Quantum Dose

PK/PD Modeling Utilizing Transformers, QIHMC, Quantum Kernels

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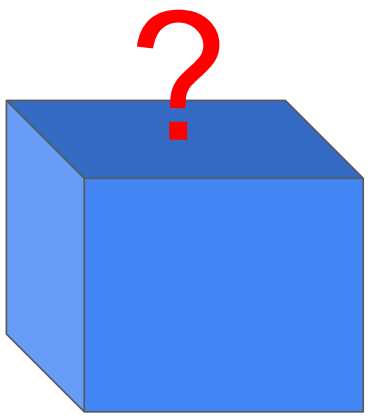
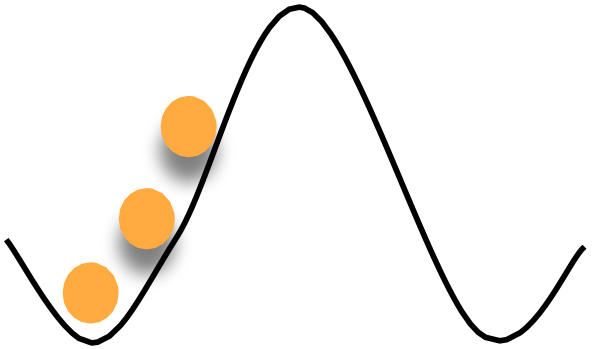
Motivation

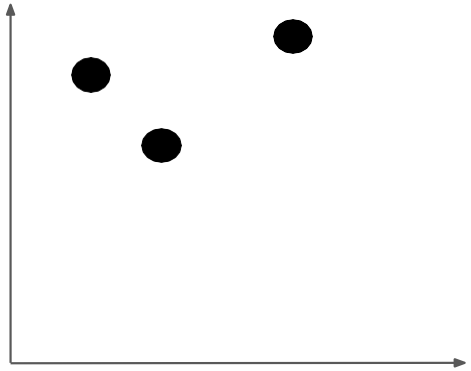
Why add "Quantumness" to the PK/PD problem?



Choice of PDE



Poor Exploration of Parameter Space



Small Dataset

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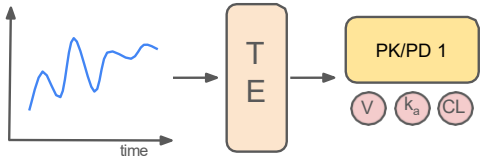
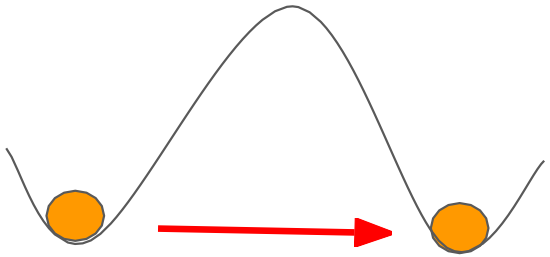
Quantum Dose Method

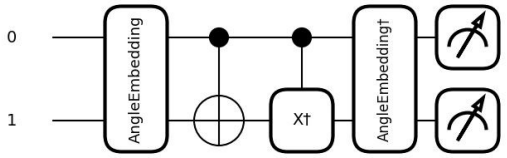
Stage 1
Transformer Encoder for PK/PD Model Identification

Stage 2
Quantum Inspired Hamiltonian Monte Carlo

Stage 3
Quantum Kernel Method for Support Vector Regression







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Advantages

Stage 1: Narrowing down the PK/PD model for improved efficiency in Stage 2/3

Stage 2: A stochastic exploration of parameter space: Tunable weight parameter to overcome large potentials

Stage 3: Quantum correlations that can't be captured by classical relationships, which potentially provide fundamental understanding from small datasets.

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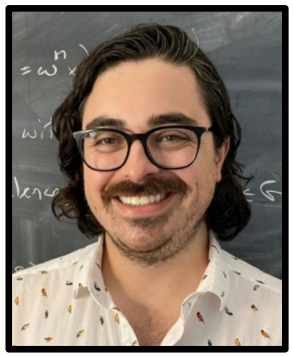
Acknowledgements

Prineha Narang



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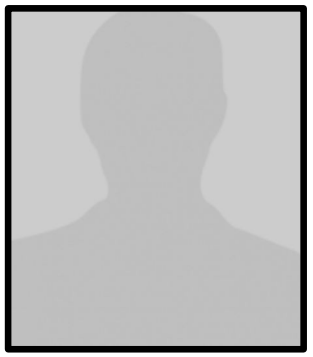

Scott Nie

Quantum Innovation Challenge Organizing Committee

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