The Journal of Open Source Software

taurex-emcee: a TauREx 3.1 plugin for the emcee sampler

Andrea Bocchieri [1], **Quentin Changeat** [2], **Lorenzo V. Mugnai** [3,4,5], **and Enzo Pascale** [1]

1 Department of Physics, La Sapienza Università di Roma, Piazzale Aldo Moro 2, Roma, 00185, Italy **2** European Space Agency (ESA), ESA Office, Space Telescope Science Institute (STScI), Baltimore, MD, 21218, USA **3** School of Physics and Astronomy, Cardiff University, Queens Buildings, The Parade, Cardiff, CF24 3AA, UK **4** Department of Physics and Astronomy, University College London, Gower Street, London, WC1E 6BT, UK **5** INAF, Osservatorio Astronomico di Palermo, Piazza del Parlamento 1, Palermo, I-90134, Italy

DOI: N/A

Software

- Review
- Repository
- Archive

Editor: Open Journals

Reviewers:

- @openjournals

Submitted: 01 January 1970
Published: 01 January 1970

Summary

taurex-emcee is a plugin for the TauREx 3.1 atmospheric retrieval framework (A. F. Al-Refaie et al., 2021) that extends the choice of sampling methods available to the user. The plugin provides an interface to the emcee sampler (Foreman-Mackey et al., 2013), a popular affine-invariant ensemble sampler widely used in the astronomy community. Running the sampler to convergence is automated through the autoemcee package, which also supports parallelization with MPI. Thus, the taurex-emcee plugin allows users to easily launch parallelized retrievals of atmospheric spectra with emcee. This enables reliable, efficient, and fast retrievals, especially when coupled with TauREx's GPU-accelerated forward models (A. Al-Refaie et al., 2020).

taurex-emcee is released under the BSD 3-Clause license and is available on GitHub. The plugin can be installed from the source code or from PyPI, so it can be installed as `pip install taurex-emcee`. The documentation is available on readthedocs, including a quick-start guide, a tutorial, a description of the software functionalities, and guidelines for developers. The documentation is continuously updated and is versioned to match the software releases.

Benchmark

Emcee vs MultiNest

Figures can be included like this:

Statement of need

Optimized sampling methods are a key component of any retrieval code. Nested samplers (F. Feroz et al., 2009; Farhan Feroz et al., 2019) are a powerful and robust sampling method, successfully applied to the retrieval of exoplanet atmospheric spectra (Barstow et al., 2020; Bocchieri et al., 2023; Changeat et al., 2020). TauREx 3.1 natively implements a suite of nested samplers, including the MultiNest sampler, or makes them available as plugins, such as the UltraNest sampler. The primary target of nested samplers is the efficient calculation of the Bayesian evidence, whilst the inference of the posterior is a by-product. This is regarded as a key advantage of nested samplers, as the evidence can be readily used for model selection. However, the evidence is not always required, and the interpretation of the

posterior from nested samplers necessitates some care. Additionally, algorithmic assumptions of nested samplers may require to tailor the priors to explore the parameter space thoroughly.

Where the inference of the Bayesian posterior is the primary target, a well-established alternative to nested samplers are a family of Markov chain Monte Carlo methods known as affine-invariant ensemble samplers (Goodman & Weare, 2010). The implementation in emcee (Foreman-Mackey et al., 2013) is a popular choice in the astronomy community, as it takes care of the heavy lifting of the sampling process, is well documented, and is straightforward to utilize. To date, the emcee sampler is not natively implemented in the TauREx 3.1 retrieval framework, nor elsewhere in other retrieval codes, to the knowledge of the authors. To fill this gap, we developed the taurex-emcee plugin, which interfaces the emcee sampler to TauREx. Key advantages of taurex-emcee are that it affords a more straightforward interpretation of the posterior and is more robust to the choice of priors. However, the current implementation is not intended to explore multimodal posteriors, for which nested samplers will inevitably be more efficient. Moreover, we caveat that it may require substantial computational time to sample high-dimensional parameter spaces with emcee, which can be mitigated by coupling taurex-emcee with TauREx's GPU-accelerated forward models (A. Al-Refaie et al., 2020).

Acknowledgements

This work was supported by the Italian Space Agency (ASI) with Ariel grant n. 2021.5.HH.0.

References

Al-Refaie, A. F., Changeat, Q., Waldmann, I. P., & al., et. (2021). TauREx 3: A Fast, Dynamic, and Extendable Framework for Retrievals. *917*(1), 37. https://doi.org/10.3847/1538-4357/ac0252

Al-Refaie, A., Changeat, Q., Venot, O., & al., et. (2020). TauREx 3.1 - Extending atmospheric retrieval with plugins. *European Planetary Science Congress*, EPSC2020–669. https://doi.org/10.5194/epsc2020-669

Barstow, J. K., Changeat, Q., Garland, R., & al., et. (2020). A comparison of exoplanet spectroscopic retrieval tools. *493*(4), 4884–4909. https://doi.org/10.1093/mnras/staa548

Bocchieri, A., Mugnai, L. V., Pascale, E., & al., et. (2023). Detecting molecules in Ariel low resolution transmission spectra. *Experimental Astronomy*, *56*(2-3), 605–644. https://doi.org/10.1007/s10686-023-09911-x

Changeat, Q., Al-Refaie, A., Mugnai, L. V., & al., et. (2020). Alfnoor: A Retrieval Simulation of the Ariel Target List. *160*(2), 80. https://doi.org/10.3847/1538-3881/ab9a53

Feroz, F., Hobson, M. P., & Bridges, M. (2009). MULTINEST: an efficient and robust Bayesian inference tool for cosmology and particle physics. *398*(4), 1601–1614. https://doi.org/10.1111/j.1365-2966.2009.14548.x

Feroz, Farhan, Hobson, M. P., Cameron, E., & al., et. (2019). Importance Nested Sampling and the MultiNest Algorithm. *The Open Journal of Astrophysics*, *2*(1), 10. https://doi.org/10.21105/astro.1306.2144

Foreman-Mackey, D., Hogg, D. W., Lang, D., & al., et. (2013). emcee: The MCMC Hammer. *125*(925), 306. https://doi.org/10.1086/670067

Goodman, J., & Weare, J. (2010). Ensemble samplers with affine invariance. *Communications in Applied Mathematics and Computational Science*, *5*(1), 65–80. https://doi.org/10.2140/camcos.2010.5.65