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REGRESSION ON INTERATOMIC DESCRIPTOR DATA: DIRECT SOLUTION STRATEGIES FOR LINEAR REGRESSION IN CPU AND MEMORY-CONSTRAINED ENVIRONMENTS

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By
Dursun Dashdamirov

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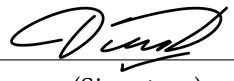
Dursun Dashdamirov		28.04.2025
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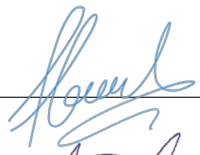
Dr. Jamaladdin Hasanov		08.08.2025
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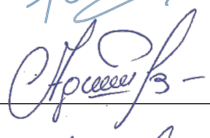
Dr. Abzatdin Adamov		08.08.2025
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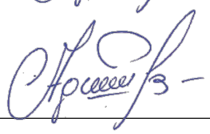
Dr. Abzatdin Adamov		08.08.2025
(Dean)		(Date)

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ABBREVIATIONS

Abbreviation	Explanation
ACE	Atomic Cluster Expansion
ASE	Atomic Simulation Environment
DFT	Density Functional Theory
FitSNAP	Fitting framework based on SNAP
GA	Genetic Algorithm
GBDT	Gradient Boosted Decision Trees
HDNNP	High-Dimensional Neural Network Potentials
HPC	High-Performance Computing
LAMMPS	Large-scale Atomic/Molecular Massively Parallel Simulator
MAE	Mean Absolute Error
MD	Molecular Dynamics
ML	Machine Learning
MLIP	Machine Learning Interatomic Potential
MPNN	Message Passing Neural Network
MSE	Mean Squared Error
PCA	Principal Component Analysis
PES	Potential Energy Surface
RAM	Random Access Memory
RMSE	Root Mean Square Error
SGD	Stochastic Gradient Descent
SHAP	Shapley Additive Explanations
SLURM	Simple Linux Utility for Resource Management
SNAP	Spectral Neighbor Analysis Potential
SOAP	Smooth Overlap of Atomic Positions
SSWRP	Stability-Weighted Square Sequence Product Aggregate Strategy
SVD	Singular Value Decomposition
VIF	Variance Inflation Factor

ABSTRACT

Molecular-dynamics (MD) simulations convert Newton's laws into atom-by-atom trajectories, from which pressure, temperature, and free energy are extracted for various experiments. While simulating any atomic environment, the most crucial feature of the atomic system is the energy. Also, it is the most challenging feature to estimate. The Machine Learning Interatomic Potentials (MLIP) solve this by fitting models to the system's definitive functions, which are utilized to make fast inferences regarding the energy of a system. The accuracy of these models depends on the domain-specific hyperparameter optimization, which is quite slow due to the use of complex deep neural networks. With this work, a new interatomic descriptor called quadratic ACE (qACE) is proposed, which surpasses the neural network's accuracy. Then, we explore and benchmark possible ways to fit a linear regression model to this computationally demanding solution in CPU and memory-bound environments. To solve the regression problem, several strategies are explored, including data reduction techniques and parallel processing. By leveraging Dask's comprehensive task scheduling infrastructure, we compute the direct least-squares regression on a 27 GB dataset in under five minutes, demonstrating both scalability and computational efficiency.

Overall, this work demonstrates that efficient feature engineering, combined with lightweight parallel regression strategies, can substitute for deep models without sacrificing accuracy or scalability.