Understanding Parameterized Quantum Circuit Learning for Quantum Chemical Applications

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Electronic Supplementary Information

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1 BSE49: Molecular Representations

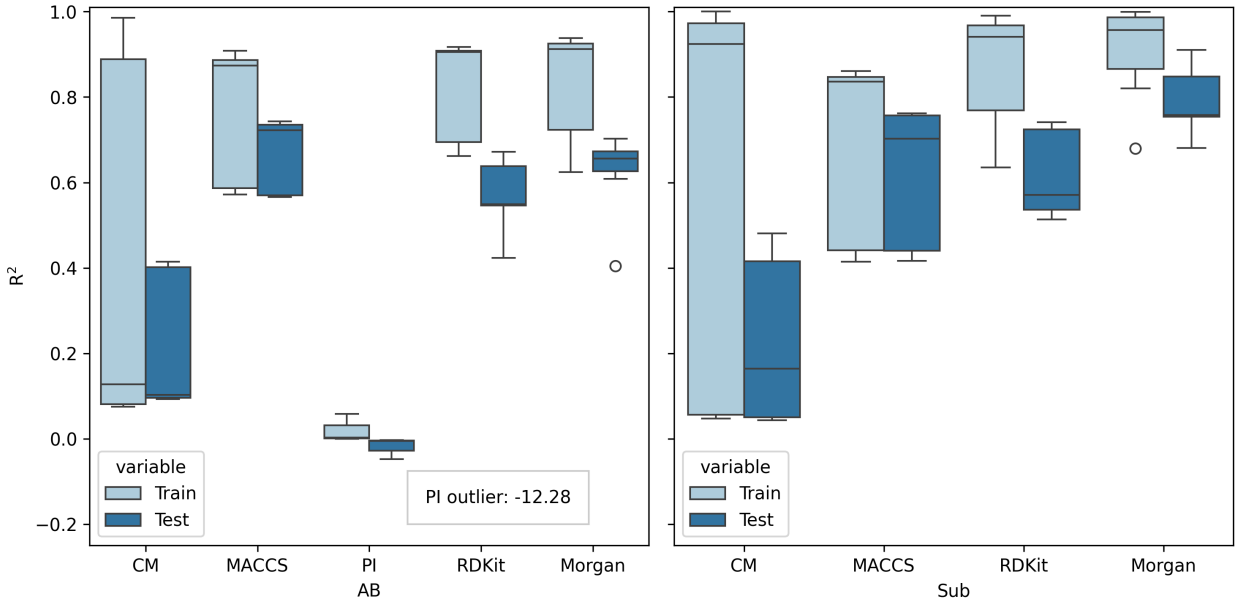
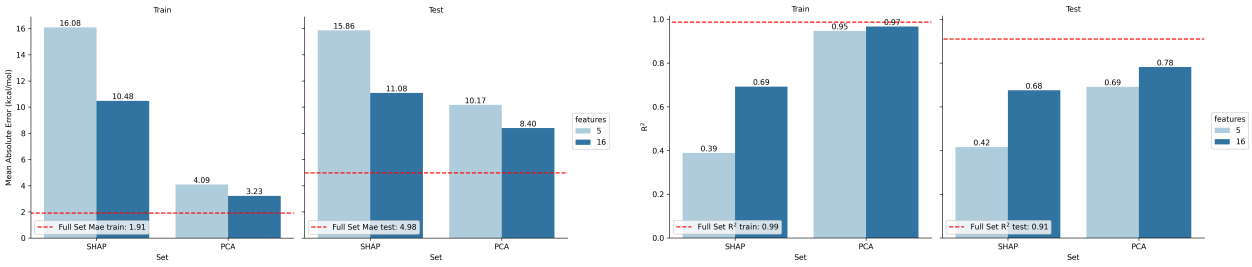


Figure S1: Coulomb matrices (CMs), Molecular ACCess Systems (MACCS), persistence images (PIs), RDKit and Morgan fingerprints. Performance of a diverse set of molecular representations R^2

2 Classical Feature Reduction



(a) (b)

Figure S2: Feature reduction of the BSE dataset represented using

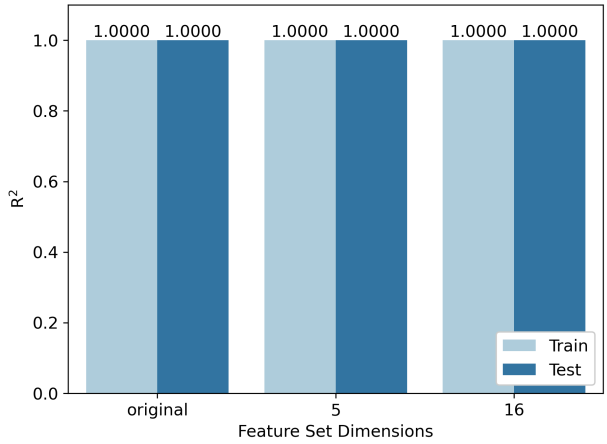


Figure S3

3 DDCC Fake Quebec

Ran using the state vector model parameters for one iteration to test the optimization and resilience levels using Fake Quebec before running on the real device

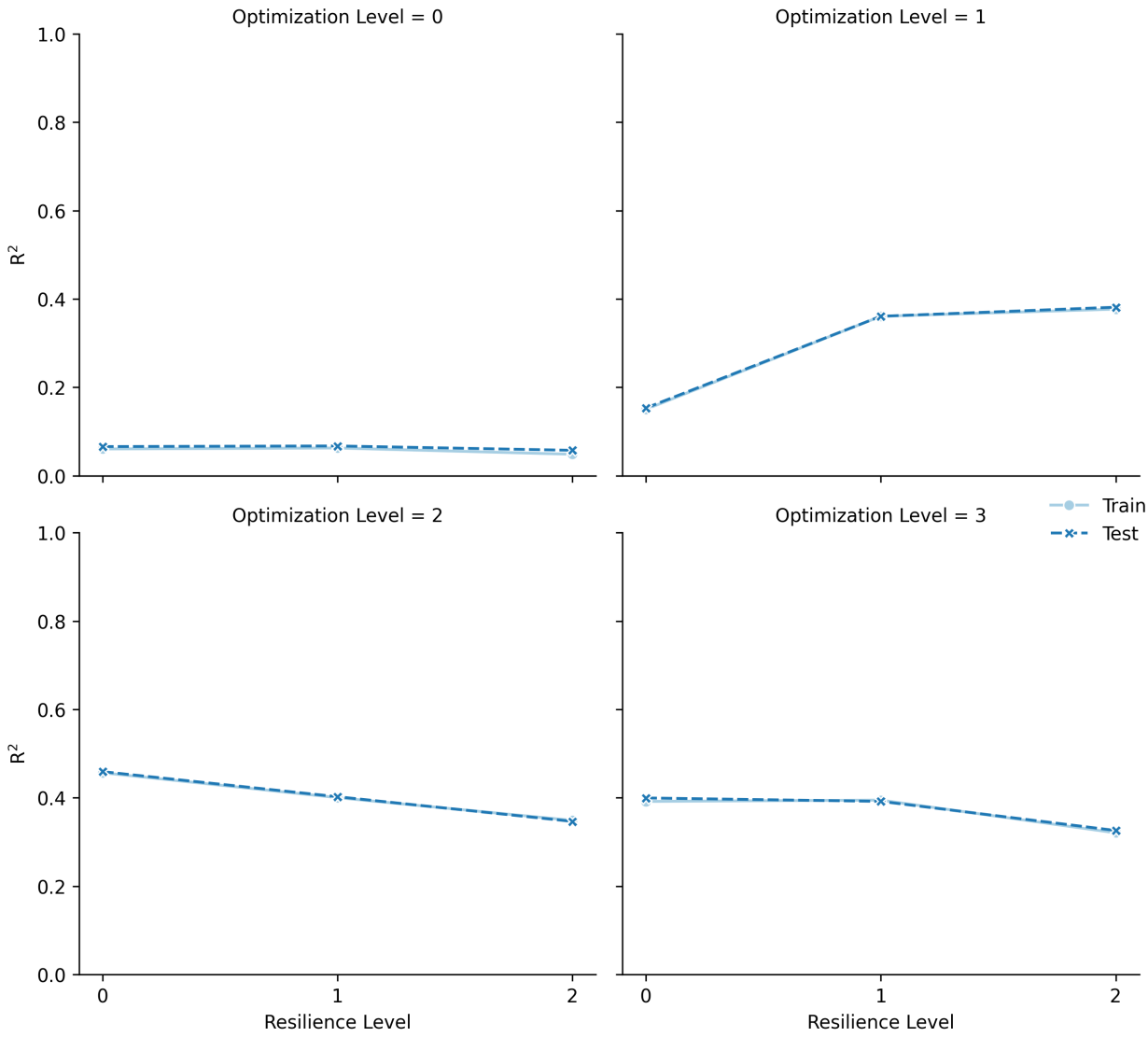

Optimization Level = 0
Optimization Level = 1
Optimization Level = 2
Optimization Level = 3
R^2
1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
Resilience Level
Train
Test

Figure S4

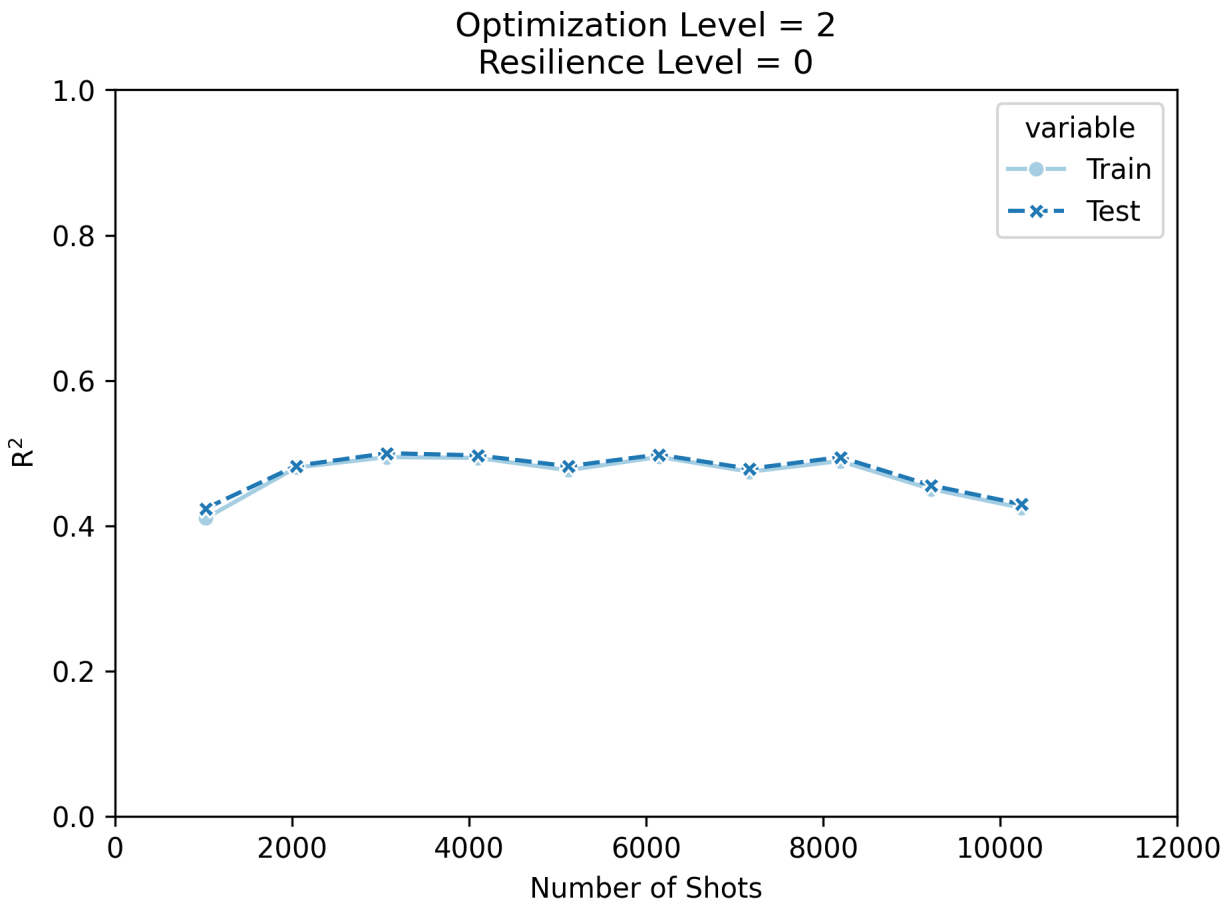


Figure S5

4 title