registers within the palette bar at the same time in the direction indicated.

`PgUp/PgDown` Changes the selected colour register intensity between maximal and minimal values.

`Ctrl-Up/Down` Changes the intensity of all RGB-registers at the same time. A polynomial of the degree specified in the menu window is used to put the intensities of the 48 RGB-registers onto a smooth curve. Position of the pointer indicates the position of the bending area on the curve.

`Alt-Up/Down` Works in the same way as the previous command but changes only the selected colour register, either red, green, or blue at the same time for all 16 palette bins.

The program is controlled by the menu environment. The following are the `Setup` menu commands:

`Polynomial degree:` *deg* `(Alt-P)` Specifies the degree of the polynomial used for the approximation of the colours by a smooth curve.

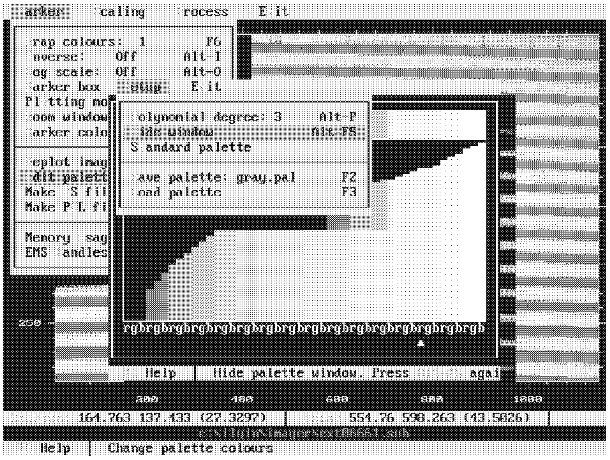

Figure 1.4: The palette editor as it seen on the imager program screen. Note the graphical movable pointer selecting one 16 VGA registers. The colours were smoothed by a polynomial of 3rd degree to obtain a grey scale palette.

`Hide window (Alt-F5)` Hides the program window, so the background image can be viewed with the new colours. The program window reappears once the key is pressed again.

`Standard palette` The command sets the standard EGA/VGA colour registers, which are normally used in the generic text mode.

`Save palette:` *name* `(F2)` Saves the current palette colours into a file with the name specified in a dialogue box. An old file with the same name is always overwritten by the new one.

`Load palette (F3)` Allows to restore a palette saved earlier. The command activates the file pickup facility (Sec. 1.6, p. 10), which displays the palette file names `*.pal` in the current `CONFIG` subdirectory. Choose the file and press `Enter` to display it. A palette can also be loaded from any other directory.

On exit from the program with `Alt-X`, the currently changed or loaded palette is saved into a file with the name specified by the `Save (F2)` menu command. If no file name was specified, the default name `def.pal` is used. The palette with the name specified is subsequently used by the calling program. For instance, an image looks more smooth with the grey scale, but the spectra might look better with the standard palette.

1.9 Make a hardcopy

1.9.1 PS-files from data displayed

The program creates a PostScript file of the graph as it is visible on the screen. The output of this program is not just a screen dump, but a real plotting of each graphical object on the screen into a PS-file, so it might create a picture with a better resolution than on the screen. The plotting is carried out in a new system of coordinates with the dimensions supplied by the program menu. The plotting mode of the graphical objects remains the same as on the screen.

One feature of the program is that it allows to reduce the output file size of two-dimensional images in case of the printer failure due to lack of memory. The program creates a binned image according to the image quality reduction factor entered with the menu command. The factor value could be any number within 10–100%. The program integrates pixels of the image within each square bin in both directions.

The program displays a menu with the commands listed:

`Output file:` *file* Changes the output PS-file name. As the default name, the program uses the file name of the displayed data (or the file name of the first data file in the list) with the extension changed to `*.ps`.

`Left margin:` *len* Gives an extra space between the left side of the paper and the left vertical axis of the plot and is given in mm. A minimal range of 5–15 mm should be enough to provide space for the title and labels of the Y-axis.

`Top margin:` *len* Gives an extra space between the top side of the paper and the top horizontal axis of the plot and is given in mm. Usually, there are no axis title and labels atop of the graph, so a minimal length of about 5 mm should be sufficient.

`Picture width:` *len* Specifies the length of the horizontal X-axis of the graph in mm. The maximal length depends on the picture orientation on the page.

`Picture height:` *len* Specifies the length of the vertical Y-axis of the graph in mm. The maximal length depends on the picture orientation on the page.

`Orient: portrait/landscape` Changes the picture orientation.

`Quality:` *percent* The command is available only for two-dimensional images and uses a graphical ruler

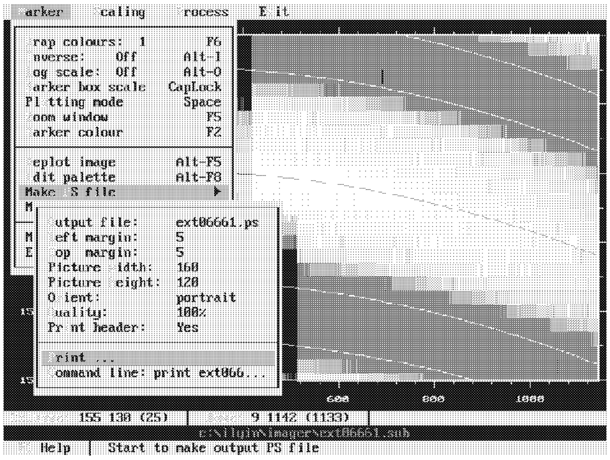

Figure 1.5: The fragment of an image showing an échelle order and its borders is transformed into a PS-file.

to make the selection. Use the `Left/Right` arrow keys to move the scale and to change the output file size as shown in the window.

`Print header: Yes/No` Prints the beginning of the FITS header if the positive answer is chosen. The number of records printed depends on the amount of space left below the picture. The command is disabled if no FITS header is associated with the graph.

`Print` Creates a PS-file with the name specified.

`Command line:` *cmd* Sends the PS-file to a printer by means of a DOS command, like `print` or `lpr`. The command might fail if not enough DOS memory is available, then exit from 3A and print from the DOS prompt.

Once the PS-file is created, it can be easily incorporated into a LaTeX file. For the PS-files used in this manual the parameters are: both margins are 5 mm (to skip Y-axis title), xy-dimension is 150×120 mm, portrait mode and print no header. The following LaTeX script is used together with the DVIPS driver `special` command:

```
\setlength{\unitlength}{1mm}
\begin{figure}
\begin{picture}(0,65)
\put(5,-82){
\special{psfile=file.ps hscale=50 vscale=50}}
\end{picture}
\hspace{5mm}
\parbox[t]{75mm}{
\caption{Caption of the figure}
\label{Label of the figure}}
\end{figure}
```

Note the scaling factor of 50% which makes the actual picture size 65 mm to include the picture itself plus an additional spacing. The second number (-82 mm) specifies the vertical position along the space allocated for the picture and it has to be negative plus an extra space. The horizontal alignement is set to 5 mm from the left border of the text.

The PS-file can be always edited with any text editor in order to remove, say, title or labels of the plot. The dots on a plot can be enlarged, as it was done in Fig. 4.1, p. 36. By using an editor find the line that looks like:

```
/dotsize {5.91} def
```

Dots of 1 mm in diameter are created with the above parameter which specifies the radius in PS-pixel units for a scale factor 100%. The resolution is 300 PS-pixels per inch (25.4 mm)

A line with the name of files printed can be found in the PS-file header.

It is also possible to create a file which can be printed on non-PS printers. The generic HP-PCL language (Hewlett-Packard Printer Command Language) is used. The program window commands are quite similar to those described. The exceptions are: it works only with two-dimensional images, and neither axes, labels nor titles can be plotted.

1.9.2 PS-files of multiple spectra

The facility is very similar to the one described previously except that it allows to make a PS-file of a number of spectra in separate boxes. The boxes can be arranged along columns and rows on the page in specified dimensions. The data are plotted from top to bottom in columns according to the order of appearance in the database. Once the page is filled up, the plot continues on the next page. *Any* number of files can be printed as highlighted in the database; note, that the output goes into a single PS-file.

The title printed atop of each box consists of the file name and the `OBJECT` record of the FITS header. The horizontal axis labels are printed, whilst the vertical ones are omitted. The plot limits are either set individually for each spectrum according to the data range or according to the one or two preset values chosen in the menu.

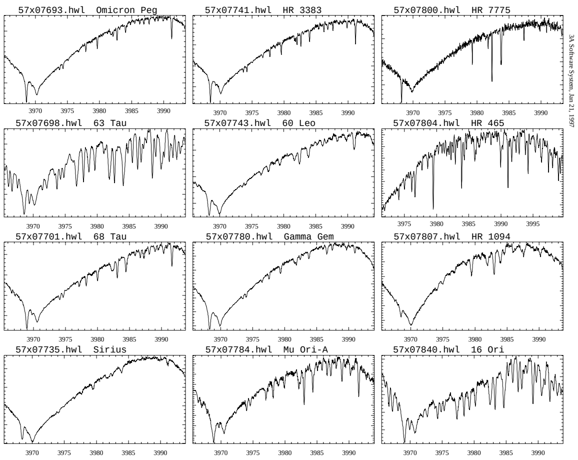

Figure 1.6: Output of the facility to print multiple files.

The program is called from the database of spectra (Sec. ??, p. ??) and it displays a menu with the commands listed:

`Output file:` *file* Changes the output PS-file name.

`Left margin:` *len* Gives an extra space between the left side of the paper and the left vertical axis of the plot and is given in mm. Labels of the vertical axes are not printed by this program, so the margin offset does not affect the figure components.

`Top margin:` *len* Gives an extra space between the top side of the paper and the top horizontal axis of the plot and is given in mm. It is also irrelevant with respect to the picture components.

`Picture width:` *len* Specifies the width of the whole composed picture in mm along the horizontal X-axis. The A4 page width is 210 mm in portrait and 297 mm in landscape modes.

`Picture height:` *len* Specifies the height of the whole composed picture in mm along vertical Y-axis. The A4 page height is 297 mm in portrait and 210 mm in landscape modes.

`Number of columns:` *ncols* Specifies the number of the horizontal boxes. The width of each box is calculated from the total specified width divided by the number of columns and the fixed interbox space.

`Number of rows:` *nrows* Specifies the number of the vertical boxes. The height of each box is calculated from the total specified height divided by the number of rows and the fixed interbox space including the title height.

`Orient: portrait/landscape` Changes the picture orientation.

`Preset X range: Yes/No` Enables to preset the interval of the data argument along the X-axis which then is used for all spectra. If disabled the individual range of arguments is used instead.

`Xmin:` *val* Sets the minimal value of the argument of data.

`Xmax:` *val* Sets the maximal value of the argument of data.

`Preset Y range: Yes/No` Enables to preset the interval of the data intensities along the Y-axis which then is used for all spectra. If disabled the individual range of intensities is used instead.

`Ymin:` *val* Sets the minimal value of the data intensities.

`Ymax:` *val* Sets the maximal value of the data intensities.

`Print` Creates a PS-file with the name specified.

`Command line:` *cmd* Sends the PS-file to a printer by means of a DOS command, like `print` or `lpr`. The command might fail if not enough DOS memory is available, then exit from 3A and print from the DOS prompt.

1.10 Printing of a table

The program is used by a number of applications working with the tables (Sec. 1.2, p. 8) in order to create a plain text file of the table contents. The program opens a menu with a number of commands to specify the printing options:

`Output file:` *name* Specifies the name of the output file where the contents of the table will be printed to. The default extension of the output file is `*.txt`.

`Page length:` *len* Specifies the length of the page for the printing files. The page break control character (`0x0C`) is added after the specified number of lines plus two lines for the table header. No page breaks occur if the parameter is zero.

`Print header: Yes/No` Specifies whether to print the header of the table or not.

`Numbering lines: Yes/No` Specifies whether to enumerate the sequential records of the table or not.

`Print selected records: Yes/No` Specifies whether to print the whole table or just the highlighted records.

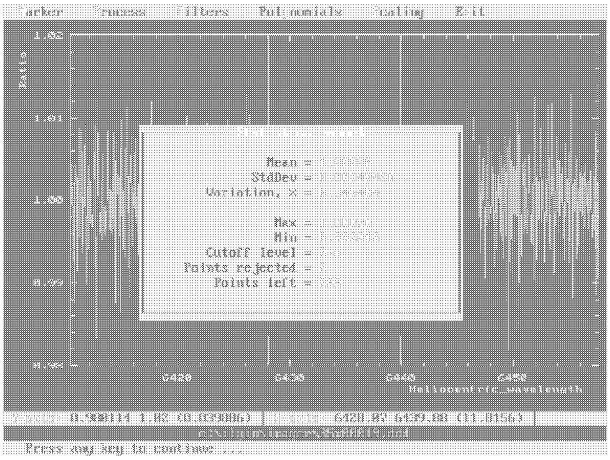

Figure 1.7: Snapshot of the statistical window called from the spectrum program. The marker box is seen as the vertical lines behind the window and indicates the range of data used.

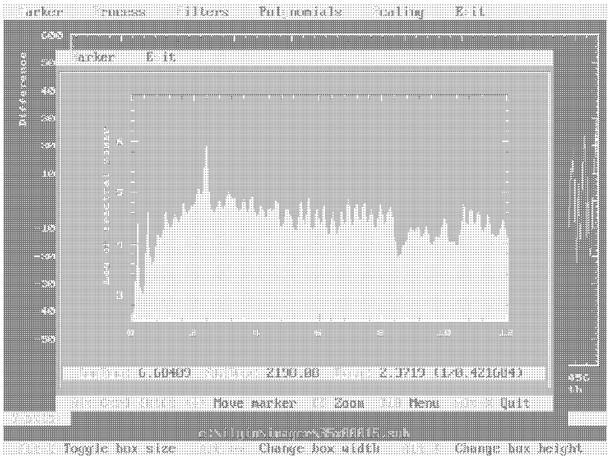

Figure 1.8: The program window of the power spectrum estimation. The peak in the plot corresponds to the periodical optical interference pattern seen in the stellar spectrum.

`Print` Starts to create an output file with the specified name.

`Command line:` *cmd* Specifies the DOS command which can be used to send the output file to a printer.

1.11 The statistical window

This program calculates the statistical parameters of one- or two-dimensional data and is mainly used for the noise estimation. The calculations are carried out within the limits of the graphical marker box and the following parameters are displayed or written into the output file:

- The mean value of the data.
- The standard deviation.
- The relative error in percent.
- The maximal value within the data region.
- The minimal value within the data region.
- The $k\sigma$-clipping input parameter used to reject the most deviating points.
- The number of points rejected after a number of iterations.
- The number of points left after no more points were rejected.

1.12 Power spectrum estimation facility

An alternative to the FFT method is used to make a fast estimation of the power spectrum of the data by the Maximum Entropy Method (Press et al. 1992, p.572). The power spectrum is approximated by a Laurent series in the z-transform domain. The number of series members is specified by the program parameter as the number of poles.

The power spectrum is estimated at each point of the frequency domain:

$$f_i = \frac{i}{n\Delta}, \quad i = 0, 1, 2, \ldots n/2$$

where n is the number of data points and Δ is the sampling interval (dispersion). The standard deviation of the data at a given frequency is estimated as:

$$\sigma = \sqrt{2P(f_i)/n}$$

The power estimate, standard deviation, frequency, and the reciprocal to the frequency, i.e. period, are printed in the message bar at the position of the graphical marker.

The larger the number of poles the higher the resolution of the power spectrum. The usual interval is 10–100. With higher resolution spurious peaks might appear.

The program is working within the menu environment. Commands of the `Marker` menu are:

`Zoom window (F5)` Enlarges the part of the power spectrum within the marker box. Press the key again to return to the original state.

`Marker colour (F2)` Changes the marker colour.

`Plot colour (F3)` Changes the colour of the power spectrum.

`Plotting mode (F4)` Changes the plotting mode of the power spectrum.

`Poles:` *num* `(Alt-W)` Specifies the number of poles, then calculates and displays the new power spectrum.

`Make PS file` Creates a PS-file of the power spectrum.

Use `Alt-X` to exit.

1.13 Histogram facility

The program allows to calculate the histogram of the data and interactively select an interval of the intensities. The histogram is mainly used for:

- The selection of a relevant interval of image intensities to enhance details.
- The separation of cosmic spikes from the normalized image intensities.

The program calculates the histogram within the region of the image specified by the position of the graphical marker box of the calling application. The ideal histogram should be calculated within a given intensity interval divided by the minimal nonzero difference of data values. In order to fit to the computer memory a much larger bin size is used, so that the maximal number of bins is 1000. Only every 3rd pixel in the region is used to find the min and max limits of data values, then the histogram calculation follows. The histogram counts the number of points falling into a separate bin of intensities.

In order to enhance the histogram resolution, the program uses the cutoff parameters supplied by the calling application. The parameters specify how many of the most deviating points should be rejected from both ends of the histogram and are given in percent of the total amount of points in the region. The program does a number of passes, i.e. rejecting and calculating with new limits of data, to achieve the amount of points rejected. The histogram is stored into a separate co-named binary file with the extension `*.hst`.

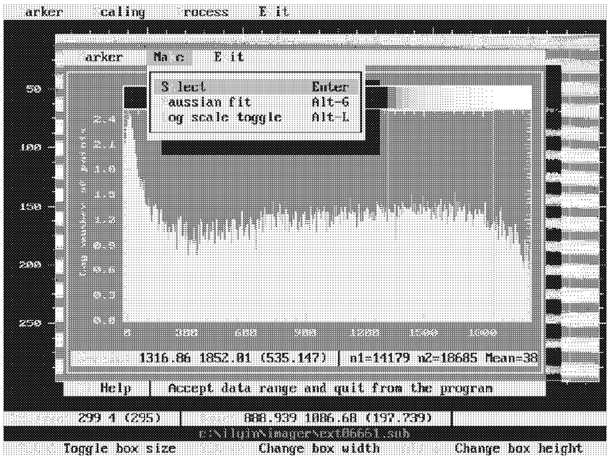

Figure 1.9: The histogram of a part of the image is displayed in the log scale of frequencies. The interval of image intensities chosen is used for the colour lookup table.

The plot of the calculated histogram follows. The horizontal bar atop of the graphical window shows how the interval of data is divided into the colours. Use the graphical marker (Sec. 1.4, p. 9) to select the relevant interval of the data values. If the limits chosen are accepted, the program updates the FITS file header, i.e. the `DATAMIN` and `DATAMAX` records are modified.

The program works within the menu environment. The following are the `Marker` menu commands:

`Wrap colours:` *num* `(F6)` Wraps the colour palette around the data limits as much as specified by the parameter. As an alternative, use the `Grey`± keys to increase or decrease the parameter. Changing the parameter causes an image replotting by the calling application on exit from the program.

`Log scale: On/Off (Alt-O)` Changes between linear and log (equal step size in the log domain) scales of the lookup table which causes a subsequent image replotting by the calling application on exit from the program.

`Zoom window (F5)` Enlarges the part of the histogram within the marker box. Press the key again to return to the original state.

`Marker colour (F2)` Changes the marker colour.

`Function colour (F3)` Changes the plotting colour of the histogram.

`Plotting mode (F4)` Changes the plotting mode of the histogram.

`Replot histogram (Alt-F5)` Replots the graph.

`Edit palette (Alt-F8)` Changes the palette colours by using the palette editor (Sec. 1.8, p. 12).

`Make PS file` Creates a PS-file of the histogram.

The next `Make` menu consists of the commands which make the histogram applicable.

`Select (Enter)` Accepts the data limits chosen with the marker box and exits from the program.

`Gaussian fit (Alt-G)` Approximates the histogram by a Gaussian curve (Sec. A.3, p. 54), and is useful for statistical estimations. The central position, maximal value, and the standard deviation ($\sigma/\sqrt{2}$) are displayed in the message bar of the graph.

`Log scale toggle (Alt-L)` Displays the histogram in the log scale, so the frequency scale (number of data points or Y-axis) can be seen in detail.

Use `Alt-X` if it makes no sense to change the data limits. There will be no action by the calling application.

1.14 Manual editing of data

The value of each pixel can be changed manually by using the data editor. The program displays a table with the number of columns and rows specified by the calling program (in the one-dimensional case the only column of the table is displayed). The number of columns is restricted by the width of the graphical screen and cannot be longer than 6. The values of the pixels are displayed in the real scale. The pixels are displayed as they are allocated in memory, i.e. the same as they are seen on the screen. The initial contents of the table corresponds to the upper left corner of the marker box. The table bar allows to select individual pixels and browse the table along image columns and rows, so the pixels beyond the initial position can be seen.

The message bar displays the position of the table bar:

- For two-dimensional images, the index number for both axes as `Col/Row`, the column and row in the physical system of coordinates as `X/Y`.
- For one-dimensional vectors, the index and the X-coordinate in physical units.

A pixel selected by the table bar can be edited with the dialogue box (Sec. 1.3, p. 8) activated by pressing `Enter`.

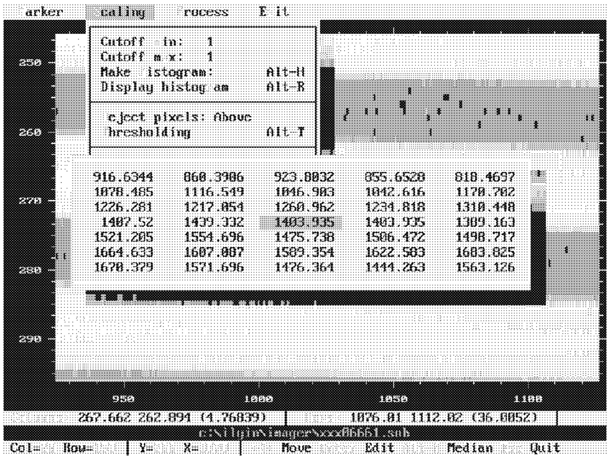

Figure 1.10: An example of the data editing window with a size of 5×7 pixels. The median value for the central pixels is calculated.

The editor works directly with the data allocated in the memory. To accept changes press `Enter` again or `Esc` to discard.

The editor can also calculate the median of the data displayed in the table. The command `Alt-M` replaces the central pixel of the table by the median and invokes the dialogue box to confirm the modification.

Use `Esc` to close the table and exit from the program.

1.15 Editor for the FITS header

This program allows to edit the FITS header of a single file. The program window contains a table with the contents of the header printed in each record (see Fig. 1.1, p. 7). The last record with the `END` FITS keyword is not printed. The table bar (Sec. 1.2, p. 8) allows to select a record and open a dialogue box (Sec. 1.3, p. 8) to edit the record components separately. The message bar displays the position of the table bar and the type of the record selected.

A number of `Edit` menu commands provide the following operations:

`Edit (F4)` Edits the record selected. Only the parameter field and comment can be modified.

`New (F5)` Creates a new record. The currently selected record is used as a template for the new one. Any field of the FITS record can be changed: the keyword, type of the record, field of the parameter, and comment. Use the `Right/Left` arrow keys and then press `Enter` to select the record type from the appearing subwindow.

`Delete (Alt-Del)` Deletes the record selected. Never delete records which are needed to open the FITS file: `SIMPLE, BITPIX, NAXIS`.

`Save (F2)` Writes the modified FITS header into the file.

`Print` Creates a plain text file from the header.

Use `Alt-X` to close the table and exit from the program. In case the header has been modified and was not saved yet with the `Save` command, a warning message appears and asks for confirmation to save the new header. Press `Enter` to save or `Esc` to keep the original (unchanged) header.

1.16 List of regions to extract

This program stores the position of different rectangular regions of the image, the associated operation, and the template of the output image file name. These parameters are stored in the table and can then be used for subsequent group operations with the images. These operations are performed by separate commands.

Coordinates of the region are given in the system of coordinates of the original image, and the graphical marker box is used to specify its position and dimension. Graphical coordinates of the marker are transformed into the physical ones with possible roundoff errors equal to the marker step size on the graphical display, which might produce an uncertainty up to a few pixels of the image. The effect can be reduced with the enlargement (zoom) of the region of the image.

The region extracted from the image can be stored into a separate file. A special template is used to construct the output file name from the name of the original image. The following table summarizes possible combinations:

	Source	Template	Destination
1.	`name.ext`	`*.*`	`name.ext`
2.	`name.ext`	`*.dat`	`name.dat`
3.	`ccd123.fit`	`ext00000.*`	`ext00123.fit`
4.	`ccd00123.fit`	`ext.dat`	`ext123.dat`

And here are some comments:

1. The output file name is the same as the original one. The output file will substitute (overwrite) the original file. Do not use this template unless it is absolutely necessary.
2. The wildcard (`*`) in the template names means that the name of the source file is used as the name of the output file. The template extension is the output file extension.
3. The wildcard (`*`) in the template extension means that the extension of the source file is used for the output file. The prefix in the template name is used as the prefix in the output file. A sequential number for the output file is taken from the source and formed with the template zero padding format.
4. The output file prefix and extension are taken from the template. A sequential number is appended to the prefix as no zero padding format is specified.

Each of the table records consists of the following fields:

`Name` Name of the region. Used to separate one region from another.

`Template` Specifies the template file name used for the construction of the output file names.

`Extract` The operation associated with the region can be selected from the window which lists the following commands:

- `sumcols` Create a summed column of the image, i.e. the horizontal cross-cut with the pixels co-added within each row (along the vertical).
- `avrcols` Create a mean column of the image, i.e. the horizontal cross-cut with the pixels averaged within each row (along the vertical).
- `sumrows` Create a summed row of the image, i.e. the vertical cross-cut with the pixels co-added within each column (along the horizontal).
- `avrrows` Create a mean row of the image, i.e. the vertical cross-cut with the pixels averaged within each column (along the horizontal).
- `subimage` Create a subset of the image. The coordinates of the resulting image are absolute and correspond to those of the original one.

`Left/Right/Top/Bottom` These fields are the coordinates of the rectangular region in the system of coordinates of the original image. The coordinates are taken from the graphical marker position, but can still be edited. The last two fields are irrelevant for a one-dimensional image.

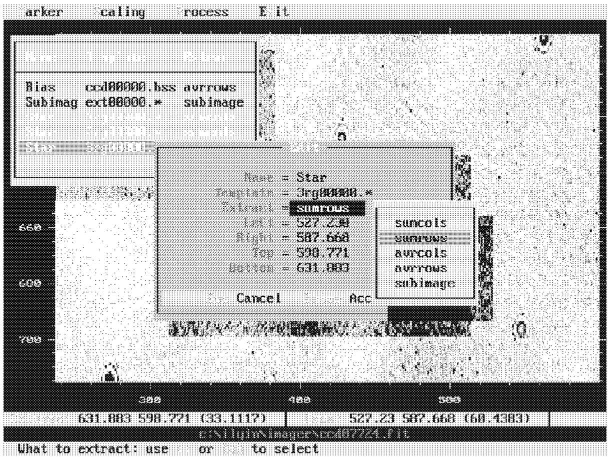

Figure 1.11: Coordinates of different regions of the image and associated operations can be stored in the list shown.

A number of keys are used to operate with the table and these are seen in the status bar at the bottom of the screen.

`F5` Create a new record. A dialogue box with the `New` title appears. The currently selected record is used as a template for the new one. The current coordinates of the graphical marker are used as the coordinates of the new region. Press `Enter` to close the dialogue box. The record created becomes highlighted.

`F4` Edit the record selected. A dialogue box with the `Edit` title appears. The coordinates of the region in the table are replaced with the current coordinates of the graphical marker. Press `Enter` to close the dialogue box. The record edited becomes highlighted.

`Ins` Marks or highlights the record.

`Del` Deletes the record selected.

`Alt` Press and hold the key, so the program window becomes hidden. Then, use the `Up/Down` arrow keys to browse the hidden table and to display the position of each region. Release the `Alt` key to let the window reappears.

`Esc` Quits the program with no action.

`Enter` Selects the record, places the graphical marker into the region, and exits from the program.

Chapter 2

The imager program

The imager program is used to display two-dimensional FITS images on the graphical screen, and perform various image processing commands in the interactive mode. The images to be displayed can be selected from the database of images.

For convenience, the CCD images are displayed so that the spectra in the image are horizontal. The spectra registered with a spectrograph are usually projected on to the CCD along the direction of the parallel transfer (which is the longest side of the CCD) in order to achieve a larger wavelength range. The image is displayed in the same way as the CCD is read out:

- The *vertical* axis is across the CCD columns and is in the direction of the serial transfer. The axis parameters refer to the FITS keywords `CRVAL1`, `CDELT1`, and `CRPIX1`.

- The *horizontal* axis is across the CCD rows and is in the direction of the parallel transfer. The axis parameters refer to the FITS keywords `CRVAL2`, `CDELT2`, and `CRPIX2`.

Note: hereafter a horizontal line is referred to as a column, and a vertical one as a row.

Once the image is displayed, the graphical marker is activated and can be controlled as described (Sec. 1.4, p. 9). The message bar of the program seen at the bottom of the screen is used to display the position and size of the graphical marker box.

The program is controlled by the menu environment and the main menu consists of the following items described in detail in the subsequent sections:

`Marker (Alt-M)` A number of commands to control the graphical marker box, and to make a hardcopy of the image.

`Scaling (Alt-S)` The menu command allows to change the interval of intensities of the image to display, create the mask image of the cosmic spikes, and edit the image pixels.

`Process (Alt-P)` A number of commands to operate with the image, including find spectral orders in the échelle image.

`Exit (Alt-X)` Exit from the program. When exiting, the program may ask for the confirmation to save a modified image after, say, trimming the spikes, geometrical transformations and so on. A message window appears on the screen offering two options: use the `Enter` key to save the modified image, or `Esc` to exit without saving any changes made with the program.

2.1 Marker menu commands

`Wrap colours:` *num* `(F6)` The selected interval of the image intensities is divided by the specified parameter, and then each subinterval is divided into the palette colours. The wrapping parameter can be changed stepwise with `Grey`±. Plot of the new image follows.

`Inverse: Yes/No (Alt-I)` Plots the image in the normal or inverse scale with the palette colour table swapped.

`Log scale: Yes/No (Alt-O)` Plots the image in linear or decadic log scale.

`Marker box scale (CapsLock)` This command is used to switch between two scale units to display the graphical marker box *position*: the actual data units (physical system of coordinates) and the index scale (pixel numbers).

`Plotting mode (F4)` Changes the plotting mode of the image pixels between two options: adjacent filled boxes, and isolated dots.

`Zoom window (F5)` Enlarges the part of the image within the marker box. Press the key again to return to the original state.

`Marker colour (F2)` Changes the colour of the marker box. Use `F2` to increase and `Ctrl-F2` to decrease the colour index.

`Replot graph (Alt-F5)` Plots the image and the attached graphical functions again.

`Edit palette (Alt-F8)` Calls the palette editor, described in Sec. 1.8, p. 12. The palette with the specified file name will be used subsequently by the program.

`Make PS file` Creates a PS-file of the image (Sec. 1.9.1, p. 13).

`Make PCL file` Creates a PCL-file of the image (Sec. 1.9.1, p. 13).

`Memory usage` Displays information about the available memory resources.

`EMS handles` Displays a table with information about the data allocated in the expanded memory (Sec. 1.7, p. 11).

2.2 Scaling menu commands

`Cutoff min:` $p1$ Specifies the amount of minimal points which will be eliminated from the histogram. The parameter is set in percent with respect to the total amount of points in the data window.

`Cutoff max:` $p2$ Specifies the amount of maximal points which will be eliminated from the histogram. The parameter is set in percent with respect to the total amount of points in the data window.

`Make histogram (Alt-H)` Calculates and displays the histogram (Sec. 1.13, p. 17) of the image area within the graphical marker box.

`Display histogram (Alt-R)` Displays the histogram calculated earlier.

`Reject pixels: Below/Above+Below/Above` Switches between three options to specify the thresholding mode.

`Thresholding (Alt-T)` Starts the thresholding facility which is used to detect pixels which are above or/and below the selected interval of intensities. The interval of intensities can be selected with the histogram facility. The output mask image $mask_i$ is calculated according to the options chosen with the previous command:

$$mask_i = \begin{cases} 1, \begin{cases} y_i > I_{\max} & \texttt{Above}\text{ option} \\ y_i < I_{\min} & \texttt{Below}\text{ option} \\ y_i < I_{\min} \text{ or} & \\ y_i > I_{\max} & \texttt{Above} + \texttt{Below}\text{ option} \end{cases} \\ 0, \quad \text{otherwise} \end{cases}$$

where y_i is the original image, and $I_{\min}, I_{\max}$ is the selected interval.

The output image is the co-named file with the extension `*.cr`. Once the image is created it is appended to the database of images and displayed on the screen. Exit from the second copy of the imager program with `Alt-X` to return to the original image.

`Patch:` *val* `(Alt-A)` Replaces pixels of the image area within the graphical marker box with the value specified by the parameter.

`Edit image data` Opens a submenu to setup the parameters of the manual editing of data (Sec. 1.14, p. 18).

- `Width of window:` w Specifies the width of the edit data window.
- `Height of window:` h Specifies the height of the edit data window.
- `Edit data (Alt-D)` Runs the program to edit the image pixels intensities manually, or to replace them with the median of the data window with the specified size. The upper left corner of the edit window corresponds to the upper left corner of the graphical marker box.

2.3 Process menu commands

`Summed/Averaged spectrum (Enter)` Creates and displays a "spectrum" (image column) or horizontal cross-section of the image by using the area within the graphical marker box. When the process menu window is displayed, the command opens a submenu which allows to choose between two options:

- `Horizontally averaged cross-cut` Creates a mean column of the image averaged over the rows.

`Horizontally summed cross-cut` Creates a summed column of the image with the pixels co-added in each row.

No dialogue follows if the spectrum is displayed by using the hotkey. In this case the previously selected option is used. Once the spectrum is created, the FITS file is added to the database of spectra and the spectrum program is invoked to display the result (Sec. 3, p. 27). The default template for the output file name is `col00000.*` (cf. Sec. 1.5, p. 9, or Sec. 1.16, p. 19), so it inherits the original image sequential number and its extension. The file prefix denotes that the axis of the spectrum is that of the image columns.

`Summed/Averaged profile (Ctrl-Enter)` Creates and displays a "profile" (image row) or vertical cross-section of the image by using the area within the graphical marker box. When the process menu window is displayed, the command opens a submenu which allows to choose between two options:

`Vertically averaged cross-cut` Creates a mean row of the image averaged over all columns.

`Vertically summed cross-cut` Creates a summed row of the image with the pixels co-added in each column.

No dialogue follows if the profile is displayed by using the hotkey. In this case the previously selected option is used. Once the profile is created, the FITS file is added to the database of spectra and the spectrum program is called to display the result (Sec. 3, p. 27). The default template for the output file name is `row00000.*` (cf. Sec. 1.5, p. 9, or Sec. 1.16, p. 19), so it inherits the original image sequential number and its extension. The file prefix denotes that the axis of the profile is that of the image rows.

`Subtract bias` The command allows to subtract the CCD overscan bias strip interactively. At first, the appropriate *averaged* column or row must be created and smoothed with a filter by the spectrum program (Sec. 3, p. 27). The command opens the file pickup facility window (Sec. 1.6, p. 10) which displays the vectors with the same sequential image number as the original one. The file selected from the table with `Enter` is used for the subtraction. The file prefix defines the subtraction mode:

`col` The horizontal column (CCD overscan by columns) is subtracted from the image column by column. The output image extension is `*.col`.

`row` The vertical row (CCD overscan by rows) is subtracted from the image row by row. The output image extension is `*.row`.

The dimension of the resulting image is defined by the length of the column or row subtracted. The output image, which has the same name as the original one and the extension as specified, is added to the database of images, and displayed instead of the original image.

`Subset of image` The command allows to extract the subset of the image within the graphical marker box in the interactive mode. The default template of the output file name is `ext00000.*`, so it inherits the sequential image number and the extension. If the original and the resulting images have the same name, then a warning message window appears which can be used to change the name, but it is possible to overwrite the original image as well. Once the subset is extracted it is added to the database of images, but the resulting image is not displayed on the screen.

`List of regions (Alt-L)` Opens a window with a table where the positions of different regions of the image can be stored (Sec. 1.16, p. 19). Use `Esc` to close the window.

`Extract regions (F8)` The command is used to extract several regions of the image at once and save them with different names, as specified with the previous command. Only the highlighted records of the table are used for this operation.

`Transformation` Opens a submenu to select a geometrical transformation of the image:

`Flip vertically` Turns the image upside down in the vertical direction around the horizontal central column.

`Flip horizontally` Turns the image in the horizontal direction around the vertical central row.

`Turn clockwise` Turns the image by 90° clockwise.

`Turn anticlockwise` Turns the image by 90° anticlockwise.

Once the operation is finished, the transformed image is displayed on the screen. The axes of the image are also transformed according to the option selected, which changes the $\mathtt{CRVAL}_i$ and $\mathtt{CDELT}_i$, $i = 1, 2$ FITS keywords. When exiting, the program asks for the confirmation to save the transformed image. The resulting image overwrites the original one.

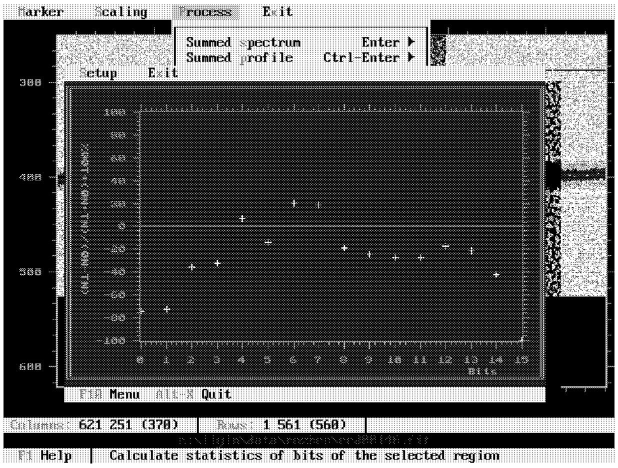

Figure 2.1: The snapshot of the program screen shows the statistics of bits taken for the whole image seen in the background. The deficit of the binary units indicates a problem with the CCD analogue-to-digital converter.

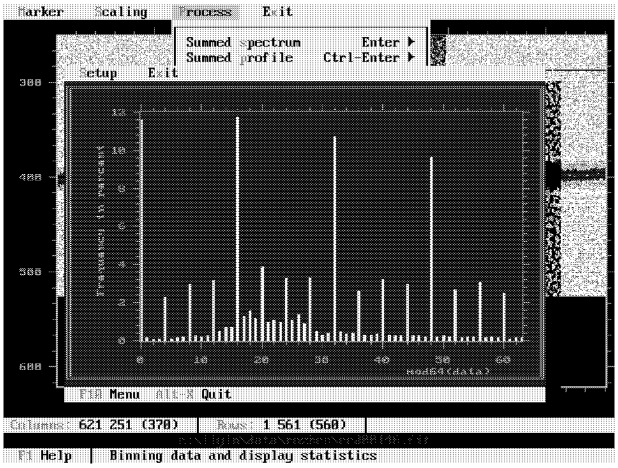

Figure 2.2: The snapshot of the program screen shows the frequency of the pixel remainders taken as modulo 64 and calculated for the whole image. The periodicity occurs at every 4th and 16th bins and indicates a problem with the CCD analogue-to-digital converter.

`Stat:` k `(Alt-Enter)` Calculates the statistical parameters of the selected region of the image within the graphical marker box and displays the report window (Sec. 1.11, p. 16). The value specified is the $k\sigma$-clipping parameter to eliminate the most deviating points.

`Bits stat` The facility is used to check the digitization error in an *integer* image, i.e. the analogue-to-digital converter error of the CCD controller. The program calculates the sums of zero and one bits in the two-byte word for every pixel within the image area bounded by the graphical marker box, and then displays the ratio for each bit:

$$f = \frac{N_1 - N_0}{N_1 + N_0}$$

If the CCD converter works properly then there should be no excess in the lower bits (i.e. $f \approx 0$).

The facility is controlled by the menu environment. The statistics can be exported into a plain text file with the name specified in the `Setup` menu command. Exit from the program with `Alt-X`.

`Bins stat:` *bin* This is the second facility to check the digitization error in an *integer* image. The program calculates the remainders $\mathrm{mod}_{bin}(p_i)$ of each pixel p_i within the image area inside of the graphical marker box with the parameter *bin* set to a power of two (2, 4, 8, 16, ...). Then the program opens a window with the plot of the relative frequency against the remainders. If the CCD converter works properly, the distribution of the frequencies should be uniform.

The facility is controlled by the menu environment. The statistics can be exported into a plain text file with the name specified in the `Setup` menu command. Exit from the program with `Alt-X`.

`Find orders:` *len* `(Alt-F7)` Detects the échelle spectral orders allocated along CCD columns of the image. The parameter specified is the binning factor across the CCD rows which is used as the step size to estimate the orders central position. Once the orders are detected, the program displays the curves which are following the central part of each order.

`Display orders (F7)` Enables or disables the plot of the spectral order curves.

`Average orders:` *num* Calculates the widths of each spectral order. The parameter specified is the échelle spectral order number of the uppermost order detected. The proper spectral order numbers are used later for the two-dimensional dispersion curve. After the orders are processed, the plot of the spectral order boundaries follows. The program creates FITS files on the output where the averaged cross-profile for each order is stored. The files are appended to the database of spectra and the default template of the name is `00w00000.dat`. The first two digits are used for the order number and the last for the sequential image number.

`Extract orders` Extracts the curved spectral orders, writes them into separate FITS files, and appends them to the database of spectra. The default template for the spectral orders is `00x00000.dat`, where the first two digits are used for the spectral order number and the last for the sequential image number.

Chapter 3

The spectrum program

The spectrum program is used to display and process one-dimensional FITS files interactively. One or several files can be picked up from the database of spectra and displayed on the same screen. Once the files are displayed, the graphical marker is activated and can be controlled as described earlier (Sec. 1.4, p. 9).

The program is controlled by the menu environment, which consists of the following items described in detail in the subsequent sections:

`Marker (Alt-M)` A number of commands related to the operational modes of the graphical marker, and to make a hardcopy of the plot.

`Process (Alt-P)` A number of commands including edit of the data pixels, calculation of statistical parameters and the power spectrum.

`Filters (Alt-F)` A number of digital filters can be used to process the spectrum and evaluate the result.

`Fit (Alt-I)` The menu offers some commands to make an approximation of the spectra by a polynomial, a smoothing spline, or a sine function.

`Scaling (Alt-S)` The scaling menu commands are used to enhance the graphical representation of the displayed spectra.

`Exit (Alt-X)` Exit from the spectrum program. When exiting, the program may ask for the confirmation to save data which were modified after, say, trimming of spikes, flipping and so on. A message window appears on the screen offering two options: use the `Enter` key to save the modified data, or `Esc` to exit without saving any changes.

3.1 Marker menu commands

`Zoom window (F5)` Enlarges the data area within the marker box. Press the key again to return to the original state.

`Marker box scale (CapsLock)` This command is used to switch between two scale units to display the graphical marker box position on the horizontal axis: the actual data units (physical system of coordinates) and the pixel (index) scale.

`Marker colour (F2)` Changes the colour of the marker box. Use `F2` to increase and `Ctrl-F2` to decrease the colour index.

`Plot colour (F3)` Changes the colour of the first plotted function. Use `F3` to increase and `Ctrl-F3` to decrease the colour index.

`Plotting mode (F4)` Changes the plotting mode of the first plotted function between six options: lines connecting the pixels, isolated dots, white dots with connecting lines, crosses, sticks, and histogram. Use `F4` to increase and `Ctrl-F4` to decrease the plotting mode.

`Shuffler (Alt-Q)` Exchanges the order (enumeration index) of the displayed spectra, so the second file goes to the first position in the list of the graphical functions and the first becomes the last. After each such action the file name of the first in the list is printed in the file name message bar. The command is used to change the first spectrum which might be used as the reference spectrum in some processes.

`Replot graph (Alt-F5)` Plots graphical functions and axes again.

`Edit palette (Alt-F8)` Calls the palette editor, described earlier (Sec. 1.8, p. 12). The palette with the specified file name will be used subsequently by the program.

`Make PS file` Creates a PS-file of the graph (Sec. 1.9.1, p. 13).

`Memory usage` Displays information about the available memory resources.

`EMS handles` Displays a table with information about the data allocated in the expanded memory (Sec. 1.7, p. 11).

3.2 Process menu commands

`Statistics:` k `(Alt-Enter)` Calculates the statistical parameters (Sec. 1.11, p. 16) of the first spectrum within the interval bounded by the marker box. The value specified is the $k\sigma$-clipping parameter to eliminate the most deviating points of data.

`Power spectrum:` *poles* `(Alt-W)` Calculates and displays the power spectrum estimation of the first function. All data points are used in the calculation regardless of the marker box size. The specified parameter *poles* is the number of poles used for the estimation (Sec. 1.12, p. 16). The period selected in the power spectrum program is stored for a subsequent fit of the data to a sine function (Sec. 3.4, p. 30).

`Histogram (Alt-H)` Calculates and displays the histogram of the first spectrum within the interval bounded by the marker box (Sec. 1.13, p. 17).

`Trim spikes (Ctrl-Enter)` Removes spikes interactively or unwanted features from the first displayed spectrum. Put the marker so that the points of data to be removed are *inside* the box. Once `Ctrl-Enter` is pressed, the points are replaced by the linear interpolation of the pixels adjacent to the marker box. On exit, the program asks for the final confirmation whether to save the modified data or not.

`Edit data:` *num* `(Alt-F4)` Calls the data editor (Sec. 1.14, p. 18) with the window length as specified by the parameter to change the pixel values of the first displayed spectrum. The uppermost number in the editor window corresponds to the left side of the marker box.

`Patch:` *val* `(Alt-A)` Substitutes all data points in the first spectrum within the marker box by the constant value specified by the parameter.

`Fixed regions list (Alt-L)` Calls the program to store coordinates of the graphical marker box (Sec. 1.16, p. 19).

`Extract regions (F8)` Extracts subsets of the displayed spectra into separate FITS files and appends them to the database of spectra. The subset positions and file name templates are defined in the list of regions (Sec. 1.16, p. 19). Only marked (highlighted) regions of the list are used for the extraction.

`Extract subset (Ctrl-F8)` Extracts subsets of the displayed spectra within the graphical marker box, writes them into separate FITS files, and appends them to the database of spectra. The default template `cut00000.*` is used to create the output file name. The command is a more simple version of the previous command (`F8`).

`Flipping` Flips the displayed spectra around the vertical central line. The axis is reversed which means in terms of the FITS header (for `CRPIX1=1`):

$$\begin{aligned} \texttt{CRVAL1}_{\text{new}} &= \texttt{CRVAL1} + (\texttt{NAXIS1} - 1) \times \texttt{CDELT1} \\ \texttt{CDELT1}_{\text{new}} &= -\texttt{CDELT1} \end{aligned}$$

`Signal/Noise ratio` Estimates the signal to noise ratio of the displayed spectra. A suitable region of the continuum within the marker box is used for the mean level estimation in *ADU*s for each spectrum separately. The CCD gain factor (e^-/ADU) should be set in the `GAIN` record (Sec. 5.6.1, p. 46) of the FITS header of the files processed. In case it is not, use the modify FITS record command (Sec. ??, p. ??) to set or modify the parameter field. If the field is not found yet, the program exits from the application. The signal-to-noise ratio is calculated as

$$\texttt{SNR} = \sqrt{\texttt{ADU} \times \texttt{GAIN}}$$

and written into the `SNR` record of the FITS header.

`Add noise` Adds normally distributed random noise to the displayed spectra. The result is written into a separate file, co-named with the original and with the extension `*.ns`, added to the database of spectra, and displayed on the screen. Use the find data range (`Alt-R`) command (Sec. 3.3, p. 29) to adjust the plots to the data window.

The program assumes that the amplitude of data is in photoelectrons c_i, so the random noise value n_i added is

$$n_i = r\sqrt{c_i}$$

where r is the normally distributed deviate with $\bar{r} = 0$ and $\sigma_r^2 = 1$ (Press et al. 1992, p.289).

3.3 Scaling menu commands

`Data max:` *max* `(Alt-2)` Determines the maximal value of the data displayed and writes it into the `DATAMAX` record of the FITS header.

`Data min:` *min* `(Alt-1)` Determines the minimal value of the data displayed and writes it into the `DATAMIN` record of the FITS header.

`Find range (Alt-R)` Finds the data amplitude of the spectra displayed within the interval of the marker box and re-displays the graph using these limits. The command is useful, when the zoom is not applicable (e.g. due to limited graphical resolution in case of large dynamic range of the displayed data), or to enhance the area of interest quickly. In order to return to the original state, expand the width of the marker box to its maximum and repeat the command again.

`Offset:` c_0 `(Ctrl-F7)` Displays the spectra separated from each other in the intensity scale by a fixed step. The displacement value is specified by the parameter. The first spectrum remains unshifted.

`Scale:` c_1 `(Alt-F7)` Displays the spectra, such that the intensities of each next spectrum, except the first, are multiplied by the same scale factor specified by the parameter.

The displacement and scale factor do not change anything in the data and do not affect any calculations; they are used only for display purposes. Both parameters may be used at the same time, so that the displayed data, except the first spectrum, are transformed according to the equation:

$$Y_i = c_0 k + c_1 y_i$$

where y_i are the points of data of the spectrum with the sequential number $k = 1, 2, \ldots$ The output of the filtering or approximation processes also cannot be offset and/or scaled, unless it is loaded as a separate file.

3.4 Fit menu commands

`Mark/unmark zones (Grey±)` Marks an interval of data within the graphical marker box. Use the plus key to include points and the minus key to exclude points from a previously selected interval. Only the first spectrum among several displayed can be used for zone selection. On exit from the program, the zones are explicitly overwritten into the file co-named with the original and the extension `*.zon`. *Hint:* To see the pixels highlighted, change the plotting mode.

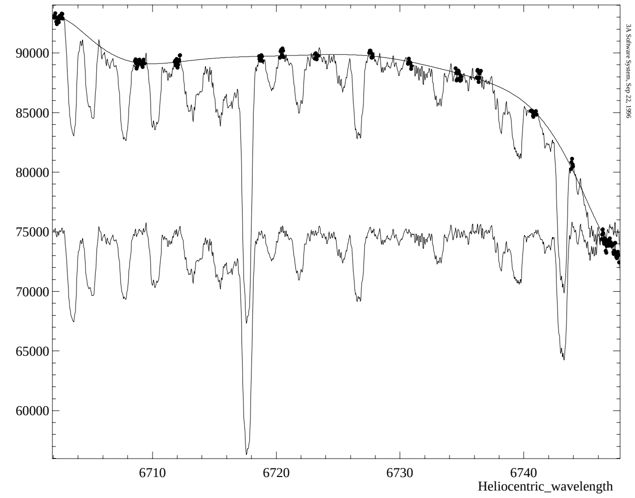

Figure 3.1: A curved spectrum was normalized by a polynomial of 9th degree which uses only the points of data marked within zones (dots on the plot). A scaling factor of 75000 was introduced to see the normalized spectrum in a similar scale as the original one.

`Read file zones (F6)` Opens the file pickup window (Sec. 1.6, p. 10) to display the files of zones saved earlier. Select a file and press `Enter`.

`Close all zones` Closes the zones currently selected in the spectrum and redisplays the graph. No file of zones is generated. Use the command to undo the current selection: the file of zones saved earlier will be preserved.

`Take ratio: Yes/No` Tells the program to take the ratio of the original data and its approximation. The ratio is written into a separate co-named file with extension `*.nor` and displayed on the same screen. Introducing a scale factor allows to see the ratio in detail, i.e. it could be displayed in a similar scale as the original data (Fig. 3.1, p. 29).

The ratio cannot be written into the same file, i.e. when the original file has already the `*.nor` extension. The file name for the result should be renamed in the dialogue box. If there are many files, a more simple solution is to change the extension of all the files with the rename command (Sec. ??, p. ??).

`Fit polynomial:` *deg* `(Alt-O)` Approximates the points of data marked within the zones by a polynomial (Sec. A.5, p. 55) of the specified degree and displays the curve.

`Fit spline:` *fac* `(Alt-D)` Approximates the points of data marked within the zones by a smoothing spline (Sec. A.6, p. 58) and displays the curve. The smoothing factor specified has the following meaning: zero results in an interpolating spline; the larger the value, the more smooth the curve.

The curve in both commands is saved into a separate file with the same name as of the original and with extension `*.pol`. The output file is sampled with the same step size as the original. The operation is performed for *all* files displayed using the same interval of zones selected in the first spectrum. The original files, as well as the resulting polynomials, and, optionally, the ratios are allocated in the expanded memory as separate entries. The maximal number of entries open at the same time is controlled by the expanded memory driver (Sec. 1.7, p. 11).

`Fit sine:` *period* `(Alt-K)` Fits a sine function with the specified period to the first spectrum (Sec. A.4, p. 55) and displays the result. The period can be obtained from the power spectrum estimation (Sec. 3.2, p. 28 and Sec. 1.12, p. 16). The result is saved into a separate file, co-named with the original, and with the extension `*.sin`. The result is sampled with the step size of the original spectrum.

`Cross-correlation (F10)` Calls the cross-correlation facility to align or to find the offsets of spectral features. The features should be marked as zones of data, see Sec. 3.4, p. 29. The facility is described in detail in Sec. 4, p. 35.

`Fit to template` Opens a submenu with the commands to setup the facility which allows to scale and transform each displayed spectrum to the first, or template, spectrum (Sec. 3.4.1, p. 30).

3.4.1 Fit spectrum to template spectrum

The program allows to find the scale factor and the offset in intensities between the reference and source (programme) spectrum. A polynomial of the specified degree n is used to fit the intensities of the selected regions of spectra:

$$I_{\rm ref} = c_0 + c_1 I_{\rm src} + c_2 I_{\rm src}^2 + \ldots + c_n I_{\rm src}^n$$

here $I_{\rm ref}$ is the intensity of the template spectrum within the intervals marked as the zones, and $I_{\rm src}$ is the intensity of the corresponding rebinned points of the programme spectrum.

The routine can also be used to estimate the *veiling* parameter which describes the reduction of the contrast

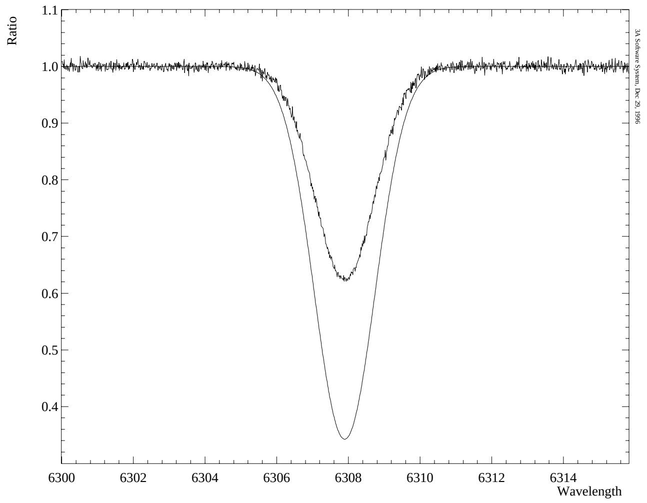

Figure 3.2: Two synthetic profiles are shown. The upper one was made from the other by adding an extra emission and the photon noise. The veiling factor 0.75 was recovered by fitting the profile to the bottom, template spectrum.

in spectral lines due to presence of some amount of extra light (like, scattered light in the spectrograph (Gray 1974), or an external continuum emission added to the spectral lines (Basri & Batalha 1990)). The parameter s is defined as:

$$s = \frac{I_{\rm ref} - I_{\rm src}}{I_{\rm src} - 1} \quad \text{or} \quad I_{\rm src} = \frac{I_{\rm ref} + s}{1 + s}$$

and it is assumed here that the spectra are normalized to their respective continua. From the latter, it can be calculated as

$$s = c_1 - 1 = -\frac{c_0}{c_0 + c_1}$$

The parameter is meaningful only if a polynomial of the first degree is used.

`Degree:` *deg* Specifies the degree of the polynomial used to fit the spectra.

`Modify data: Yes/No` Choose whether to do the polynomial transformation of the programme spectra or not. In case of a positive answer the spectra are transformed and displayed to show the quality of the fit. On exit from the spectrum program a message window appears to confirm whether to save the modified spectra or not.

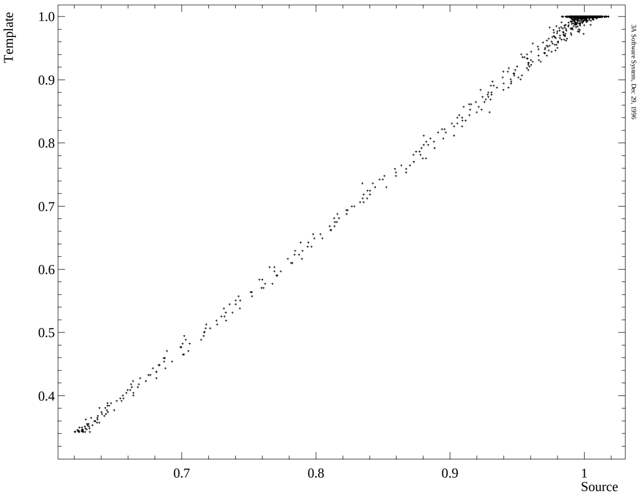

Figure 3.3: Intensities of the programme spectrum are ploted against the intensities of the template spectrum for each pixel. A straight line fitted to the points is used to derive the veiling factor.

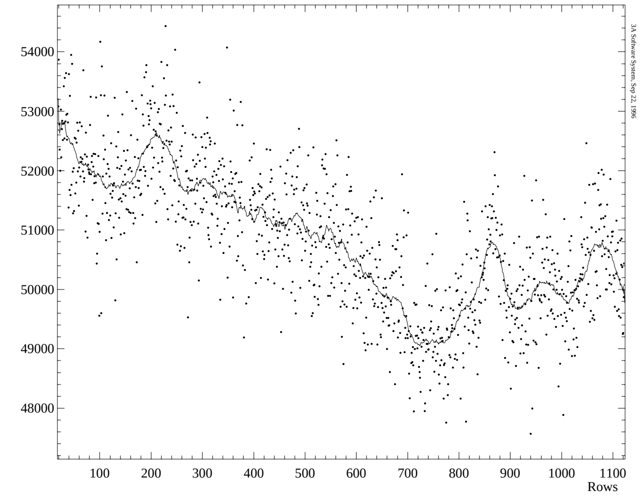

Figure 3.4: A column of the CCD image with artifacts. The trimmed mean filter was applied with the parameters 45:9+9. The filter was chosen because it gives a more smooth curve than the median filter does, it is not affected by the spikes as the average or the Gaussian filters.

`Display coeffs: Yes/No` The command allows to display the coefficients of the polynomial fit and the veiling parameter after the spectra are processed.

`Start processing (Alt-F9)` Activates the procedure.

3.5 Filter menu commands

The filter menu commands allows to smooth the first spectrum displayed and see the result. A similar filter menu in the database allows to process (with subsequential normalization or taking difference) many spectra marked in the database table.

`Median filter:` *n* `(Alt-E)` Runs the median filter with the window length specified in pixels and displays the first spectrum smoothed. The median is taken at the midpoint of the *sorted* window w:

$$\mathrm{med} = w_{n/2}, \quad n \text{ odd}$$

$$\mathrm{med} = (w_{n/2-1} + w_{n/2})/2, \quad n \text{ even.}$$

At the data array ends, the median is computed with reducing window size. The smoothed curve is saved into a separate file co-named with the original, but with extension `*.med`. The output file data format remains the same as that of the original.

`Average filter:` *len* `(Alt-V)` Runs the average filter with the window length as specified in pixels and displays the first spectrum smoothed. At the data array ends, the average is calculated with reducing window size. The smoothed curve is saved into a separate file co-named with the original, but with extension `*.avf`. The output file data format remains the same as that of the original.

`Trimmed mean filter (Alt-T)` Opens a menu of commands to specify the parameters and run the trimmed mean filter (Pasian 1991). The points of data in the window of specified size are sorted and the specified number of points from the minimal and maximal ends are eliminated. The rest is averaged. The filter behaves like the average filter if no points are eliminated, and like the median filter if all points except the central one are eliminated.

`Window length:` *len* Specifies the length of the filter window in pixels.

`First cut:` *num*1 Specifies the number of the minimal data points eliminated.

`Last cut:` *num*2 Specifies the number of the maximal data points eliminated.

`Start processing` Filters the first spectrum and displays the result.

The smoothed curve is saved into a separate file co-named with the original, but with extension `*.tmf`. The output file data format remains the same as that of the original.

`Gaussian filter (Alt-G)` Opens a menu of commands to specify the parameters and run the Gaussian filter. In addition to the normal mode, the filter can work in the rejective mode in order to make a smooth approximation of the upper or lower parts of the spectrum. The data y_i are filtered, and after that a new array of data is created according to the option selected:

$y_i^{\mathrm{new}} = \min(y_i, f_i)$ the points of data above the filtered curve f_i are eliminated.

$y_i^{\mathrm{new}} = \max(y_i, f_i)$ the points of data below the filtered curve f_i are eliminated.

In the next pass, the new data array is used for the filtering as many times as specified by the number of iterations. The smaller the filter length the more flexible the resulting curve, and the more iterations the smoother the curve.

`Window length:` *len* Specifies the FWHM of the Gaussian in real scale (as opposed to the index scale).

The half width of the convolution window is set to 4σ of the Gaussian (Sec. A.3, p. 54). If the specified window length is too small, then a warning message appears which points out the minimal FWHM allowed for the spectrum with the given dispersion. The minimal window length is calculated so, that the number of points of the convolution window is at least three. The warning message cancels the application.

At the ends of the spectrum, the boundary effects are eliminated by convolution with reducing effective window size, while keeping *len* constant.

`Num of iterations:` *num* Specifies the number of the subsequent passes of the filter.

`Cut direction: None/Above/Below` Specifies the elimination direction:

- `None` Does a normal convolution with the Gaussian the specified number of times.
- `Above` Indicates that the points above the curve are eliminated after each iteration and the curve is approaching the bottom part of the spectrum.
- `Below` Indicates that the points below the curve are eliminated after each iteration and the curve is approaching the upper part of the spectrum.

`Start processing` Filters the first spectrum and displays the result.

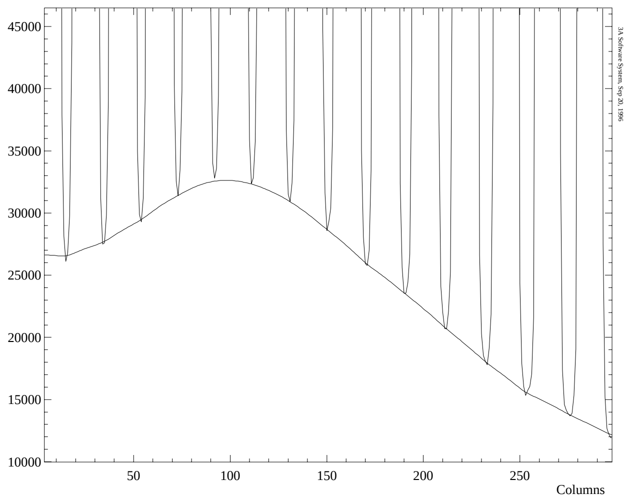

Figure 3.5: An enlarged part of the cross-order cut of an échelle image. A Gaussian filter with 7 pixels FWHM was used 99 times with the cut points *above* option. The resulting curve shown is used to estimate the interorder background variations.

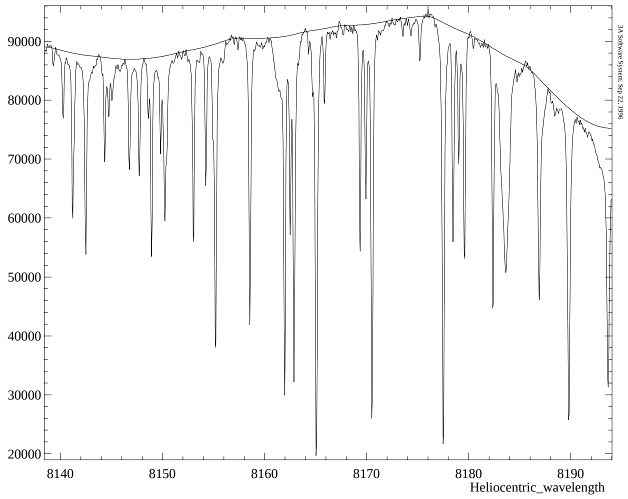

Figure 3.6: A spectrum with sharp telluric lines was filtered with the Gaussian of 31 pixels FWHM. The spectral lines were eliminated after 33 subsequent passes of the filter with the cut points *below* option and such a pseudo-continuum is shown by the smooth curve.

The smoothed curve is saved into a separate file conamed with the original, but with extension `*.gss`.

`Spinning up` Opens a menu of commands to specify the parameters and run the convolution filter to produce the rotational broadening of spectral lines. According to Gray (1988, p.1-26), the rotation profile in the discrete case

$$G(x_i) = \frac{2(1-\epsilon)\sqrt{1-x_i^2} + \pi\epsilon(1-x_i^2)/2}{\pi(1-\epsilon/3)n}$$

is a function of the normalized argument $-1 \leq x_i \leq +1$ $(-n < i < +n)$, where n is the total number of pixels within the rotational profile and the argument is computed as

$$x_i = \frac{\Delta\lambda}{\lambda_c v/c} \cdot i$$

where $\Delta\lambda$ is the dispersion of the spectrum, λ_c is the central wavelength, v is the projected stellar rotational velocity in km s^{-1}, c is the speed of light. ϵ is the limb darkening coefficient in the approximation

$$I(\theta) = I_0\,(1 - \epsilon + \epsilon\cos\theta)$$

The function G is normalized to the number of discrete points n in order to have $\int G(x)dx = 1$.

The central wavelength λ_c is taken at the mid-point of the spectrum. The program can distinguish between spectra in the wavelength and radial velocity scales according to the axis units (`WAVELENGTH`, `HELIOCENTRIC_WAVELENGTH`, or `RVEL` are the possible combinations). In the latter case, the argument of the rotation profiles is gived as

$$x_i = \Delta v \cdot i$$

where Δv is the step size of a spectrum given in the radial velocity scale.

In case, the radial velocity parameter is set too small, a warning message appears which is points out the minimal possible value for the spectrum with the given step size. The minimal width is calculated so, that the length of the rotation profile is at least three points ($n = 1$). The warning message cancels the application.

`Rotational velocity:` *vel* Specifies the projected rotational velocity in km s^{-1}.

`Limb darkening:` ϵ Specifies the limb darkening coefficient. In the real world $0 \leq \epsilon \leq 1$, but other values are also allowed.

`Start processing` Filters the first spectrum and displays the result.

Chapter 4

Cross-correlation facility

The facility is basically designed to align spectral features in the programme spectrum to those of the reference or template spectrum. As the reference spectrum the first in the sequence of displayed spectra is used. Two or more spectra can be cross-correlated at once. The first spectrum is the uppermost spectrum selected in the database of spectra and, optionally, their order can be changed by using the shuffler command (Sec. 3.1, p. 27) of the spectrum program.

The cross-correlation program is called from the spectrum program (Sec. 3.4, p. 30) and works interactively. After the lines are aligned to the reference spectrum the offset can be introduced into each programme spectrum, so that the spectra are properly shifted for the following data reduction processes. With another option, these offsets can just be stored into a separate records of the FITS header of each file without changing the positions of the spectra. There are no constraints on the axis units of the spectra: it can be pixels, wavelengths, radial velocities or any other. The only requirement is that the step size is positive, i.e. the argument of the data is increasing (not the case for swapped spectra (Sec. 3.2, p. 28)).

One or more features chosen in highlighted zones of data (Sec. 3.4, p. 29) are used for the cross-correlation of the spectra. Zones are always selected in the first, reference spectrum. The cross-correlation function is calculated at different offsets of the program spectrum with respect to the reference spectrum. The coefficient of the cross-correlation function for a given offset is calculated (Press et al. 1992, p.636) as:

$$r = \frac{\sum(a_i - \bar{a})(b_i - \bar{b})}{\sqrt{\sum(a_i - \bar{a})^2 \sum(b_i - \bar{b})^2}} \tag{4.1}$$

which is equivalent to the following equation (Bevington 1969, p.121), more suitable for computational purposes:

$$r = \frac{n\sum a_i b_i - \sum a_i \sum b_i}{\sqrt{n\sum a_i^2 - \left(\sum a_i\right)^2}\sqrt{n\sum b_i^2 - \left(\sum b_i\right)^2}} \tag{4.2}$$

where a_i is the reference spectrum taken within intervals of zones:

$$x_i \in [x_{k_0}, x_{k_1}]\,[x_{k_2}, x_{k_3}]\,\ldots$$

x_i is the argument of the reference spectrum, and k_j are the indices (pixel numbers) of the reference spectrum intervals. Points of the programme spectrum b_i are calculated by linear interpolation of the intensities of adjacent pixels at each point $x_i + t$, where t is the displacement called the *lag*. The mean values $\bar{a}$ and $\bar{b}$ are calculated for each lag and n is the number of overlapped points of data within the intervals of zones.

A positive lag shifts the programme spectrum to the *left* (to the blue) with respect to the reference spectrum. The correlation function ranges from +1, when the spectra are fully correlated, to –1, when they are fully anti-correlated at the given offset, and the zero level indicates no correlation.

What is displayed Once the program is activated, the cross-correlation function is calculated and displayed within the maximal interval of lags. The positive wing of the lag is calculated up to the maximal distance between the rightmost pixel of the programme spectrum and the leftmost point of the first zone of the reference spectrum. The negative wing is calculated up to the maximal absolute distance between the leftmost pixel of the programme spectrum and the rightmost point of the last zone of the reference spectrum. The resolution can then be enhanced by recalculating the cross-correlation function within a smaller region of lags specified by position and width of the graphical marker box.

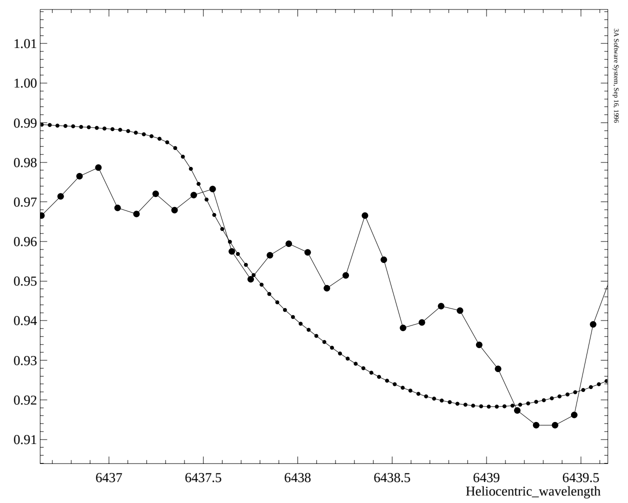

Figure 4.1: A very enlarged part of the edge of a spectral line of the programme and the reference spectrum (smooth line) with different dispersions. At the initial zero offset shown, intensities of the programme spectrum are interpolated for each corresponding point of the reference spectrum and the correlation coefficient is calculated. In the next step, the programme spectrum is shifted by the step size of the reference spectrum if the pixel resolution mode is chosen.

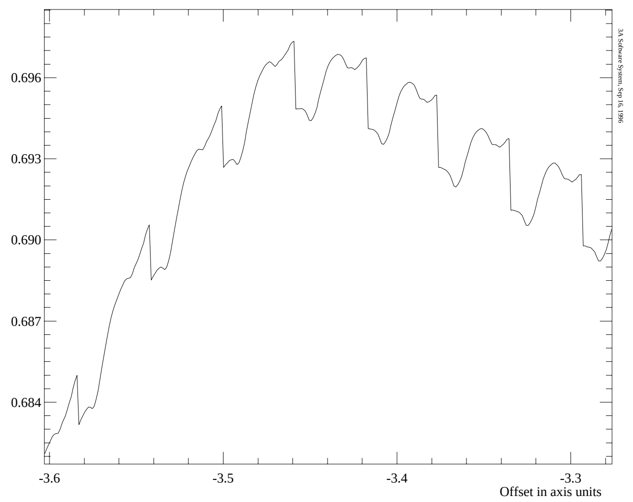

Figure 4.2: A saw-edged fine structure of the enlarged part of the cross-correlation function of two noisy spectra. The distance between two maxima is the step size of the reference spectrum.

The function can be calculated with a different step size according to the resolution mode options of the program. With the first, *subpixel* resolution mode, the step size is calculated by division of the interval of lags into a number of bins specified by the user. With the second, *pixel* resolution mode, the step size is taken as the minimal step size of the reference and the programme spectra. Subpixel resolution mode allows to plot the function much faster within a broad interval of the offsets.

How to find the maximum Three methods are used for finding the position of the cross-correlation maximum.

- In the first method, the maximum is *searched* by direct computation of the function using Brent's method of parabolic interpolation (Press et al. 1992, p.402). The scope of the search is defined by the position of the graphical marker box and the initial guess is set to the maximum of the discrete, displayed function within the interval. Obviously, the result is *not* the position of maximal point of the function on the screen, but the position of the real maximum achieved by subsequent division of the searching interval regardless of the step size or resolution mode selected.

- In the second method, the cross-correlation function is *approximated* by a polynomial of user specified degree within the interval given by the marker box. The cross-correlation maximum is calculated as a root of the polynomial's first derivative and the initial guess is set to the maximum of the discrete, displayed function. Laguerre's method (Press et al. 1992, p.371) is used for solving the polynomial root finding problem. The method depends on the resolution mode selected and explicitly uses the data which are displayed on the screen within the marker box.

- The last method assumes that the cross-correlation peak is a symmetrical function and a Gaussian is used to fit the data. The position of the Gaussian maximum is interpreted as the offset of the function. This method is the most robust technique for the centering of symmetrical functions. The method depends on the resolution mode selected and explicitly uses the data which are displayed on the screen within the marker box.

The offsets found are listed in the table together with the position in index (pixel) scale calculated with the step size (dispersion) of each spectrum. The program allows to display individual cross-correlation functions by browsing the table. The position of the offset found is shown by the vertical graphical marker line.

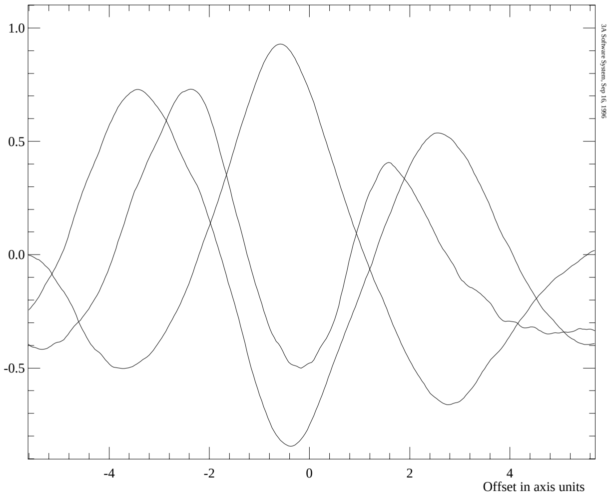

Figure 4.3: The cross-correlation functions are calculated for the spectrum of the close double-lined binary star ER Vul at three different phases. The Sun spectrum was used as a template, spun up to 77 km s^{-1}.

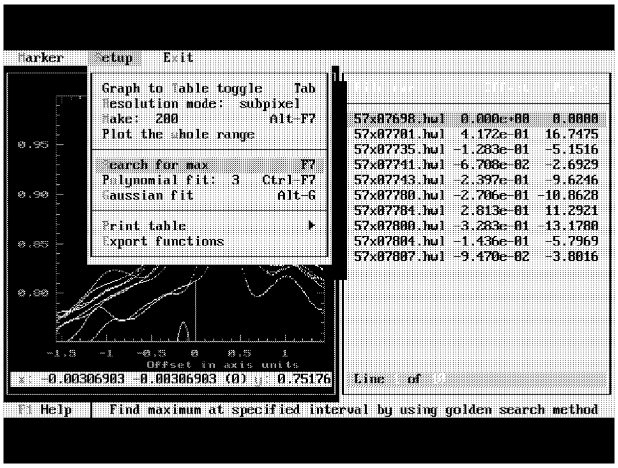

Figure 4.4: Snapshot of the program menu. The cross-correlation function of several spectra is calculated in subpixel resolution mode within an interval of lags and shown in the graph. Offsets are found using the search algorithm and the results are shown in the table.

Danger of ripples Great care should be taken concerning the undersampling problem of the method. Ripples can be easily seen on the cross-correlation function calculated with a small step size within a narrow interval of lags in the subpixel resolution mode. The origin of the ripples is the random noise component of the spectra. The amplitude of the ripples is strongly decreasing with a square law when the spectra are smoothed by a filter. Still, the ripples can affect the offset finding procedures. For the polynomial fit, it can sometimes shift the position of maximum simply because the ripples might not be symmetrical at the ascending and descending wings of the curve. For the search method, the procedure can fail by stopping just at some local maximum. The ripples are most conspicuous on the cross-correlation functions with smooth-shaped features produced by shallow and broad spectral lines. In such a case, the only way to do measurements correctly is to use the pixel resolution mode with a subsequent polynomial fit, but not the searching method which will be affected by the ripples anyway (if there are any). Spectra with sharp lines produce a sharply shaped cross-correlation peak which is not affected by the ripples due to the steep slope. In this case, the undersampling mode could work much better because it produces a smooth maximum and both methods should give the same offset.

How to save the result There are a few ways to store the offsets found. If the spectra should be physically shifted, then the reference pixel number `CRPIX1` of the FITS header should be changed, so the program *accumulates* a new value to the original one:

$$\texttt{CRPIX1}_{\rm new} = \texttt{CRPIX1} + \texttt{OFFSET/CDELT1}$$

by using the `CDELT1` value of the FITS header as the dispersion (step size) of the spectrum and `OFFSET` is the cross-correlation offset in axis units introduced by this program as a new FITS record. The `OFFSET` record can be accumulated or overwritten. It is always possible to undo (reset) any shifts introduced if these two records are modified at the same time (Sec. ??, p. ??).

Another way of storage is to be chosen when the spectra should not be changed in their positions. Then, the offsets can be stored into indexed `OFFSET`i keywords, where i is an index specified by the user. For instance, the offset of the blueshifted cross-correlation component can be stored as `OFFSET1` and the redshifted as `OFFSET2`. Additionally, two other records are created by the program: `NZONES`i is the number of separate zones (features) used and `CROCOR`i is the value of the cross-correlation function at the given offset. The occurance of the index i depends on the storage mode selected.

The same records are created in the FITS header of the reference spectrum according to the storage mode of the programme spectra.

4.1 Marker menu commands

`Zoom window (F5)` Enlarges the data area displayed within the marker box. Return to the original state by pressing `F5` again.

`Marker colour (F2)` Changes the colour of the marker box. By pressing `F2` the colour index is increased, whilst `Ctrl-F2` has the opposite effect.

`Plot colour (F3)` Changes the colour of the function plot. By pressing `F3` the colour index is increased, whilst `Ctrl-F3` decreases the colour index.

`Plotting mode (F4)` Changes the plotting mode of the function currently selected from the table. Use `F4` to increase, and `Ctrl-F4` to decrease the plotting mode. Use `Tab` to activate and move the table bar and then change the mode of the selected function.

`Replot graph (Alt-F5)` Replots the graph as it is, so each plot in the list is redrawn with subsequent replotting of the axes.

`Edit palette (Alt-F3)` Call of the palette editor described in Sec. 1.8, p. 12. The palette with the specified name will be used in the following calls of the cross-correlation program.

`Make PS file` Creates a PS-file from the graph as it is seen on the screen (Sec. 1.9.1, p. 13).

4.2 Setup menu commands

`Graph to Table toggle (Tab)` This command activates either the graphical marker or the table bar. If the table bar is not visible, then the graphical marker is activated and can be moved. Otherwise, the table can be browsed by using the `up` and `down` arrow keys. Switching to the table changes the plot and the marker box position. The position of the table bar defines single or multiple operational modes. If the first record in the table is selected, which is the reference spectrum, then the cross-correlation functions of all spectra are displayed and the maxima of all functions can be found at once. The position of the bar apart from the first spectrum states the single operational mode, so the individual function is displayed and can be used separately. When in the table, the vertical marker line shows the position of the offset field of the selected record. Once the cross-correlation function is recalculated being in single mode, the functions of all other spectra should be re-calculated as well. To do that, go to the first record to get into multiple mode and repeat the operation.

`Resolution mode: pixel/subpixel` If the `pixel` option is chosen, the program calculates the function with the step size taken as the minimal of the dispersions of the reference and the programme spectra. The second option allows to divide the interval chosen into as many points as specified by the following command.

`Make:`*bins* `(Alt-F7)` This command calculates the cross-correlation function for the selected interval of data arguments and then plots the new function(s). The interval of arguments is selected by the graphical marker, so the new function is calculated from the left to the right of the box. If the marker box is set to a vertical line, then the limits of data in the current plotting window are used instead. If the resolution mode is `subpixel` the number of bins is required (a reasonable range is 100–300), which is used to calculate the new step size. This is not required for the `pixel` resolution mode option.

`Plot the whole range` This command calculates and displays the cross-correlation function for the initial interval of offsets, as it was when entering the program, but the current resolution mode and number of bins are used. This helps to redo the selection of the offset interval.

`Search for max (F7)` Used for searching the maximum of the function(s) within the interval of lags defined by the marker box. The search algorithm works in the subpixel mode, regardless of the resolution mode chosen. For each subsequent spectrum, the program prints the offset found into the table and displays its position by the vertical graphical marker.

`Polynomial fit:`*deg* `(Ctrl-F7)` The points of the data within the interval of lags bounded by the marker box are approximated by a polynomial of specified degree (required parameter *deg*) sequentially for each cross-correlation function. The minimum order of the polynomial is two. The root of the first derivative of the polynomial is used as the offset value. The initial guess for the root finding problem is the maximal data point within the interval. The routine uses the data calculated with the selected resolution mode and displayed on the screen.

`Gaussian fit (Alt-G)` The points of the data within the marker box are approximated by a Gaussian and the central position is used as the offset of the cross-correlation peak. The routine uses the data calculated with the selected resolution mode and displayed on the screen.

`Print table` The command opens a submenu with the table printing command options (Sec. 1.10, p. 15). This can be used to create a plain text file of the table contents.

`Export functions` Transfers the cross-correlation functions into separate FITS files for further analysis. The functions are exported as they are seen on the screen and written into co-named files with the extension `*.ccf`. The files are appended to the database of spectra.

4.3 Exit menu commands

`Save changes and exit (F8)` Modifies the reference pixel value and the offset of each FITS file used for cross-correlation according to the options set below. The database fields with the same name are updated, too. Only with this exit command, the spectra are redisplayed afterwards according to the offsets found. The command is enabled after one of the offset finding procedures was activated.

`Save changes and stay (Alt-F8)` Works exactly as the previous one with the exception that it does not exit from the program and the spectra remain unshifted. This is useful when the positions of different cross-correlation maxima should be measured and saved as a separate `OFFSET` keywords. The command is enabled after one of the offset finding procedures was activated.

`Exit without changes (Ctrl-F8)` Exit from the program without any changes in the FITS headers and in the database fields. The spectra are redisplayed, as they were before.

`CRPIX1: accumulate/no changes` The two options how to modify the reference pixel value can be interchanged by pressing `Enter`. With the first option, the offset calculated in pixels (index scale) is added to the `CRPIX1` value, so the spectrum becomes physically shifted. With the second option, the spectrum remains unshifted as it was before entering the program.

`OFFSET: accumulate/overwrite` The two options how to modify the supplementary record `OFFSET` can be interchanged by pressing `Enter`. If the first option is selected, the offset is added to the present value of the record with the same name. Otherwise, the record will be created or overwritten.

`Index:` *num* This allows to create indexed `OFFSET`*i* keywords ($i = 1, 2, 3\ldots$) to store different offsets into separate FITS records, as specified in the previous command. The command is disabled in case the option for `CRPIX1` is `accumulate`. In this case, the offset is stored into the `OFFSET` record without index.

4.4 Operational sequence

Here is a summary of the basic operational sequence of the program:

1. Display the marked spectra, select zones in the reference spectrum and run the cross-correlation program by pressing `Alt-F10`.
2. The program starts to plot the cross-correlation functions within the whole possible interval of lags. The plot can be stopped at any moment by `Esc`. The subpixel mode can plot faster but can omit important details due to reduced resolution (depending on the number of bins chosen).
3. Put the graphical marker around the maximum of interest and use the `Make (Alt-F7)` command to see the area in detail. In subpixel mode the number of bins is required (100–300 is reasonable).
4. Use either `Search for max (F7)`, or `Polynomial fit (Ctrl-F7)`, or `Gaussian fit (Alt-G)` to find the position of the maximum of each spectrum. If the multiple operation is not possible (i.e. the initial guess defined by the marker box position is not suitable for the all functions), then it can be done individually for each spectrum. Use `Tab` to go to the table and browse the records to display and find the offset for each function separately. To activate the graphical marker press `Tab` again.
5. Check that the offsets are found correctly by browsing the table, the vertical marker line shows the position of the maximum of each function.
6. Press `Alt-X` to enter into the exit menu and select the options concerning the `CRPIX1` and `OFFSET` records.
7. In case of re-entry to the program being in the spectrum program: the spectra might be shifted if the `Save and exit (F8)` command was used before. The cross-correlation function will be shifted to zero offset accordingly, even if the reference pixel value was not changed.

Chapter 5

The observations

The program is used as the control software to carry out astrophysical observations with a spectrograph installed at the telescope. The program provides the following general purpose functions:

- Hardware control of the spectrograph units.
- Hardware control of the CCD detector attached to the spectrograph.
- Software control of the specific observational functions, the acquired data flow, storage, and archiving.

The hardware control is performed by means of the instrument specific software drivers designed with the standard protocol of the input/output parameters. The control program then can operate as an instrument independent software with any kind of similar equipment controlled by the standard drivers. The operating system environment variable `INSTRUME` (setup during 3A installation) is pointing to the directory with the instrument control software drivers and some of the default files. Changing the variable allows to change the instrument connected to the same computer without any modification of the control program.

To create these drivers the échelle spectrograph SOFIN was used as prototype. Any other instrument, which has some devices not remotely controlled, use dummy software drivers. The description of the control program is given in instrument-independent form. The instrument specific descriptions and setup are given in the respective manuals.

Here is the list of the standard drivers performing all the possible functions of any spectrograph.

`ONLINE` Checks that the hardware control device is online with the computer.

`BEAM` Changing the light source to render it into the entrance slit of the spectrograph.

`LAMP` Switches on and off the comparison spectrum or flat field lamp.

`SHUTTER` Opens and closes the shutter of the spectrograph.

`DISPER` Positions the dispersion and cross-dispersion units of the spectrograph, sets the optical filter, and changes the entrance slit width.

`XM` Operates the photon counter (exposuremeter): starts and stops the integration, and reads the accumulated counts.

`TVF` Controls the guiding TV camera: opens or closes the shutter, and inserts the grey filter.

`SM` Operates the Stokesmeter unit.

`CLAMP` Controls the auxiliary light source (LED) used for the CCD calibration.

A similar approach is used to control the CCDs: the control program is a CCD independent software and communicates with the specific drivers by the standard protocol. Any CCD connected to the same computer can be inserted into the setup of the control program by pointing to another directory of the control software. The following list shows the software drivers used to operate the CCD from the control program:

`INITCCD` Initializes the controller.

`CLEANCCD` Cleans the CCD in order to remove residual charge from the chip (usually, it is done by fast readout with the substrate offset increased, so that the charge is pulled out to the surface level).

`READCCD` Reads the CCD and writes the image into a FITS file.

`CCDTEMP` Displays the temperature.

`CCDCABLE` Checks the data transmission line.

`CCDBIAS` Auxiliary program to control the CCD setup.

`CCDVOLTS` Displays the voltage setup.

Some of the drivers are not implemented in the particular CCD systems.

The control program consists of the following commands that appear in the main menu and are described in separate sections:

`Setup` Opens a submenu with the auxiliary commands to setup the instrument and CCDs.

`Bias frame` Opens another menu level with the commands used to obtain a CCD bias frame.

`Comparison spectrum` Contains a number of commands to setup and acquire the comparison spectrum.

`Flat field` Contains the commands to setup and make an exposure of the flat field lamp image.

`Object` The menu consists of the commands which provide observations of the object.

5.1 Setup menu

The following commands are listed in the setup menu:

`Detector` Opens a submenu to choose the CCD used for observations, initialize the electronics and others.

`Instrument` This submenu commands are used to initialize the instrument electronics, for focussing and TV control.

`File naming` Used to specify the CCD image file names.

`Identification` Specifies general information about observations.

5.1.1 Detector setup menu

`Configuration:` *name* Opens a window with a table where the CCD configuration can be selected, changed, and stored.

`Initialize CCD` Initializes the CCD controller which was selected with the previous command.

`Voltage setup` Displays the CCD control voltages setup table.

`Temperature` Displays the CCD temperature.

`Clean CCD:` *num* Starts to clean the CCD the specified number of times. The same number of sequential cleanings is used at the beginning of each following exposure. A zero value disables the operation.

`CCD bias:` *num* Auxiliary command used to change or inspect the setup of the programmable CCD controller. The parameter specifies a number of serial transfers in each cycle of a loop, after which the average and standard deviation of the pixel intensities are printed.

`Check cable` Performs a test which checks the reliability of the data transmission line. How to switch into the echo mode depends on the particular CCD electronics.

`CCD calibration` Opens a submenu with the commands used to obtain a series of uniformly illuminated CCD images of different intensities by means of the external light source which is controlled by the program.

`Low level:` *min* Specifies the minimal brightness of the LED in percent of its maximum.

`High level:` *max* Specifies the maximal brightness of the LED in percent of its maximum.

`Number of levels:` *num* Specifies the number of different illumination levels.

`Number of exposures:` *rep* Specifies the number of exposures at the same illumination level.

`Exposure time:` *time* Sets the exposure time which is the same for each exposure.

`Start sequence` Starts the series of $num \times rep$ exposures. To interrupt the sequence use `Esc`. The CCD is read out after each exposure and the images are added to the database. The FITS object name is `FF`*num*, where *num* is the illumination level in percent.

5.1.2 Instrument setup menu

`Initialize devices` Parks the instrument devices, so that each of them is moving or set to the initial zero home position: all shutters are closed, the lamps are off, the entrance slit is closed, the grating and the cross-dispersion prism are at the end switch. The command must be used to reset the devices of the remotely controlled instrument after powering on before any further operations.

`Preset devices` Works similarly as parking, but then sets the device positions to those that were stored in the program setup file (useful in case of a power failure).

`ICCD camera:` *state* Opens a submenu with the following commands to operate the guiding (intensified) TV CCD camera: `Close`, `Open` shutter, and `Grey filter`. Once the operation is completed, the current state of the device is printed instead of the *state* parameter.

`Focussing` Opens a submenu with the commands used to find the optimal focus of the spectrograph. The comparison spectrum lamp is used to provide a series of exposures at different foci. The program changes the grating angle after each exposure to separate the comparison lines on the image, and finally reads the CCD once the specified number of exposures is done. At the end, the grating is returned to the original position.

  `Spectral region:` *name* Allows to pickup a name from the database and to setup the instrument to the chosen spectral region,

  `Filter number:` *num* Allows to pickup a name and to setup the specified filter.

  `Slit width:` w Changes the entrance slit width as specified in microns.

  `Exposure time:` *time* Changes the exposure time of the comparison spectrum.

  `Shift value:` Δx Specifies the amount of stepping drive units to change the grating angle after each exposure.

  `Waiting time, sec:` Δt Introduces a delay between exposures to allow for a manual change of the focus.

  `Number of exposures:` *num* Specifies the total number of successive exposures of the comparison lines at the different foci.

  `Start exposures` Starts the sequence of exposures. The message bar of the program menu window displays the current exposure number. The next exposure can be started either by pressing `Enter` or it starts automatically after the delay time is over. To stop the series of exposures press `Esc`. The CCD image is read out and displayed on the screen. The new image is added to the database with the object name `Focussing` in the FITS header.

`Stokesmeter, steps:` *num* Sets up the Stokesmeter quarter-wave plate position. A zero angle initializes the device.

5.1.3 File naming setup menu

`Image number:` *num* Specifies the current sequential number of the image. The image number increments after each readout of the CCD. It is important to check (at the beginning of the observing run or after a computer crash) that the image number is greater than the last image number in the database of images. Otherwise, the database record for a new image would overwrite the older contents.

`Template:` *tmp* Specifies the template to construct the name of image files. The default template is `ccd00000.fit`; any other choice should be in agreement with the 3A file name conventions (Sec. 1.5, p. 9).

5.1.4 Identification setup menu

The following commands specify general information which will be written into the FITS header of each CCD image created by the control program. The default parameters of the first two commands are taken from the `defaults.lst` setup file (Sec. 5.6.3, p. 47) in the directory pointed to by the `INSTRUME` environment variable.

`Telescope:` *name* Specifies the name of the telescope.

`Instrument:` *name* Specifies the name of the acquisition instrument.

`Observer:` *name* Specifies the observer(s).

`Comments:` *name* Specifies some observer's comments.

5.2 Bias frame menu

`Exposure time:` *time* Specifies the exposure time for the dark CCD image. A zero exposure time provides a bias frame.

`Number of frames:` *num* Specifies the number of sequential exposures.

`Start series` Starts the series. The timer window appears to show the dark exposure status. Use `Esc` for a premature stop of the exposure and break of the sequence. After each exposure the CCD is read out and the images are added to the database with the FITS header object name `Dark frame` or `Bias frame`, respectively.

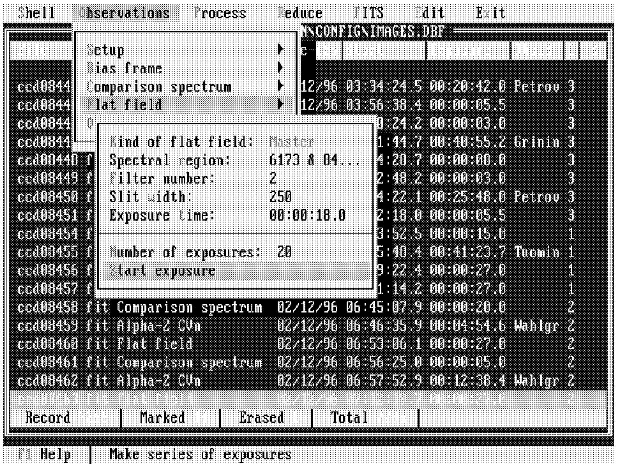

Figure 5.1: A snapshot of the flat field menu of the control program.

5.3 Comparison spectrum menu

`Spectral region:` *name* Allows to pickup a name from the database and to setup the instrument to the selected spectral region.

`Filter number:` *num* Allows to pickup a name from the table and to setup the specified optical filter.

`Slit width:` *w* Changes the entrance slit width of the spectrograph as specified in microns.

`Exposure time:` *time* Changes the exposure time of the comparison spectrum.

`Start exposure` Starts the comparison spectrum exposure. The guiding TV camera shutter is closed during the exposure. The timer window appears to show the exposure status. Use `Esc` for a premature stop of the exposure. The program reads out the CCD and appends the new image to the database with the FITS object name `Comparison spectrum`.

5.4 Flat field menu

`Kind of flat field:` `Normal/Master` Switches between two kinds of flat fields and their setup parameters. Each of the two has its own slit width, exposure time, and number of exposures which are stored in separate fields of the database of the spectral regions. The slit width for the normal flat field is the same as for the object exposure. A number of master flat fields can be obtained with a different slit width and exposure time.

`Spectral region:` *name* Allows to pickup a name from the database and to setup the instrument to the selected spectral region.

`Filter number:` *num* Allows to pickup a name from the table and to setup the specified optical filter.

`Slit width:` *w* Changes the entrance slit width of the spectrograph as specified in microns.

`Exposure time:` *time* Changes the exposure time of the flat field.

`Number of exposures:` *num* Sets up the number of successive exposures of the flat field lamp.

`Start exposure` Starts a series of flat field exposures. The timer window appears to show the exposure status. Use `Esc` for a premature stop of the exposure and a break of the sequence. The program reads out the CCD after each exposure and appends the image to the database with the FITS object name `Flat field`.

5.5 Object menu

`Object name:` *name* Specifies the name of the object which can be picked up from the database of objects.

Once the object is selected, a program window appears to select the identifier of the observing programme. As opposed to the observer name, the identifier gives the name of the principal investigator of a given observation and can be used to separate images later from one another by using the introduced FITS and database field `OBSID`. Details on how to add a new identifier are given in Sec. 5.6.5, p. 48.

`Spectral region:` *name* Allows to pickup a name from the database and to setup the instrument to the selected spectral region.

`Filter number:` *num* Allows to pickup a name from the table and to setup the specified optical filter.

`Slit width:` *w* Changes the entrance slit width of the spectrograph as specified in microns.

`Exposure time:` *time* Changes the exposure time of the object. The exposure time counter is locked while the dialogue box is displayed, so that the exposure cannot be ended during the dialogue.

`Num of exposures:` *num* Sets up the number of successive exposures of the object. The program takes the same precautions as in the previous command.

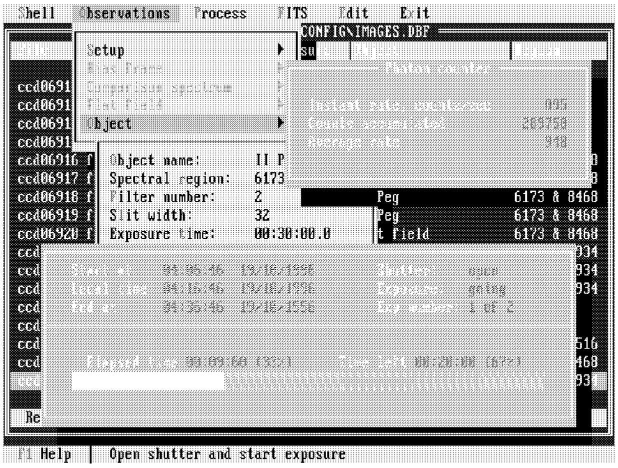

Figure 5.2: The snapshot of the control program screen after the object exposure has started shows the exposure watch window and the photon counter window.

`Start exposure(s)` Starts the exposure(s). The watch window appears and shows the exposure status. The exposuremeter window appears, too, and shows the amount of photons accumulated (if the device is implemented in the instrument). Press `Esc` to close the windows. The program will stop the exposure automatically when the time is over.

During the exposure it is allowed to:

- Change the time to prolong or shorten the exposure.
- Pickup another object from the database. The exposure time remains unchanged.
- Suspend and resume, prematurely stop, or abort the exposure.
- Watch the exposure status.
- Exit from the object menu and from the control program, and even to reboot the computer.

During the object exposure it is not allowed to (most of these commands are simply disabled by the software control):

- Start the exposure again.
- Change the spectral region.
- Clean the CCD or make calibration exposures.
- Stay in the database of objects or spectral regions at the end of the exposure (in order to have enough DOS memory for the read CCD program).

Exit from the object menu deactivates the exposure timer, which is the software counter controlled by the system clock. Once the object menu is entered again, the software timer is re-activated to monitor the end of exposure, and the time left is taken as the difference between the end time and the actual time. It implies that it is impossible for the program to end the exposure and read out the CCD while not being in the object menu. If the object menu is re-entered after the exposure time is finished, the program ends the exposure immediately.

At the end the program reads out the CCD and appends the image to the database with the object name as specified. The exposure time in the FITS header keyword `EXPOSURE` is the effective total exposure time while the shutter was open, which ensures a correct value for postponed, suspended, resumed, or prematurely stopped exposures. The start and end times remain the UT when the shutter was opened and closed for the first/last time.

`Suspend exposure` Allows a temporary stop of the exposure by closing the spectrograph shutter. The command does not change the exposure time, only the end of exposure becomes accordingly later.

`Resume exposure` Resumes a suspended exposure by opening the shutter.

`Prematurely stop` Allows to stop the exposure and read out the CCD image. A warning message appears asking to confirm the action by `Enter`. To disregard use `Esc`.

`Abort exposure` Stops the exposure and does not read the CCD. A warning message appears asking to confirm the action by `Enter`. To disregard use `Esc`.

`Watch window` Shows the exposure status window: the local time of the start and end of the exposure, the elapsed time, and the time left, the status of the exposure (suspended or going) and the shutter (closed or opened). The window can be closed at any time by `Esc`.

5.6 Details of the control program

5.6.1 Contents of the FITS header

The table shows the general FITS records that appear in any two-dimensional image, with the default values given in brackets:

`SIMPLE`	Standard FITS format (`T`).
`BITPIX`	Two bytes per pixel (16).
`NAXIS`	Two-dimensional image (2).
`NAXIS1`	Number of columns of the image.
`NAXIS2`	Number of rows of the image. These two parameters specify the size of the CCD readout region which possibly includes the bias overscan areas.
`BSCALE`	Scaling factor of the FITS pixel values (1).
`BZERO`	Offset of the FITS pixel values (+32768). The transformation Real=FITS $\times$ Bscale + Bzero converts the signed integer pixel value stored in the FITS file into the unsigned integer obtained from a 16-bit ADC.

The following table shows the parameters specific for the CCD readout region. The values are counted from 1, not from 0.

`CRVAL1`	Starting column number of the CCD readout region.
`CRVAL2`	Starting row number of the CCD readout region
`CDELT1`	Step size which is the CCD binning factor along the columns (1).
`CDELT2`	Step size which is the CCD binning factor along the rows (1).
`CRPIX1`	Column number to which `CRVAL1` refers (1).
`CRPIX2`	Row number to which `CRVAL2` refers (1).
`CTYPE1`	Name of the first axis (`COLUMNS`).
`CTYPE2`	Name of the second axis (`ROWS`).
`BUNIT`	Physical unit of the pixel values (`ADU`).

The following parameters are specific for the CCD camera being used:

`CCDHEAD`	Identification name of the CCD camera used.
`CCDCOLS`	Specifies the length of the CCD serial register as it is defined in the CCD configuration file.
`CCDROWS`	Specifies the number of CCD pixels in the parallel transfer direction.
`COMMENT`	The full CCD voltage setup: `VOD`, `VRD`, `VOG` and so on (implemented for the Astromed-3200 programmable CCD camera).
`CCDTEMP`	CCD temperature in K at read out.
`GAIN`	CCD gain factor e^-/ADU. The parameter is the preset value and specified in the select CCD program.
`DATE`	Local date the file was written.

The following parameters are common for the FITS images and can be changed in the setup menu:

`TELESCOP`	Data acquisition telescope.
`INSTRUME`	Data acquisition instrument.
`OBSERVER`	Name of the observer(s) or identification.
`COMMENT`	Observer's comments.

The following parameters appear in the object, comparison spectrum, and flat field images and specify the instrument setup:

`REGION`	Spectral region name as it is defined in the database of regions.
`GRATING`	Dispersion unit position in stepping drive units.
`PRISM`	Cross-dispersion unit position in stepping drive units.
`FILTER`	Optical filter number with its name in the comment field.
`CAMERA`	Optical camera number. The parameter can be changed only in the database of spectral regions.
`SLIT`	Entrance slit width of the spectrograph in microns.

The following FITS records appear in every image:

`DATE-OBS`	UT date when the exposure was started.
`START`	UT when the shutter was opened.
`EXPOSURE`	The effective total exposure time while the shutter was open.
`STOP`	UT when the shutter was closed.

The next records are specific for the object FITS file and are calculated for the midpoint of the effective exposure time:

`OBJECT`	Object name as selected from the database.
`LST`	Local siderial time.
`JD-OBS`	Julian Date.
`HJD-OBS`	Heliocentric Julian Date.
`EQUINOX`	Equinox.
`RA`	Right ascension of the object.
`DEC`	Declination of the object.
`HA`	Hour angle.
`ZA`	Zenith distance.
`AIRMASS`	Air mass.
`PHASE`	Phase of the object. Present, if the period and the initial epoch are given in the database of objects.

`EARTHVEL`	The projected sum of the radial and rotation velocities of the Earth on the line of sight in km sec^{-1}. Positive towards the object.
`COUNTS`	Photon counts accumulated/1000. Present, if the exposuremeter is implemented in the instrument.

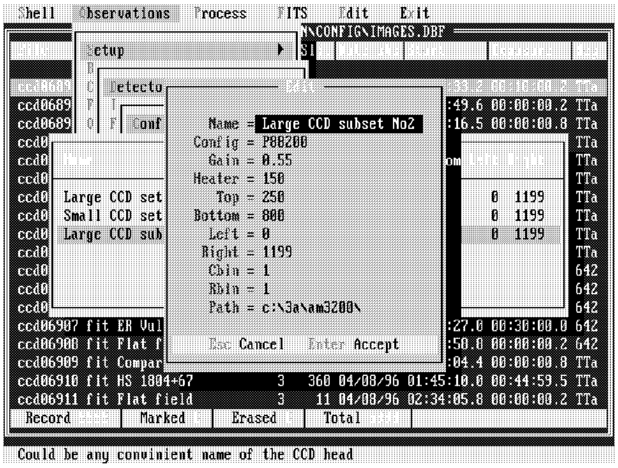

Figure 5.3: The CCD selection program with the edit window open in order to change the CCD readout region.

5.6.2 The CCD configuration

The facility allows to change the CCD configuration. The program window contains a table which consists of the following fields:

`Name` The identification name of the CCD configuration which allows to separate one setup from another; therefore, the name should be unique in the table.

`Config` The name of the configuration file which defines the voltage setup for the given CCD. The name is defined by the CCD control software.

`Gain` The estimate of the CCD gain factor e^-/ADU for the given configuration. The value is written into the FITS header of each image taken with the given CCD.

`Heater` The CCD preset temperature in K. The parameter is used to setup the CCD temperature control unit during initialization of the electronics.

`Top` The first column of the CCD readout region. All values are counted from zero.

`Bottom` The last column of the CCD readout region.

`Left` The first row of the CCD readout region.

`Right` The last row of the CCD readout region.

`Cbin` The CCD binning factor in direction of the serial transfer across the columns. The default value is one.

`Rbin` The CCD binning factor in direction of the parallel transfer across the rows. The default value is one.

`Path` Points to the directory where the CCD control programs are situated.

A number of keys, which are displayed in the window status bar, are used to operate the table:

`F4` Edit the selected record by using a dialogue box.

`F5` Create a new record in the table. The record currently selected is used as a template for the new one, which can be edited by a dialogue box. The name of the new CCD setup should be different from the old ones.

`Alt-Del` Deletes the record selected from the table.

`Alt-R` Changes the readout region of the CCD. The program reads the graphical marker box position of the latest image displayed, and puts them into the readout region fields of the currently selected record. A dialogue box appears for editing. As an alternative to this command, the readout region can be simply edited by `F4`.

`Esc` Exits from the program without changing the previously selected CCD setup.

`Enter` Selects the new CCD configuration from the table, checks that the software exists in the path pointed to, and exits from the program.

5.6.3 The default parameters file

All parameters of the current observing setup are stored in the local `CONFIG` subdirectory. The default parameters file is used in case the control program is started in a newly created empty working directory. The defaults have typical parameters specific for the given observing site. The observer should not make any changes in the file and it is the responsibility of the site manager to keep it suitable for all new observers.

A plain text file with the name `defaults.lst`, which can be edited by any text editor, is stored in the directory pointed to by the `INSTRUME` environment variable and contains lines like the following

```
Nordic Optical Telescope
SOFIN spectrograph
0 0 1199 769 1 1 0.55 150 P88200 c:\3a\am3200\ Large CCD
0 0 1199 297 1 1 0.53 150 P88100 c:\3a\am3200\ Small CCD
```

The first two lines are used for the telescope and instrument specification. The last two lines shown here are used by the CCD configuration program and the number of such lines can be as large as needed. The line consists of the following parameters: the first row (`Left`), the first column (`Top`), the last row (`Right`), and the last column (`Bottom`) of the CCD readout region, the binning factor (`Cbin` and `Rbin`), the gain factor (`Gain`), the CCD preset temperature (`Heater`), the CCD configuration file (`Config`), the CCD control software directory (`Path`), and the identification name of the CCD setup (`Name`).

5.6.4 The filter list

A plain text file with the name `filters.lst`, which can be edited by any text editor, is stored in the directory pointed to by the `INSTRUME` environment variable. The file contains information about the filters used in the spectrograph and is used by the control program to pickup the filter by its name from the list and setup the filter according to its number. An example for the file is:

```
1  Open
2  3000 - 25000 Neutral
3  8500 - 25000 Infrared
4  7000 - 25000 Red
5  6000 - 25000 Orange
6  5000 - 7000  Green
7  Closed
```

The first integer number is the filter number which is used by the device driver to setup the filter. The same number is stored in the database ob the spectral regions and displayed in the menu command. The rest of each line is the identification of the filter which can be up to 38 characters in length. The filter number with its name is printed in the FITS header of the CCD image in the `FILTER` record.

5.6.5 The observing programme identifier

A plain text file called `obsid.lst` is stored in the directory pointed to by the `INSTRUME` environment variable. To add, remove, or modify records of the list any convenient text editor can be used (being in the Norton Commander use `F4` or `Alt-F4` shortcuts). The format of the field is rather simple. Any kind of abbreviation of the investigator name with a length of up to six characters can be used, so that it could be recognizable for other people. Any printable characters are valid, except the white space which is used as a separator for the rest of the line, which can be 70 characters long and it contains the first and last names of the principal investigator of the observing project, and the affiliation.

The identifier selection program uses the standard control keys (Sec. 1.2, p. 8) to browse the table and select a record. It is also key sensitive, so the table bar moves to the record if its first letters are typed. The record selected with `Enter` becomes first in the list, so the most frequently used records are always on top of the table list.

5.6.6 Entering the control program

When the user enters into the observations menu from the database, the program checks the functionality of the control hardware and the software setup:

- Checks that the databases of objects, observing sites, and spectral regions exist in the path specified in the database of images.
- Checks that the `INSTRUME` environment variable is defined and the directory it points to exists. Checks that the control hardware is powered on and is online with the computer.
- Checks the setup parameters of the program. The missing parameters are taken from the defaults file. In such a case, the CCD setup window appears asking to select or create a new configuration.
- Checks that the observing site name is not missing. Otherwise, the database of sites appears in order select the proper observing site.
- Checks that the current sequential image number is not less than the number of records in the database of images. Otherwise, a warning message appears which suggests to modify the image number in order to avoid overwriting of older database records with the forthcoming images.

5.6.7 Exposure control sequence

The following description is a general sequence of the remotely controlled operations which are performed to obtain a calibration image:

- Checks that the shutter is closed.
- Turns off the intensified guiding TV CCD camera.

- Moves the beam switch to the correspondent position to render the beam of the flat field or comparison spectrum lamp to the entrance slit.
- Positions the grating and the cross-dispersion units to the selected spectral region, sets up the specified filter and the entrance slit width.
- Makes a single or a series of exposures as follows:
  - Checks that there is enough disk space to allocate the new image and that the image with the same name does not exist in the current directory.
  - Cleans the CCD the specified number of times.
  - Switches on the lamp.
  - Opens the shutter.
  - Activates the time counter, and the status window pops up.
  - Reads out the CCD, writes the file to the disk, and appends the image record to the database.
- Turns the beam switch back to the initial position.
- Returns the guiding TV camera back to the original state.
- Displays the latest image obtained on the screen.

The object exposure is very similar to the sequence described. The exceptions are:

- The shutter of the guiding TV camera remains unchanged.
- The shutter of the photon counter (exposuremeter) opens and closes together with the spectrograph shutter.

Chapter 6

The database of images

6.1 Shell menu commands

6.2 Observations

The command allows to open a menu to carry out observations with a remotely controlled spectrograph on the telescope. The menu can be opened if the corresponding control software is installed and the control equipment is connected to the computer. The detailed description of the observation menu commands is given in Chap. 5, p. 41.

6.3 Process menu commands

6.4 Reduction menu commands

6.4.1 Multiorder operations

The facility is similar to the arithmetical operations with the images except that not the images itself but the correspondent spectral orders are used instead in the operations. This allows to process in the same manner many spectral orders from different images by one command.

As a possible alternative to the facility, the pair operations command of the database of spectra can be used which provides similar operations with only pairs of spectra arranged in the database. The most simple alternative is to use the arithmetical operation commands with the spectra.

The file name of the spectral order (like, `34x12345.dvd`) being processed is constructed from the following three components:

- The sequential spectrum number is taken from the corresponding number of the images as they are marked or selected from the database.
- The prefix of the spectral order (which is equal to the échelle order number) is formed from the table of the spectral order parameters for the corresponding image.
- The file extension of the spectral orders being processed is specified by the corresponding menu command.

The images itself are not needed to be present on the disk, but the relevant records should be present in the database and the corresponding files with the extension `*.spp` should be in the current directory.

All implemented operations are divided into three groups:

`Sum/Average/Product` Performing the operation with the spectral orders of the specified extension for the series of images marked in the database. The file extension of the processed spectral orders can be specified with the menu command for the extension of the first operand. The resulting files inherit the sequential number of the first marked image and the extension `*.sum`, `*.avr`, or `*.mul`.

`Ratio/Difference` Divides or subtracts spectral orders of many marked images (as the first operand) by the spectral orders of a single selected image (as the second operand). The corresponding file extensions of the processed spectral orders can be specified with the menu commands. The resulting files inherit the sequential number of each marked image and the extension `*.dvd` or `*.sub`. The second operand image selection is asked for once the procedure has been started.

`CrossCorr` Identifies spectral lines of the marked comparison spectra images by using a template image with the lines identified and selected as the second operand. The file extension of the spectral orders from the marked images is specified by the first operand extension command. The template spectrum image selection is asked for once the procedure has been activated.

The program cross-correlates each order of the marked images with the corresponding order of the template image. Once the offset is established, the program determines the line positions based on the intervals taken from the table of the spectral line parameters of the template. The lines located are assigned to the corresponding wavelength from the template table. The resulting table of the spectral line identification (`*.slp`) is then created for each comparison spectrum order of each marked image. The tables prepared can be already used for the two-dimensional dispersion curve calculation by means of merging identified spectral orders.

`First operand ext:` *ext*1 Selects the file extension of the spectral orders of the first operand.

`Second operand ext:` *ext*2 Selects the file extension of the spectral orders of the second operand.

`Take: Sum/Aver/Product/Ratio/Diff/CrossCorr` Selects the kind of operation from the list of alternatives.

`Start processing` Starts processing the marked records for the first group of operations, or asking to select the image to be used as the second operand or the reference image. Make the selection and press `Enter` to start processing. The `Esc` key disregards the application.

6.5 FITS menu commands

6.6 EDIT menu commands

Appendix A

Mathematical notes

A.1 Propagation of errors

A.1.1 The variance

The variance of a function $f(x)$ of the arguments $x = (x_0, x_1 \ldots, x_n)$ randomly distributed with the variance $\sigma^2(x_i)$ and *uncorrelated* between each other (Bevington 1969, p.60) is

$$\sigma^2(f(x)) = \sum_{i=0}^{n} \left[\frac{\partial f(x_i)}{\partial x_i}\right]^2 \sigma^2(x_i) \qquad \text{(A.1)}$$

In the other words, the standard deviation (σ) of a function is the length of its vector in n-dimensional space.

Some relations are often used in practice and derived from Eq. A.1:

$$\sigma^2(u \pm v) = \sigma_u^2 + \sigma_v^2$$

$$\sigma^2(u \times v) = v^2\sigma_u^2 + u^2\sigma_v^2$$

$$\sigma^2(u/v) = \left(\frac{u}{v}\right)^2 \left[\frac{\sigma_u^2}{u^2} + \frac{\sigma_v^2}{v^2}\right]$$

$$\sigma^2(v \pm const) = \sigma_v^2$$

$$\sigma^2(v \times const) = \sigma_v^2\, const^2$$

A.1.2 The signal-to-noise ratio

Let s be a positive signal with the noise level σ. Then the signal-to-noise ratio is defined as

$$r(s) = \frac{s}{\sigma}$$

The following shows how the ratio is changing for different combinations of two signals:

$$r(s_1 \pm s_2) = \frac{(s_1/s_2 \pm 1)\, r_1}{\sqrt{(s_1/s_2)^2 + (r_1/r_2)^2}}$$

$$r(s_1 \times s_2) = r(s_1/s_2) = \frac{1}{\sqrt{1/r_1^2 + 1/r_2^2}}$$

$$r(s \times const) = r(s)$$

$$r(s \pm const) = r(s)\left(1 \pm \frac{const}{s}\right)$$

A.1.3 The relative error

Similarly, the relative error is

$$\delta(s) = \frac{\sigma}{s}$$

and some useful relations are

$$\delta^2(s_1 \pm s_2) = \frac{\sigma_1^2 + \sigma_2^2}{(s_1 \pm s_2)^2}$$

$$\delta^2(s_1 \times s_2) = \delta^2(s_1/s_2) = \delta_1^2 + \delta_2^2$$

$$\delta(s \pm const) = \frac{\delta(s)}{1 \pm const/s}$$

$$\delta(s \times const) = \delta(s)$$

A.2 Fit data to a quadratic parabola

Given tabulated function (x_i, y_i, ω_i), $i = 0, 1 \ldots, N-1$, with the weights

$$\omega_i = \frac{1}{\sigma_i^2}$$

are the inverse variance of the measurements y_i. Fit the data to the parabola

$$y = c_0 + c_1 x + c_2 x^2 \tag{A.2}$$

The system of normal equations:

$$\begin{bmatrix} s_0 & s_1 & s_2 \\ s_1 & s_2 & s_3 \\ s_2 & s_3 & s_4 \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix} \tag{A.3}$$

with the notations

$$\begin{array}{llll} s_0 = \sum \omega_i & s_1 = \sum \omega_i x_i & s_2 = \sum \omega_i x_i^2 & s_3 = \sum \omega_i x_i^3 \\ y_0 = \sum \omega_i y_i & y_1 = \sum \omega_i x_i y_i & y_2 = \sum \omega_i x_i^2 y_i & s_4 = \sum \omega_i x_i^4 \end{array}$$

The solution of normal equations

$$\begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} = \frac{1}{\Delta} \begin{bmatrix} s_2 s_4 - s_3^2 & s_2 s_3 - s_1 s_4 & s_1 s_3 - s_2^2 \\ s_2 s_3 - s_1 s_4 & s_0 s_4 - s_2^2 & s_1 s_2 - s_0 s_3 \\ s_1 s_3 - s_2^2 & s_1 s_2 - s_0 s_3 & s_0 s_2 - s_1^2 \end{bmatrix} \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix}$$

where

$$\Delta = \Delta_0 + \Delta_1$$

$$\Delta_0 = s_0 s_2 s_4 - s_0 s_3^2 - s_2^3 \qquad \Delta_1 = 2 s_1 s_2 s_3 - s_1^2 s_4$$

Each of the coefficent of the parabola is determined with the sums over the data points. Uncertainity in the data points contributes a small fraction to the uncertainity of the parameter determination. According to the error propagation equation (A.1), the contribution is the standard deviation of the individual measurement times the effect which that point has on the parameter determination.

The errors of the coefficient determination includes the diagonal elements of the solution matrix:

$$\begin{aligned} \sigma_{c_0}^2 &= \left(s_2 s_4 - s_3^2\right)/\Delta \\ \sigma_{c_1}^2 &= \left(s_0 s_4 - s_2^2\right)/\Delta \\ \sigma_{c_2}^2 &= \left(s_0 s_2 - s_1^2\right)/\Delta \end{aligned} \tag{A.4}$$

A great simplification of the equations can be achieved together with the reduction of roundoff errors if the weighted mean point of the data argument is removed:

$$t_i = x_i - x_c \qquad x_c = \frac{s_1}{s_0} = \frac{\sum \omega_i x_i}{\sum \omega_i}$$

which leads us to find the parameters of the parabola

$$y_i = d_0 + d_1 t_i + d_2 t_i^2$$

Using a similar notations of the sums over the argument t_i and setting the sum $s_1 = 0$, the coefficients of the parabolic fit are

$$d_2 = \frac{1}{\Delta_0}\left(s_0 s_2 y_2 - s_0 s_3 y_1 - s_2^2 y_0\right)$$

$$d_1 = \frac{1}{s_2}\left(y_1 - d_2 s_3\right) \qquad d_0 = \frac{1}{s_0}\left(y_0 - d_2 s_2\right)$$

with the errors $\sigma_{d_2}^2$, $\sigma_{d_1}^2$, and $\sigma_{d_0}^2$ are calculated according to Eq. A.4.

The coefficients of the parabola with the argument unscaled (A.2) are

$$c_0 = d_0 - d_1 x_c + d_2 x_c^2 \quad c_1 = d_1 - 2 d_2 x_c \quad c_2 = d_2$$

with the errors after the transformation

$$\sigma_{c_0}^2 = \frac{1}{s_0} + \frac{x_c^2}{s_2} + \left(x_c^2 + \frac{s_3}{s_2} x_c - \frac{s_2}{s_0}\right)^2 \sigma_{d_2}^2$$

$$\sigma_{c_1}^2 = \frac{1}{s_2} + \left(\frac{s_3}{s_2} + 2 x_c\right)^2 \sigma_{d_2}^2$$

$$\sigma_{c_2}^2 = \sigma_{d_2}^2$$

The root mean square (in square) of the fit is

$$(\text{rms})^2 = \frac{N}{s_0} \frac{1}{N-3} \sum_{i=0}^{N-1} \omega_i \left[y_i - y(x_i)\right]^2$$

A.3 Fit data to a Gaussian curve

The Gaussian curve

$$y(x) = y_0 \exp\left[-\left(\frac{x - x_0}{\sigma}\right)^2\right]$$

has the full width at half maximum

$$\text{FWHM} = \sigma\sqrt{\ln 16} \approx 1.665\sigma$$

and the integral

$$\int_{-\infty}^{+\infty} y(x)dx = y_0\sigma\sqrt{\pi} = y_0\sqrt{\frac{\pi}{\ln 16}} \times \mathrm{FWHM}$$

In order to approximate the data by a Gaussian curve, the model is transformed into the linear form:

$$\ln y = c_0 + c_1 x + c_2 x^2$$

The variance of the measurements y_i under the assumption of Poisson noise is $\sigma^2(y_i) = y_i$. According to Eq. A.1, the variance after the transformation becomes

$$\sigma^2(\ln y_i) = 1/y_i$$

which is used as the inverse weight $1/\omega_i$ for the parabolic fit.

Once the cofficients of the parabolic fit are obtained, the Gaussian parameters are calculated with the equations:

$$\sigma^2 = -\frac{1}{c_2} \qquad x_0 = -\frac{c_1}{2c_2} \qquad \ln y_0 = c_0 - \frac{c_1^2}{4c_2}$$

and the uncertainty of the Gaussian parameters:

$$\sigma_\sigma^2 = -\frac{\sigma_{c_2}^2}{4c_2^3} \qquad \sigma_{x_0}^2 = \sigma^4\left(\frac{1}{4}\sigma_{c_1}^2 + x_0^2\sigma_{c_2}^2\right)$$

$$\sigma_{y_0}^2 = y_0^2\left(\sigma_{c_0}^2 + x_0^2\sigma_{c_1}^2 + x_0^4\sigma_{c_2}^2\right)$$

A.4 Fit data to a sine function

The model of a periodical process with the known period P and given points of data (x_i, y_i), $i = 0, 1 \ldots, N-1$, is:

$$y_i = Y_0 \sin\left(2\pi(\phi + \frac{x_i}{P})\right) + C \qquad \text{(A.5)}$$

or in other terms:

$$y_i = A\sin t_i + B\cos t_i + C \qquad \text{(A.6)}$$

$$A = Y_0\cos(2\pi\phi) \quad B = Y_0\sin(2\pi\phi)$$

$$t_i = 2\pi\frac{x_i}{P}$$

The system of the normal equations is:

$$\begin{cases} As_2 + Bu_0 + Cs_0 = s_1 \\ Au_0 + Bc_2 + Cc_0 = c_1 \\ As_0 + Bc_0 + CN = u_1 \end{cases}$$

where the sums are defined as:

$$s_2 = \sum \sin^2 t_i,\ \ s_1 = \sum y_i \sin t_i,\ \ s_0 = \sum \sin t_i,$$

$$c_2 = \sum \cos^2 t_i,\ \ c_1 = \sum y_i \cos t_i,\ \ c_0 = \sum \cos t_i,$$

$$u_0 = \sum \sin t_i \cos t_i,\ \ u_1 = \sum y_i,$$

Introducing

$$Q = c_0 s_0 - N u_0 \qquad R = Nc_2 - c_0^2$$

$$S = Nc_1 - c_0 u_1 \qquad D = \frac{R(Ns_1 - s_0 u_1) + QS}{R^2(Ns_2 - s_0^2) - Q^2}$$

the solution is:

$$A = RD \qquad B = QD + S/R$$

$$C = \frac{1}{N}(u_1 - As_0 - Bc_0)$$

$$\tan\phi = B/A \qquad Y_0 = \sqrt{A^2 + B^2}$$

A.5 Chebyshev polynomial approximation

A given weighted tabulated function (x_i, y_i, ω_i), with the normalized argument $x_i \in [-1, +1]$, $i = 0, 1 \ldots, N-1$, is approximated by a polynomial of degree n

$$f_n(x) = \left[\sum_{i=0}^{n} d_{n,i} T_i(x)\right] - \frac{1}{2}d_{n,0} = {\sum_{i=0}^{n}}' d_{n,i}\ T_i(x) \quad \text{(A.7)}$$

where the prime indicates a sum whose first term is halved and $T_i(x)$ are the Chebyshev polynomials calculated with the recurrence

$$T_0(x) = 1$$

$$T_1(x) = x$$

$$T_{i+1}(x) = 2xT_i(x) - T_{i-1}(x)$$

The weights are chosen so that they are a fraction of the population variance:

$$\mathcal{D}[y_i] = \frac{\sigma^2}{\omega_i}$$

A.5.1 Coefficients of the approximation

The method to obtain polynomials which are orthogonal on the arbitrary chosen set of the arguments was developed by Clenshaw (1960) and reviewed by Seber (1977).

The coefficients $d_{n,i}$ are calculated by the recurrence formula:

$$d_{k,i} = d_{k-1,i} + F_k c_{k,i} \quad \text{or} \quad d_{n,i} = \sum_{k=i}^{n} c_{k,i} F_k \qquad (A.8)$$

with

$$\begin{aligned} c_{k+1,0} &= 2c_{k,1} - 2A_{k+1}c_{k,0} - B_k c_{k-1,0} \\ c_{k,k} &= 2 \\ c_{k+1,i} &= c_{k,i+1} + c_{k,i-1} - 2A_{k+1}c_{k,i} - B_k c_{k-1,i} \\ &\quad i = 1, 2 \ldots, k-1 \end{aligned}$$

which produces a triangular matrix of the coefficients:

$$\begin{pmatrix} c_{00} & 0 & 0 & 0 & 0 & 0 \\ c_{10} & c_{11} & 0 & 0 & 0 & 0 \\ c_{20} & c_{21} & c_{22} & 0 & 0 & 0 \\ c_{30} & c_{31} & c_{32} & c_{33} & 0 & 0 \\ & & \cdots & & & \\ c_{n,0} & c_{n,1} & c_{n,2} & c_{n,3} & \ldots & c_{n,n} \end{pmatrix}$$

The coefficients A_k, B_k, and F_k, with the index $k = 0, 1 \ldots, n$, are the sums of the Chebyshev polynomials:

$$A_{k+1} = \frac{1}{H_k} \sum_{i=0}^{N-1} \omega_i x_i p_k^2(x_i) \qquad B_k = \frac{H_k}{H_{k-1}}$$

$$H_k = \sum_{i=0}^{N-1} \omega_i p_k^2(x_i) \qquad F_k = \frac{1}{H_k} \sum_{i=0}^{N-1} \omega_i y_i p_k(x_i)$$

with the Chebyshev polynomials

$$p_k(x) = {\sum_{i=0}^{k}}' c_{k,i}\, T_i(x)$$

which are orthogonal with their weights

$$\sum_{i=0}^{N-1} \omega_i p_k(x_i) p_m(x_i) = 0 \qquad \text{for} \quad k \neq m$$

According to the recurrence relation (A.8), the function $f_n(x)$ can be expressed as the sum

$$f_n(x) = \sum_{k=0}^{n} F_k p_k(x)$$

which follows the relation

$$f_k(x) = f_{k-1}(x) + F_k p_k(x)$$

The first terms of the sums are

$$H_0 = \sum_{i=0}^{N-1} \omega_i \qquad A_1 = \frac{1}{H_0} \sum_{i=0}^{N-1} \omega_i x_i$$

$$F_0 = \frac{1}{H_0} \sum_{i=0}^{N-1} \omega_i y_i \qquad f_0(x) = H_0 F_0^2$$

A.5.2 Calculating the recurrence polynomials

The sum of the Chebyshev polynomial series

$$p_k(x) = {\sum_{i=0}^{k}}' h_i\, T_i(x)$$

with the function $T_i(x)$ obeying the recurrence relation can be effectively calculated by using Clenshaw's recurrence formula (Press et al. 1992, p.181 and Seber 1977). By introducing extra variables g_i, $i = k+2, k+1, k \ldots, 0$, which are calculated according to the recurrence formula:

$$g_i = 2x g_{i+1} - g_{i+2} + h_i$$

with the starting values $g_{k+1} = g_{k+2} = 0$, the polynomial sum is

$$p_k(x) = \frac{1}{2}(g_0 - g_2)$$

A.5.3 Residuals of the approximation

The residual sum of squares

$$\chi_k^2 = \sum_{i=0}^{N-1} w_i \left[y_i - f_k(x_i)\right]^2$$

at different degrees are related as so that

$$\chi_{k-1}^2 = \chi_k^2 + H_k F_k^2$$

The root mean square of the polynomial fit is

$$(\text{rms})^2 = \frac{\chi_n^2}{N-n-1} \cdot \frac{N}{H_0}$$

In fact, according to (A.8), the coefficients of the vector $\mathbf{d} = [d_{n,i}]$ are correlated with each other and the elements of the symmetrical dispersion matrix $\mathcal{D}[\mathbf{d}]_{n\times n}$ consist of the covariances

$$\mathrm{Cov}(d_{n,i}, d_{n,k}) = \frac{\chi_n^2}{N-n-1} \sum_{m=0}^{n} \frac{c_{m,i} c_{m,k}}{H_m}$$

A.5.4 Power series

For the given coefficients $d_{n,i}$ of the polynomial series find the coefficients a_i of the power series, so that

$$f_n(x) = {\sum_{i=0}^{n}}' d_{n,i} T_i(x) = \sum_{i=0}^{n} a_i x^i$$

Let the polynomials $T_k(x)$ be the power series with unknown $b_{k,i}$:

$$T_k(x) = \sum_{i=0}^{k} b_{k,i} x^i$$

Then, according to the reccurence (A.8)

$$\sum_{i=0}^{k+1} b_{k+1,i} x^i = \sum_{i=0}^{k} 2 b_{k,i} x^{i+1} - \sum_{i=0}^{k-1} b_{k-1,i} x^i$$

which gives the relation between the coefficients of the same powers of x:

$$b_{k+1,i} = 2b_{k,i-1} - b_{k-1,i} \qquad k = 2, 3 \ldots, n$$

$$b_{k+1,0} = -b_{k-1,0} \qquad k = 2, 3 \ldots, n$$

$$b_{k,k} = 2b_{k-1,k-1} \qquad k = 1, 2 \ldots, n$$

with the initial values $b_{0,0} = 0.5$, $b_{1,0} = 0$, $b_{2,0} = -1$, and $b_{1,1} = 1$.

The triangular matrix of the coefficients $\mathbf{B} = [b_{k,i}]$ for the first few degrees looks familiar:

	x^0	x^1	x^2	x^3	x^4	x^5	x^6
T_0	0.5						
T_1	0	1					
T_2	−1	0	2				
T_3	0	−3	0	4			
T_4	1	0	−8	0	8		
T_5	0	5	0	−20	0	16	
T_6	−1	0	18	0	−48	0	32

Then, the vector of the unknown coefficients $\mathbf{a} = [a_{n,i}]$ is

$$\mathbf{a} = \mathbf{B}' \cdot \mathbf{d} \qquad \text{or} \qquad a_{n,i} = \sum_{k=i}^{n} b_{k,i} d_{n,k}$$

The dispersion matrix of the coefficients $a_{n,i}$ is

$$\mathcal{D}[\mathbf{a}] = \mathbf{B}' \cdot \mathcal{D}[\mathbf{d}] \cdot \mathbf{B}$$

A.5.5 Scaling the argument of the power series

The original argument of the data $X_i \in [X_{\min}, X_{\max}]$ have to be normalized into $x_i \in [-1, +1]$ as follows

$$x_i = -\frac{X_{\max} + X_{\min}}{X_{\max} - X_{\min}} + \frac{2X_i}{X_{\max} - X_{\min}} = A + BX_i$$

The power series of the Chebyshev approximation with the scaled argument x_i is transformed into one with the unscaled argument X_i with the unknown coefficients q_k:

$$\sum_{k=0}^{n} a_k x^k = \sum_{k=0}^{n} a_k (A + BX)^k = \sum_{k=0}^{n} q_k X^k$$

The vector of the coefficients $\mathbf{q} = [q_k]$ is

$$\mathbf{q} = \mathbf{E} \cdot \mathbf{a}$$

where the triangular matrix $\mathbf{E}_{n\times n} = [e_{i,k}]$ consist of the binomial coefficients:

$$e_{i,k} = B^k \frac{i!}{k!\,(i-k)!} A^{i-k} \qquad \text{for} \quad i \geq k$$

The dispersion matrix of the coefficients $\mathbf{q}$ is

$$\mathcal{D}[\mathbf{q}] = \mathbf{E} \cdot \mathcal{D}[\mathbf{a}] \cdot \mathbf{E}'$$

A.5.6 Two-dimensional Chebyshev polynomials

Given a surface (x, y, z) with the cross-sections along y-axis approximated by the Chebyshev polynomials of degree n_x at the points y_m, $m = 0, 1 \ldots, M$:

$$P(x, m) = {\sum_{i=0}^{n_x}}' p_{im} T_i(x)$$

Then, the coefficients p_{im} can be approximated in the cross-direction for indices $i = 0, 1 \ldots, n_x$ by the polynomials on degree n_y ($n_y < M$) with the y_m as the argument of the fit:

$$Q(i, y) = \sum_{k=0}^{n_y}{}' q_{ik} T_k(y)$$

The matrix q ($n_x \times n_y$) is used for the polynomial evaluation of the surface:

$$f(x, y) = \sum_{i=0}^{n_x}{}' \left[\sum_{k=0}^{n_y}{}' q_{ik} T_k(y) \right] T_i(x)$$

as well as, if the argumens are interchanged:

$$f(x, y) = \sum_{k=0}^{n_y}{}' \left[\sum_{i=0}^{n_x}{}' q_{ik} T_i(x) \right] T_k(y)$$

A.6 Cubic spline approximation

For the given tabulated function (x_k, y_k), $k = 0, 1 \ldots, n-1$, the interpolating cubic spline (Press et al. 1992, p.113) is a set of piecewise cubic polynomials joined at the distinct points x_k, also known as the knots. The polynomial on the interval $[x_i, x_{i+1}]$ is

$$s_i(p) = a_i + b_i p + c_i p^2 + d_i p^3$$

where

$$p = \frac{x - x_i}{h_i} \qquad h_i = x_{i+1} - x_i$$

with the following boundary conditions:

$$\begin{matrix} s_i(0) = y_i & s_i''(0) = y_i'' \\ s_i(1) = y_{i+1} & s_i''(1) = y_{i+1}'' \end{matrix} \qquad s_i'(1) = s_{i+1}'(0)$$

The solution can be written as:

$$s_i(p) = q y_i + p y_{i+1} + Q y_i'' + P y_{i+1}'' \qquad \text{(A.9)}$$

where

$$q = 1 - p$$

$$P = \frac{1}{6}(p^3 - p) h_i^2 \qquad Q = \frac{1}{6}(q^3 - q) h_i^2$$

and

$$s_i'(p) = \frac{y_{i+1} - y_i}{h_i} - h_i \left[\frac{3q^2 - 1}{6} y_i'' - \frac{3p^2 - 1}{6} y_{i+1}'' \right]$$

$$s_i''(p) = q y_i'' + p y_{i+1}''$$

$$s_i'''(p) = \frac{y_{i+1}'' - y_i''}{h_i}$$

The polynomial coefficients are given by

$$d_i = \frac{h_i^3}{6} s_i'''(0) = \frac{h_i^2}{6}(y_{i+1}'' - y_i'')$$

$$c_i = \frac{h_i^2}{2} s_i''(0) = \frac{h_i^2}{2} y_i''$$

$$a_i = y_i$$

$$b_i = h_i s_i'(0) = y_{i+1} - (a_i + d_i + c_i)$$

The second derivatives can be found from the system of linear equations:

$$\begin{cases} 0 & + \hat{u}_0 y_0'' & + \hat{v}_0 y_1'' & = D_0 \\ v_{i-1} y_{i-1}'' & + u_i y_i'' & + v_i y_{i+1}'' & = D_i \\ \hat{v}_{n-2} y_{n-2}'' & + \hat{u}_{n-1} y_{n-1}'' & + 0 & = D_{n-1} \end{cases} \qquad \text{(A.10)}$$

where $i = 1, 2 \ldots, n-2$.

$$v_i = \frac{h_i}{6} \qquad u_i = \frac{h_{i-1} + h_i}{3}$$

$$D_i = \frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}} = y_i' - y_{i-1}'$$

One has $n - 2$ equations with n unknowns y_i''. The unknowns y_0'' and y_{n-1}'' can be found according to the boundary conditions:

I $s_0'(0) = a \quad s_{n-1}'(1) = b$
$\hat{u}_0 = h_0/3 \quad \hat{u}_{n-1} = h_{n-2}/3$
$\hat{v}_0 = v_0 \quad \hat{v}_{n-1} = v_{n-1}$
$D_0 = y_0' - a \quad D_{n-1} = b - y_{n-1}'$

II $s_0''(0) = a \quad s_{n-1}''(1) = b$
$\hat{u}_0 = \hat{u}_{n-1} = 1$
$\hat{v}_0 = \hat{v}_{n-2} = 0$
$D_0 = a \quad D_{n-1} = b$

The smoothing spline $\tilde{s}$ is the interpolating spline which goes through the smoothed points of noisy data and minimizes the functional (de Boor 1978, Voskoboynikov et al. 1984)

$$\chi^2(\tilde{s}) = \sum_{i=0}^{n-1} \frac{[\tilde{s}(x_i) - y_i]^2}{\sigma_i^2} + \alpha \int_{x_0}^{x_{n-1}} [\tilde{s}''(x)]^2 \, dx$$

The smoothing parameter $\alpha \geq 0$ governs the tradeoff between the fit and smoothness of the curve. Small values of α favor jagged curves that follow the data points closely: choosing $\alpha = 0$ means that the spline becomes interpolating and goes through the points of data. Large values of α favor smoother curves that do not adhere so closely to the data.

The minimum of the functional is achieved if the spline goes through the new points of data calculated according to the following relations:

$$\begin{aligned} \tilde{y}_0 &= y_0 - \alpha\sigma_0^2 \, y_0''' \\ \tilde{y}_i &= y_i - \alpha\sigma_i^2 \, \left(y_i''' - y_{i-1}'''\right) \\ \tilde{y}_{n-1} &= y_{n-1} + \alpha\sigma_{n-1}^2 \, y_{n-2}''' \end{aligned} \tag{A.11}$$

where the third derivative is calculated from the second

$$y_i''' = \frac{y_{i+1}'' - y_i''}{h_i}$$

Replacing y_i by the $\tilde{y}_i$ on the right hand side of the system of equations (A.10), a new, 5-diagonal system of linear equations (A.12) is obtained.

$$A_i = \frac{\sigma_i^2 + \sigma_{i+1}^2}{h_i^2} \qquad B_i = \frac{\sigma_{i+1}^2}{h_i h_{i+1}}$$

$$u_i = \frac{h_{i-1} + h_i}{3} + \alpha\left[A_{i-1} + 2B_{i-1} + A_i\right]$$

$$v_i = \frac{h_i}{6} - \alpha\left[B_{i-1} + A_i + B_i\right]$$

$$w_i = \alpha B_i$$

with the elements are set to zero at the ends:

$$A_{-1} = B_{-1} = h_{-1} = 0$$

$$A_{n-1} = B_{n-2} = B_{n-1} = h_{n-1} = 0$$

Thus, one has $n-2$ equations with n unknowns y_i''. Two unknowns y_0'' and y_{n-1}'' can be found from one of the kinds of boundary conditions:

I	$s_0'(0) = a$	$s_{n-1}'(1) = b$
	$D_0 = y_0' - a$	$D_{n-1} = b - y_{n-1}'$
	$\hat{u}_0 = u_0$	$\hat{v}_0 = v_0$
	$\hat{w}_0 = w_0$	$\hat{u}_{n-1} = u_{n-1}$
	$\hat{v}_{n-2} = v_{n-2}$	$\hat{w}_{n-3} = w_{n-3}$
II	$s_0''(0) = a$	$s_{n-1}''(1) = b$
	$\hat{u}_0 = 1$	$\hat{v}_0 = v_0 = 0$
	$\hat{w}_0 = w_0 = 0$	$\hat{u}_{n-1} = 1$
	$\hat{v}_{n-2} = v_{n-2} = 0$	$\hat{w}_{n-3} = w_{n-3} = 0$
	$D_0 = a$	$D_{n-1} = b$
VI	$s_0''(0) = as_0''(1)$	$s_{n-1}''(1) = bs_{n-1}''(0)$
	$\hat{u}_0 = 1$	$\hat{v}_0 = v_0 = -a$
	$\hat{w}_0 = w_0 = 0$	$\hat{u}_{n-1} = 1$
	$\hat{v}_{n-2} = v_{n-2} = -b$	$\hat{w}_{n-3} = w_{n-3} = 0$
	$D_0 = 0$	$D_{n-1} = 0$

Combining interpolation equation (A.9) with the smoothed values as in (A.11), one can get general form of the smoothing spline formule:

$$\tilde{s}_0(p) = s_0(p) - \alpha\sigma_0^2 \, [(q-p)y_0''' + py_1''']$$

$$\tilde{s}_i(p) = s_i(p) - \alpha\sigma_i^2 \, \left[(q-p)y_i''' - qy_{i-1}''' + py_{i+1}'''\right]$$

$$\tilde{s}_{n-2}(p) = s_{n-2}(p) - \alpha\sigma_{n-2}^2 \, \left[(q-p)y_{n-2}''' - qy_{n-3}'''\right]$$

In practice, however, it is worthwhile first to calculate the smoothed points of data $\tilde{y}_i$ by using equation (A.11), and then to use interpolation spline equation (A.9) as the folloing:

$$\tilde{s}_i(p) = q\tilde{y}_i + p\tilde{y}_{i+1} + Qy_i'' + Py_{i+1}''$$

$$\left\{\begin{array}{llllll} 0 & +\ 0 & +\ \hat{u}_0 y''_0 & +\ \hat{v}_0 y''_1 & +\ \hat{w}_0 y''_2 & = D_0 \\ 0 & +\ v_0 y''_0 & +\ u_1 y''_1 & +\ v_1 y''_2 & +\ w_1 y''_3 & = D_1 \\ w_{i-2} y''_{i-2} & +\ v_{i-1} y''_{i-1} & +\ u_i y''_i & +\ v_i y''_{i+1} & +\ w_i y''_{i+2} & = D_i \\ w_{n-4} y''_{n-4} & +\ v_{n-3} y''_{n-3} & +\ u_{n-2} y''_{n-2} & +\ v_{n-2} y''_{n-1} & +\ 0 & = D_{n-2} \\ \hat{w}_{n-3} y''_{n-3} & +\ \hat{v}_{n-2} y''_{n-2} & +\ \hat{u}_{n-1} y''_{n-1} & +\ 0 & +\ 0 & = D_{n-1} \end{array}\right. \tag{A.12}$$

where $i = 2, 3 \ldots, n-3$.

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