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

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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 a number of tools for the analysis of spectra from any (sub)stellar object, regardless of the observational method used to obtain the spectra (direct imaging or not) and the format of the spectra (multi-band photometry, low-resolution or medium-resolution spectrum, or a combination thereof). Although implemented with the characterization of directly imaged substellar companions in mind, the main routines in `special` (e.g. Bayesian retrieval of model parameters though MCMC or nested samplers, or best-fit template search) can also be applied to the spectrum of any object, provided a relevant grid of models or library of templates for the fit.

`special` shares similar basic utilities as offered in `splat` (Burgasser & Splat Development Team, 2017), such as dereddening, spectral indices calculation, model grid fitting through MCMC and template fitting. However, a number of features are currently unique to `special`, such as (i) Bayesian inference through nested samplers; (ii) inclusion of non-grid parameters for model fits (e.g. extinction, extra blackbody components, specific emission lines); (iii) inclusion of relative extinction and flux scaling, and handling of spectral coverage mismatches when searching for the best-fit template in a library; (iv) empirical estimation of spectral correlation between channels of an integral field spectrograph, which is relevant to the directly imaged companions for which uncertainties in the spectrum capture correlated residual speckle noise (Greco & Brandt, 2016); and (v) compatibility of all `special` fitting routines with combined spectra (i.e. obtained with multiple instruments with potentially different resolving powers or photometric filters).

The main available features of the package are listed below:

- calculation of the spectral correlation between channels of an integral field spectrograph (IFS) datacube (Delorme et al., 2017; Greco & Brandt, 2016);
- 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 either photo-/atmospheric model grids or a blackbody model, including additional parameters such as (extra) black body component(s), extinction,

total-to-selective extinction ratio or specific emission lines.

- 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):

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

where $\mathbf{F}_{\rm obs}$ and $\mathbf{F}_{\rm mod}$ 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.

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). It is available on GitHub, Binder and the documentation of `special`.

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