

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Machine learning for many-Body physics¹ LOUIS-FRANCOIS ARSENAULT, Department of Physics, Columbia University, New York, New York 10027, USA, ALEJANDRO LOPEZ-BEZANILLA, Materials Science Division, Argonne National Laboratory, 9700 S. Cass Avenue, Lemont, IL 60439, USA, O. ANATOLE VON LILIENFELD, Institute of Physical Chemistry, Department of Chemistry, University of Basel, Klingelbergstrasse 80, CH-4056 Basel, Switzerland, ANDREW J. MILLIS, Department of Physics, Columbia University, New York, New York 10027, USA — We investigate the application to many-body physics of Machine Learning (ML) methods for predicting new results from accumulated knowledge. We show that ML can be used efficiently for the Anderson impurity model (AIM)[1] and present preliminary results on its use as a solver for dynamical mean field theory (DMFT). We establish that the best representation of the Green's function for ML is by parametrizing it as an expansion in term of Legendre polynomials [1]. In DMFT applications, a key issue is the choice of descriptor, the data representation used as input for ML, which is not dependent on the impurity solver. Different parametrizations are examined. The ability to distinguish metallic and Mott insulating solutions is analysed.

[1] L.-F. Arsenault et al., PRB 90, 155136 (2014)

¹DOE No. 3F-3138

Louis-Francois Arsenault
Department of Physics, Columbia University, New York, New York 10027, USA

Date submitted: 14 Nov 2014

Electronic form version 1.4