Machine Learning in Quantum Mechanics

Normalizing Flows for Computing Molecular Vibrational Wave Functions

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HELMHOLTZ

DESY.

Overview

> Introduction

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- Introduction
- Physics

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- Machine Learning

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- Mathematics

Introduction

The Challenge

- Solving Schrödinger's Equation is **hard**
- Usually turn to numerical approximations
- …but numerics have limitations
- The Curse of Dimensionality

$$E_{t,ij} = \sum_{k,l} \sum_{\lambda_i,\lambda_i'} \rho_{\lambda_1,\lambda_1'}(e_1^-)\rho_{\lambda_2,\lambda_2'}(e_2^-)[T_{ij}^{\lambda_1\ \lambda_2}(\tilde{\chi}_k^0)] \cdot [T_{ij}^{\lambda_1'\lambda_2'}(\tilde{\chi}_k^0)]^*$$

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Thank you!

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