Machine learning assisted prediction of correlation structure in strongly correlated systems

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The active-space quantum chemical methods could provide a very accurate description of strongly correlated electronic systems. The proper choice of the active space is crucial, but a non-trivial task. Recently, we developed the neural network (NN) based approach for automatic selection of active spaces, focused on transition metal systems.[1]

In the most recent work, we have trained a new Ml model which predicts a mutual information. This is a complex quantity, much more difficult to predict than one-site entropies. The mutual information carries important information about correlation structure inside systems. We show the performance on selected systems, where we utilized the mutual information for two important tasks - to determine bonding or ordering of orbitals for accurate DMRG calculations.

References

[1] Pavlo Golub, Andrej Antalik, Libor Veis, and Jiri Brabec, J. Chem. Theory Comput. 2021, 17, 10,6053–6072

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