Fighting the Curse of Dimensionality

Machine Learning for High Dimensional Potential Energy Functions

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Setting

Problem

Given some ensemble of N nuclei with positions $x_i \in \mathbb{R}^3$ and atomic numbers $Z_i \in \mathbb{N}$, find the ensemble's electronic energy $E = E(\{(x_i, Z_i)\}_{i=1,\dots,N})$ and its derivatives with respect to the atoms' positions.

In theory, this is can be achieved by solving the electronic Schrödinger equation

$$H^{(e)} \left|\Phi\right\rangle = E \left|\Phi\right\rangle .$$

Dimension Reduction

- The original problem is very high dimensional, as we want to handle tens or hundreds of thousands of particles.
- Move to "site energies" V with

$$E = \sum_i V(Dx_i),$$

where Dx_i is the neighborhood of atom i.

Invariants

Analogously to the previous talk, the site energies obey invariants

- with respect to Euclidean transformations of the neighborhood and
- with respect to permutation of chemically equivalent atoms.

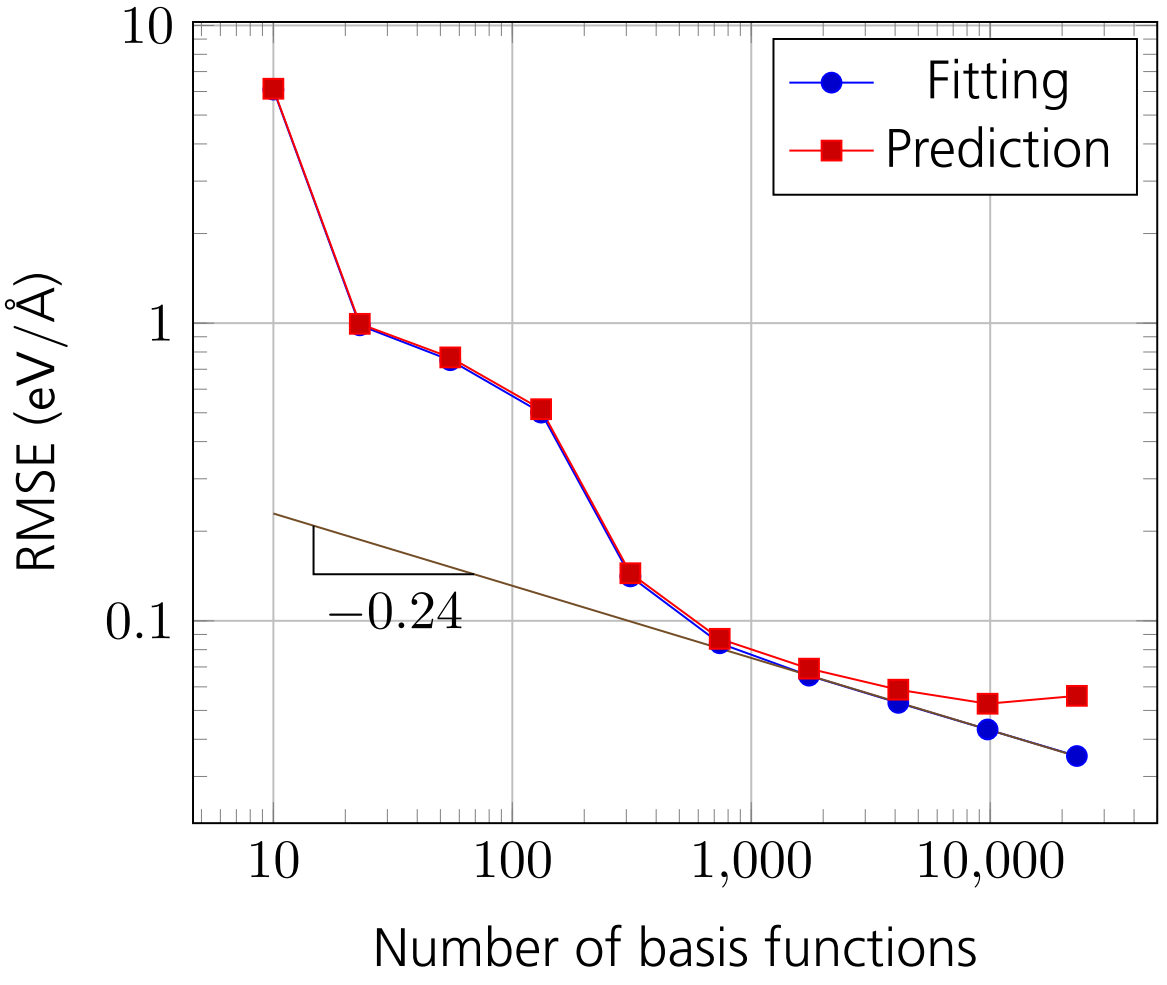
Descriptors

- To employ ML techniques for learning V, we need to map atomic neighborhoods to some tuple of real numbers.
- Key challenge: choose such maps (aka. *descriptors*) such that
  - they guarantee the neighborhoods' invariants,
  - they can tell different neighborhoods apart, and
  - they can be evaluated efficiently.

Existing Machine Learning Potentials

- Gaussian approximation potentials, using spherical harmonics and Gaussian kernels. (Bartók)
- Neural network potentials, using a set of *atom-centered symmetry functions* and feed-forward neural networks. (Behler)
- Moment tensor potentials, using invariant polynomials. (Shapeev)

Fitting and Prediction Error for Tungsten Dataset



Conclusion

- Express high-dimensional global problem through smaller local problems.
- Encode known properties in descriptors of the local problem.
- Last, apply machine learning to find good approximations.

Thank you for your attention!

Questions?