Atmospheric Retrievals with petitRADTRANS

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Summary

`petitRADTRANS` (pRT) is a fast radiative transfer code used for computing emission and transmission spectra of exoplanet atmospheres. These spectra can be used as a forward model for fitting data using monte carlo techniques, commonly referred to as an atmospheric retrieval. The retrieval module of pRT combines fast pRT with the `MultiNest` (F. Feroz et al., 2009; Farhan Feroz et al., 2019; F. Feroz & Hobson, 2008) and `Ultranest` (Buchner et al., 2014) nested sampling codes, allowing for fast atmospheric retrievals on a large range of different types of exoplanet data.

Statement of need

Atmospheric retrievals are a cornerstone of exoplanet atmospheric characterisation. pRT is a powerful and user-friendly tool, and is unique in its abilities to characterise exoplanets in both emission and transmission. Various thermal structures, chemistry and cloud parameterisations and opacity calculation methods (correlated-k and line-by-line) can be combined and used to statistically identify the most favoured model for a given atmosphere. With increasing volumes of both ground- and space-based spectra available, it is necessary for exoplanet researchers to have access to a range of characterisation tools.

petitRADTANS Retrieval Module

The `Retrieval` module combines the `RadTrans` forward modelling class with a nested sampler via a likelihood function to perform an atmospheric retrieval. Datasets, priors and other retrieval hyper parameters are set through the `RetrievalConfig` class, while the `models` module includes a range of complete atmospheric models that can be fit to the data. Users can also define their own model function, making use of temperature profiles from the `physics` module and chemistry parameterisations from the `chemistry` module.

Multiple datasets can be included into a single retrieval, with each dataset receiving its own RadTrans object used for the radiative transfer calculation, allowing for highly flexible retrievals where multiple spectral resolutions, wavelength ranges and even atmospheric models can be combined in a single retrieval. Each dataset can also receive scaling factors (for the flux, uncertainties or both), error inflation factors and offsets. The model functions are used to compute a spectrum $\vec{S}$, which is convolved to the instrumental resolution and binned to the wavelength bins of the data using a custom binning function to account for non-uniform bin sizes. The resulting spectrum compared to the data with flux $\vec{F}$ and covariance $\mathbf{C}$ in the likelihood function:

$$-2\log\mathcal{L} = \left(\vec{S} - \vec{F}\right)^T \mathbf{C}^{-1} \left(\vec{S} - \vec{F}\right) + \log\left(2\pi \det\left(\mathbf{C}\right)\right). \quad (1)$$

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39 The second term is included in the likelihood to allow for uncertainties to vary as a free
40 parameter during the retrieval, and penalizes overly large uncertainties.

41 pRT can compute spectra either using line-by-line calculations, or using correlated-k tables for
42 defining the opacities of molecular species. We include up-to-date correlated-k line lists from
43 Exomol (Chubb et al., 2020; McKemmish et al., 2016; Polyansky et al., 2018; Tennyson &
44 Yurchenko, 2012) and HITEMP (Rothman et al., 2010), with the full set of available opacities
45 listed in the online documentation. The exo-k package is used to resample the the correlated-k
46 opacity tables to a lower spectral resolution in order to reduce the computation time (Leconte,
47 2021). Combining the c-k opacities of multiple species requires mixing the distributions in g
48 space. Previously, this was accomplished by taking 1000 samples of each distribution. This
49 sampling process resulted in non-deterministic spectral calculations, resulting in unexpected
50 behaviour from the nested sampling process, as the same set of parameters could result in
51 varying log-likelihood. This has been updated to fully mix the c-k distributions. Considering
52 the first species, the second species is added in, and the resulting grid is sorted. The cumulative
53 opacity grid is then mixed with the next species, a process which iterates until every species
54 with significant opacity contributions ($>0.1\%$ of the current opacity in any bin) is mixed in to
55 the opacity grid. Once complete, the resulting grid is linearly interpolated back to the 16 g
56 points at each pressure and frequency bin as required by pRT. This fully deterministic process
57 stabilized the log-likelihood calculations in the retrievals, and resulted in a $5\times$ improvement in
58 the speed of the c-k mixing function.

59 Included in pRT is an option to use an adaptive pressure grid with a higher resolution around
60 the location of the cloud base, and a lower resolution elsewhere. The higher resolution grid is
61 10 times as fine as the remaining grid, and replaces one grid cell above and below the cloud
62 base layer, as well as the cloud base layer cell itself. This allows for more precise positioning of
63 the cloud layers within the atmosphere.

64 Finally, photometric data are fully incorporated into the retrieval process. As with spectroscopic
65 data, a model is computed using a user-defined function. This model spectrum is then
66 multiplied by a filter transmission profile from the SVO database using the `species` package
67 (Stolker et al., 2020). This results in accurate synthetic photometry, which can be compared
68 to the values specied by the user with the `add_photometry` function.

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