Fit\_ATRAN README

Alex Reedy, Randolf Klein 2017-10-19

**Installing Fit\_ATRAN**

1. Obtain Fit\_ATRAN procedures and data.
2. Change the path to the IDL-save files in atran\_transmission.pro to match your installation directory!!!
3. Add the Fit\_ATRAN installation directory to your IDL !PATH variable.
4. Execute procedures using the calls outlined below. They are as follows:
   1. Fit\_atran\_baseline\_parallel.pro to fit just an ATRAN-baseline
   2. Fit\_atran\_base\_and\_line\_parallel.pro to fit an ATRAN-baseline and a Gaussian emission line simultaneous.

**Notes**

1. The fitting routines use data from the atmospheric model ATRAN. ATRAN was developed and kindly provided to the SOFIA program by Steve Lord. The reference for ATRAN is Lord, S. D., 1992, NASA Technical Memorandum 103957. The current version uses the 2000/2001 version of the HITRAN database. Users of these routines are requested to reference the Lord technical memorandum and this web site in any publications.
2. Contained in atran\_transmission.pro, there are two restore procedures in which the path must be changed to match that of your machine (see item (2) of “Installing Fit\_ATRAN”. If this is not changed you will receive an error message

% Compiled module: FIT\_ATRAN\_BASELINE\_CALLBACK.

Error encountered: Attempt to subscript PARAMS with <INT      (       1)> is out of range.

1. For all FIX\_ keywords *in* base\_and\_line, the default is unrestricted unless stated otherwise below. If given one value, it’s fixed to that value. If given two then those two are the range of values. If given 3 the middle value is the starting value and the other denote the range. If one of the range limits is nan (!value.f\_nan) the fitting range is unbounded on that side.
2. For now only the base\_and\_line-routines accept mpfitfun keywords that are passed down to mpfitfun to change the default behavior of the fitting routine.

**To Do**

* Port the common treatment of the FIX\_ keywords in the base\_and\_line routines to the baseline routines. That should also allow keywords to be passed down to mpfitfun in the baseline routines.
* Fully debug /no\_parallel in fit\_atran\_baseline\_parallel.
* Introduce scale\_err into fit\_atran\_baseline\_parallel.pro.

**CO153 Example Call Using fit\_atran\_baseline\_parallel.pro**

1. Estimate baseline regions using Fluxer. Note down the wavelengths.

[152.91] [153.18] [153.37] [153.66]

1. Calling the procedure like in the example code below. Some parameters may be fixed like the zero point in this example.

IDL> fit\_atran\_baseline\_parallel,’F0310\_FI\_IFS\_04004934\_RED\_WXY\_100872-200647.fits’,$

‘CO153\_atran\_fit’,[[152.91,153.18],[153.37,153.66]],/no\_zero

1. Example output for running fit\_atran\_baseline\_parallel.pro
2. There should now be six additional .fits files in your directory, one for each fitted or fixed parameter containing the map for that parameter.



(Procedure 1): Fit\_atran\_baseline\_parallel.pro

**PURPOSE**

Fits a baseline using an ATRAN model to all spectra in a data cube from a (FIFI-LS) fits-file using parallel processing. The baseline is fitted in the wavelength range specified in the call (base\_wavel). The baseline has the following form:

(cont+(wave-wave0)\*slope)\*atran\_transmission(wave,alt,pwv,za,/smoothed,/interpol)+zero

The parameters for baseline are:

* the continuum level (cont),
* its slope (slope), and
* the data’s zero level (zero).

The atmospheric transmission model by ATRAN has the parameters:

* altitude (alt), [not fitted, taken from header]
* water vapor (pwv), and
* zenith angle (za). [not fitted, take from header]

The variable wave denotes the wavelength for which the baselines are calculated. The parameter wave0 is the wavelength were the slope pivots around and is fixed to the median of the fitted wavelengths.

The fitted parameters are written out to fits-files. Two more files are written out each containing a cube with the baselines and the original cube minus the baseline.

The fitted parameters can be fixed or limited with keywords.

**SYNTAX**

fit\_atran\_baseline\_parallel,*fn\_cube*,*out\_prefix*,*base\_wavel*,$

[CUBE\_EXT=],[ERR\_EXT=],[PWV\_FIT],[CONT\_FIT=],[ZERO\_FIT=],[SLOPE\_FIT=],$

[BASELINED],[BASELINES],[ZA],[ALT],[CLIP= ],[/NO\_ZERO],[FIX\_PWV= ],$

[FIX\_SLOPE=],[/NO\_PARALLEL],[CPUS=],[JOBS\_PER\_CPU= ]

**ARGUMENTS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Format |
| fn\_cube | File name of cube | ‘\_\_\_\_.fits’ |
| out\_prefix | Prefix for output files | ‘\_\_\_\_\_’ |
| base\_wavel | [2,N] describing the wavelength range of baseline fit. (Taken from Fluxer) | [[x0,x1],[y0,y1]] |

**KEYWORDS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Default |
| CUBE\_EXT | Cube extension | 3rd (uncorrected) |
| ERR\_EXT | Error extension | 4th |
| PWV\_FIT | Water vapor map | Output keyword |
| CONT\_FIT | Continuum map | Output keyword |
| ZERO\_FIT | Zero map | Output keyword |
| SLOPE\_FIT | Slope map | Output keyword |
| BASELINE | Baseline cube | Output keyword |
| BL\_SUBTRACTED | Baseline subtracted cube | Output keyword |
| ZA | Zenith angle from header | Output keyword |
| ALT | Altitude from header | Output keyword |
| CLIP | Find median / good fit | If non-zero, limits the fitting range of the fitting value to +/- clip value. If not set the range of the zero value is not limited. |
| NO\_ZERO | Fix zero value to 0 | 0 |
| FIX\_PWV | Fix water vapor | If not set water vapor is limited between 1-50. If set water vapor is fixed that value, must be between 1 – 50. |
| FIX\_SLOPE | Fix the slope | If not set, slope is not fixed. If set to a value, then this value is the slope. To set a range for the slope, set the keyword to a 2-element. |
| NO\_PARALLEL | No parallel processing | 0 |
| CPUS | How many CPUS are used | 4 |
| JOBS\_PER\_CPU | How many jobs per CPU | 8 |

(Procedure 2): Fit\_atran\_baseline.pro

**PURPOSE**

Called by fit\_atran\_baseline\_parallel, but can also be called directly. Fits a baseline using an ATRAN model to all spectra in a data cube.

**SYNTAX**

fit\_atran\_baseline,*cube*,*err\_cube*,header,*base\_idx*,$

[PWV\_FIT],[CONT\_FIT],[ZERO\_FIT=],[SLOPE\_FIT=],[BL\_SUBTRACTED=],$

[BASELINES=],[ZA=],[ALT=],[CLIP=],[NO\_ZERO=],[FIX\_PWV=],[FIX\_SLOPE=],$

[STATUS],[\_EXTRA=]

**ARGUMENTS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Format |
| cube | Data cube to be fitted | 3D array |
| Err\_cube | Error cube for the data cube | 3D array |
| header | Primary fits header with NAXIS keywords matching the cubes. | String array |
| base\_idx | Indices of wavelength that are to be used in baseline fitting. | [i1,i2,…,iN] |

**KEYWORDS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Default |
| PWV\_FIT | Water vapor map | Output keyword |
| CONT\_FIT | Continuum level map | Output keyword |
| ZERO\_FIT | Zero level map | Output keyword |
| SLOPE\_FIT | Slope map | Output keyword |
| BL\_SUBTRACTED | Cube with baseline subtracted | Output keyword |
| BASELINES | Cube with baselines | Output keyword |
| ZA | Zenith angle from header | Output keyword |
| ALT | Altitude from header | Output Keyword |
| CLIP | Find median | If non-zero, limits the fitting range of the fitting value to +/- clip value. If not set the range of the zero value is not limited. |
| NO\_ZERO | No zero value | 0 (Boolean) |
| FIX\_PWV | Fix water vapor | If not set water vapor is limited between 1-50. If set water vapor is fixed that value, must be between 1 – 50. |
| FIX\_SLOPE | Fix slope | If not set, slope is not fixed. If set to a value, then this value is the slope. To set a range for the slope, set the keyword to a 2-element. |
| STATUS |  | Returns the status of mpfitfun |
| \_EXTRA |  | Keywords passed to mpfitfun |

(Procedure 3): Fit\_atran\_base\_and\_line\_parallel.pro

**PURPOSE**

Fits a Gaussian emission line plus a high-resolution baseline using an ATRAN model smoothed to spectral resolution to all spectra in a data cube from a (FIFI-LS) fits-file using parallel processing. The baseline and line is fitted in the wavelength range specified in the call (fit\_wavel). The fitted function has the following form:

line = fltarr(n\_elements(wave)) ; creates the array for the emission line

z=(wave-p\_center[0])/p\_width[0] ; argument for the gauss

calc=where(abs(z) lt 6.79) ; to improve cacluation time and avoid underflows

A0=p\_flux[0]/(p\_width[0]\*sqrt(2.\*!pi)) ; scaling of the flux argument

line[calc]=A0\*exp(-0.5\*z[calc]^2) ; Gaussian line

; multiply the continuum and line with the atmospheric transmisson

spectrum=(p\_cont+ line)\*atran\_transmission(wave,p\_alt,p\_pwv,p\_za)+p\_z

;calculate the width of the kernel to smooth the model spectrum

dlam=(wave[-1]-wave[0])/(n\_elements(wave)-1)

lam=(wave[-1]+wave[0])/2.

sigma=(lam/dlam)/p\_R/2.35482

;smooth the model spectrum and return the result

return,p\_z+gauss\_smooth(spectrum,sigma,/edge\_tru,/nan,$

width=min([6.\*sigma,.9\*n\_elements(spectrum)]))

The parameters for baseline and emission line are:

* the continuum level (p\_cont),
* the zero level (p\_z),
* the intrinsic line width (p\_width),
* the line center (p\_center),
* the line flux (p\_flux).

The atmospheric transmission model by ATRAN has the parameters:

* altitude (alt), [not fitted, taken from header]
* water vapor (pwv), and
* zenith angle (za). [not fitted, take from header].
* The resolution (p\_R) is the parameter used to smooth the model spectrum.

The variable wave denotes the wavelength for which the baselines are calculated.

The fitted parameters are written out to fits-files. Two more files are written out each containing a cube with the fitted function and the residuals.

The fitted parameters can be fixed or limited with keywords. Fitting all keywords for a large cube can take very long. With the sub\_cube-keyword a spatial subsection can be selected to be fitted. On that sub-cube, one can test which parameters can fixed, which must be free or restricted for the fit. Once the number of parameters for the fit is reduced ideally to just the continuum and the line flux, the full cube can be fitted in a relatively short time. For how to fix the parameters, look at the keywords for fit\_atran\_base\_and\_line.pro. They will be passed down.

**SYNTAX**

fit\_atran\_base\_and\_line\_parallel,fn\_cube,out\_prefix,fit\_wavel,$

[SUB\_CUBE=],[CUBE\_EXT=],[ERR\_EXT=],[SCALE\_ERR=],[/NO\_PARALLEL],$

[CPUS=],[JOBS\_PER\_CPU=],[\_EXTRA]

**ARGUMENTS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Format |
| Fn\_cube | File name of cube | ‘\_\_\_\_.fits’ |
| Out\_prefix | Prefix for the output files | ‘ ‘ |
| Fit\_wavel | Array of wavelength interval denoting fitting range | [x0,x1] |

**KEYWORDS**

|  |  |  |  |
| --- | --- | --- | --- |
| Name | Definition | | Default |
| SUB\_CUBE | | 2x2 array with indices to select subcube to be fitted: [[x0,x1],[y0,y1]] | If not set then whole cube will be fitted |
| CUBE\_EXT | | Extension of fits file with fluxes to fit | 3rd extension |
| ERR\_EXT | | Extension of fits file with flux uncertainties | 4th extension |
| SCALE\_ERR | | Scale the flux with this value to estimate error instead of using uncertainty extension |  |
| NO\_PARALLEL | | No parallel processing | 0 (Boolean) |
| CPUS | | How many cpus to be used | 4 |
| JOBS\_PER\_CPU | | How often to task each CPU | 8 |
| \_EXTRA | | Passed first to fit\_atran\_base\_and\_line then mpfitfun |  |

(Procedure 4): Fit\_atran\_base\_and\_line.pro

**PURPOSE**

Fits a Gaussian emission line plus a high-resolution baseline using an ATRAN model smoothed to spectral resolution to all spectra in a data cube from a (FIFI-LS) fits. The routine fit\_atran\_base\_and\_line\_parallel calls this routine, but it can also be called directly.

**SYNTAX**

fit\_atran\_base\_and\_line,*cube*,*err\_cube*,*fit\_wavel\_idx*,$

[ALT\_FIT=],[PWV\_FIT=],[CONT\_FIT=],[ZERO\_FIT=],[FLUX\_FIT=],$

[CENTER\_FIT=],[WIDTH\_FIT=],[RES\_FIT=],[RESIDUALS=],$

[BASE\_AND\_LINE=],[ZA=],[FIX\_ALT=],[FIX\_PWV=],[FIX\_ZERO=],$

[FIX\_CENTER=],[FIX\_WIDTH=],[FIX\_RESOLUTION],[STATUS],$

[FIX\_CONT=],[FIX\_FLUX=],[\_EXTRA]

**ARGUMENTS**

|  |  |  |
| --- | --- | --- |
| Name | Definition | Format |
| cube | Data cube to be fitted | 3D array |
| err\_cube | Error cube for the data cube | 3D array |
| Header | Primary fits header with NAXIS keywords matching the cubes. | String array |
| Fit\_wavel\_idx | Indices of wavelength that are to be used in baseline fitting. | [i1,i2,…,iN] |

**KEYWORDS**

|  |  |  |  |
| --- | --- | --- | --- |
| Name | Definition | | Default |
| ALT\_FIT | | Altitude map | Output keyword |
| PWV\_FIT | | Water vapor map | Output keyword |
| CONT\_FIT | | Continuum map | Output keyword |
| ZERO\_FIT | | Zero map | Output keyword |
| FLUX\_FIT | | Line flux map | Output keyword |
| CENTER\_FIT | | Line center map | Output keyword |
| WIDTH\_FIT | | Intrinsic line width map | Output keyword |
| RES\_FIT | | Resolution map | Output Keyword |
| RESIDUALS | | The residuals of the baseline and line subtract | Output Cube |
| BASE\_AND\_LINES | | Contains the baseline and the line | Output Cube |
| ZA | | Zenith Angle | Out |
| FIX\_ALT | | Fix the altitude | If not set, the fit is restricted to the altitude from the header. If fitted, can range from 38000 to 45000 to vary the amount of dry atmosphere. |
| FIX\_PWV | | Fix the water vapor | [1,7,50] |
| FIX\_ZERO | | Fix the zero level | Fixed to 0 |
| FIX\_CENTER | | Fix the line center | Unrestricted |
| FIX\_WIDTH | | Fix the intrinsic line width | Unrestricted |
| FIX\_RESOLUTION | | Fix the resolution | [500,1000,2000] |
| FIX\_CONT | | Fix the continuum flux | [0,median(cube)>0,!values.f\_nan], i.e. must be non-negative starting with the median of the cube if positive otherwise starting with 0 |
| FIX\_FLUX | | Fix the line flux | [0,!values.f\_nan], i.e. must be non-positve |
| STATUS | |  | Returns the status of mpfitfun |
| \_EXTRA=EXTRA | |  | Passed to mpfitfun |