

ExaMiniMD

	base	norm	poly
	(1562, 21)	(1562, 21)	(1562, 253)
Random Forest Regressor	0.732664193	0.793603084	0.366890571
Bayesian Ridge	0.307756732	0.403984823	0.500059676
SVR RBF	-0.135880024	-0.135686792	-0.142561288
SVR poly 1	-0.126490846	-0.125976458	-0.142927947
SVR poly 2	-0.14445748	-0.143431834	-0.143149637
SVR poly 3	-0.129263498	-0.129190228	-0.143565874
SVR sigmoid	-0.13000108	-0.129527472	-0.143423841
Linear SGD Regressor	0.221632858	0.359253608	-5.40035E+14
1-NN Regressor	0.367107084	0.304131568	0.395624225
2-NN Regressor	0.609903365	0.525537524	0.593242722
3-NN Regressor	0.671833323	0.618137749	0.640664003
4-NN Regressor	0.700854864	0.656493371	0.671178626
5-NN Regressor	0.707915126	0.680321377	0.666687502
6-NN Regressor	0.710922018	0.692181235	0.670626618
7-NN Regressor	0.705068932	0.695910513	0.665738518
1 PLS Regression	0.240744462	0.245383016	0.127370886
2 PLS Regression	0.375592003	0.383252959	0.152992308
3 PLS Regression	0.284778196	0.387041444	0.190119149
4 PLS Regression	0.242763526	0.364700751	0.231752265
Decision Tree Regressor	0.465568922	0.586909588	0.036563739
1 MLP Regressor relu	0.36016759	0.038285367	0.360396233
1 MLP Regressor identity	0.141517218	0.065186375	0.325163783
1 MLP Regressor logistic	-0.307721818	-0.301958435	-0.309733148
1 MLP Regressor tanh	-0.314342737	-0.298735969	-0.303211819
2 MLP Regressor relu	0.670730938	0.616675788	0.2852946
2 MLP Regressor identity	0.188442077	0.395497888	0.379647481
2 MLP Regressor logistic	-0.309037559	-0.306756485	-0.311393304
2 MLP Regressor tanh	-0.307939686	-0.302698889	-0.303243399
3 MLP Regressor relu	0.657077043	0.747587443	0.307125095
3 MLP Regressor identity	0.219022702	0.399394624	0.402910755
3 MLP Regressor logistic	-0.313593043	-0.313573747	-0.313118712
3 MLP Regressor tanh	-0.305475402	-0.303159011	-0.303135536
4 MLP Regressor relu	0.660902472	0.733524815	0.305694608
4 MLP Regressor identity	0.244919296	0.400679277	0.391428336
4 MLP Regressor logistic	-0.314412205	-0.314410783	-0.312049389
4 MLP Regressor tanh	-0.31316086	0.303192246	-0.30687163
5 MLP Regressor relu	0.661044698	0.688208932	0.356655583
5 MLP Regressor identity	0.247392674	0.401802767	0.38269591
5 MLP Regressor logistic	-0.314123267	-0.314122718	-0.311917623
5 MLP Regressor tanh	-0.313966338	-0.303232349	-0.303304571
6 MLP Regressor relu	0.613428274	0.672639948	0.324908173
6 MLP Regressor identity	0.296030441	0.400481181	0.388943333
6 MLP Regressor logistic	-0.31443382	-0.314433774	-0.313740696
6 MLP Regressor tanh	-0.307008812	-0.303073084	-0.303180037
7 MLP Regressor relu	0.721817927	0.703173623	0.45865547
7 MLP Regressor identity	0.297576354	0.400210995	0.463587083
7 MLP Regressor logistic	-0.314324193	-0.31432419	-0.314667097
7 MLP Regressor tanh	-0.311494424	-0.303207903	-0.303218486
8 MLP Regressor relu	0.633618262	0.715461133	0.45311566
8 MLP Regressor identity	0.278230753	0.397626729	0.408632904
8 MLP Regressor logistic	-0.314596686	-0.314596686	-0.312952078
8 MLP Regressor tanh	-0.306986244	-0.303362573	-0.303176553
9 MLP Regressor relu	0.695899895	0.675906718	0.407981449
9 MLP Regressor identity	0.277142611	0.405559063	0.415426692
9 MLP Regressor logistic	-0.313099923	-0.313099922	-0.316341175
9 MLP Regressor tanh	-0.303301562	-0.303301325	-0.3032179768
10 MLP Regressor relu	0.697750441	0.724049516	0.392120052
10 MLP Regressor identity	0.275876747	0.406803013	0.393678148
10 MLP Regressor logistic	-0.31222043	-0.31222043	-0.314481521
10 MLP Regressor tanh	-0.308011171	-0.303171343	-0.303258251

SWFFT

	base	norm	poly
	(1618, 7)	(1618, 7)	(1618, 36)
0.773893103	0.466321999	0.768365766	
0.116693646	0.104908667	0.241554132	
-0.017999624	-0.018214607	-0.016919815	
-0.015667768	-0.018503565	-0.003018618	
0.004299923	-0.015586346	0.053558902	
0.039700812	-0.018019803	0.168092353	
-0.019544249	-0.018731357	-0.016706519	
0.116253053	0.112473612	0.221376314	
-0.146776915	-0.362223465	-0.253639875	
0.222837234	0.052260528	0.264000531	
0.275830152	0.116816051	0.323749123	
0.267897322	0.159843328	0.279488046	
0.316067235	0.204969371	0.371750835	
0.31873803	0.264421641	0.3391312	
0.319817192	0.252547872	0.344394446	
0.11818297	0.108804241	0.196858163	
0.116590962	0.109471845	0.233939369	
0.116477713	0.109498948	0.228810849	
0.116504176	0.10950024	0.229221337	
0.706744772	-0.002902105	0.653430439	
0.131939728	0.04697183	0.252832297	
0.115226455	0.046076042	0.24401984	
-0.002870644	-0.00331181	-0.002462966	
-0.002725814	-0.002014774	-0.002797012	
0.350777046	0.231654069	0.513012555	
0.116526427	0.108929624	0.232535155	
-0.003964092	-0.003665409	-0.005731755	
-0.004155649	-0.002508126	-0.006532709	
0.574850136	0.232826148	0.507547721	
0.118301803	0.108437011	0.232715174	
-0.007956199	-0.007942338	-0.007607194	
-0.00609808	-0.004732506	-0.004474352	
0.587395591	0.180372777	0.540498616	
0.115247294	0.109580637	0.230717528	
-0.00896257	-0.008960441	-0.008217155	
-0.006890548	-0.003560948	-0.006516782	
0.613499161	0.198310042	0.546287197	
0.117978713	0.109282225	0.225320145	
-0.00815554	-0.008155465	-0.007940113	
-0.005738436	-0.005743009	-0.005549735	
0.663531518	0.261978768	0.499473414	
0.110215401	0.106712979	0.234739514	
-0.00816883	-0.008168829	-0.007933491	
-0.005746587	-0.005749519	-0.005730032	
0.688547515	0.122370456	0.482713602	
0.1173259	0.110405329	0.220594931	
-0.008415364	-0.008415363	-0.008081911	
-0.005753421	-0.005756942	-0.005767619	
0.545606624	0.180382637	0.508354661	
0.118428457	0.106614093	0.230356021	
-0.008283131	-0.00828313	-0.00849232	
-0.005715079	-0.00571617	-0.005714283	
0.571388871	0.270346834	0.382705235	
0.115179568	0.104931341	0.239383747	
-0.008612067	-0.008612067	-0.007855291	
-0.005750321	-0.005752884	-0.005789497	
0.667368104	0.141418761	0.464959168	
0.114063477	0.102655397	0.23150956	
-0.008751273	-0.008751273	-0.008595119	
-0.005791864	-0.005794156	-0.005725702	

NEKbone

	base	norm	poly
	(1579, 12)	(1579, 12)	(1579, 91)
0.987550752	0.961175425	0.983676451	
0.753037023	0.792200928	0.928062273	
0.697806037	0.673379979	0.349620153	
0.700084911	0.74004849	0.506908346	
0.134835615	0.139800799	0.298368932	
0.523825521	0.586308741	0.192477663	
0.672104169	0.726383397	0.490134864	
0.752966947	0.792282003	0.927943305	
0.691180236	0.678619129	0.69151092	
0.784803476	0.772570749	0.759549548	
0.81258348	0.812460521	0.794122366	
0.827723074	0.832492201	0.802000385	
0.827509393	0.835130115	0.803734156	
0.832325442	0.837826199	0.801657841	
0.839435085	0.842470356	0.797520222	
0.688530285	0.754428332	0.685547515	
0.739719973	0.787792059	0.863759533	
0.752306383	0.792045991	0.913120579	
0.75299082	0.792178295	0.924910383	
0.982973318	0.932128581	0.977391578	
0.943922423	0.928821728	0.940640684	
0.752793106	0.792293061	0.927976906	
0.861801076	0.852595789	0.950414287	
0.960217312	0.92040598	0.930030764	
0.947754064	0.939572785	0.92192882	
0.752478868	0.792487633	0.92725614	
0.948540176	0.904152315	0.916486297	
0.959878515	0.961924671	0.918969823	
0.937344636	0.929437046	0.917727918	
0.751427749	0.791779638	0.924459492	
0.957651743	0.902657262	0.905089446	
0.945039777	0.959728858	0.920001908	
0.929023526	0.926091211	0.917804436	
0.75140987	0.792381052	0.926612709	
0.572931175	-0.003248922	0.917501817	
0.943835376	0.949973488	0.92531092	
0.92974628	0.92505743	0.918711316	
0.750561757	0.791407014	0.927255536	
-0.002906833	-0.002907061	-0.003191628	
0.947825714	0.946275149	0.925498262	
0.930585198	0.925324263	0.915875112	
0.75206996	0.788754232	0.923944051	
-0.002894507	-0.002894522	-0.003033339	
0.94177433	-0.003085608	0.92967725	
0.931410474	0.924212497	0.914034857	
0.74583252	0.791928864	0.921952445	
-0.003216815	-0.003216817	-0.003128295	
0.943603021	-0.003144193	0.927283586	
0.933713931	0.919469891	0.916357953	
0.74779763	0.788615303	0.924072382	
-0.002840383	-0.002840383	-0.003109842	
0.94160496	-0.003187306	0.9316586	
0.933040149	0.929443529	0.91930292	
0.74510536	0.77952027	0.91716362	
-0.003159196	-0.003159196	-0.002967624	
0.940689812	-0.003214355	0.556713816	
0.933138197	0.928039941	0.916655366	
0.743397833	0.775902013	0.922837546	
-0.00316001	-0.00316001	-0.003126391	
0.93848226	-0.003010219	0.371413844	