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Machine Learning of Quantum Forces: building accurate force fields for molecular dynamics simulation via "covariant" kernels. ALDO GLIELMO, King's College London, Physics Department, PETER SOLLICH, King's College London, Mathematics Department, ALESSANDRO DE VITA, Kings College London, Physics Department — In recent years, Machine Learning algorithms have proven successful in the construction of data-driven force fields that bridge the gap between accurate (but slow) quantum chemical calculations and the fast (but unreliable) classical interatomic potentials. Such schemes learn either the local energy of a specific atom [Behler et al. PRL (2007), Bartók et al. PRL, 2010] or its relative force [Li et al. PRL, 2015]. Within Learn On The Fly (LOTF) [Csányi et al. PRL, 2004] simulations, the second approach is particularly suited since it guarantees reference accuracy on database entries. I will discuss a novel scheme [Glielmo et al. PRB, submitted] to accurately predict atomic forces as vector quantities, rather than sets of scalar components, by Gaussian Process (GP) Regression. This is based on matrix-valued kernel functions, to which we impose that the predicted force rotates with the target configuration and is independent of any rotations applied to the configuration database entries. We show that such "covariant" GP kernels can be obtained by integration over the elements of the rotation group SO(n). The accuracy of our kernels in predicting quantum forces in real materials is investigated by tests on pure and defective Ni and Fe crystalline systems.

Aldo Glielmo
King's College London, Physics Department

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