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Hermes: A Repository for Autonomous Materials Science

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In this work we present Hermes, a code repository designed to facilitate the development of autonomous materials science. Many common machine learning algorithms have biases or assumptions that do not account for the physics of many materials science problems. It is therefore often necessary to adapt common machine learning tools into physics-informed algorithms. The idea behind Hermes is to bring together the otherwise disparate efforts in creating these physics-informed machine learning tools into a modular and composable repository. Hermes includes machine learning methods useful for materials science applications such as analyzing measurements and autonomous research campaigns as well as methods for communicating with instruments (or computational methods) and FAIR-ly archiving results. Hermes provides a common syntax and modular tool set to easily construct data analysis pipelines –from controlling the instrument, through all the analysis steps, making predictions, choosing the next experiment to perform, and saving the results along the way. In this way Hermes can be used for: autonomously identifying phase maps with x-ray diffraction, autonomously discovering magnetic ordering temperatures with neutron diffraction, efficiently controlling neutron spin wave echo measurements, and discovering optimal materials with the joint inference of structural and property measurements.

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