Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Machine Learning for Dynamical Mean Field Theory[1] LOUIS-FRANCOIS ARSENAULT, Department of Physics, Columbia University, New York, NY 10027, USA, ALEJANDRO LOPEZ-BEZANILLA, Physical Sciences and Engineering, Argonne National Laboratory, Argonne, Illinois 60439, USA, O. ANATOLE VON LILIENFELD, Department of Chemistry, University of Basel, Basel, Switzerland, P.B. LITTLEWOOD, Physical Sciences and Engineering, Argonne National Laboratory, Argonne, Illinois 60439, USA, ANDY MILLIS, Department of Physics, Columbia University, New York, NY 10027, USA — Machine Learning (ML), an approach that infers new results from accumulated knowledge, is in use for a variety of tasks ranging from face and voice recognition to internet searching and has recently been gaining increasing importance in chemistry and physics [1]. In this talk, we investigate the possibility of using ML to solve the equations of dynamical mean field theory which otherwise requires the (numerically very expensive) solution of a quantum impurity model. Our ML scheme requires the relation between two functions: the hybridization function describing the bare (local) electronic structure of a material and the self-energy describing the many body physics. We discuss the parameterization of the two functions for the exact diagonalization solver and present examples, beginning with the Anderson Impurity model with a fixed bath density of states, demonstrating the advantages and the pitfalls of the method.

[1] J. Chem. Theory Comput., 9 3404 (2013)

[1]DOE contract DE-AC02-06CH11357

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

Date submitted: 15 Nov 2013 Electronic form version 1.4