Tata Institute of Fundamental Research
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Internal Webinar

Iterative Solvers for Local Kernel Ridge Regression

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Machine Learning (ML) methods have now become the mainstay of computational chemistry research. ML has found diverse applications, ranging from predicting yields of reactions to understanding electron dynamics in molecules. As ML methods are growing, so are their computational requirements. Vast majority of ML research utilizes Kernel Ridge Regression method with underlying Cholesky Factorization based solver. As kernel matrices are dense, the choices of solvers are rather limited. However, it can be demonstrated that iterative solvers can provide an alternative to Cholesky factorization based solvers. Iterative solvers can converge faster and are more scalable for well-behaved kernel matrices and hence can meet the modern day requirements of the KRR based ML methods. As a proof of concept, I would demonstrate how local descriptors can simplify complexity of infinite chemical space and in tandem with a Conjugate Gradient based solver, can yield a highly accurate NMR machine with accuracy rivaling DFT methods.

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11:30 AM