Understanding Parameterized Quantum Circuit Learning for Quantum Chemical Applications

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Electronic Supplementary Information

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1 BSE49: Molecular Representations

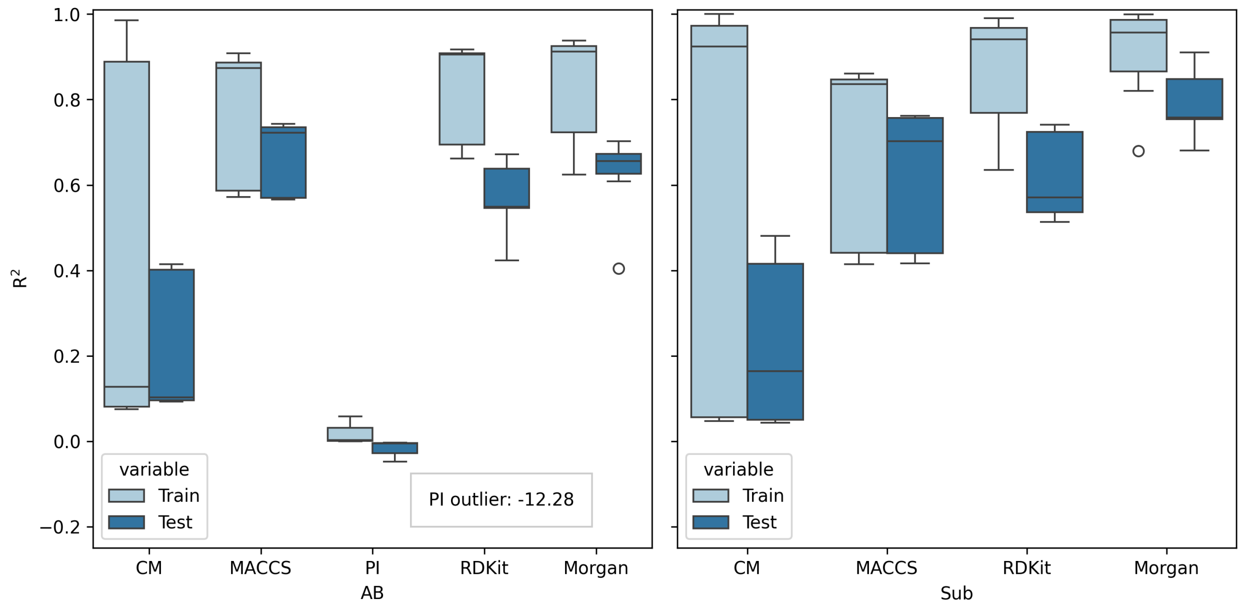
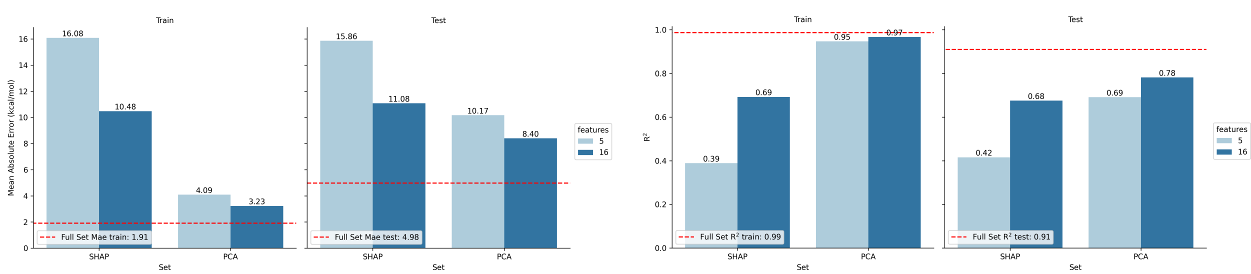


Figure S1: Coulomb matrices (CMs), Molecular ACCess Systems (MACCS), persistence images (PIs), RDKit and Morgan fingerprints. Performance of a diverse set of molecular representations R^2

2 Classical Feature Reduction



(a) (b)

Figure S2: Feature reduction of the BSE dataset represented using

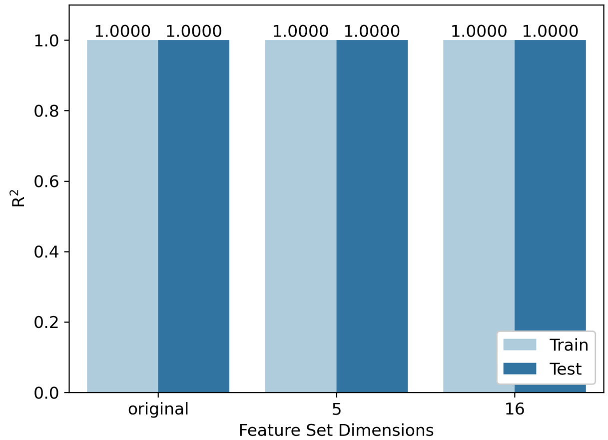


Figure S3

3 BSE49 5 Qubit Learning Curve Data

ratio	model	Train	Test
0.1	M-M-CZ_HWE-CNOT	0.2015	0.1303
	elastic	0.1787	0.1229
	gpr	0.3254	0.2147
	grad	0.9010	0.3352
	knn	0.9998	0.3963
	krr	0.4242	0.2811
	lasso	0.1786	0.1229
	rfr	0.8896	0.4220
	ridge	0.1789	0.1226
	svr	0.4020	0.2719
0.3	M-M-CZ_HWE-CNOT	-0.0172	-0.0088
	elastic	0.2099	0.2012
	gpr	0.4211	0.3857
	grad	0.8896	0.5215

	knn	0.9998	0.5837
	krr	0.4967	0.4385
	lasso	0.2094	0.2002
	rfr	0.9455	0.5589
	ridge	0.2100	0.2015
	svr	0.4881	0.4287
0.5	M-M-CZ_HWE-CNOT	0.1715	0.1792
	elastic	0.1960	0.2050
	gpr	0.4383	0.4377
	grad	0.9350	0.5721
	knn	0.9998	0.6222
	krr	0.4724	0.4612
	lasso	0.1954	0.2039
	rfr	0.9453	0.5970
	ridge	0.1961	0.2055
	svr	0.4754	0.4628
0.7	M-M-CZ_HWE-CNOT	0.1908	0.2064
	elastic	0.1623	0.1785
	gpr	0.4347	0.4516
	grad	0.9624	0.5957
	knn	0.9998	0.6366
	krr	0.4577	0.4714
	lasso	0.1617	0.1770
	rfr	0.9483	0.6430
	ridge	0.1623	0.1791
	svr	0.4577	0.4709
0.8	M-M-CZ_HWE-CNOT	0.1559	0.1727

elastic	0.1656	0.1828
gpr	0.4445	0.4607
grad	0.9531	0.6030
knn	0.9999	0.6725
krr	0.4596	0.4727
lasso	0.1651	0.1812
rfr	0.9462	0.6400
ridge	0.1657	0.1834
svr	0.4578	0.4671

4 DDCC 5 Qubit Learning Curve Data

ratio	model	Test	Train
0.1	A2_HWE-CNOT	0.4502	0.4434
	elastic	0.9874	0.9877
	gpr	1.0000	0.9997
	grad	1.0000	0.9999
	knn	1.0000	1.0000
	krr	0.9999	0.9997
	lasso	0.9873	0.9877
	rfr	1.0000	0.9999
	ridge	0.9898	0.9901
	svr	0.9985	0.9982
0.3	A2_HWE-CNOT	0.4341	0.4270
	elastic	0.9873	0.9875

	gpr	1.0000	1.0000
	grad	1.0000	1.0000
	knn	1.0000	1.0000
	krr	0.9999	0.9999
	lasso	0.9872	0.9874
	rfr	1.0000	1.0000
	ridge	0.9897	0.9899
	svr	0.9990	0.9989
0.5	A2_HWE-CNOT	0.8310	0.8308
	elastic	0.9875	0.9875
	gpr	1.0000	1.0000
	grad	1.0000	1.0000
	knn	1.0000	1.0000
	krr	0.9999	1.0000
	lasso	0.9875	0.9874
	rfr	1.0000	1.0000
	ridge	0.9899	0.9899
	svr	0.9994	0.9994
0.7	A2_HWE-CNOT	0.7162	0.7093
	elastic	0.9874	0.9875
	gpr	1.0000	1.0000
	grad	1.0000	1.0000
	knn	1.0000	1.0000
	krr	1.0000	0.9999
	lasso	0.9874	0.9875
	rfr	1.0000	1.0000
	ridge	0.9898	0.9899

	svr	0.9995	0.9995
0.8	A2_HWE-CNOT	0.8470	0.8492
	elastic	0.9875	0.9874
	gpr	1.0000	1.0000
	grad	1.0000	1.0000
	knn	1.0000	1.0000
	krr	0.9999	1.0000
	lasso	0.9874	0.9873
	rfr	1.0000	1.0000
	ridge	0.9899	0.9898
	svr	0.9995	0.9995

5 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

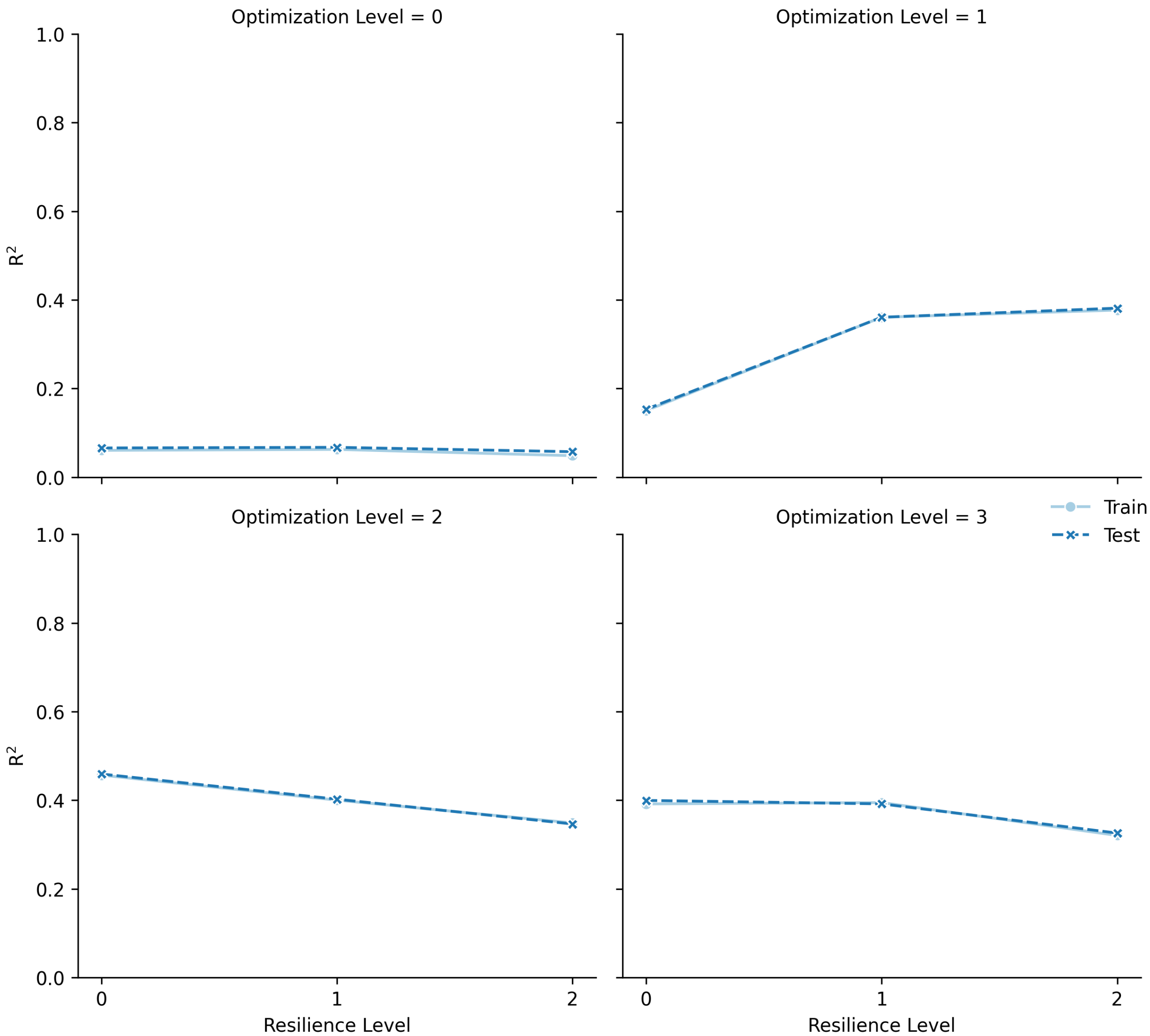

Optimization Level = 0
Optimization Level = 1
Optimization Level = 2
Optimization Level = 3
R²
1.0
0.8
0.6
0.4
0.2
0.0
0
1
2
Resilience Level
Train
Test

Figure S4

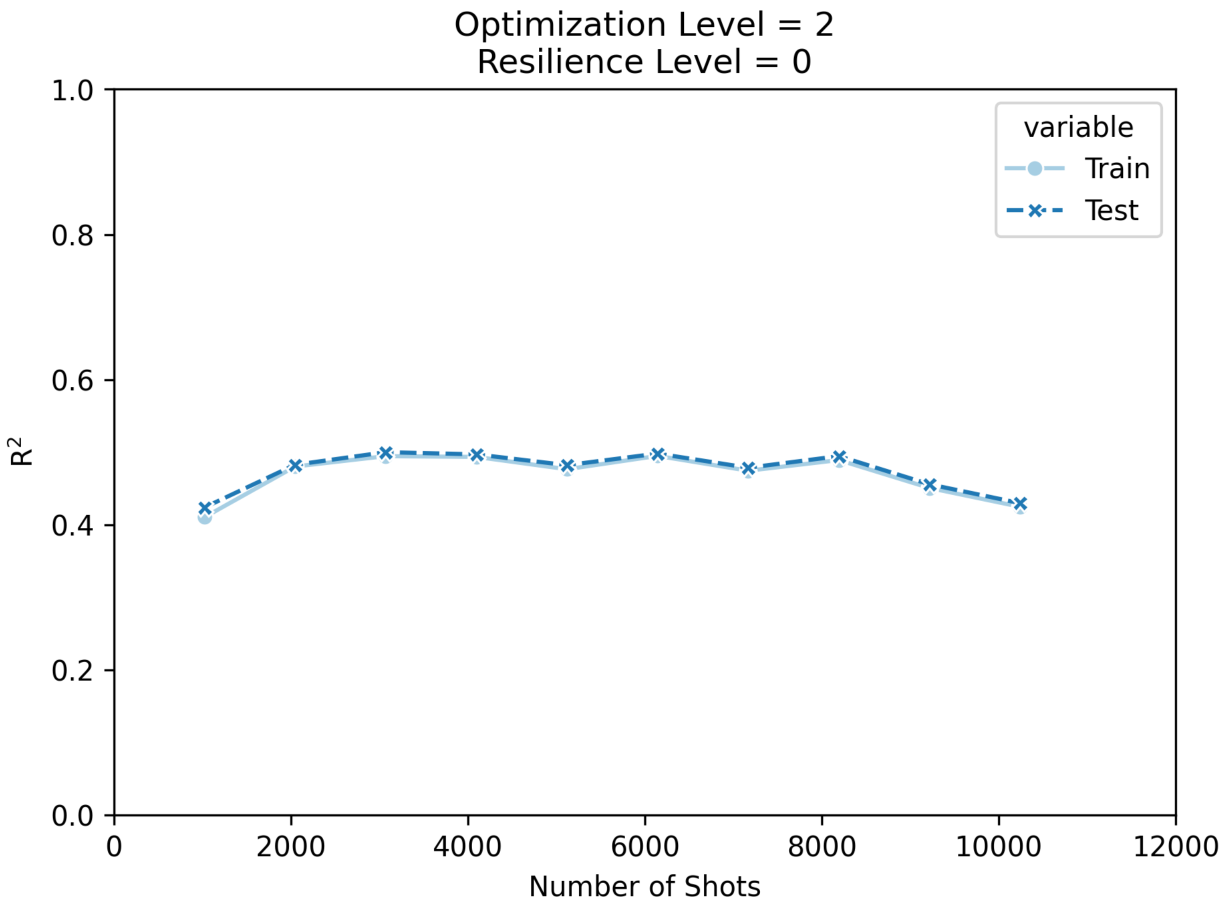

Optimization Level = 2
Resilience Level = 0
variable
Train
Test
1.0
0.8
0.6
0.4
0.2
0.0
R^2
0
2000
4000
6000
8000
10000
12000
Number of Shots

Figure S5