

FITLYMAN: A Midas Tool for the Analysis of Absorption Spectra

A. FONTANA, Osservatorio Astronomico di Roma, Italy

P. BALLESTER, ESO-Garching

Introduction

The introduction of echelle spectrographs on 4-m telescopes has allowed the observation of faint objects ($m < 18$) with high resolution ($R = \lambda / \Delta\lambda > 20,000$). In the study of the interstellar and intergalactic medium, where the absorption lines from tenuous and relatively cold ($T \leq 5 \times 10^4$ K) clouds are sought in the spectrum of bright background sources, this resolution allows the observation of narrow lines with an instrumental FWHM lower than their intrinsic width. This

makes it possible to independently derive the column density N and the Doppler width b from line profile fitting, rather than from the curve of growth analysis. Typical applications of these techniques are the study of the Galactic clouds, which trace the gas content and the metallicity inside the Galaxy, and of the absorption systems found in the spectra of high redshift quasars, which trace the evolution of primordial structures.

The fit of heavy element systems may require the simultaneous fit of different lines spread all over the spectrum. For

these lines, it is often necessary to test different configurations (i.e. number of components and constraints on them) before a satisfying fit is achieved. In the analysis of the Lyman- α forest, on the contrary, hundreds of independent lines are fitted, which must be identified by the user himself. In any case, a significant fraction of the time required for this analysis is spent in user interaction rather than in computing time.

Three different approaches to this problem are known: (a) interactive construction of a Voigt profile until a

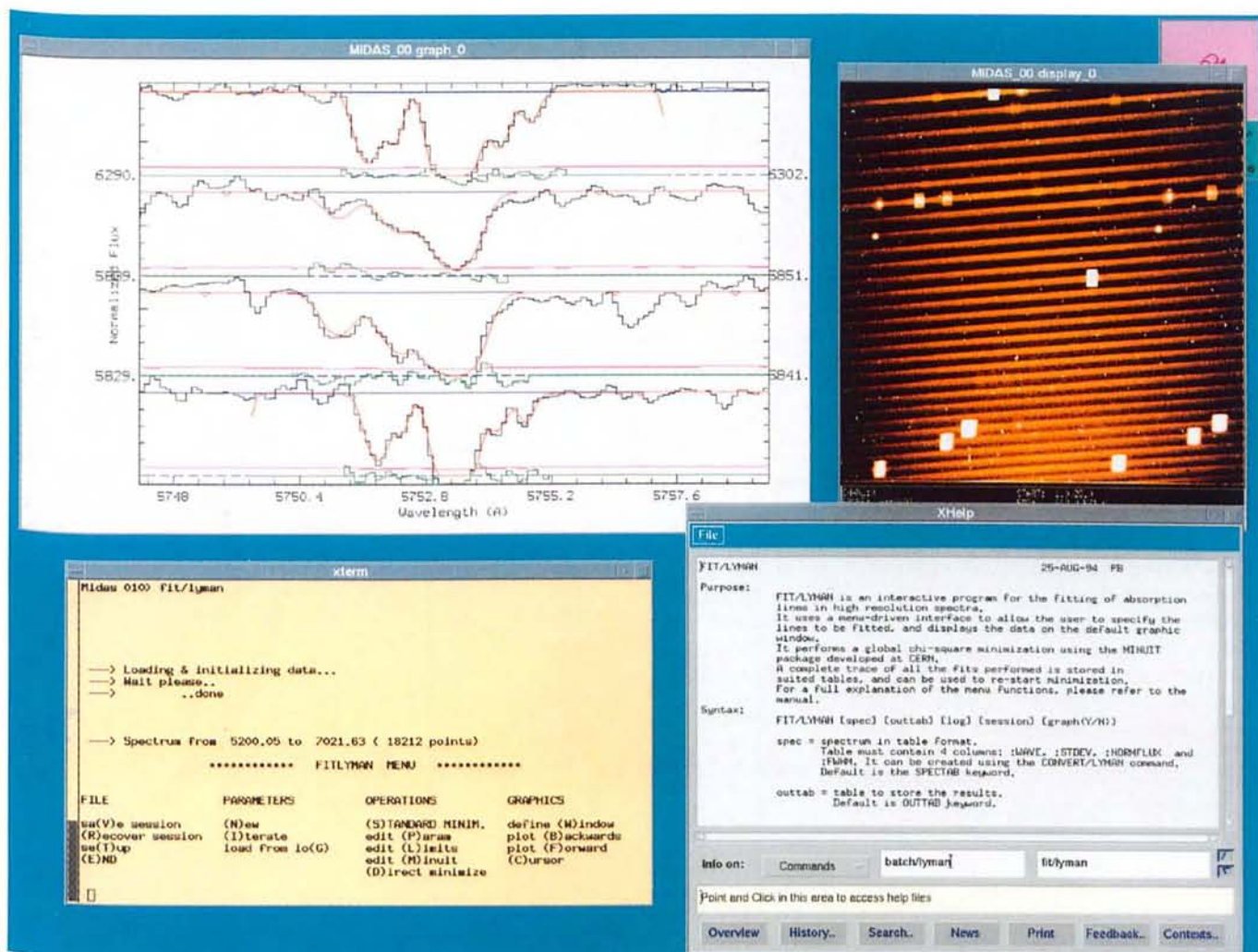


Figure 1: Example of a FITLYMAN session. The Main Menu is shown in the bottom left window. The graphic window over it displays a fit performed on a complex metal system at $z = 2.768$. Lines fitted are, from the top, Al1670, CIV1550, CIV1548, SiII1526. The CIV doublet has been fitted with three components, lower ionisation elements with five. Data from Giallongo et al., 1993, and J. Wampler.

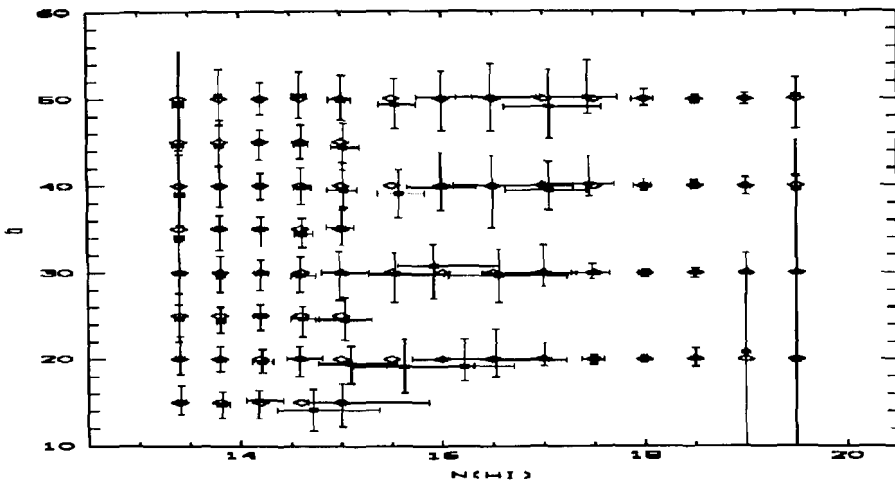


Figure 2: Results of a set of simulated fits. Squares represent the mode value (i.e. the most probable value) of the median value of the b , N values obtained by the fitting procedure, and the error bars show the region where 68% of the points are found, representing an estimate of the observed scatter. Lozenges are the "true" parameters of the line.

satisfactory solution has been achieved (Mar & Bailey, 1995); (b) construction of a photo-ionisation model, from which the relevant absorption lines are computed (e.g. using the Midas context Cloud) and finally compared with the data (Wampler et al., 1995); (c) fit of a Voigt profile by numerical minimisation of χ^2 (Carswell et al., 1991, Giallongo et al., 1993).

Even though the two former methods have the advantage of being more intuitive and easier to implement, the latter approach is usually preferred, since it is more objective, testable through numerical simulations, provides an accurate estimate of the errors, and is usually faster.

While the reduction of echelle spectra to 1D calibrated spectra may be accomplished with several standard astronomical packages (such as the MIDAS Echelle context), no similar tool exists for the fit of their absorption features. The lack of a software tool properly tailored for all the different aspects of this problem has moved us to the realisation of FITLYMAN, a new package available in the Lyman context of the Midas 94NOV release, that we present in this paper.

This code is the evolution of a former version, developed at the Osservatorio Astronomico di Roma (Giallongo et al., 1993). It allows the fit of Voigt profiles to a large number of absorption lines in a normalised spectrum through the numerical minimisation of χ^2 . Its main features are flexibility in specifying the line configuration, a fast user interface, and full documentation on the fit as performed.

Special care has been taken to maximise the efficiency of the user operations: FITLYMAN provides recursivity and allows recovery of previous configurations.

Main Features

We describe here the most important features of FITLYMAN: for a more complete description of the commands and algorithms please refer to the ESO Midas User's Manual.

- Each absorption line is modelled by a Voigt profile, whose parameters are the central wavelength λ_c , the column density N and the Doppler broadening b . The line profile $I(\lambda)$ for a spectrum $I_0(\lambda)$ is $I(\lambda) = I_0(\lambda)e^{-\tau(\lambda)}$ where the optical depth is

$$\tau(\lambda) = \frac{N f_0 f \sqrt{\pi} c \lambda_0^{-8}}{b \sqrt{2} m^2} H(a, u). H(a, u) \text{ is the}$$

Voigt function, defined as:

$$H(a, u) = \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{a^2 + (u-y)^2}$$

whose parameters a and u are given by:

$$a = \frac{\Gamma \lambda_0}{4\pi b \lambda_0^3}; \quad u = \frac{(\lambda_c - \lambda)c}{b \lambda_0 \sqrt{2} m^2}$$

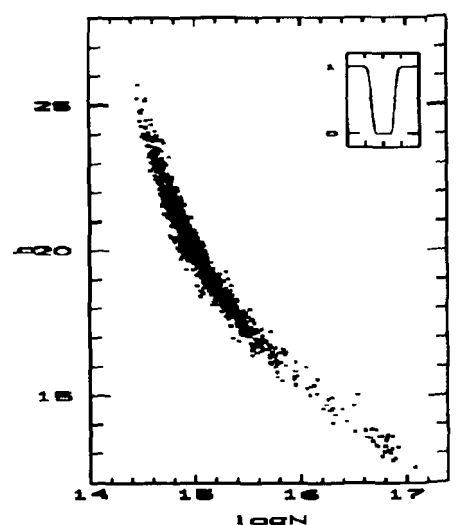
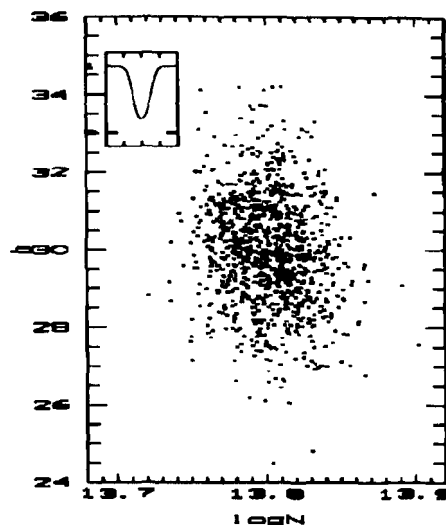


Figure 3: Values of Doppler parameter b and column density N obtained by the fitting procedure for 1000 lines of $b = 30$ and $\log N = 13.8$ (left) and for 1000 lines of $b = 20$ and $\log N = 15$ (right). Small boxes show the respective line profile

Here, r_0 is the classical radius of the electron, c is the speed of light, λ_c , f and Γ are the three parameters associated with the observed transition (i.e. rest frame central wavelength, oscillator strength and damping coefficient, respectively).

In general, the Doppler broadening of a line is due either to the intrinsic thermal broadening $b_K = (2kT/m)^{0.5}$ or to a turbulent motion of the gas $b_T = \sqrt{2}\sigma_T$, where σ_T is the inner velocity dispersion. When transitions from different ions are observed, it is possible to constrain the two cases: for the thermal component of the broadening, indeed, the b -values of different atoms scale with the masses as $b_{\text{ion1}}/b_{\text{ion2}} = (m_{\text{ion2}}/m_{\text{ion1}})^{0.5}$, while in the turbulent case they remain essentially equal. To allow for a complete analysis of the physical conditions of the absorbing clouds, both types of b -values can be accounted for in computing the line profile: each line is thus parameterised by four different parameters (λ_c , N , b_K , b_T), and the Voigt profile is computed using a b -value $b = (b_K^2 + b_T^2)^{0.5}$. This unique feature, combined with the possibility of constraining the different parameters in a flexible way (see below), allows for the simultaneous fitting of different ionic transitions to yield meaningful values for both the turbulent and thermal broadening.

- An extensive set of atomic parameters is supplied: it allows for the fitting of several ionic transitions found in absorption spectra, and can be easily expanded by the user him/herself.

- It is possible to simultaneously fit lines from different ions, or from different transitions of the same ion, specifying several links (relations) among them which reflect the physical condition in the cloud responsible for the absorption. The lines can be forced to share the same

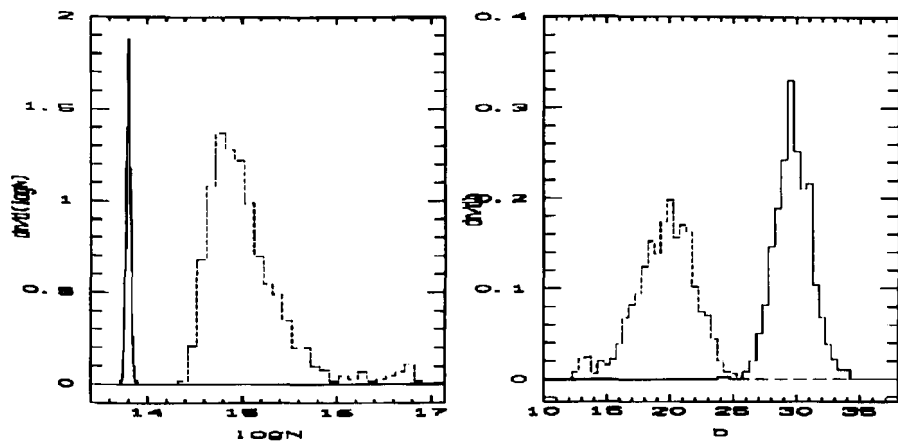


Figure 4: Distribution of Doppler parameter b (right) and column density N (left) obtained by the fitting procedure for 1000 lines with $S/N = 10$. Solid line is for lines of $b = 30$ and $\log N = 13.8$, and dashed line is for $b = 20$ and $\log N = 15$. Solid line on the left panel has been divided by 10 for illustrative purposes.

velocity relative to the earth (redshift), and/or the same column density N , and/or the same b value, and/or the same temperature T by properly scaling ($b\kappa$) with the ion masses. Any combination of lines and links is allowed, the only limit being the maximum number of independent parameters which the programme can handle (currently 100). In general, the number of free parameters depends on the kind and number of links imposed: for instance, when the lines are forced to have the same absorption redshift, there is only one actual free parameter (i.e. the redshift), not one for any individual central wavelength.

The absolute freedom in specifying links with these rules is a powerful tool when the ionisation and metallicity of a system is investigated, and also to correct for possible systematic errors: for instance, two lines far away in the spectrum (e.g. Si II1260 and Si II1526) might be forced to have the same b and N but different redshifts, to allow for some wavelength calibration uncertainties.

The input data have to be stored into a Midas table, containing wavelength, normalised flux, standard deviation and instrumental FWHM for each pixel. A tool for the conversion of the usual image data to this format is supplied. Both pixel size and resolution can vary along the spectrum. Gaps may exist in the spectrum, provided that they do not fall in fitted regions.

The numerical minimisation is performed using the MINUIT package, developed at CERN. It allows for the simultaneous minimisation of up to 100 free parameters (equivalent to at least 33 independent absorption lines). The user can choose among different minimisation algorithms or strategies. For instance, some parameters may be fixed at the first iteration, to find a reasonable “first guess” solution, and then released to achieve the final result. This procedure is particularly useful to find meaningful solutions in

complex situations. The original MINUIT package can also be used in interactive mode: since this option is not compatible with the Midas command language, it has been disabled in FITLYMAN. Nevertheless, all its relevant functions can be invoked from the User Interface: this solution also eliminates the necessity of learning the MINUIT command language.

MINUIT may perform an accurate error analysis, by computing either the covariance matrix and/or more detailed statistics, as non parabolic errors or scans and contour levels in the χ^2 space.

In principle, the results of each minimisation depend on several parameters, which specify: (a) the line configuration, (b) the spectrum regions where the χ^2 is computed and (c) the MINUIT commands used. To keep track of these parameters, each minimisation is associated with a unique identifier, whose value is stored in the output table. At the same time, the full initial configuration, together with the same identifier, is stored in three “log” tables. Later, these tables can be either consulted for the interpretation of the results, or used to re-start the

minimisation. Furthermore, a batch procedure (BATCH/LYMAN) allows for the automatic, non-interactive fit of a whole spectrum using the configurations stored in the “log” tables.

The FITLYMAN User Interface has been designed to satisfy two different – and almost opposite – requirements: it must allow the user to handle and modify all the parameters needed for the minimisation, reducing the requested time as much as possible. To fulfill the Midas requirements about compatibility with any kind of terminal and environment, we have designed a menu-driven User Interface which uses both the standard I/O devices (keyboard + screen) and the standard Midas graphics window.

A Main Menu introduces the user to all the functions available in the programme, such as modifying the input parameters, loading/saving previous configurations, modifying the set-up options of the programme, or accessing the graphics device. The parameters which specify a line configuration may be entered or modified either by answering a sequence of questions that guide the user to the correct sequence of operations (to be preferred when new lines are defined), or by directly accessing their values (to modify a few parameters).

The input spectrum and the fitted profile are plotted on the active graphics window. Optionally, the standard deviation and/or the residuals may be plotted as well. The cursor in the graphics window may be used to enter the wavelengths needed to specify some parameters (e.g. “first guess” central wavelength or the intervals over which the χ^2 is computed).

An example of a working session with FITLYMAN is shown in Figure 1.

Performance and Examples

To investigate the accuracy and stability of the results obtained with

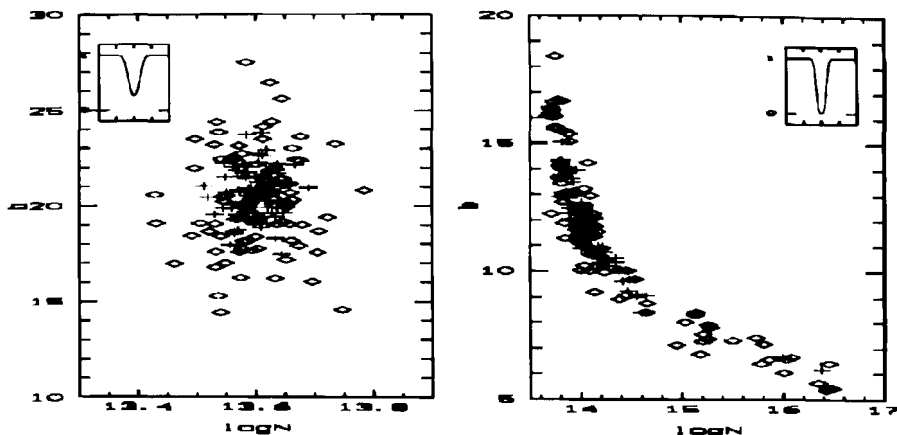


Figure 5: Values of Doppler parameter b and column density N obtained by the fitting procedure for 100 lines at different S/N ratio. Lozenges are for $S/N = 5$, crosses for $S/N = 10$. Left: an unsaturated line of $b = 21$ and $\log N = 13.6$; right: a saturated line of $b = 12$ and $\log N = 13.8$. Small boxes show the respective line profile.

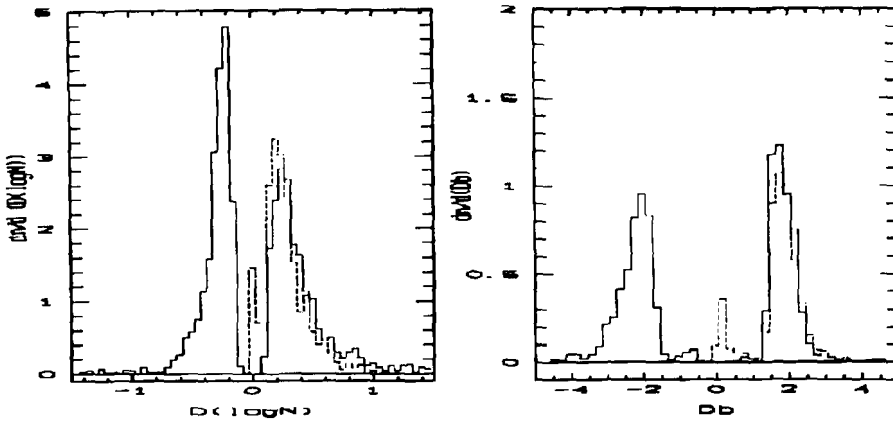


Figure 6: Distribution of statistical errors computed by MINUIT. Left: errors on column density; right: errors on Doppler parameter. Solid line is from the MINOS procedure, dashed line from the HESSE procedure. Note that a fraction of errors estimated with HESSE are implausibly small. Data are for 1000 saturated lines of $b = 20$ and $\log N = 15$.

FITLYMAN, we have performed extensive tests on simulated data. Clearly, these tests cannot span the whole range of resolution and signal-to-noise ratio available: anyway, since the test data were entirely generated and analysed with the programmes available in the LYMAN context, we strongly invite every user to perform similar tests to evaluate the possible systematic effects on his/her data.

Stability

Concerning the stability of the algorithm we found that, when single lines have been fitted, the results have proven to be remarkably insensitive to the “first guess” values used in the minimisation. Even implausible initial values usually converge to the correct values, the only cost being extra computing time. When more complex situations – i.e. severe blends of many lines – are to be fitted, it may be necessary to provide reasonable initial values to obtain the correct answer.

This behaviour is due to the complex shape of the χ^2 hyper-surface in the parameter space, that may present local minima for unphysical solutions.

Noise effects

To explore the influence of noise on the fitted values we have defined a grid of N and b values, and for each pair we have computed and fitted 100 HI lines with central wavelength 5000 Å (i.e. with $z \approx 3.11$) and $S/N = 10$. Figure 2 shows the results obtained for b and N (the central wavelength has always been found with great accuracy). Four regions can be identified. For unsaturated lines (leftmost points) the mode value is quite close to the “true” value, with a small and symmetric scatter around it. As the central flux of the line reaches zero, the spread around the “true” value becomes

larger and usually asymmetric: in some cases there is a measurable shift of the mode value, even if it is always well within the observed 68% spread. At higher column densities, however, the line shape becomes unambiguously defined by the appearance of the Lorentzian wings, and the fit becomes much more precise. Finally, for the highest column densities the line width becomes too large for the Doppler broadening to be effective, and b becomes practically undetermined. Clearly, the values of column density and Doppler parameter for which the lines saturate or the damping wings appear, depend on the considered ionic transition.

We have investigated in more detail two cases, which may represent most of the typical situations: an unsaturated Lyman- α line ($b = 30$, $\log N_{\text{HI}} = 13.8$) and a moderately saturated one ($b = 20$, $\log N_{\text{HI}} = 15.0$). In Figure 3 the results of 1000 simulated fits for each line are reported in the $N-b$ plane, while in Figure 4 their b and N distributions are shown. For the unsaturated line the b and N values are essentially uncorrelated (see Figure 3,

left panel), and the fitted values are distributed around the “true” values according to Gaussian statistics (Fig. 4). For saturated lines the $b-N$ correlation is quite strong, and the uncertainties on N are much greater. The fitted values are thus distributed along the curve of constant equivalent width, as shown in Figure 3 (right panel). The observed band N distributions are rather asymmetric, with a tail extending far away from the mode value (Figs. 4a, b). In any case, most of the fitted values are still confined in a region close to the “true” values.

Different levels of S/N ratio do not seem to change the results outlined here qualitatively. As an example, in Figure 5 we report (in the $N-b$ plane) the results of 100 simulated fits with $S/N = 10$ (crosses) and $S/N = 5$ (lozenges) for two different lines. At lower S/N the spread of the fitted values obviously increases, but this is entirely consistent with the increased uncertainties on the equivalent width. No systematic effect seems to arise as a pure effect of lower S/N.

Summarising, the effect of noise on the fitting of isolated lines is mainly a spread of the fitted values, without any severe systematic effect. For saturated, but not damped, lines the spread is wider, and occurs along the curves of constant equivalent width, which is an integral quantity poorly affected by noise fluctuations. This gives a characteristic anticorrelation in the b and N plane. We stress that these simulations do not take into account other processes that may alter the fit (Rauch et al., 1993), such as selection effects in the identification of the lines, line blending and a wrong choice of the limits of minimisation (see below).

Error estimate

We have hence tested the MINUIT ability in giving realistic estimates on the statistical errors on fitted values. Errors

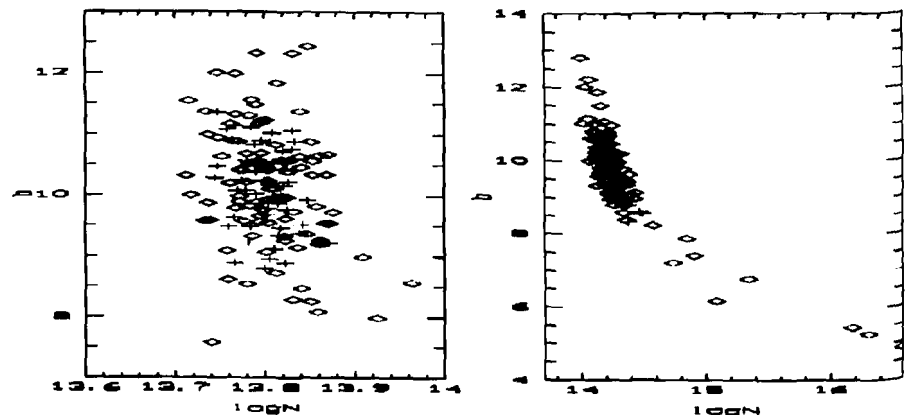


Figure 7: Values of Doppler parameter b and column density N obtained by the fitting procedure on CIV doublets. Lozenges are for individually fitted lines, crosses are for the same lines when the fit is on the two lines simultaneously. Left: $b = 10$ and $\log N_{\text{CIV}} = 13.8$; right: $b = 10$ and $\log N_{\text{CIV}} = 14.2$.

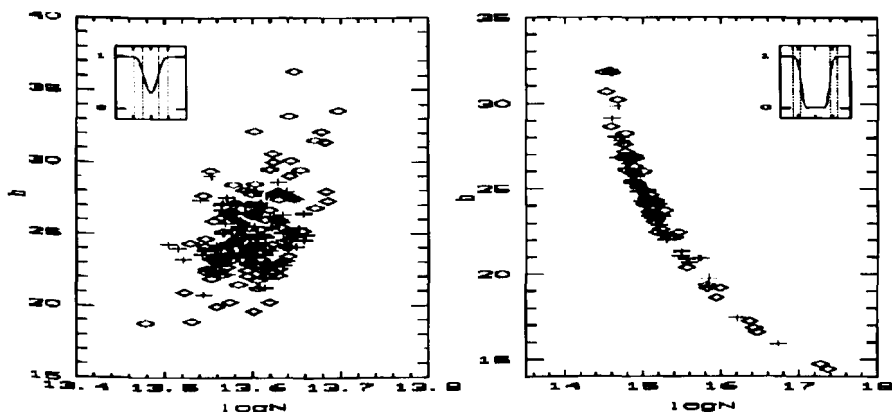


Figure 8: Values of Doppler parameter b and column density N obtained by the fitting procedure on Ly α lines with different fit intervals. Lozenges are for limits set at half intensity of the line, crosses are for the same lines when the fit is over the whole line width. Left: $b = 25$ and $\log N_{\text{HI}} = 13.6$; right: $b = 25$ and $\log N_{\text{HI}} = 15$. For clarity, on the right only 50 representative points are plotted. Small boxes show the respective line profile, with the different intervals considered.

may be computed by MINUIT either by inverting the covariance matrix (*HESSE* command) or by scanning the χ^2 hypersurface around the minimum (*MINOS* command) until a 1σ offset has been reached. In Figure 6 we plot the observed distributions of the errors obtained with both methods for 1000 simulated lines of $b = 20$ and $\log N = 15$. The peak value of the distributions is in good agreement with the observed dispersion in fitted values (see Fig. 4). Clearly *HESSE*, due to its symmetric nature, cannot account for the asymmetric distributions such as those shown in Figure 4. This is better accomplished by *MINOS*, as is shown in Figure 6, where the two error distributions are compared: as can be seen, the peaks and the shapes of the *MINOS* errors are not symmetric. We have also found out that both of them are sometimes inaccurate: the first one, for inexplicable reasons, provides implausibly small values in a significant fraction ($\sim 15\%$) of the lines (see Fig. 6, dotted line), while the second is not computed in a small fraction of cases ($\sim 5\%$). Thus, we suggest the performance of both computations, to check for consistency of the results.

Fit of metal systems

We have also verified that the simultaneous fit of different metal lines does significantly increase the precision attainable in the fit. We have performed a set of fits on simulated CIV doublet spectra, again for different values of b and N , at $S/N = 10$. A self-explanatory example for two of them is reported in Figure 7. The results of our simulation clearly indicate that the simultaneous fit of different ionic transitions should be exploited whenever possible.

Limits of the fit region

As has been pointed out by Rauch et al. (1993), great care must be taken when choosing the limits on which the χ^2 is computed.

Following Rauch, we quantified the systematic effects by fitting the same set of lines with different limits, repeating this test for different b and N values. When the limits are chosen inside the line (i.e. before the line has reached the continuum) two effects arise. The first is an increase in the noise on the equivalent

width, due to the reduced number of pixels: this reflects into a larger dispersion of the fitted values. Furthermore, severe systematic effects may appear, in particular in the fits of saturated lines, which depend strongly on the line profile close to the continuum level. Thus, *the limits must always be chosen as wide as possible*, in order to follow the line profile up to the continuum. Two examples of the simulated fits are shown in Figure 8.

Improvements

The Lyman context is still an evolving tool. Some improvements are already being implemented, and will be released with the future versions of Midas. Among these, the possibility of drawing plots in the velocity space, and more commands for the research of metallic systems. The convenience of a GUI version is currently being evaluated.

We are grateful to D. Trevese and L. Camurani for having supplied the first version of the code, and E. Giallongo and P. Petitjean for useful suggestions and discussion.

References

- Carswell, R. F., Lanzetta, K. M., Parnell H. C., Webb J. K., 1991, *ApJ* **371**, 36.
- Cristiani, S., D'Odorico, S., Fontana, A., Giallongo, E., Savaglio, S.: 1995, to be published in *Monthly Notices of the Royal Astronomical Society* (ESO Preprint 1054).
- Giallongo, E., Cristiani, S., Fontana, A., Trevese, D.: 1993, *ApJ* **416**, 137.
- Mar, D.P. & Bailey, G. 1995, *ProcASA*, in press.
- Rauch, M., Carswell, R. F., Webb J. K., Weymann, R. J. 1993 *MNRAS*, **260**, 589.
- Wampler, E.J., Chugai, N.N., Petitjean, P.: 1995, to be published in *Astroph. Journal*, April 20. (Eso Preprint 1045).

P. Ballester
e-mail: pballest@eso.org

Astronomers in Chile Meet at ESO in Vitacura

BO REIPURTH, ESO-Chile

During September 1994 the Astronomy Support Department of ESO-Chile moved its offices and facilities from the La Silla observatory to ESO's Vitacura premises in Santiago. Here a new institute of astronomy has emerged and is now successfully operating. For the past two decades ESO astronomers have had their work place at La Silla and have conse-

quently been fairly isolated. With our move to Santiago this situation has significantly improved, and ESO is now able to a much larger degree to be a partner in the wider astronomical activities in Chile.

To celebrate ESO's new presence in Santiago and to further the possibilities for increased scientific ties between the various astronomical institutions in Chile, a

three-day workshop *Astronomy in Chile* was held 18–20 April in Vitacura. All astronomers working in Chile were invited, and the workshop gave the about 50 attendees an opportunity to learn about the wide range of astronomical interests currently pursued within Chile. Except the staff working those days at La Silla, Cerro Tololo and Las Campanas, and those