

Jun Dai

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Work Experience

Graduate Research Assistant, University of British Columbia, Vancouver, BC September 2018 - Present

- Developed optimization methods for quantum circuits to construct quantum regression models
- Explored importance of entanglement for quantum regression models
- Developed ML-based algorithms for auto-tuning and gate pattern optimization of quantum dot-based quantum simulators
- Illustrated automated algorithms for fitting potential energy surfaces that reduced errors by 37.5%
- Demonstrated possibility of extrapolation of potential energy surfaces
- Applied Bayesian machine learning methods to correct approximate quantum dynamics calculations
- Explored applications of infinite-wide neural networks for quantum problems
- Mentored and trained graduate students

Graduate Teaching Assistant, University of British Columbia, Vancouver, BC September 2018 - Present

- Taught university-level labs for over 100 students
- Organized tutorials of quantum mechanics for over 50 students

Education

Doctor of Philosophy: Chemistry, University of British Columbia, Vancouver, BC September 2018 - June 2023

- Thesis: Applications of classical and quantum machine learning for quantum problems
- Relevant coursework: CPSC 532M Machine Learning and Data Mining, CPSC 540 Machine learning, PHYS 500 Quantum Mechanics, PHYS 502 Condensed Matter Physics I

Bachelor of Science: Materials and Nanosciences, University of Waterloo, Waterloo, ON September 2014 - June 2018

- Dean's Honours List
- Term Dean's Honours List Winter 2017

Publications

1. J. Dai, R. Krems (2019). "Interpolation and extrapolation of global potential energy surfaces for polyatomic systems by Gaussian processes with composite kernels," J. Chem. Theory Comput.
2. A. Jasinski, J. Montaner, R. C. Forrey, B. Yang, P. Stancil, N. Balakrishnan, J. Dai, R. A. Vargas-Hernandez, R. Krems (2020). "Machine learning corrected quantum dynamics calculations," Phys. Rev. Research
3. J. Dai, R. Krems (2022). Quantum Gaussian process model of potential energy surface for a polyatomic molecule," J. Chem. Phys.
4. L. Szulakowska, J. Dai. Bayesian autotuning of Hubbard model quantum simulators, arXiv:2210.03077
5. J. Dai, R. Krems. Interpolation and extrapolations of quantum physical systems with neural network Gaussian process, arXiv:2304.05528
6. Quantum enhanced basis expansion, (in preparation)

Presentations

1. Gaussian processes for system-agnostic construction of high-dimensional PES with sparse ab initio data, DAMOP 2020
2. Machine-learning-corrected quantum dynamics calculations, DAMOP 2020

Skills

- Python
- Julia
- C
- Qiskit
- JAX
- TensorFlow
- Pytorch
- Markov chain Monte Carlo
- High-Performance Computer Systems
- Exact diagonalization
- Discrete variable representations
- Simulation of second-quantized models
- Machine learning
- Deep learning
- Bayesian optimization

- Kernel optimization
- Quantum computing
- Quantum information
- Quantum machine learning
- Quantum simulation
- Quantum kernel optimization
- Expert in Bayesian inference
- Expert in theory of machine learning
- Communication
- Creative problem solving
- Research project development
- Analytical writing and presentation

References

- Professor Roman Krems, Supervisor, Email: rkrems@chem.ubc.ca
- Professor Mark Thachuk, Email: thachuk@chem.ubc.ca
- Professor Rodrigo Alejandro Vargas Hernandez, Email: vargashr@mcmaster.ca