Rebuttal for ICML'25 Submission #3922

Submission #3922 Authors

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Table 1: **The RMSE result on correlation prediction of $|\psi_{\mathrm{HB}}\rangle$ with varied N and n_{sft}.** M is fixed to 64. `ResXXX-a-b-cxd-e` represents neural network `MLP` (`CNN`) that composed of $d+3$ in the order a-,b-, d layers of c-, and e-width fully connected (convolutional) layers with residual connection. The best results are highlighted in **boldface** while the second-best results are distinguished in underlined.

Methods	$N=48$			$N=63$			$N=100$			$N=127$		
	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$
CS	0.21113			0.21257			0.21399			0.21447		
ResMLP-128x2	0.08282	0.07752	0.06616	0.12055	0.08776	0.07086	0.10848	0.08158	0.07405	0.10091	0.10083	0.08245
ResMLP-128x3	0.06214	0.04853	0.04494	0.07256	0.05506	0.04467	0.07740	0.06496	0.07098	0.08535	0.08280	0.08691
ResMLP-128x4	0.05428	0.03825	0.03524	0.06463	0.04435	0.03833	0.07532	0.05952	0.06010	0.07971	0.09173	0.08608
ResMLP-128x5	0.07228	0.04721	0.03764	0.07308	0.05957	0.05091	0.08046	0.07146	0.07174	0.08408	0.08650	0.08458
ResCNN-32-64	0.07160	0.04723	0.03795	0.07176	0.04066	0.03042	0.06549	0.04566	0.03464	0.06468	0.03189	0.07404
ResCNN-32-64-128	0.08089	0.03422	0.03435	0.09003	0.03401	0.03159	0.07603	0.03245	0.03295	0.08420	0.03179	0.03025
ResCNN-32-64-128x2	0.06484	0.04899	0.03456	0.06621	0.03608	0.03100	0.06436	0.03425	0.02808	0.07441	0.03196	0.05221
ResCNN-32-64-128x2-64	0.17049	0.15600	0.16109	0.18302	0.13459	0.14636	0.13584	0.14809	0.11732	0.17961	0.09261	0.12525
LLM4QPE-T	0.05189	0.03368	0.03197	0.06111	0.03364	0.02863	0.05050	0.03227	0.02726	0.05079	0.03184	0.02634
RBFK	0.05452	0.04176	0.04101	0.04726	0.03829	0.03922	**0.04096**	0.03299	0.03282	**0.03850**	0.03115	0.03086
Lasso	**0.04221**	**0.02636**	0.02489	0.04856	**0.02791**	**0.02326**	0.04219	**0.02602**	0.02646	0.04137	0.03292	**0.02083**
Ridge	0.04247	0.02884	**0.02475**	**0.04216**	0.02816	0.02402	0.04191	0.02711	**0.02251**	0.04110	**0.02620**	0.02161

Table 2: **The RMSE result on correlation prediction of $|\psi_{\mathrm{TFIM}}\rangle$ with varied N and n_{sft}.** M is fixed to 64. `ResXXX-a-b-cxd-e` represents neural network `MLP` (`CNN`) that composed of $d+3$ in the order a-,b-, d layers of c-, and e-width fully connected (convolutional) layers with residual connection. The best results are highlighted in **boldface** while the second-best results are distinguished in underlined.

Methods	$N=48$			$N=63$			$N=100$			$N=127$		
	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$	$n_{\mathrm{sft}}=20$	$n_{\mathrm{sft}}=60$	$n_{\mathrm{sft}}=100$
CS	0.20924			0.20990			0.21092			0.21180		
ResMLP-128x2	0.07899	0.06371	0.05524	0.07986	0.05279	0.04283	0.08293	0.05303	0.04630	0.07908	0.05006	0.04333
ResMLP-128x3	0.06080	0.05664	0.06074	0.06514	0.06928	0.06914	0.06301	0.06358	0.07317	0.06324	0.06510	0.07327
ResMLP-128x4	0.05912	0.05794	0.05980	0.05899	0.05705	0.06163	0.05678	0.05628	0.06977	0.05535	0.06496	0.07197
ResMLP-128x5	0.07422	0.06545	0.05739	0.07341	0.06921	0.069215	0.06648	0.06556	0.07044	0.06941	0.07222	0.06867
ResCNN-32-64	0.12845	0.15039	0.08935	0.12227	0.16686	0.10315	0.10084	0.08879	0.05177	0.10495	0.08535	0.04647
ResCNN-32-64-128	0.13545	0.17135	0.12004	0.12545	0.17026	0.11778	0.11433	0.11267	0.05027	0.13312	0.03562	0.05347
ResCNN-32-64-128x2	0.13624	0.17178	0.12015	0.12608	0.17103	0.13809	0.12221	0.11046	0.06586	0.13757	0.10498	0.05556
ResCNN-32-64-128x2-64	0.13719	0.16750	0.14122	0.13184	0.16034	0.14158	0.12356	0.14996	0.11282	0.11823	0.03601	0.03785
LLM4QPE-T	0.05088	0.03493	0.03006	0.05252	0.03566	0.03082	0.05217	0.03476	0.03012	0.05259	0.03641	0.03084
Lasso	0.04624	0.03219	0.02812	0.04633	0.03930	0.02859	**0.04073**	**0.03256**	0.02899	0.04583	**0.03283**	0.02932
Ridge	**0.04473**	**0.03173**	**0.02807**	**0.04561**	**0.03226**	**0.02839**	0.04598	0.03277	**0.02883**	**0.04570**	0.03285	**0.02911**

Table 3: The RMSE results on correlation prediction of $|\psi_{\mathrm{HB}}\rangle$ with varied N. Training set and testing set are both have 10^4 samples, with noise-free labels ($M \to \infty$). The best results are highlighted in **boldface**.

$M \to \infty$	$N = 8$	$N = 10$	$N = 12$	$N = 16$	$N = 25$	$N = 31$
`Ridge`	**0.00367**	**0.00444**	**0.00566**	**0.00636**	**0.00599**	**0.00579**
`ResMLP-128x4`	0.03961	0.03677	0.03460	0.03129	0.02769	0.02625
`ResCNN-32-64-128x2`	0.02056	0.03710	0.03432	0.03050	0.02582	0.02381
`LLM4QPE-F`	0.04666	0.04385	0.03969	0.03728	0.03083	0.02951

Table 4: The RMSE results on correlation prediction of $|\psi_{\mathrm{HB}}\rangle$ with varied training size n. System size $N = 8$. The number of testing set is fix to 2×10^4. Labels are noise-free ($M \to \infty$). The best results are highlighted in **boldface**.

$M \to \infty$	# Params	$n = 10^2$	$n = 10^3$	$n = 10^4$	$n = 10^5$
`Ridge`	< 0.01M	**0.00780**	**0.00528**	**0.00367**	**0.00660**
`ResMLP-128x4`	0.09M	0.04219	0.04172	0.03961	0.03956
`ResCNN-32-64-128x2`	1.14M	0.01987	0.02078	0.02056	0.02054
`LLM4QPE-F`	9.89M	0.03966	0.04304	0.04916	0.04659

Table 5: The RMSE results of `LLM4QPE-F` on correlation prediction of N-qubit $|\psi_{\mathrm{HB}}\rangle$, with embedding M_{emb} random measurement outcomes. Training set and testing set are both have 10^4 samples, with noise-free labels ($M \to \infty$).

	$N = 8$	$N = 10$	$N = 12$	$N = 16$	$N = 25$	$N = 31$
$M_{\mathrm{emb}} = 1$	0.04666	0.04385	0.04126	0.03728	0.03083	0.03125
$M_{\mathrm{emb}} = 8$	0.04746	0.04926	0.03969	0.03984	0.03408	0.02951
$M_{\mathrm{emb}} = 64$	0.04795	0.04791	0.04785	0.04043	0.03637	0.03524
$M_{\mathrm{emb}} = 512$	0.04913	0.04521	0.04506	0.03905	0.03406	0.03268

Table 6: The RMSE results of `LLM4QPE-F` on correlation prediction of N-qubit $|\psi_{\mathrm{HB}}\rangle$, with embedding M_{emb} real measurement outcomes over the finetuning phase. testing size is set to 200. M is fixed to 512.

	$N = 63$			$N = 100$			$N = 127$		
	$n_{\mathrm{sft}} = 20$	$n_{\mathrm{sft}} = 60$	$n_{\mathrm{sft}} = 100$	$n_{\mathrm{sft}} = 20$	$n_{\mathrm{sft}} = 60$	$n_{\mathrm{sft}} = 100$	$n_{\mathrm{sft}} = 20$	$n_{\mathrm{sft}} = 60$	$n_{\mathrm{sft}} = 100$
$M_{\mathrm{emb}} = 1$	0.02555	0.02104	0.02019	0.02307	0.01872	0.01760	0.02239	0.01739	0.01635
$M_{\mathrm{emb}} = 8$	0.02556	0.02106	0.02019	0.02309	0.01873	0.01760	0.02242	0.01739	0.01635
$M_{\mathrm{emb}} = 64$	0.02556	0.02104	0.02019	0.02309	0.01872	0.01759	0.02239	0.01739	0.01636
$M_{\mathrm{emb}} = 512$	0.02560	0.02104	0.02019	0.02309	0.01872	0.01759	0.02240	0.01740	0.01635

Table 7: The RMSE results of `Ridge` on predicting correlation of N-qubit $|\psi_{\mathrm{HB}}\rangle$ and $|\psi_{\mathrm{TFIM}}\rangle$. The input dimension d is both fixed to 20. Regularization of Ridge is set to $\lambda = 1$.

Dataset	$N = 63$					$N = 100$					$N = 127$				
	$n = 20$	$n = 40$	$n = 60$	$n = 80$	$n = 100$	$n = 20$	$n = 40$	$n = 60$	$n = 80$	$n = 100$	$n = 20$	$n = 40$	$n = 60$	$n = 80$	$n = 100$
HB	**0.09998**	0.10555	0.09941	0.09322	0.08782	**0.10015**	**0.10395**	0.09867	0.09278	**0.08692**	**0.09964**	0.10491	**0.09898**	**0.09241**	**0.08680**
TFIM	0.10185	**0.10333**	**0.09845**	**0.09189**	**0.08565**	0.10093	0.10436	**0.09847**	**0.09193**	0.08824	0.10148	**0.10372**	0.10106	0.09426	0.08716

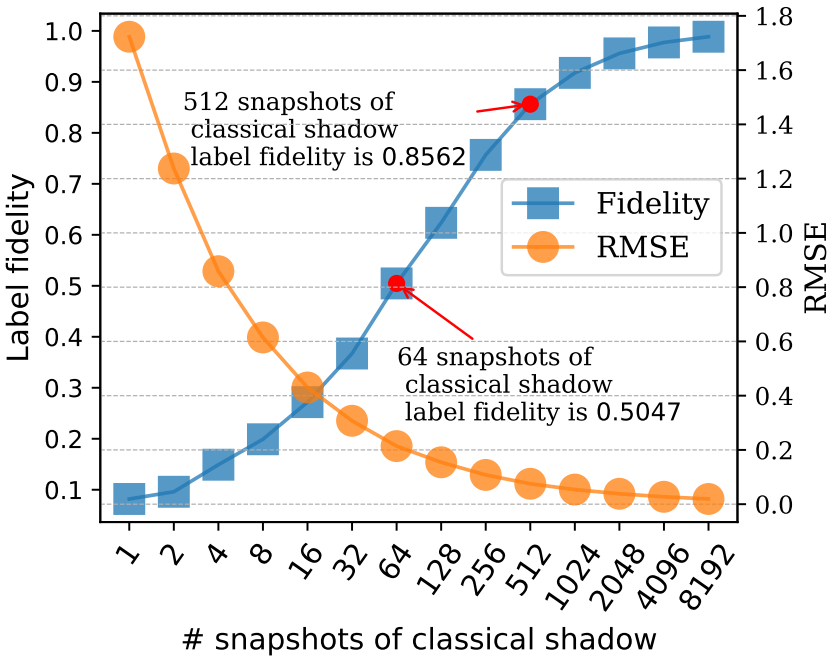

Figure 1: **Logarithmically** scaling behavior of label fidelity with **exponentially** increased measurement snapshots in dataset generation.

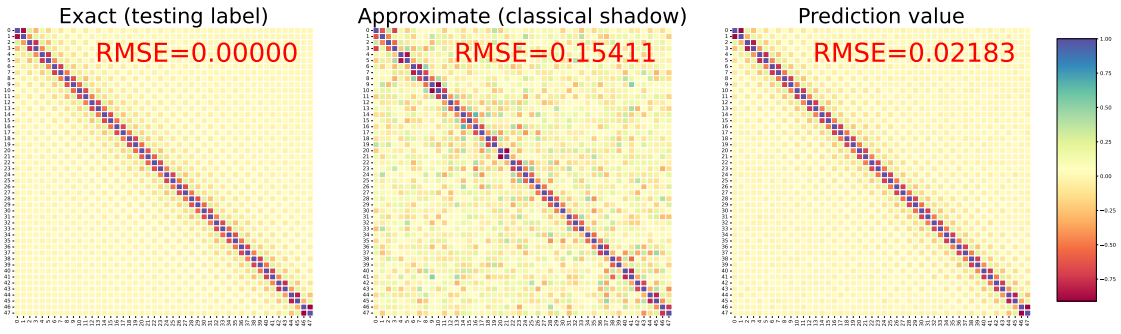

Figure 2: **A case of comparison between `Ridge` and baseline (`CS`) on predicting C_{ij} with a 48-qubit** $|\psi_{\mathrm{HB}}\rangle$. We take one Hamiltonian sample as an example, the left is the exact ground truth, the middle is the estimation by `CS`, and the right is the estimation by `Ridge`, where RMSE is 0.15411 and 0.02183, respectively.