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Subject: Manual of Band Shape Fitting method

1. Introduction

Band Shape Fitting is a method to differentiate infilling by fluorescence and deepening by oxygen absorption in O2 bands. The method is designed for the retrieval of F from towers, where atmospheric correction is needed.

The algorithm is describe in detail in a paper by C. van der Tol et al.. This document is a user manual for the code.

The code is written in Matlab2017a.

2. The main code

The main script of the altorithm is `retrievalF.m`

This function uses:

Set_parameters.m: to specify the shoulder locations of the bands

Cost4F: the cost function

iFLD: for comparison, the function also applies the iFLD method

The main function is `retrievalF.m`. This function contains the full algorithm.
This function requires as input:

- The wavelength of the measurement, which must include the range from the left to the right shoulder of both bands (O2A or O2B). This must be a vertically oriented array.
- The corresponding spectrum of measured irradiance E (in the same unit as piL). This must be a vertically oriented array.
- The corresponding spectrum of measured upwelling radiance piL (in the same unit as E). This must be a vertically oriented array.
- Options for the iteration (such as the stopping criterion) for the function 'lsqnonlin', notably:
```
opt          = optimset('MaxIter',30,'TolFun',1E-4);
```
- The prior value of the relative atmospheric path length a
- The cosine of the solar zenith angle
- The cosine of the viewing angle of L
- The weight of the prior value of a (between 0 and inf, use '0' as default value)
- A structure of parameters that includes at the left and right shoulder wavelengths of the band of both bands (see function 'parameters' below).

The output of the function is two structures, O2A and O2B, containing:

- wl: the wavelengths of the measurement within the band ranges
- F: the retrieved fluorescence
- E: the measured downwelling irradiance
- piL: the measured upwelling radiance times pi
- piLr: the measured upwelling radiance times pi, less the fluorescence
- normpiL: the upwelling radiance normalized by the shoulders
- normE: the donwelling irradiance normalized by the shoulders
- a: the retrieved atmospheric optical path length
- EXITFLAG: the output flag of the Matlab buitin function 'lsqnonlin'
- iFLD: the fluorescence of the iFLD method (for comparison to the BSF method)

The function is called as follows:
```
[O2A, O2B]     =
retrievalF(wl,E,piL,opt,aprior,cos_sza,cos_vza,priorweight,p);
```

The supporting function set_`parameters.m` specifies the left and right shoulders of the O2A and O2B band. The other lines in this function are not needed for BSF, but they are parameters for the iFLD method, and they are included for completeness. In the script of the paper, these are used to calculate iFLD fluorescence for the same measurements.

parameters.wl_left   = [759, 686.5]; % just left, used in BSF

parameters.wl_right   = [768, 688.1]; % just right, used in BSF

parameters.wl_in   = [761,686.9]; % next 6 coefficients are all used in iFLD

parameters.wl_out   = [755,686.5];

parameters.wl_left0   = [750,680];

parameters.wl_left1   = [755,686.5];

parameters.wl_right0   = [772,688.1];

parameters.wl_right1   = [777,690];

The function `cost4F` which is called by `retrieval` contains the cost function to be minimized. This code subtracts fluorescence (as input) from the measured radiance, then carried out linear regress of log radiance versus log irradiance, uses the slope of the linear regression to model the upwelling radiance, and finally calculates the difference between modelled and measured upwelling radiance. This difference is a vector with the dimensions of the wavelengths of the measurements in the band. The difference between the prior value of the atmospheric path length 'a' and the slope of the linear regression is added with a weight 'w' (see the paper for details).

The use is as follows:

```
[e,a,ymod] = cost4F(F,input)
```

Where the input is:
F is the fluorescence in the same unit as the irradiance, and input a structure containing the following (all are calculated within `retrievalF.m`):
Logx : the logarithm of the normalized irradiance
Y: the upwelling radiance
cos_sza: the cosine of the solar zenith angle
cos_vza: the cosine of the viewing zenith angle
fwlf: a function that describes the shape of the fluorescence spectrum over the O2 band
normpiL: the spectral shape of the upwelling radiance interpolated between the shoulders of the O2 band

The output includes the cost function 'e' ('e' stands for error here), the slope of the regression 'a', and the modelled upwelling radiance without fluorescence ymod.

Other supporting functions are provided to apply the model. These are not essential, but they are useful to prepare inputs for the model.

3. Other supporting functions

The model was applied to sample FLOX box data using: `master_selecteddays`. This function loads FLOX box L1b data, prepares the input for BSF, estimates prior values for the atmospheric optical path length, and saves the output data. It also contains a section in which SCOPE can be run (which in turn uses `ephoton` and `e2phot`). The function `master_selecteddays` carried out all time series simulation that are presented in the paper.

The function `plot_F_final` reproduces nearly all figures of the paper.

The function `plot_barometric` reproduces figure 3 of the paper.

The supporting functions used in `master_selecteddays` are:

`readFXBox:` a function that scans a FLOXboxfile, and returns the data as matlab variables. Usage:
`[wl, data, time] = readFXBox(filename)`
`calczenithangle:` a function that calculates the solar zenith angle from the geographical location and the date and time.
`set_parameters:` a function that specifies the wavelengths of the shoulders of the O2 bands.
`Barometric`: contains the barometric equation, which in turn uses `set_constants`.

The function `run_and_plot_sensitivity` carries out a sensitivity analysis of BSF and plots a figure for the paper.