Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Machine learning properties of materials and molecules with entropy-regularized kernels[1] MICHELE CERIOTTI, EPFL - Lausanne, ALBERT BARTK, GBOR CSNYI, University of Cambridge, SANDIP DE, EPFL - Lausanne — Application of machine-learning methods to physics, chemistry and materials science is gaining traction as a strategy to obtain accurate predictions of the properties of matter at a fraction of the typical cost of quantum mechanical electronic structure calculations. In this endeavor, one can leverage general-purpose frameworks for supervised-learning. It is however very important that the input data – for instance the positions of atoms in a molecule or solid – is processed into a form that reflects all the underlying physical symmetries of the problem, and that possesses the regularity properties that are required by machine-learning algorithms. Here we introduce a general strategy to build a representation of this kind. We will start from existing approaches to compare local environments (basically, groups of atoms), and combine them using techniques borrowed from optimal transport theory, discussing the relation between this idea and additive energy decompositions. We will present a few examples demonstrating the potential of this approach as a tool to predict molecular and materials' properties with an accuracy on par with state-of-the-art electronic structure methods.

[1]MARVEL NCCR (Swiss National Science Foundation) and ERC StG HBMAP (European Research Council, G.A. 677013)

Michele Ceriotti
EPFL - Lausanne

Date submitted: 10 Nov 2016 Electronic form version 1.4