FEATURE SELECTION FOR NEURAL NETWORK POTENTIALS

The Adaptive Group Lasso

Johannes Sandberg, Institute for Materials Physics in Space, 10.09.2024

Introduction

Feature Selection for High-Dimensional Neural Network Potentials with the Adaptive Group Lasso

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Abstract. Neural network potentials are a powerful tool for atomistic simulations, allowing to accurately reproduce *ab initio* potential energy surfaces with computational performance approaching classical force fields. A central component of such potentials is the transformation of atomic positions into a set of atomic features in a most efficient and informative way. In this work, a feature selection method is introduced for high dimensional neural network potentials, based on the Adaptive Group Lasso (AGL) approach. It is shown that the use of an embedded method, taking into account the interplay between features and their action in the estimator, is necessary to optimize the number of features. The method's efficiency is tested on

Background

- Descriptor-based MLIPs require careful design of input features
- Large Featuresets:
  - Contain more information
  - Increase computational demand
  - Potentially contributes to overfitting

Feature Selection

- Filter Methods
  - Optimizing some criterion over dataset
  - No knowledge of estimator
- Wrapper Methods
  - Search method over feature subsets
- Embedded Methods
  - Select features during training

1: I. Lemhadri, et al, *J. Machine Learn. Research* **22** (2021)

Previous Work

- Unsupervised Filter Methods
  - G. Imbalzano, *et al*, *J. Chem. Phys.* **148** (2018)
- Supervised Filter Method
  - R. K. Cersonsky, *et al*, *MLST* **2** (2021)
- Embedded Methods for Linearized Potentials
  - A. Seko, *et al*, *Phys. Rev. B* **90** (2014)
  - M. Benoit, *et al*, *MLST* **2** (2021)

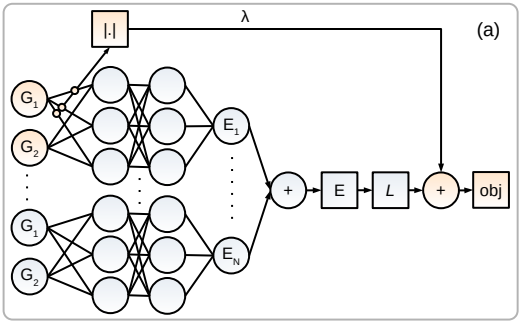
Embedded Methods for NNs

- Lasso not directly suitable for NNs
  - L1 regularization shrinks individual weights
- Group Lasso
  - Group input weights by feature $w^0_{i,[:]}$
  - Regularize with euclidean norm of each group

Group Lasso Penalty

$$obj(W) = L(W) + \lambda \sum_{i}^{D} \|w^0_{i,[:]}\|$$

Adaptive Group Lasso



- Initial training to obtain weights $\hat{w}$ used to adapt penalty in second training run

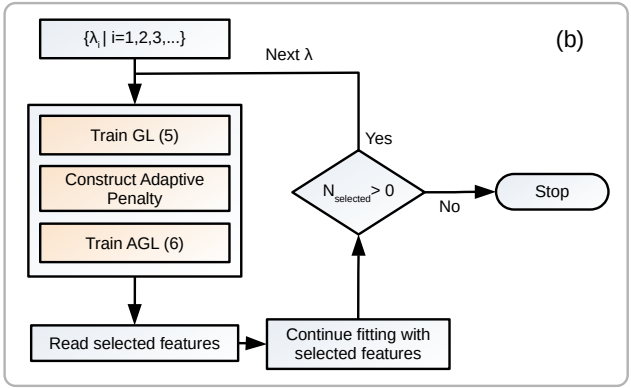
Adaptive GL Penalty

$$obj(W) = L(W) + \lambda \sum_{i}^{D} \frac{\|w^0_{i,[:]}\|}{\|\hat{w}^0_{i,[:]}\|}$$

1: V. Dinh, L. S. T. Ho, *NeurIPS* (2020)

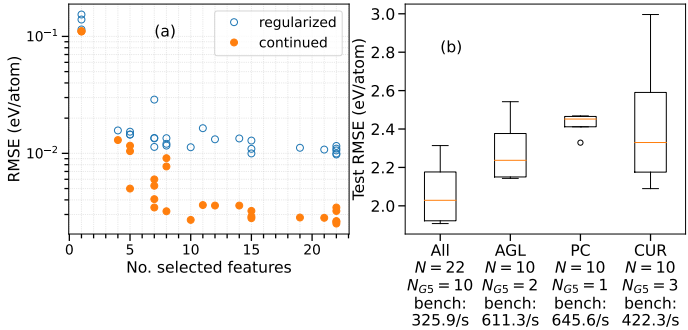
Overview: Test Cases

- Aluminium
  - Relatively low angular dependence
- Boron
  - Complicated structure, with highly directional bonds

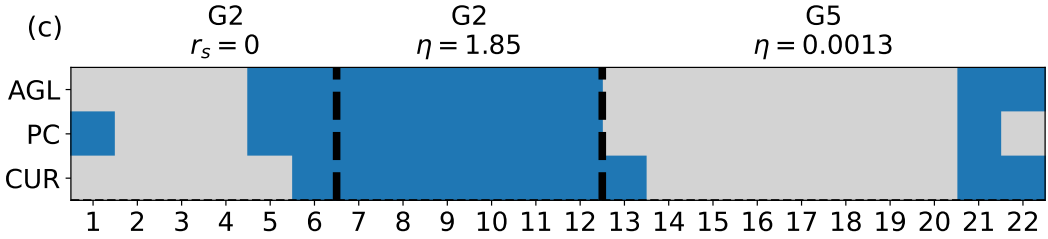


Aluminium

- Atom-Centered SFs
  - 12 Radial
  - 10 Angular
- Plateau in selection curve
- Favors radial features

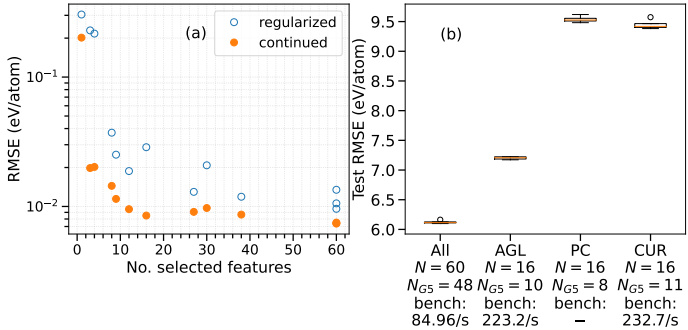


AI - Selected Features

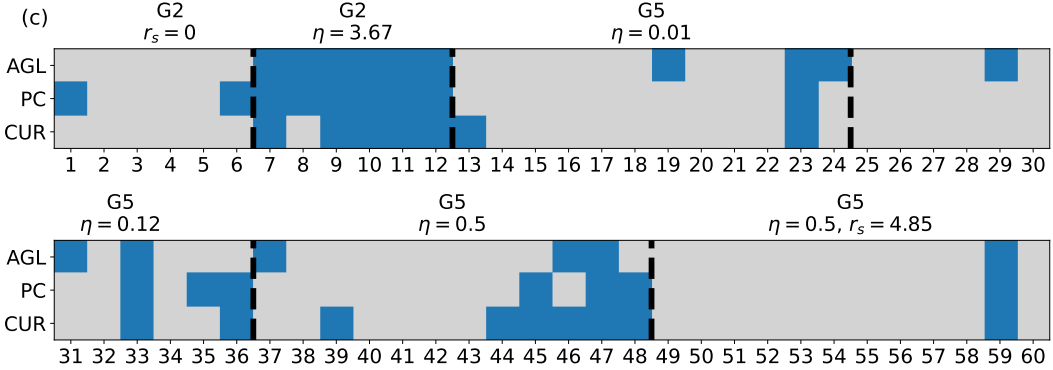


Boron

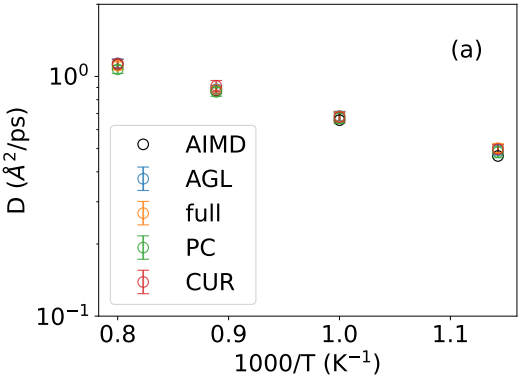
- ACSFs less well suited for this system
  - Worse baseline performance compared to Aluminium
- Outperforms PC and CUR

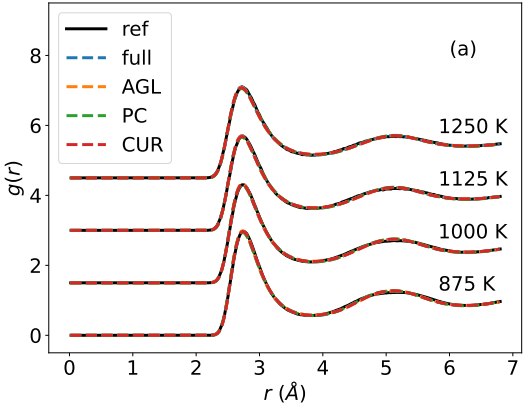


Boron - Selected Features

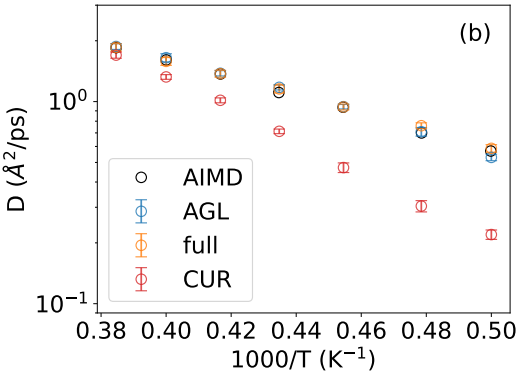


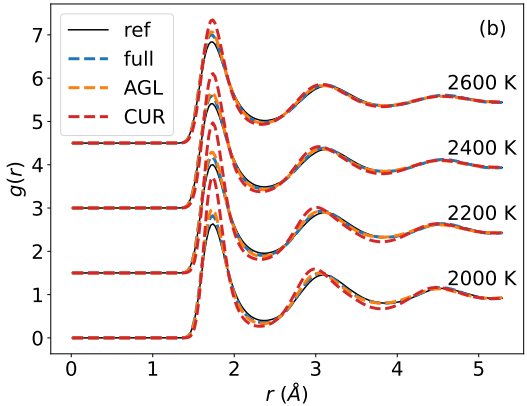
Simulation Results for Aluminium





Simulation Results for Boron





Outlook

- Extension to Multicomponent systems
  - Species-dependent regularization
- Usage with second order optimization methods
- Possible applications to Sparsification