

Appendix C

Xvoigt

This Appendix contains a copy of the user documentation for the Xvoigt line-fitting software which was developed by me, with help from Geoff Bailey. This version of the documentation is for Version 3.0 of Xvoigt, dated 25 July, 1994.

Xvoigt has been described in the paper: Mar and Bailey (1995).

C.1 Introduction

Xvoigt is a program which allows the interactive fitting of Voigt profiles to atomic absorption lines in astronomical spectra. It is designed for use under the X Window System¹, running on a UNIX² operating system.

This document assumes you have access to a working copy of Xvoigt on your computer system. If not, information on getting a copy and installing Xvoigt can be found in Section C.10.

Please read the disclaimer notice in Section C.2.2 before using Xvoigt.

C.1.1 The Philosophy of Xvoigt

Xvoigt is an *interactive* program. This means the human user is required to make judgements on the appropriateness of the fits it produces. In a day and age where automation and objectivity are seen as virtuous (at least in science), this may seem like a step backwards. After all, many researchers regularly use automated line-fitting programs to analyse their data. So why use Xvoigt?

Automated line-fitting programs can do well with data of high signal-to-noise ratios. However, when one is dealing with data of signal-to-noise ratio ~ 10 or less, the ability of such programs to distinguish reality from noise-related effects is not so clear. Here is where experience and the processing power of the human brain come into their own.

¹X Window System is a trademark of the Massachusetts Institute of Technology.

²UNIX is a trademark of Bell Laboratories.

Another advantage of analysing your data manually is that you are *involved* with the process all the way. A result produced by an automatic program at a formal significance level of 99.99% is all well and good, but someone should actually *look* at the fit at some stage!

Having made these points, I hope you use your experience and best judgement to determine whether or not Xvoigt is an appropriate tool for analysing your data.

C.2 Release Notes

C.2.1 Copyright

The Xvoigt program and all accompanying documentation are Copyright 1994, David Mar. Permission is granted to distribute the material, provided no charge is levied. Permission is granted for users to modify the program code for personal use, but I would greatly appreciate it if modified versions of Xvoigt were *not* distributed.

C.2.2 Disclaimer

Although I have taken great care to ensure that Xvoigt produces physically correct outputs, I cannot guarantee any of the results, nor accept liability for any erroneous results which may occur.

I have tested results from Xvoigt against the established programs ALAS and APIG, and in all of my tests the results produced were identical. Perhaps the best guarantee I can give is that I am using results from Xvoigt as part of my PhD thesis.

Xvoigt compiles on a Sun³ machine using the GNU C compiler gcc. Xvoigt is written in ANSI C, so the default Sun C compiler cc cannot be used without various ANSI-enabling options (at least on my system). I have not explored these options, since I find gcc's default behaviour nicer.

I have not tried compiling Xvoigt on other machines, and have little idea of how portable it might or might not be. If you successfully port Xvoigt to a different machine, please notify me so I can include the information in future releases.

C.2.3 Bug Reports

If you uncover any bugs in Xvoigt—particularly any which cause it to produce incorrect output—please report them to me, preferably by e-mail. I also welcome any comments, or suggestions for extra features.

³Sun is a trademark of Sun Microsystems.

C.3 Preparing to Use Xvoigt

In this manual it is assumed that you have some familiarity with UNIX and the X environment and know how to do the following:

- Work with directories and pathnames of files.
- Use the mouse or trackball to move the pointer around the screen and click various areas.
- Select specific windows and manipulate them by moving, resizing, etc.

If you need any help with these points, it is probably best to ask a friendly local with more experience at using UNIX and X.

Before running Xvoigt, it is important to make sure that your spectral data exist in files in the correct format. The data must be:

- listed in plain ASCII files;
- normalised;
- listed with a pair of numbers on each line, representing the wavelength and normalised intensity respectively, separated only by white space (blanks or tabs);
- listed in order of increasing wavelength.

The Figaro routine `alasoout` produces output in a format suitable for use in Xvoigt.

If your data have been recorded in a redshifted frame, there is no need to convert the wavelengths to the rest frame. Xvoigt automatically calculates and takes redshifts into account for you.

If you have non-overlapping data in several separate files (high resolution echelle data with inter-order gaps, for example), it is a good idea to concatenate them together into one large file. This will save you having to load several different data files each time you run Xvoigt. You can also combine overlapping data, but it's up to you how to deal with the overlapping regions (by averaging the intensities or whatever)—just make sure the result is monotonically increasing in wavelength.

If you have overlapping data which you *do not wish to combine* for some reason (comparing fits on high and low resolution data of the same wavelength region, for example), then leave them in separate files, to be loaded into Xvoigt individually. You only need to leave files separate if they overlap; if you have non-overlapping data of different resolutions you may as well concatenate them together to save yourself some time later.

Since Xvoigt requires full path names of any data files which you want to use and which are not in your current working directory, it is simplest to change into a working directory which contains all the relevant files before beginning your Xvoigt session.

Sections C.4 and C.5 explain in detail how to invoke and use Xvoigt. If you would prefer to follow a tutorial session with sample data, you can skip straight to Section C.6 and return to Sections C.4 and C.5 later.

C.4 Invoking Xvoigt

To run Xvoigt, simply make sure that the Xvoigt executable is accessible from your working directory and type the command `xvoigt`. If you store the executable in another directory which is not included in your search path, then you will have to type the full path name.

Xvoigt begins by prompting for a file name. Type in the name of the first file you want to analyse.

```
Enter normalised spectrum file name : somedata.dat
```

Xvoigt then reads the data, which may take several seconds if the file is large. It then prompts for a central wavelength. Type in the *observed* wavelength of the first line you wish to analyse. *If the line is redshifted, this will not be equal to the rest wavelength.*

```
Enter observed central wavelength of line (Angstroms) : 1234.567
```

Xvoigt prompts for the instrumental b value at this wavelength. This is related to the full-width at half-maximum resolution by

$$b = \frac{\text{FWHM}}{2\sqrt{\ln 2}} \simeq 0.60056 \text{ FWHM}. \quad (\text{C.1})$$

```
Enter instrumental b value [= FWHM/(2 sqrt(ln 2))] (km/s) : 4.5
```

Xvoigt asks for an identification of which particular absorption line you are analysing. It uses this information to determine both the line's redshift and its quantum line strength parameters. You can enter either the line's rest, vacuum wavelength (truncated to a whole number) or a special ID code (listed in Section C.9). Xvoigt will either confirm your selection, or inform you that you have selected a line which it does not know.

```
Enter absorption line ID or rest, vacuum wavelength.
('?' for list of known lines, '.' to define your own) : 1215
```

```
Selected line is H I 1215.6701
```

If you type a question mark at this prompt, Xvoigt will print a list of all the lines it knows. If you type a dot, you can define a line which Xvoigt does not already know. You will need to know the accurate wavelength and the f_k^1 , q_k and q_1 numbers of the atomic transition to define lines in this way. See Section C.7 for more details on defining your own lines. Once a line is selected, Xvoigt automatically calculates the redshift.

Finally, Xvoigt prompts for a velocity scale range to use for its initial graphics plot. The plot will be centred at the wavelength you entered previously, and extend to \pm the velocity range you enter here. The total range of the plot is therefore twice the velocity you enter.

```
Enter half-velocity range (km/s) : 200
```

Xvoigt now performs some calculations and then generates a new window, in which it will display graphics. Position the window where it is convenient on your screen, preferably in such a way that you can still see as much of the window in which you invoked Xvoigt as possible. Messages are printed to this window, so it is a good idea not to obscure the bottom portion of it. From now on, this window will be called the *message window*.

The graphics window will contain the section of spectrum from the data file you have selected, plotted as a histogram, with an initial Voigt profile plotted over the top. You are now ready to analyse the line you have chosen.

C.5 Interacting with Xvoigt

Most of the interaction with Xvoigt is via the mouse (or trackball). The keyboard is also used to type in certain values or names, and can be used as an alternative for issuing many of the mouse-driven commands. This section will explain all of the Xvoigt commands and how to use them.

C.5.1 Scroll-Bars

The basic manipulation of the absorption cloud model is done using the three scroll-bars below the graph display in the main window.

By using the mouse to drag the square white “slider” in each scroll-bar, you can modify the velocity dispersion b , the cloud’s velocity offset v , and its column density (displayed logarithmically as $\log N$). The calculated Voigt profile shown in the graph changes immediately to reflect the new parameter values. You can also change the parameter values by clicking inside the left or right arrows at the ends of the scroll-bars. Each click increments or decrements the parameter by a fixed step size. Holding the mouse button down in one of these arrows gives continuous incrementing or decrementing until the button is released.

The current values of the parameters are displayed above the appropriate scroll-bars, near the centre of each bar. These values update automatically whenever changes are made. The minimum and maximum values available from the scroll-bar are displayed to the left and right of the current value, respectively.

If you need a parameter value outside the current range of its scroll-bar, there are two ways to get it. You can place the slider at the end of the bar closest to the value you want (either by dragging it or holding down the mouse button with the

pointer on a scroll arrow), and then use the scroll arrow to increase/decrease the value further. The current value will change, and so will the minimum/maximum values of the scroll-bar.

Alternately, you can click the mouse pointer on the “coarse” button below the scroll bar. This will increase the range of the scroll-bar by a factor of ten (or two in the case of $\log N$). (NB: The way in which the scroll bar ranges increase is a little non-intuitive. A little experimentation should make it clear how it works. This will be changed in the near future to a hopefully more intuitive method.) If you need to, you can keep clicking the button to multiply the range further. Then simply move the slider to the required parameter value. Be careful with large scroll-bar ranges, because the parameter adjustments become very sensitive to the slider position. If you wish to decrease the slider range again for finer adjustments, simply click the “fine” button under the appropriate scroll bar. This decreases the range by a factor of ten (or two for $\log N$). You can use these buttons at any time for fine-tuning of parameter values.

There are keyboard equivalents for both of these commands. With the mouse pointer positioned *in the relevant scroll bar*, hitting the ‘i’ key increases the range and hitting the ‘m’ key decreases it.

C.5.2 Equivalent Width and Residual Calculations

Displayed in the graphics window are the equivalent widths of both the calculated profile and the data shown and the sum of the squares of the residuals between the calculated profile and the data file points. These values appear below the graph and above the scroll-bars. They are also updated automatically when the cloud model parameters are changed.

There are three equivalent widths shown. The one labelled **Full EW** is integrated across the entire theoretical profile displayed. If your profile is so wide that it extends beyond the limits of the graph (for example, with a strongly damped line), then the equivalent width only includes the part of the line within the graph borders.

The equivalent widths labelled **Prof EW** and **Data EW** are the widths of the theoretical profile and the real data respectively, integrated over a more restricted range. This range is initially set to cover the whole graph display as well but this can be changed. This is useful so that you can avoid including large amounts of continuum or adjacent absorption lines in the equivalent width calculation.

If you click with the mouse pointer inside the graph area, a vertical line will appear. This now indicates the leftmost data point which will be included in the equivalent width calculation. You can switch to positioning the rightmost point marker by clicking the “R marker” button to the side of the graph display. Now any clicks in the graph area will reposition the right marker. Note that the “R marker” button changes to read “L marker”. Click on the “L marker” button to switch back to adjusting the left marker.

If you want finer control over the positioning of the markers, the “Move left” and “Move right” buttons will move the currently selected marker by one data point to

the left or right, respectively. The markers are actually positioned *between* data points, so that any points between the markers are included in the calculations and there is no ambiguity about points positioned on a marker. This may not be apparent if the number of data points displayed approaches or exceeds the number of screen pixels across the graph. In this case, moving a marker by one data point with the “Move” buttons may result in no movement across the screen, but in Xvoigt’s memory the marker has actually been moved by one data point. If a marker is moved off the edge of the display, it reverts to the default of including points all the way to the graph edge.

Each of these commands can be also issued from the keyboard. Hitting the ‘r’ key selects the right marker, ‘e’ selects the left marker (note the behaviour is different to the single “R/L marker” button). The ‘j’ and ‘k’ keys move the selected marker left and right just like the “Move” buttons.

The number labelled **Residual** is the sum of the squares of the differences between the theoretical profile and the data points, at the wavelengths given by the data points. The residual calculation limits are also dependent on the positions of the graph markers, again allowing regions of continuum or neighbouring absorption to be excluded.

C.5.3 Residual Display

You can also display the residuals from profile fitting by clicking the “Residual” button. This changes the graphics display to show the residual data after the fitted profile has been subtracted away. The fitted profile itself remains visible for reference. You can still alter the cloud model while in residual mode, and watch the changes in the residual data as you do so. The display may flicker when doing this—this is because the calculations involved are much more numerous than when in normal mode and the screen cannot update as often. In residual mode the “Residual” button changes to read “Profile”. Clicking on the “Profile” button switches back into normal profile-fitting mode. Residual mode cannot be accessed with a keyboard command.

C.5.4 Adding More Clouds to the Model

Often a single Voigt profile is insufficient to fit the observed line profile adequately. Xvoigt allows you to add further cloud components to the model, calculating the composite profile for you.

To add a new cloud to the model, click the “Add cloud” button. A new profile with default cloud parameters is added to the original profile. You may now manipulate the parameters of the new cloud with the scroll-bars.

While changing the new cloud, the old cloud remains unaffected. You can see which cloud you are currently modifying, and how many clouds are in the model altogether, by checking the cloud number which is displayed at the top of the main

graph area. There is a vertical line at the bottom of the graph which shows the position of the centre of the individual profile you are now considering.

If you wish to switch back to the previous cloud to modify its parameters some more, click the “Prev cloud” button. Note that the “Add cloud” button then changes to read “Next cloud”. Clicking on “Next cloud” switches you to the ‘next’ cloud in the model; *i.e.* the cloud numbered one higher than the currently considered cloud. You can switch between clouds as often as you like. To add further clouds to the model, click “Next cloud” until you reach the last cloud in the model. The button will change to read “Add cloud” again and you can click it to do so.

If you accidentally add more clouds than are necessary, or if you decide that you prefer your fit with fewer clouds, you can delete the current cloud by clicking the “Zap cloud” button. Xvoigt will first prompt with a message in the message window to make sure you want to remove this cloud. Be careful! Once you have zapped a cloud, you cannot recover its parameters except by adding a new cloud and using the scroll-bars again. If you really want to remove the cloud, *select the message window* and type ‘y’ as your answer, otherwise (if you clicked the “Zap cloud” button accidentally, or just change your mind) select that window and type ‘n’.

Again, all these commands are available from the keyboard. The “Add/Next cloud” function is accessed by positioning the mouse pointer in the main graph area and hit the ‘i’ key. (Note that this is the same key used to increase the range of scroll-bars. The difference in behaviour is determined by the pointer position.) The “Prev cloud” function is accessed by hitting the ‘m’ key with the mouse pointer in the main graph area. (Again, this key doubles for use with the scroll-bar ranges.) You can zap the current cloud by hitting ‘z’ on the keyboard (this also prompts to make sure).

C.5.5 Analysing Several Ion Transitions at Once

Often there will be more than one atomic transition from a particular ion you are examining in the spectrum. Xvoigt allows you to analyse several different transitions simultaneously, applying the same cloud model to each and checking all of the lines to see how well the model matches the data.

Once you have selected your first atomic transition and are ready to fit your cloud model, you can add another transition to the analysis by clicking the long “Add new ion” button near the top of the button area.

You will be prompted for the instrumental b value at the wavelength of the new line. Then you will be asked which transition the new line is. This works in the same way as selecting the initial transition. Once you have chosen a transition, Xvoigt automatically calculates the correct wavelength to display, using the same redshift as the first line you defined.

The new section of spectrum is displayed, complete with the same cloud model as before. The atomic ion and wavelength of the current transition are displayed in a highlighted button near the top of the button area. You can change the current

transition by clicking on a button with the name of a different transition in it. There are also square “check boxes” next to each ion button. These indicate which ions are “switched on” in the current redshift model. It is possible to have ions loaded into Xvoigt, but not currently being used — this is indicated with an empty check box. Ions with check boxes on will be plotted as Voigt profiles on the screen, those with the check boxes off will not. You can toggle the check boxes by clicking in them. Note that the *same* cloud model applies to all the transitions selected. Changes made while looking at one transition will affect the model for all the transitions.

(Important note: If you are examining a close doublet, for example, and both lines in the doublet fall on the screen, Xvoigt will *not* display the fit to both lines simultaneously while you are examining the cloud concerned. This is something I definitely want to fix in the next release of Xvoigt. However, you *can* see the effect of both the doublet lines when you switch to a different cloud, or to a different redshift model. The simplest way to see the profiles of both pairs of a doublet simultaneously is to use a “dummy” cloud in the model with column density low enough to make no difference to the other fits. Adjust the relevant cloud and switch back and forth with the dummy cloud to see what the doublet looks like.)

The left and right markers for residual calculation limits, however, *do* change from transition to transition. You should set them up appropriately for each transition — they will be saved as you change between transitions. This is so that you can treat each section of spectrum individually to get the best results out of the residual calculations. Note that when you change transitions, the left residual marker is selected automatically for the new transition, so you will have to select the right marker first if you want to change its position.

These commands are available from the keyboard by hitting the ‘a’ key to add a new transition, and hitting the ‘c’ key, which cycles through the full list of transitions one by one.

C.5.6 Overlaying Data from Several Transitions

It is often useful to overlay the spectral data from several atomic transitions on a common velocity scale, so that homologous or analogous lines can be compared in structure. To activate this feature, click on the “Overlay” button. The data from the current transition remain on screen, possibly in a different colour, and the theoretical profile disappears. You can now select additional transitions to plot overlaid on the same velocity scale by clicking the appropriate transition buttons in the top right corner of the window. The data from the selected transitions appear on the plot, in different colours on colour monitors so they can be distinguished. The colour coding is shown by coloured highlighting of the appropriate transition buttons.

You can switch any given transition on or off individually by clicking its button. (You can also use the check boxes, but remember that these control which ions are plotted as Voigt profiles when you switch back to normal mode.) To switch back to non-overlay mode and continue profile fitting, click the “Overlay” button — whose

name has changed to read “Normal” — again. You can combine overlay and residual modes to examine the fitting residuals of several transitions together if you wish. Overlay mode cannot be accessed by keyboard commands.

C.5.7 Adding Extra Models

Sometimes there will be several lines from different ions at different redshifts either overlapping or very close together. You can analyse all of these simultaneously by adding new cloud models at different redshifts.

To add a new model, click the “Add model” button. You will be prompted for an observed wavelength, an instrumental b value, and an ion transition ID. Xvoigt then adds a new “z=” button with the redshift of the new model, and displays the relevant data and profiles on the screen, beginning with a default Voigt profile as usual. If the profiles from the other redshift models are in the wavelength region shown on the screen, then they will be shown, and a composite profile of several different ions at several different redshifts can be built up if necessary.

The redshift model currently being considered is shown with a highlighted button. You can switch to other redshift models by clicking on the appropriate buttons. Note that the ion check boxes may not be the same for each model. Xvoigt remembers which ions are checked for each model individually, and uses that knowledge to work out for which ions Voigt profiles should be plotted.

C.5.8 Saving and Loading Models

Once you are happy with a cloud model, you can save the relevant data to a file for reference, or for loading back into Xvoigt later.

To save the details of a cloud model, select the redshift model you wish to save and click the “Save Model” button. The message window will prompt you for a file name. Select that window and type one in. If no file with that name exists, Xvoigt will create it and save the model parameters in it. If you provide the name of an existing file, Xvoigt will append the model data to that file; this is useful because it allows you to keep all the models for a single spectrum in the one file.

Xvoigt saves cloud models as ASCII data, with one cloud per line, in the following format:

```
1 4530.6114 34.00 15.400 H_I 1215.6701 3.80
1 4528.7331 8.00 12.700 H_I 1215.6701 3.80
1 4532.4293 34.00 13.600 H_I 1215.6701 3.80
2 4532.9480 8.00 13.833 C_IV 1550.7700 3.80
```

The columns are, in order:

- A reference number which identifies all of the clouds in a given model.
- The observed wavelength of the cloud.

- The b value of the cloud.
- The $\log N$ value of the cloud.
- The ionic species of the cloud.
- The rest wavelength of the transition for that species.
- The instrumental b value at the observed wavelength.

These data files can be reformatted either manually or by using a simple program (such as an `awk` script) to produce tables suitable for publishing.

When a model is saved, Xvoigt assigns to all the clouds of that model a common reference number, so the model can be identified later. If the model is appended to an existing file, the number chosen is the next integer greater than the largest already in the file. In the example above, there are two cloud models, the first consisting of three H I $\lambda 1215$ clouds and a C IV $\lambda 1550$ cloud.

Later, you can load saved models into Xvoigt from these files. Click on the “Load Model” button and a prompt will appear in the message window requesting a file name. When you type a name, Xvoigt will ask for a cloud model reference number—you should make sure you know which one to use! Xvoigt will then load the data from the file, adding the model as a new redshift system.

Note that when you save a model, the file only contains the ionic transition information for one transition. When the data are reloaded, you can always add any other transitions you wish by selecting them from the set of ion buttons. If you wish to save the data for several transitions in the one redshift system (so you have all the observed wavelength information, for example), you can select each ion in turn and use the “Save Model” command repeatedly.

C.5.9 Working on Several Data Files

Normally you would have all of your data in one file. However, if you wish to examine the fits to data in several different files, you can do that by adding new files to the analysis.

To add a new file, click on the “Add file” button. You will be prompted for the file name, and Xvoigt will dutifully load the file if it finds it.

When working with several files, you can switch between them at will by clicking on the appropriate “File (number)” button. The currently used file has its button highlighted for reference. When you switch between different ions or redshift models, Xvoigt remembers which file was last associated with each particular combination of model and ion, so when you switch back you will be looking at the same data as the previous time.

C.5.10 Saving Profiles

If you are happy with the result of your profile fitting, you can save the calculated Voigt profile to a file so that you can refer to it later, or use it as input to some other program.

Click on the “Save Prof” button. The message window will prompt you for a file name. Select the window and type in a name. Xvoigt will save the calculated Voigt profile to that file. If the file name you give already exists, Xvoigt will check to see if you wish to overwrite the existing file before writing anything. The file is saved in the same sort of format as input files, with wavelengths and normalised intensities as pairs of numbers, one per line. The keyboard equivalent of the “Save Prof” command is hitting the ‘w’ key.

C.5.11 Producing a Hard Copy

Xvoigt can also produce a hard copy version of your fitted profile, residual data, or overlaid transition plots. Simply configure the graphics area to look the way you want it, then click the “Hard copy” button. You will be prompted for a file name in the message window; select that window and type one in. You will also be prompted for a plot title; enter any descriptive text you wish — it will appear at the top of the hard copy plot. Xvoigt will then produce a PostScript⁴ output file in the file name you have specified. If a file with that name already exists, Xvoigt will ask you if you wish to delete it.

The PostScript output file can be printed on any PostScript printer, viewed with a software PostScript viewer, or included as a graphic in some other document. PostScript output produced by Xvoigt fully conforms to Adobe System’s specifications for Level 1 Conforming PostScript.

C.5.12 Other Commands

If at any stage you wish to change the range of the graph display, you can click the “New range” button. A prompt will appear in the message window asking for a new half-velocity range. Select the window and type in your new range. The graph will update instantly to the new range. Changing the range does not affect the cloud model in any way. If the residual limit marker points move off screen, then the markers are reset to the edge of the display (and a warning is printed in the message window), otherwise they stay at the points set. This command’s keyboard equivalent is hitting the ‘v’ key.

Another useful command is accessed by clicking the “Wavelength” button. This changes the x-axis labels on the graph display to wavelength units. The button name also changes, to “Velocity”, and can be used to switch back to velocity units. Switching between these labels has no effect on anything else. The keyboard equivalent is the ‘t’ key.

The button labelled “Dots” can be used to change the data histogram plot to one which uses dots to represent the data values. You may find this useful, although I always prefer to look at histograms. When in dotted mode, the button changes to

⁴PostScript is a registered trademark of Adobe Systems Incorporated.

read “Histogram”, and can be clicked to change the data back to a histogram plot. This can also be done using the ‘d’ key.

If you want to work on a new absorption system in the same data file, click the “New model” button. It clears all of the current cloud models completely and allows you to start afresh in a new section of spectrum. If you wish to reset Xvoigt and start from scratch with a new data file, click the “Reset” button. Both of these commands issue appropriate prompts in the message window, beginning with a warning that all data on the current models will be lost and the option to abort the command. You will have to select that window and answer them. The keyboard equivalents are the ‘l’ key for a new model, and ‘f’ for reset.

The ‘h’ (or ‘help’) key causes a list of all the command keys and their actions to be printed to the message window. This command has no button (since if you are using the buttons you shouldn’t need reminding!).

C.5.13 Quitting Xvoigt

When you are finished using Xvoigt, simply click the “Quit” button. A prompt appears in the message window to confirm that you want to quit. Select that window and type ‘y’ if you do want to quit, or ‘n’ if you don’t (because you clicked “Quit” accidentally, for example). If you do quit, Xvoigt will close the graphics window and return a UNIX system prompt for you in the message window. You can also quit by hitting the ‘q’ key.

If worst comes to worst and Xvoigt starts doing strange things which you don’t understand, you can usually kill it by selecting the message window and hitting `ctrl-c`, the standard UNIX escape sequence.

C.6 A Tutorial

This section will take you step by step through an Xvoigt session with the sample data which accompanies this manual. Make sure you have the files `sample.dat` and `sample.model` in your working directory, and type `xvoigt`. Answer the prompts as follows:

```
Enter normalised spectrum file name : sample.dat
Enter observed central wavelength of line (Angstroms) : 4529
Enter instrumental b value [= FWHM/(2 sqrt(ln 2))] (km/s) : 3.8
Enter absorption line ID or rest, vacuum wavelength.
('?' for list of known lines, '.' to define your own) : c4a
Selected line is C IV 1550.7700
Enter half-velocity range (km/s) : 400
```

Xvoigt will generate a new window, which you can position as you wish. Make sure you can still see the bottom of the original window, since Xvoigt prints messages

to that window. The original window is referred to as the *message window*, while the new window is the *main window*.

In the main window, you will see a portion of spectrum, and an initial Voigt profile in the centre. The C IV $\lambda 1550$ line is the deep absorption line on the right side. The first thing to do is move the cloud in velocity until it matches the wavelength of the absorption.

Click once on the “coarse” button underneath the central scroll bar. This scroll bar controls the cloud’s Doppler velocity, and we need to increase the range of the bar to move the cloud far enough. Drag the scroll bar slider to the right end of the bar. The Voigt profile on the screen will move across to the 200 km s^{-1} mark on the x-axis. This is not quite far enough, so click a few times on the right arrow at the end of the scroll bar, or hold the mouse button down and watch the Voigt profile move across until it lines up with the absorption at a bit beyond 250 km s^{-1} .

Now make the profile a bit narrower by adjusting the b scroll bar to a value of about 8. Increase the strength of the profile on the $\log N$ bar to about 13.8. You should now have a reasonable fit to the absorption line.

The deep line at the far left is the matching C IV $\lambda 1548$ line. Add this line to the analysis by clicking on the “Add new ion” button and answering the prompts in the message window as follows:

```
Enter instrumental b value [= FWHM/(2 sqrt(ln 2))] (km/s) : 3.8
Enter absorption line ID or rest, vacuum wavelength.
('?' for list of known lines, '.' to define your own) : c4b
Selected line is C IV 1548.2020
```

A new button appears, showing the ion, and the data on the screen move to show the fit to the 1548 line. (The data are truncated to show only a small spectral region, so don’t worry about the lack of data to one side.) Click on the C IV 1550.77 button to switch the view back. Unfortunately, the current version of Xvoigt will not show both of these profiles simultaneously while you are examining this cloud model—this will be rectified in the future!

But now let’s fit the other absorption lines. They are Lyman α lines at a higher redshift. I have saved some parameters into a file, so you can load them without having to play with the scroll bars. Click on the “Load model” button and answer the prompts as follows:

```
Load cloud model from file:
Enter file name to use : sample.model
Enter cloud model reference number : 1
Loading...
Cloud model loaded from file: sample.model
```

Xvoigt loads three clouds at a redshift of 2.7, adding a new button to the array of redshift model buttons. It also asks you for some instrumental b value information

(since it needs it to calculate profiles), but you will not be looking at the particular wavelengths it asks about, so you can type in any number. You can see the clouds immediately on the screen, and also both of the CIV clouds. The fits should look okay, but could do with some fine tuning. By now you should have something which looks a bit like the screen dump shown in the accompanying PostScript file, `sample.ps`.

Try clicking the “Residual” button. The screen changes to show the residual data after the fitted profiles have been subtracted. It should be a uniform noise about 1, but you should see clearly that there are one, maybe two or more, other lines present which have not been fitted. When you are done looking at the residual, click the same button (now marked “Normal”) to return to normal mode.

Let’s see what the Lyman β lines for these same clouds look like. Click the “Add new ion” button, this time entering 4.0 for the instrumental b value, and ‘lyb’ as the absorption line ID. Xvoigt will ask for a few other instrumental b values—it doesn’t matter what you enter for those. Then it will show you a different region of data, with the Lyman β equivalents of the three Lyman α lines. This spectral region is very noisy, but you should be able to see that the strongest cloud matches the data quite well.

Click the “Overlay” button. The Voigt profiles disappear, and the data plot changes colour. Now click the H I 1215.67 button to see an overlaid plot of the two Lyman data regions in different colours. You can see the good wavelength match between the strong absorption lines, confirming that this is a high-redshift hydrogen cloud.

This tutorial shows just a sample of what Xvoigt can do. Continue playing with the data provided if you like. Experimentation is a good way to learn about a new program! Then read the detailed sections on how to use Xvoigt for more information.

C.7 Defining Your Own Lines

Xvoigt allows you to define your own absorption lines, and saves the line definitions for you automatically so you can use them again next time you use Xvoigt. To define your own absorption line, simply add a new ion to your analysis (using the “Add new ion” button). When Xvoigt asks for a line wavelength or ID code, type a dot ‘.’. This will allow you to define your own line by answering the prompts.

```
Manual line data definition...
Enter a name for this line : Bi II
Give a nickname for this line : bill
Enter this line’s accurate vacuum wavelength : 2345.678
Enter this line’s f1k : 0.3183
Enter this line’s qk : 6
Enter this line’s q1 : 2
This definition saved in your personal ion data file.
```

Xvoigt saves this data in a file called `.xvoigt_data` in your home directory. You can override the default directory and file name by defining an environment variable `XVOIGT_HOME` to be equal to the full path and file name you prefer, for example

```
XVOIGT_HOME = /home-users/fred/programs/xvoigt/.xvoigt_data .
```

If you wish to override the default in this way, it is best to define the environment variable `XVOIGT_HOME` in a file which is executed automatically every time you log in. If you don't know how to do this, a local UNIX expert is your best bet.

Whatever file name you use, you can examine and edit it directly. Here is a short sample of what such a file looks like:

```
U XCIX- uranus 1234.789 2.345000E-01 6 2
Np C- neptune 2345.678 1.234000E-01 6 2
Pl CI- pluto 9876.543 9.876000E-01 6 2
```

On each line, the text *up to but not including* the minus sign “-” is the name of the atomic species, the next word is the nickname, and the numbers are vacuum wavelength, f_k^1 , q_k , and q_1 respectively. The minus sign is required after the species name as a signal to Xvoigt, since the species name often has spaces in it. The nickname is not allowed to contain any spaces. If you feel like it, you can edit out lines you no longer need, or change ones which are defined incorrectly, and you can add your own lines directly to this file rather than entering them via Xvoigt. Just make sure to follow the format in the above example. (The f_k^1 values do not have to be in exponential notation; 0.2345 would be acceptable, for example. Xvoigt just writes them that way to maintain precision, but you need not do so.)

C.8 Keyboard Command Summary

The mouse-activated buttons should be the easiest way to access all the commands in Xvoigt, but here is a full summary of the keyboard commands in case you prefer to use them.

- i (“up”)**: With the mouse pointer in the main graphics area of the window, this key causes the current cloud number to be incremented by one, adding an extra cloud to the model if necessary. If the pointer is within a cloud parameter scroll-bar, this key increases the range of that scroll-bar by a factor of ten (or two for $\log N$).
- m (“down”)**: With the mouse pointer in the main graphics area of the window, this key causes the current cloud number to be decremented by one. If the pointer is within a cloud parameter scroll-bar, this key decreases the range of that scroll-bar by a factor of ten (or two for $\log N$).

- f** (“**reset**”): Prompts for a new spectrum data file in the message window. Select this window and type in a new data file name. Xvoigt will also request a new central wavelength, instrumental b value, and velocity range.
- l** (“**new model**”): Prompts for a new central wavelength in the message window. Select this window and type in the observed wavelength. Xvoigt will also request a new instrumental b value and velocity range.
- v** (“**velocity**”): Prompts for a new velocity range in the message window. Select this window and type in the new range. Changing the velocity range only does not destroy the current cloud model. To restart fitting with a new cloud model, use the ‘l’ key and re-enter the central wavelength.
- z** (“**zap**”): Removes the currently selected cloud from the cloud model. Any higher numbered clouds in the model are shuffled down to fill the gap in the cloud numbering sequence. The currently selected cloud number remains the same, unless the highest numbered cloud was the one removed. In this case, the current cloud number decreases by one.
- a** (“**add ion**”): Adds a new ion species to the cloud analysis, allowing simultaneous fitting of different lines at the same redshift with the same cloud model. A prompt appears in the message window, asking for a file name. Select this window and type the name of the file in which data appropriate for the next line in the analysis are stored. If the file has already been read by Xvoigt, it will not bother reading it again, otherwise it will read the contents of the given file. A prompt is then given for the instrumental b value at the appropriate wavelength, and another to identify the line being examined. The graphics window will then change to display the new line with the same cloud model, calculating the wavelength from the redshift.
- c** (“**change ion**”): Cycles the display between the ion species which are currently in the analysis.
- e** (“**left marker**”): Selects the left residual marker for movement by either mouse clicking in the main graph area or by using the ‘j’ and ‘k’ keys.
- r** (“**right marker**”): Selects the right residual marker for movement by either mouse clicking in the main graph area or by using the ‘j’ and ‘k’ keys.
- j** (“**left**”): Moves the currently selected residual marker one data point to the left.
- k** (“**right**”): Moves the currently selected residual marker one data point to the right.
- d** (“**data**”): Toggles the data display between histogram and dots.
- s** (“**save model**”): Saves the current cloud model data to a file.
- p** (“**load model**”): Loads a cloud model from a saved data file.

-
- w** (“**save prof**”): Saves the calculated profile of the current cloud model to a file. A prompt for the file name appears in the message window. Select this window and type in a file name. The profile is saved as pairs of numbers, one pair per line, which are the velocity and intensity coordinates, in increasing velocity order.
- h** (“**help**”): Prints a summary of all the command keys and their functions to the message window.
- q** (“**quit**”): Quits the program, killing the Xvoigt graphics window and returning control to the message window.

C.9 Known Atomic Lines

Ion	Code Name	$\lambda/\text{\AA}$	f_k^1	q_k	q_1
H I	lyalpha	1215.6701	0.41640	6	2
H I	lybeta	1025.7223	0.07912	6	2
H I	lygamma	972.5368	0.02900	6	2
H I	lydelta	949.7431	0.01394	6	2
H I	lyepsilon	937.8035	0.007804	6	2
H I	lyzeta	930.7483	0.004816	6	2
H I	lyeta	926.2257	0.003183	6	2
H I	lytheta	923.1504	0.002216	6	2
H I	lyiota	920.9631	0.001605	6	2
H I	lykappa	919.3514	0.001200	6	2
H I	lylambda	918.1294	0.00092	6	2
H I	lymu	917.1806	0.0007226	6	2
H I	lynun	916.429	0.00058	6	2
H I	lyxi	915.824	0.00047	6	2
H I	lyomicron	915.329	0.00039	6	2
H I	lypi	914.919	0.00032	6	2
H I	lyrho	914.576	0.00027	6	2
D I	dalpha	1215.3394	0.4165	6	2
D I	dbeta	1025.4432	0.07912	6	2
D I	dgamma	972.2722	0.02901	6	2
D I	ddelta	949.4847	0.01395	6	2
C I	c1a	1656.9283	0.1405	3	1
C I	c1b	1560.3092	0.08041	3	1
C I	c1c	1328.8332	0.05804	3	1
C I	c1d	1280.1353	0.02432	3	1
C I	c1e	1277.2454	0.09665	3	1
C I	c1f	1260.7355	0.03937	3	1
C I	c1g	1193.0308	0.0447	3	1
C I	c1h	1157.9097	0.02178	3	1
C II	c2a	1334.5323	0.1278	4	2
C II	c2b	1036.3367	0.1231	2	2
C III	c3a	977.020	0.762	3	1
C IV	c4a	1550.770	0.09522	2	2
C IV	c4b	1548.202	0.1908	4	2

Ion	Code Name	$\lambda/\text{\AA}$	f_k^1	q_k	q_1
N I	n1a	1200.7098	0.04423	2	4
N I	n1b	1200.2233	0.08849	2	2
N I	n1c	1199.5496	0.1328	6	4
N I	n1d	1134.9803	0.04023	6	4
N I	n1e	1134.4149	0.02683	4	4
N I	n1f	1134.1653	0.01342	2	2
N II	n2a	1083.990	0.1031	3	1
N II	n2b	915.612	0.1449	3	1
N III	n3a	989.799	0.1066	4	2
N V	n5a	1242.804	0.07823	2	2
N V	n5b	1238.821	0.157	4	2
O I	o1a	1302.1685	0.04887	3	5
O I	o1b	1039.2304	0.009197	3	5
O I	o1c	1025.7618	0.0203	3	5
Na I	nad1	5897.5581	0.318	2	2
Na I	nad2	5891.5833	0.6311	4	2
Mg I	mg1a	2852.9642	1.83	3	1
Mg II	mg2a	2803.531	0.3054	2	2
Mg II	mg2b	2796.352	0.6123	4	2
Al II	al2a	1670.7874	1.833	3	1
Si I	si1a	2515.0725	0.1622	3	1
Si I	si1b	1845.5202	0.2291	3	1
Si II	si2a	1808.0126	0.005527	4	2
Si II	si2b	1526.7066	0.2303	2	2
Si II	si2c	1304.3702	0.1473	2	2
Si II	si2d	1260.4221	1.007	4	2
Si II	si2e	1193.2897	0.4991	2	2
Si II	si2f	1190.4158	0.2502	4	2
Si II	si2g	1020.6989	0.02828	2	2
Si II	si2h	989.8731	0.133	4	2
Si III	si3a	1206.500	1.669	3	1
Si IV	si4a	1402.770	0.255	2	2
Si IV	si4b	1393.755	0.514	4	2
S I	s1a	1807.3113	0.1105	5	3
S I	s1b	1425.0299	0.1918	7	5

Ion	Code Name	$\lambda/\text{\AA}$	f_k^1	q_k	q_1
K I	k1a	7701.093	0.3393	2	2
K I	k1b	7667.021	0.6816	4	2
Ca I	ca1a	4227.918	1.753	3	1
Ca II	cah	3969.591	0.3145	2	2
Ca II	cak	3934.777	0.6346	4	2
Ti II	ti2a	3384.740	0.3401	6	4
Cr II	cr2a	2066.161	0.06982	4	6
Cr II	cr2b	2062.234	0.1049	6	6
Cr II	cr2c	2056.254	0.1403	8	6
Fe II	fe2a	2600.1729	0.2239	10	10
Fe II	fe2b	2586.6500	0.06457	8	10
Fe II	fe2c	2382.765	0.3006	12	10
Fe II	fe2d	2374.4612	0.02818	8	10
Fe II	fe2e	2344.214	0.1097	8	10
Fe II	fe2f	1608.4511	0.06194	8	10
Fe II	fe2g	1260.533	0.025	8	10
Fe II	fe2h	1144.9379	0.105	12	10
Fe III	fe3a	1122.526	0.07884	10	8
Ni I	ni1a	2320.744	0.6851	11	9
Ni I	ni1b	2311.669	0.3765	9	9
Ni II	ni2a	1751.910	0.0638	8	6
Ni II	ni2b	1741.549	0.1035	6	6
Ni II	ni2c	1709.600	0.06884	6	6
Ni II	ni2d	1454.842	0.05954	6	6
Ni II	ni2e	1370.132	0.1309	4	6
Ni II	ni2f	1317.217	0.1458	8	6
Zn II	zn2a	2062.664	0.2529	2	2
Zn II	zn2b	2026.136	0.5150	4	2

The lines are listed in increasing order of atomic number and ionisation, then by decreasing order of wavelength. The code names are defined to be the atomic abbreviation in lower case letters, followed by the ionisation state as a digit, and a letter in alphabetical order starting with the highest wavelength for that ion. The only exceptions are:

- the hydrogen and deuterium Lyman sequences, labelled respectively ‘ly’ and ‘d’ followed by the appropriate greek letter spelt out in full;
- the sodium D lines, labelled ‘nad1’ and ‘nad2’;
- and the calcium H and K lines, labelled ‘cah’ and ‘cak’.

C.10 Installing Xvoigt

This appendix describes the procedures for installing Xvoigt on your computer system. You must make sure the system is running UNIX.

If the code for Xvoigt is not available on your system, you can get it by anonymous ftp from the following site:

```
ftp://suphys.physics.su.oz.au/pub/mar/xvoigt
```

This directory contains the following files:

```
manual.shar.Z (The latest version of the documentation.)  
xvoigt.shar.Z (The latest version of the program.)
```

These files are both in compressed binary format, so be sure to set binary transfer mode in ftp before transferring them.

If you cannot access the ftp site, contact me by e-mail at mar@physics.su.oz.au and I will send you an archived file containing all the relevant material.

Depending on how you receive the Xvoigt program source code, you may be able to skip the first one or more steps below. In particular, if you ftp the code you can begin at step 3.

Before you start, it is strongly suggested that you create a new directory, in which all of the Xvoigt files will be stored. Once you have done this, move all your Xvoigt related files there, and then follow the following steps.

1. If you have received the code by e-mail or some other method in several uuencoded parts, you will need to strip off the message headers and concatenate the parts into a single file, leaving no blank lines between. If the code is in a single uuencoded file, there is no need to strip any initial header — the uudecode command will do that automatically.
2. If you have a single uuencoded file, simply type

```
uudecode <filename>
```

This will create a compressed file called `xvoigt.shar.Z`
3. If you have the compressed file `xvoigt.shar.Z`, then type

```
uncompress xvoigt.shar.Z
```

This will create the shell archive file `xvoigt.shar`
4. If you have the shell archive file `xvoigt.shar`, then type

```
sh xvoigt.shar
```

This will extract several source code files and a Makefile from the shell archive file.

5. If you have all the source code files and the Makefile, then type

```
make
```

This will compile the source code and create the executable file `xvoigt` for you. If your system is not a Sun, then you may need to make some changes to the Makefile first. I am not a guru when it comes to these matters, so you are better off asking a local expert at your site.

You can now run Xvoigt.

If you have any problems with the above procedures, it is probably easiest to ask a friendly local UNIX expert for help.

C.11 Known Bugs

I know of one bug in Xvoigt which could cause it to produce physically incorrect results. When the same ionic transition is entered twice in two separate ion selection buttons, with different instrumental resolutions, Xvoigt may sometimes use the “wrong” instrumental resolution for that transition, and not the one you might expect. To avoid this problem, make sure you do not enter the same transition with different instrumental resolutions as two of the ion selection buttons.

I know of no bugs which could cause the program to crash or hang.

If you find any bugs of any sort, please report them to me.

Some slightly weird and non-intuitive behaviour concerning the selection of ions, files, and models may be apparent when changing these while in Overlay and/or Residual modes, but none of this should effect the actual results produced by Xvoigt.

When in Residual mode, it is possible for the residual data to extend beyond the confines of the graphics area of the main window. This is not so much a problem as an aesthetic nuisance. I will fix this when I learn about graphics clipping in X.

C.12 Future Developments

Plans for future releases include:

- An option to change manually the y-range of the graphics display, rather than relying on the current auto-scaling.
- Adding vertical tick marks at the centres of all of the clouds on screen, and highlighting the current cloud in some way.
- Changing the velocity scroll bar so that it toggles to a wavelength bar when the graph display is in wavelength units.
- Adding a facility to measure the signal-to-noise ratio of regions of data.
- The ability to delete ions, files, and models from the analysis without having to reset and hence lose information.

- The ability to show the changes in all ions of a given cloud as its parameters are varied.