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TwoFitlines: An Spectrum and Line Analysis Tool

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Abstract. Twofitlines is a tool developed within IRAF, optimized to be used with data containing multiple spectra along the spatial axis of the detector. A given spectral feature can be decomposed in one or several Gaussian components. The results are obtained in handy graphical and text formats. The error in the fitted parameters is estimated by successive fits to Montecarlo simulated spectra. An extra capability allows to measure useful asymmetry parameters for non-resolved spectral features.

1. Motivation

Twofitlines is a task developed to facilitate the analysis of spectroscopic data, containing multiple spectra along the spatial axis of the detector. These type of data are produced by longslit, multislits or fiber spectrographs. The basic requirements to build such tool were:

- A given spectral feature can be modeled using one or more components (currently only Gaussian profiles are available),
- The fitting model should be easily and interactively configurable,
- It should keep memory of the best fitting model when moving across the spectra,
- The continuum can be modeled separately from the spectral features, which is especially important when measuring faint emission or absorption lines,
- Close spectral features could be modeled simultaneously. The variation of Gaussian parameters for the various lines can be constrained in different ways,
- It should be used in a similar way in both interactive and background modes.

2. How was it done?

There exist tools in IRAF which allows to measure spectral line features using different profiles, for instance *splot*, *fitprofs,* and *specfit*. These three tasks cover most of the above requirements, although each of them has its own limitations. Some time ago, we decided to take what was considered the best from each task and put it together into a unique task. The final result closely resembles those mentioned tasks. The programming language is SPP, and it is structured as a mini–package in IRAF called **twofitlines**, although the task actually doing the work is called **fitlines**. The tool is available at the ftp address `ftp://ftp.iac.es/pub/users/jacosta/twofitlines.tar.gz`.

```
a  - Define the relation between components of the fit
b  - Fit the continuum and put the value at the limits of the fitting region
c  - Modifies the number of components, define wc[i], sig[i], fix[i]
d  - Add new components, define wc[i], sig[i], fix[i]
e  - Exit and save the last fit
f  - Make and plot the fit
g  - Print initial values for Gaussian model fit
i  - Calculate the flux by direct integration
k  - Save initial values for Gaussian model fit as a record in the database
l  - Define the limits of the line
n  - Sets a new fitting region
o  - Change interactively center for each Gaussian component
p  - Change interactively sigma for each Gaussian component
q  - quit  without saving the last fit
r  - Redraw the region to be fit
s  - Save the last fit
t  - Calculates the asymmetry parameters of a given profile
w  - window the graph
I  - Interrupt
A  - Auto expand around the marked region
S  - Smooth the data via a boxcar. The box size is given.
Z  - Zoom the graph by a factor of 2 in x
,  - Shift the graph to the left
.  - Shift the graph to the right
<space> - Cursor position and flux
?  - This display

COLON  COMMANDS
:fitcont            - Enable/disable continuum fitting
:sigma <value>      - Default sigma value
:rms <value>        - Default rms value, used if continuum fitting is disable
:errors <value>     - Set errors estimator [none|uniform|Poisson]
:fluxcalib <value>  - Set mode of calibration flux factor  [none|estimate|given]
:cts_flux <value>   - Set calibration flux factor
:fit_type <value>   - Change fitting algorithm [simplex|marquadt]
:gain   <value>     - Gain (CCD parameters)
:ron <value>        - Readout noise (CCD parameters)
```

Figure 1. List of available parameters in interactive modes.

3. Program Features

Spectra can be read from images in a variety of IRAF formats for spectroscopic data.The basic input parameters are a fitting region, a list of initial positions and widths, plus some constrains. The program can be used in both interactive or background modes. The main features of *fitlines* are described below:

1. Two minimization algorithms can be selected, Levenberg–Marquadt or Simplex;
2. The uncertainty of model parameters is determined by a number of repeated fits to simulated data in the following way:
   i. An specified model with a given number of components is fit to the selected spectral region, obtaining the best fitting model parameters;
   ii. Random Gaussian noise is added to each pixel value as computed from the best fitting model. Two type of noises can be added: the noise amplitude is uniform along the spectrum, or based in Poisson statistics;
   iii. A new model is fitted to the simulated spectrum, taking as starting values those recently obtained. The new parameter models are saved temporarily. After a number of tries the error of each fitting parameter is computed as the standard deviation.
3. Output results in non-interactive mode can be saved in graphical and text formats for later inspection;
4. Initial values for a fit can be read from a database file. This file can be manually edited or directly created from a successful fit. This is very useful for non-interactive processing of large amount of data.

3.1. Interactive Commands

A variety of commands are available in interactive mode, which allow to perform any model fit, output the results and saving the parameters to be used as initial values for next fitting operations (see Figure 1).

3.2. Outputs

The results of the fitting process are the computed parameters (line center, amplitude and width), the flux and the equivalent width for each component. The flux included within the limits of the selected spectral feature is also computed by simply adding each spectrum bin after continuum subtraction. The goodness of the fit can be easily assessed from the comparison of the total flux which results from the addition of all model components and the direct sum just mentioned. The reliability of each model component is also inferred from the S/N ratio, i.e. the line peak to the continuum noise ratio (see Figure 2).

3.3. Parameter Constrains

Sometimes it is worth to set relationships in between some components parameters, e.g. if two emission lines are expected to come from the same region the width could be the same, or to fix the ratio between intensity of line sets, give same center offsets to line sets. One of the remarkable features of **fitlines** is the capability to set model fit constrains in a flexible and interactive way. At the moment there are four ways of setting constrains for each parameter group: (1) all vary freely; (2) all are fixed to the initial values; (3) only the value for one component varies and the others are offset/scaled by a the initial values; and (4) for each component one parameter can be set to vary independently, fixed to a specific value or to be tight to another component. An example of the last type is presented in Figure 2. The emission line complex Hα+[NII]$\lambda\lambda 6548, 6584$ is modeled including physical constrains. There are two components per line of similar width plus a broad one for Hα. The kinematically coupled components obey the following conditions: same line width, constant wavelength offset, and constant flux ratio for [NII]$\lambda\lambda 6548, 6584$.

3.4. Parameterizing Line Profiles

Spectral features show in many occasions complex line profiles, or relatively smooth asymmetric profiles which reflect the complex internal velocity field of the emission source or the poor spectral or spatial resolution of our spectra. In these cases the decomposition into a number of Gaussian components does not produce a set of meaningful parameters. More general approaches have been proposed (Whittle 1985; Heckman et al. 1981), such as measuring the width, the center and asymmetry at different heights of the profile. The two above parameterizations are included in the program fitlines and can be applied to any 1-D or 2-D spectrum.

References

Heckman, T. M., Butcher, H. R., Miley, G. K., & van Breugel, W. J. M 1981, ApJ, 247, 403

Whittle, M. 1985, MNRAS, 213, 1

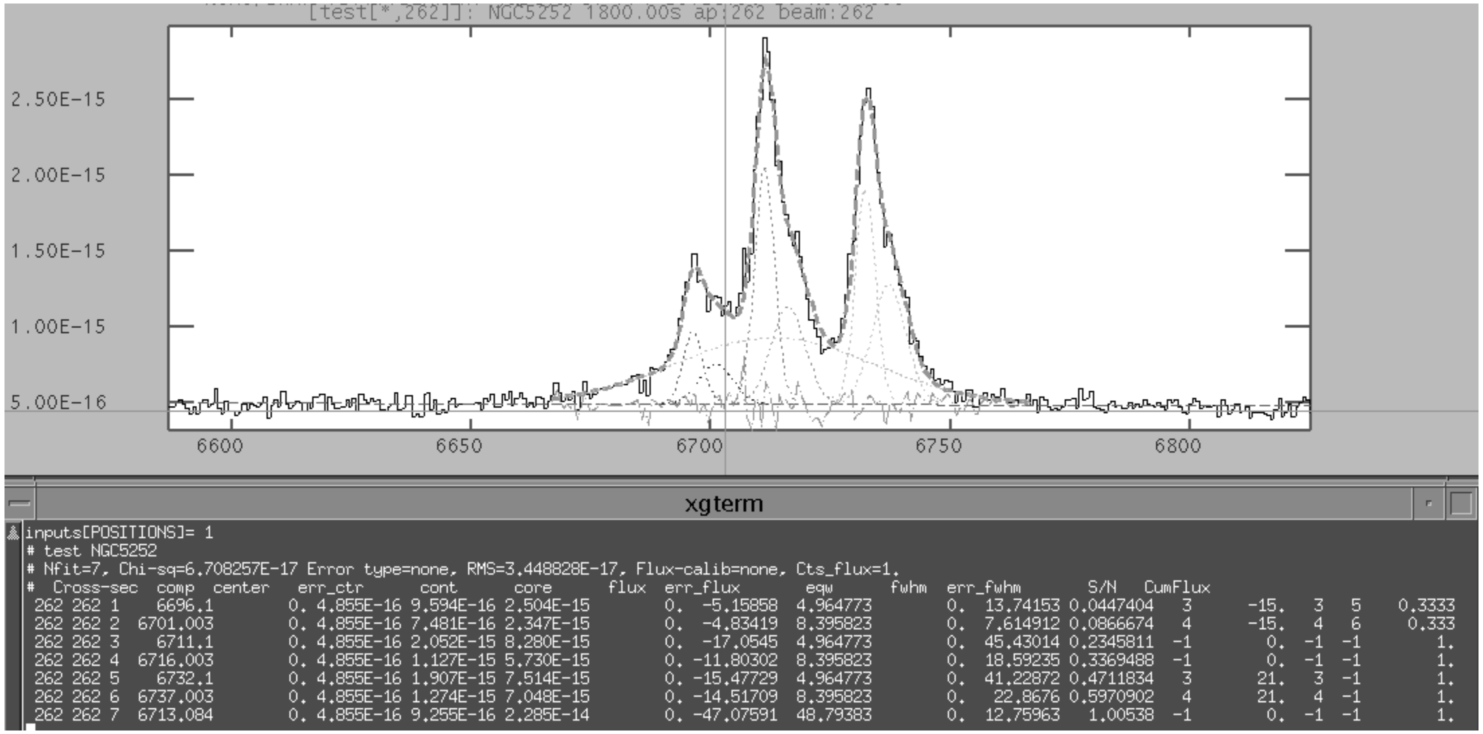

Figure 2. The emission line complex Hα+[NII]$\lambda\lambda$6548, 6584 is modeled including physical constrains (detailed description in text).