Alchemical and structural distribution based representation for improved QML

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We introduce a representation of any atom in any chemical environment for the automatized generation of universal kernel ridge regression-based quantum machine learning (QML) models of electronic properties, trained throughout chemical compound space. The representation is based on Gaussian distribution functions, scaled by power laws and explicitly accounting for structural as well as elemental degrees of freedom. The elemental components help us to lower the QML model's learning curve, and, through interpolation across the periodic table, even enable "alchemical extrapolation" to covalent bonding between elements not part of training. This point is demonstrated for the prediction of covalent binding in single, double, and triple bonds among main-group elements as well as for atomization energies in organic molecules. We present numerical evidence that resulting QML energy models, after training on a few thousand random training instances, reach chemical accuracy for out-of-sample compounds. Compound datasets studied include thousands of structurally and compositionally diverse organic molecules, non-covalently bonded protein side-chains, (H2O)(40)-clusters, and crystalline solids. Learning curves for QML models also indicate competitive predictive power for various other electronic ground state properties of organic molecules, calculated with hybrid density functional theory, including polarizability, heat-capacity, HOMO-LUMO eigenvalues and gap, zero point vibrational energy, dipole moment, and highest vibrational fundamental frequency
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