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SpecpolFlow: a new software package for spectropolarimetry using Python

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Summary

Spectropolarimetry, the observation of polarization and intensity as a function of wavelength, is a powerful tool in stellar astrophysics. It is particularly useful for characterizing stars and circumstellar material, and for tracing the influence of magnetic fields on a host star and its environment. Maintaining modern, flexible, and accessible computational tools that enable spectropolarimetric studies is thus essential. The SpecpolFlow package is a new, completely Pythonic workflow for analyzing stellar spectropolarimetric observations. Its suite of tools provides a user-friendly interface for working with data from an assortment of instruments and telescopes. SpecpolFlow contains tools for spectral normalization and visualization, the extraction of Least-Squares Deconvolution (LSD) profiles, the generation and optimization of line masks for LSD analyses, and the calculation of longitudinal magnetic field measurements from the LSD profiles. It also provides Python classes for the manipulation of spectropolarimetric products. The SpecpolFlow website includes an array of tutorials that guide users through common analysis procedures using the software. SpecpolFlow is distributed as a free, open-source package, with fully documented tools (via an API and command line interface) which are actively maintained by a team of contributors.

Statement of need

Spectropolarimetry is an essential observational technique in stellar astrophysics, which is used to study the surface properties of stars and their environments. Symmetry-breaking phenomena like stellar magnetic fields leave an imprint on polarized spectra. Magnetic fields are present in most classes of stars throughout their evolution (Donati & Landstreet, 2009; Mestel, 2012). Cool stars (with convective envelopes) display a wide range of observed field strengths, driven by variations in their internal dynamos (Reiners, 2012). Nearly 10% of hot stars (with radiative envelopes) also harbour strong magnetic fields (Grunhut et al., 2017; Sikora et al., 2019). Furthermore, magnetic fields are found in evolved giants and compact stellar remnants such as white dwarfs and pulsars (Ferrario et al., 2015). Spectropolarimetry is a valuable tool for characterizing the strength, orientation, and topology of these fields. Therefore the maintenance and dissemination of computational tools enabling this technique

are a key element of research.

Spectropolarimetric studies of stellar magnetic fields typically leverage the splitting of spectral lines due to the Zeeman effect (e.g., Landstreet, 2015). The Zeeman split components of a line are polarized and shifted in wavelength proportionally to field strength. These shifts in wavelength are typically undetectable due to other line broadening processes (except for very strong fields) but the changes in polarization remain detectable. In practical observations this polarization signal is often below the noise level for an individual line, thus it is important to combine information from many spectral lines. The Least-Squares Deconvolution (LSD, Donati et al., 1997; Kochukhov et al., 2010) approach is the most widely used method for detecting such polarization signatures. LSD is a multi-line technique that produces a pseudo-average line profile at increased signal-to-noise. LSD models the spectrum as the convolution of a set of delta functions (the 'line mask') with a common line shape (the 'LSD profile'). This model is fit to an observation, using a weighted linear least-squares approach, to derive the LSD profile. An estimate of the surface-averaged line-of-sight component of the field (the 'longitudinal field', $\langle B_z \rangle$) can then be computed from the circular polarization and intensity LSD profiles. Modelling the variation of $\langle B_z \rangle$ as the star rotates enables further characterization, such as determining the stellar rotational period and simple models of the magnetic topology.

Several successful programs supporting spectropolarimetric analyses exist in the literature, although they are often proprietary and poorly documented. There is currently no publicly available software that provides the full toolset needed to analyze reduced spectropolarimetric observations and produce magnetic field measurements. The original LSD code by Donati et al. (1997) is efficient and effective, written in C, but it is both proprietary and undocumented. A more recent program, `iLSD`, is an Interactive Data Language (IDL) interface around a Fortran core implementing LSD (Kochukhov et al., 2010). This code includes additional features such as the reconstruction of multiple line profiles from the same spectrum, or an optional Tikhonov regularization of the LSD profiles. However, `iLSD` is also proprietary and has very limited documentation. Some additional support codes (e.g., to read and write LSD profiles, to create line masks, or to combine observations) have been written in a variety of languages and passed down from person to person. While these codes are scientifically relevant, they often lack documentation, version control, active maintenance, and generally they are neither publicly available nor open source. Factors like these negatively impact accessibility, serving as a significant barrier to both learning and research reproducibility.

Overview of SpecpolFlow

The SpecpolFlow package is a modernized, unified revitalization of the tools that have preceded it. The software is open source, well documented, and the code itself is extensively commented and designed to be readable. SpecpolFlow produces results that are consistent with previous proprietary codes implementing similar algorithms. It produces LSD profiles that are consistent with the code of Donati et al. (1997) and `iLSD`, and it produces $\langle B_z \rangle$ values that are consistent with the code of Wade et al. (2000).

SpecpolFlow provides a toolkit with an ensemble of Python functions that:

- Convert observed spectra into a common file format
- Continuum normalize spectra, with an interactive graphical interface
- Generate line masks for LSD from lists of atomic transitions
- Clean line masks interactively to remove problem lines or adjust line depths
- Calculate LSD profiles
- Calculate line bisectors
- Calculate radial velocities
- Calculate $\langle B_z \rangle$ values

The continuum normalization routine follows the algorithm briefly described in Folsom et al. (2008) and Folsom (2013), and implements an interactive graphical interface with the Tkinter

and Matplotlib packages. Line masks can be generated from line lists in the Vienna Atomic Line Database (Ryabchikova et al., 2015) "extract stellar" "long" format. If necessary, effective Landé factors are estimated using LS, J_1J_2, and J_1K coupling schemes (Landi Degl'Innocenti & Landolfi, 2004; Martin et al., 1978). The LSD calculation follows the method of Donati et al. (1997), with details from Kochukhov et al. (2010). It relies on NumPy (Harris et al., 2020) and makes careful use of NumPy's sparse arrays for efficiency. The interactive line mask cleaning tool uses Tkinter and Matplotlib for the interface. This tool can remove lines from the mask, and automatically fit line depths using a reference observed spectrum, following Grunhut et al. (2017) with some optimizations. The line depth fitting routine inverts the linear least squares problem in LSD, and instead fits line depths given an observation and LSD profile. That LSD profile must be approximately correct, calculated using a mask (or part of a mask) with dominantly acceptable lines. Line depth fitting remains a weighted linear least squares problem, similar to the LSD calculation, and can be solved efficiently using spare matrix operations. Radial velocities are calculated by fitting a Gaussian to an LSD profile by default, although calculating from first moments is also supported. The $\langle B_z \rangle$ calculation uses the first moment technique applied to LSD profiles (Donati et al., 1997; Kochukhov et al., 2010; Rees & Semel, 1979).

SpecpolFlow enables users to build their own custom workflow from the available classes and functions, which can enhance scientific archiving and reproducibility. This is also valuable for training or involving students in projects. SpecpolFlow's website includes an extensive set of tutorials that explain the use of the package and demonstrate some common analysis cases. These tutorials, in the form of Jupyter Notebooks, can flexibly be used within a classroom or workshop setting.

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