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special: A Python package for the spectral characterization of directly imaged low-mass companions

Valentin Christiaens [1]

1 Space sciences, Technologies & Astrophysics Research Institute, Université de Liège, Belgium

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Summary

Recent technological progress in high-contrast imaging has allowed the spectral characterization of directly imaged giant planet and brown dwarf companions at ever shorter angular separation from their host stars, hence opening a new avenue to study their formation, evolution, and composition. In this context, `special` is a Python package that was developed to provide the tools to analyse the low- to medium-resolution optical/IR spectra of these directly imaged low-mass companions.

Statement of need

`special` provides the following tools for the analysis of measured spectra:

- calculation of the spectral correlation between channels of an integral field spectrograph (IFS) datacube (Greco & Brandt, 2016; **Delorme:2017?**);
- calculation of empirical spectral indices for MLT-dwarfs (Allers et al., 2007; Gorlova et al., 2003; Slesnick et al., 2004), enabling their classification;
- fitting of input spectra to different (user-provided) grids of models, with the possibility to include additional parameters such as extra blackbody component(s) and extinction;
- estimating most likely model parameters in a Bayesian framework, using either MCMC (Goodman & Weare, 2010) or nested (Buchner, 2021a; Feroz et al., 2009; Mukherjee et al., 2006; Skilling, 2004) samplers to infer their posterior distributions;
- searching for the best-fit template spectrum within a given template library, with up to two free parameters (flux scaling and relative extinction).

The MCMC sampler relies on `emcee` (Foreman-Mackey et al., 2013, 2019), while two options are available for nested sampling: `nestle` (Barbary, 2013) and `ultranest` (Buchner, 2021b). The samplers have been adapted for flexibility - they are usable on any grid of input models provided by the user, simply requiring a snippet function specifying the format of the input. Moreover they can sample the effect of blackbody component(s) (either as a separate model or as extra components to an atmospheric model), extinction, and different extinction laws than ISM. The samplers can accept either uniform or Gaussian priors for each model parameter. In the case of the MCMC sampler, a prior on the mass of the object can also be provided if surface gravity is one of the model parameters. The code also considers convolution and resampling of model spectra to match the observed spectrum. Either spectral resolution or photometric filter transmission (or combinations thereof for compound input spectra) can be provided as input to the algorithm, for appropriate convolution/resampling of different parts of the model spectrum. The adopted log-likelihood expression can include i) spectral covariance between measurements of adjacent channels of a given instrument, and ii) additional weights that are proportional to the relative spectral bandwidth of each measurement, in case these are obtained from different instruments (e.g. photometry+spectroscopy):

$$\log \mathcal{L}(D|M) = -\frac{1}{2}\left[\mathbf{W}(\mathbf{F}_{\mathrm{obs}} - \mathbf{F}_{\mathrm{mod}})^T\right]\mathbf{C}^{-1}\left[\mathbf{W}^T(\mathbf{F}_{\mathrm{obs}} - \mathbf{F}_{\mathrm{mod}})\right] \quad (1)$$

where $\mathbf{F}_{\mathrm{obs}}$ and $\mathbf{F}_{\mathrm{mod}}$ are the fluxes of the observed and model spectra respectively, $\mathbf{C}$ is the spectral covariance matrix, and $\mathbf{W}$ is the vector of weights $w_i \propto \Delta\lambda_i/\lambda_i$, with $\Delta\lambda_i$ the width of spectral channels (for integral field spectrograph points) or the FWHM of photometric filters.

Finally, a jupyter notebook tutorial illustrates most available features in `special` through their application for the analysis of the composite spectrum of CrA-9 B/b (Christiaens et al., 2021).

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