

Rebuttal for ICML'25 Submission #3922

Submission #3922 Authors

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Table 1: **The RMSE result on correlation prediction of $|\psi_{\text{HB}}\rangle$ 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	$N = 48$			$N = 63$			$N = 100$			$N = 127$		
	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$
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	<u>0.04726</u>	0.03829	0.03922	0.04096	0.03299	0.03282	0.03850	<u>0.03115</u>	0.03086
Lasso	0.04221	0.02636	<u>0.02489</u>	0.04856	0.02791	0.02326	0.04219	0.02602	<u>0.02646</u>	0.04137	0.03292	0.02083
Ridge	<u>0.04247</u>	<u>0.02884</u>	0.02475	0.04216	<u>0.02816</u>	<u>0.02402</u>	<u>0.04191</u>	<u>0.02711</u>	0.02251	<u>0.04110</u>	0.02620	<u>0.02161</u>

Table 2: **The RMSE result on correlation prediction of $|\psi_{\text{TFIM}}\rangle$ 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	$N = 48$			$N = 63$			$N = 100$			$N = 127$		
	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$
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	<u>0.03566</u>	0.03082	0.05217	0.03476	0.03012	0.05259	0.03641	0.03084
Lasso	<u>0.04624</u>	<u>0.03219</u>	<u>0.02812</u>	<u>0.04633</u>	0.03930	<u>0.02859</u>	0.04073	0.03256	<u>0.02899</u>	<u>0.04583</u>	0.03283	<u>0.02932</u>
Ridge	0.04473	0.03173	0.02807	0.04561	0.03226	0.02839	<u>0.04598</u>	<u>0.03277</u>	0.02883	0.04570	<u>0.03285</u>	0.02911

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

$M \rightarrow \infty$	$N = 8$	$N = 10$	$N = 12$	$N = 16$	$N = 25$	$N = 31$
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 $|\psi_{\text{HB}}\rangle$ with varied training size n . System size $N = 8$. The number of testing set is fix to 2×10^4 . Labels are noise-free ($M \rightarrow \infty$). The best results are highlighted in **boldface**.

$M \rightarrow \infty$	# 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 $|\psi_{\text{HB}}\rangle$, with embedding M_{emb} random measurement outcomes. Training set and testing set are both have 10^4 samples, with noise-free labels ($M \rightarrow \infty$).

	$N = 8$	$N = 10$	$N = 12$	$N = 16$	$N = 25$	$N = 31$
$M_{\text{emb}} = 1$	0.04666	0.04385	0.04126	0.03728	0.03083	0.03125
$M_{\text{emb}} = 8$	0.04746	0.04926	0.03969	0.03984	0.03408	0.02951
$M_{\text{emb}} = 64$	0.04795	0.04791	0.04785	0.04043	0.03637	0.03524
$M_{\text{emb}} = 512$	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 $|\psi_{\text{HB}}\rangle$, with embedding M_{emb} real measurement outcomes over the finetuning phase. testing size is set to 200. M is fixed to 512.

	$N = 63$			$N = 100$			$N = 127$		
	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$	$n_{\text{sft}} = 20$	$n_{\text{sft}} = 60$	$n_{\text{sft}} = 100$
$M_{\text{emb}} = 1$	0.02555	0.02104	0.02019	0.02307	0.01872	0.01760	0.02239	0.01739	0.01635
$M_{\text{emb}} = 8$	0.02556	0.02106	0.02019	0.02309	0.01873	0.01760	0.02242	0.01739	0.01635
$M_{\text{emb}} = 64$	0.02556	0.02104	0.02019	0.02309	0.01872	0.01759	0.02239	0.01739	0.01636
$M_{\text{emb}} = 512$	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 $|\psi_{\text{HB}}\rangle$ and $|\psi_{\text{TFIM}}\rangle$. The input dimension d is both fixed to 20. Regularization of Ridge is set to $\alpha = 1$.

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