AKPIK 2: Machine Learning Prediction and Optimization Tasks

Time: Tuesday 9:30–10:30 Location: H5

AKPIK 2.1 Tue 9:30 H5

Attention space geometry — •Claudius Gros — Institute for Theoretical Physics, Goethe University Frankfurt

Attention involves comparing query and key vectors in terms of a scalar product, $\mathbf{Q} \cdot \mathbf{K}$, together with a subsequent softmax normalization. Classicaly, parallel/orthogonal/anti-parallel queries and keys lead to large/intermediate/small attention weights. Here we study expressive attention (EA), which is based on $(\mathbf{Q} \cdot \mathbf{K})^2$, the squared dot product. In this case attention is enhanced when query and key are either parallel or anti-parallel, and suppressed for orthogonal configurations. For a series of auto-regressive prediction tasks, we find that EA performs at least as well as the standard mechanism, dot-product attention (DPA). Increasing task complexity, EA is observed to outperform DPA with increasing margins, which also holds for multi-task settings. For a given model size, EA manages to achieve 100% performance for a range of complexity levels not accessible to DPA.

AKPIK 2.2 Tue 9:45 H5

Global Opimization of Atomic Structures in Extra Dimensions — •Casper Larsen[1], Sami Kaappa[2], Andreas Vishart[3], Thomas Bligaard[4], and Karsten Jacobsen[5] — [1]Technical University of München — [2]Tampere University — [3]Technical University of Denmark — [4]Technical University of Denmark — [5]Technical University of Denmark

This work formulates an approach to global optimization of atomic structures by use of an atomic descriptor extending the atoms with additional nonphysical degrees of freedom. These include chemical identity coordinates, atomic existence, and hyperspatial coordinates, all of which can be energetically minimized separately or simultaneously. The minimization is performed on a surrogate potential energy surface generated by Gaussian process regression trained on DFT calculations as part of a Bayesian optimization algorithm, where it is assured that all relaxational end states and training points are physically valid. The method is shown to successfully interpolate energy and force predictions from a training set of physically valid structures to structures with nonphysical coordinates. The inclusion of extra degrees of freedom significantly improves the efficiency of optimization of both clusters and bulk materials by circumventing energy barriers encountered in the conventional potential energy surface.

AKPIK 2.3 Tue 10:00 H5

Co-orchestration of multiple instruments for automated exploration of structure-property relationships in combinatorial libraries — •Boris Slautin[1], Utkarsh Pratiush[2], Ilia Ivanov[3], Yongtao Liu[3], Rohit Pant[4], Xiaohang Zhang[4], Ichiro Takeuchi[4], Maxim Ziatdinov[5], and Sergei Kalinin[2,5] — [1]University of Duisburg-Essen, Essen, Germany — [2]University of Tennessee, Knoxville USA — [3]Oak Ridge National Laboratory, Oak Ridge, USA — [4]University of Maryland, College Park, USA — [5]Pacific Northwest National Laboratory, Richland, USA

The advancement of combinatorial synthesis techniques has significantly accelerated the development of novel materials. However, closing the loop in materials design requires powerful approaches for characterizing the synthesized libraries. This is a non-trivial task, as characterization often involves revealing multiple methods.

We present a multimodal co-orchestration framework for autonomous combinatorial library characterization through the simultaneous coordination of various tools (e.g., Raman spectroscopy, SPM). The multimodal co-orchestration enables the real-time utilization of acquired knowledge about one property to accelerate the exploration of other properties measured by different methods. The capabilities of the proposed framework were validated by the co-orchestrating of the SPM and Raman techniques in the Sm-BiFeO3 combinatorial library. The workflow confirms its effectiveness in optimizing the exploration trajectory. The proposed framework is general and can be extended to multiple modalities and arbitrary dimensionality of signals.

AKPIK 2.4 Tue 10:15 H5

Data nexus vista: A research assistance framework for physics-informed descriptor engineering — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

In today's fast-paced world, accurate modeling and prediction of complex systems are more crucial than ever, particularly for advancing modern technologies. In energy storage, for example, the design of materials with tailored properties for sustainable, next-generation devices is a critical goal. However, the vast materials space and intricate nature of materials data poses serious challenges for experimental and computational explorations, often likened to searching for a needle in a haystack. To address this, we present "Data Nexus Vista," a flexible framework for descriptor engineering. The framework offers four core functionalities: (1) adaptive preprocessing protocols for defining physically meaningful data transformations; (2) a feature selection interface that incorporates physics-based rules for improved interpretability; (3) diverse correlation analysis tools to uncover underlying physical mechanisms; and (4) workflows for developing interpretable models that balance physical validity with statistical robustness. By enabling thorough exploration of data-physical phenomena connections, this user-guided, modular approach ensures scientific rigor while addressing uncertainties in complex systems. Moreover, its adaptable design allows seamless application across diverse domains, from energy storage, surface science to nonlinear optical properties, advancing both scientific discovery and practical innovation.