Understanding Machine-learned Density Functionals[1] LI LI, JOHN SNYDER, Department of Physics and Astronomy, University of California, Irvine, MATTHIAS RUPP, Department of Chemistry, University of Basel, KLAUS-ROBERT MÜLLER, Machine Learning Group, Technical University of Berlin, KIERON BURKE, Department of Chemistry, University of California, Irvine — Recently, some of us applied machine learning (ML) in a completely new approach to approximating density functionals [1,2]. In a proof of principal, kernel ridge regression was used to approximate the kinetic energy of non-interacting fermions confined to a 1d box as a functional of the electron density [1]. In that work, a modified orbital-free DFT scheme was able to produce highly accurate self-consistent densities and energies, which were systemically improvable with additional training data. In this work, we explore the properties of the ML approximated functional derived in [1]. In particular, we investigate the use of various kernels and their properties and compare various cross validation methods. We discuss the issue of functional derivatives in greater detail, explain how a modified constraint to the standard Euler equation enables highly accurate self-consistent densities, and derive a projected gradient descent algorithm using local principal component analysis. Finally, we explore the use of a sparse grid representation of the electron density and its effects on the method.

[1] J. C. Snyder, et al. Phys. Rev. Lett., 108, 253002 (2012).
[2] J. C. Snyder, et al. accepted to J. Chem. Phys. (2013).

Li Li
Department of Physics and Astronomy, University of California, Irvine

Date submitted: 15 Nov 2013   Electronic form version 1.4