

Supplementary Materials for a Review of R Neural Network Packages (with NNbenchmark): Accuracy and Ease of Use

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1 Additionnal materials for all packages

1.1 Result for dataset `mDette`

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Table 1: Result for mDette

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlr	41. default	0.1400	0.4500	0.3100	0.3497	2.7841	0.522
rminer	45. default	0.2335	0.3147	0.0812	0.2456	1.2905	0.248
nnet	42. default	0.2650	0.4735	0.2085	0.3557	2.0121	0.078
validann	56. BFGS	0.2730	0.4266	0.1536	0.3155	1.9320	1.712
	57. CG	0.3813	0.4231	0.0418	0.3165	1.8043	11.228
	58. L-BFGS-B	0.4455	1.5927	1.1472	1.1539	8.9132	1.828
	59. Nelder-Mead	3.1073	3.5453	0.4380	2.7197	17.3854	2.126
	60. SANN	3.3417	4.0522	0.7105	2.9633	19.6574	0.172
MachineShop	32. default	0.2570	1.2314	0.9744	0.9854	8.0327	0.076
traineR	55. default	0.4539	0.5799	0.1260	0.4649	2.6448	0.078
radiant.model	44. default	0.2621	0.5412	0.2791	0.4096	2.1475	0.112
monmlp	34. BFGS	0.3732	0.4512	0.0780	0.3380	1.8359	0.298
	35. Nelder-Mead	3.0247	3.4557	0.4310	2.5277	18.0917	1.100
CaDENCE	12. optim	0.3277	2.5664	2.2387	1.2936	17.3208	7.072
	14. Rprop	4.6664	5.7488	1.0824	3.4794	31.0108	17.178
	13. psoptim	3.1663	3.6338	0.4675	2.1362	22.3798	11.258
h2o	24. first-order	0.3696	0.3789	0.0093	0.2948	1.3228	6.274
EnsembleBase	23. default	0.8770	13.9426	13.0656	11.3013	47.5398	0.026
caret	15. default	0.3175	0.3514	0.0339	0.2681	1.8536	0.252
brnn	11. Gauss-Newton	0.4578	1.9537	1.4959	1.4572	11.8945	0.216
qrnn	43. default	0.3632	0.7514	0.3882	0.4482	6.6249	0.518
RSNNS	51. Rprop	0.7757	1.2553	0.4796	0.9246	7.6985	0.692
	52. SCG	0.4652	1.7312	1.2660	1.2784	7.8765	1.156
	53. Backpropagation	0.4789	0.5588	0.0799	0.4219	2.0582	0.638
	47. BackpropChunk	0.5892	0.7126	0.1234	0.5252	2.8993	0.702
	48. BackpropMomentum	0.6547	0.7744	0.1197	0.5909	3.1612	0.688
	49. BackpropWeightDecay	0.6328	0.7698	0.1370	0.5856	3.0364	0.654
	46. BackpropBatch	1.9746	2.0170	0.0424	1.5451	10.0256	6.752
	50. Quickprop	7.1667	7.3190	0.1523	6.0055	29.6111	7.460
automl	8. adam	0.4255	0.6160	0.1905	0.4710	3.2585	9.584
	9. RMSprop	0.4821	0.6996	0.2175	0.5006	3.8172	8.632
	10. trainwpso	2.7275	4.9634	2.2359	3.7904	24.2831	13.696
deepnet	20. BP	0.5308	0.6403	0.1095	0.5135	2.7237	0.648
neuralnet	38. rprop+	0.4859	0.5467	0.0608	0.4149	2.3410	3.836
	37. rprop-	0.5338	2.0473	1.5135	1.4437	12.5391	6.318
	40. slr	0.5494	0.5688	0.0194	0.4293	2.4012	6.914
	39. sag	2.1196	8.1656	6.0460	6.5262	36.2385	12.916
	36. backprop	8.1656	8.1656	0.0000	6.5262	36.2385	14.200
keras	28. adamax	0.6492	0.6952	0.0460	0.5462	4.1959	4.386
	27. adam	0.7615	1.0487	0.2872	0.7949	6.3699	2.068
	29. nadam	1.0271	1.2485	0.2214	0.9787	4.9790	3.422
	26. adagrad	1.5412	2.2114	0.6702	1.5982	12.7204	18.384
	25. adadelta	2.0733	2.3080	0.2347	1.5890	13.7080	29.372
	31. sgd	0.5726	2.3026	1.7300	1.6878	10.2998	8.816
	30. rmsprop	2.6780	3.2516	0.5736	2.3382	16.3052	1.836
AMORE	2. ADAPTgdwm	0.3972	0.4012	0.0040	0.3084	1.7312	0.184
	1. ADAPTgd	0.4391	0.4564	0.0173	0.3246	2.0005	0.128
	4. BATCHgdwm	1.8586	1.9806	0.1220	1.4990	11.2445	1.862
	3. BATCHgd	1.8688	1.8999	0.0311	1.5158	8.6487	1.870
minpack.lm	33. default	0.6081	0.6081	0.0000	0.4989	1.9776	0.242
ANN2	6. rmsprop	1.9463	2.0761	0.1298	1.5240	12.6858	0.206
	5. adam	1.7980	2.0396	0.2416	1.5178	11.5812	0.218
	7. sgd	1.2208	2.0228	0.8020	1.4953	8.6218	0.204
deepdive	16. adam	3.0971	3.0971	0.0000	2.0640	18.6373	0.738
	19. rmsProp	2.7205	2.7205	0.0000	1.8705	16.1780	0.758
	18. momentum	4.1990	4.1990	0.0000	3.1011	18.5512	7.434
	17. gradientDescent	4.4310	4.4310	0.0000	3.2628	20.7622	7.266
snnR	54. default	1.9864	1.9864	0.0000	1.5889	8.8501	0.140
elmNNRepp	21. extremeML	7.3193	7.6899	0.3706	5.9574	32.3344	0.004
ELMR	22. extremeML	6.3469	7.2310	0.8841	5.5344	32.0052	0.018

Note: Statistics over 10 runs.

1.2 Result for dataset mFriedman

Table 2: Result for mFriedman

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.0045	0.0061	0.0016	0.0048	0.0196	0.762
rminer	45. default	0.0095	0.0112	0.0017	0.0088	0.0373	0.286
nnet	42. default	0.0091	0.0120	0.0029	0.0094	0.0404	0.102
validann	56. BFGS	0.0096	0.0688	0.0592	0.0500	0.1513	2.500
	57. CG	0.0163	0.0184	0.0021	0.0145	0.0580	25.592
	58. L-BFGS-B	0.0211	0.0256	0.0045	0.0208	0.0865	2.702
	59. Nelder-Mead	0.0991	0.1082	0.0091	0.0820	0.3701	6.334
	60. SANN	0.1414	0.1485	0.0071	0.1149	0.5629	0.204
MachineShop	32. default	0.0085	0.0116	0.0031	0.0092	0.0360	0.106
traineR	55. default	0.0112	0.0263	0.0151	0.0209	0.0954	0.094
radiant.model	44. default	0.0084	0.0150	0.0066	0.0106	0.0664	0.122
monmlp	34. BFGS	0.0132	0.0139	0.0007	0.0110	0.0465	0.308
	35. Nelder-Mead	0.1155	0.1219	0.0064	0.0960	0.3777	1.084
CaDENCE	12. optim	0.0160	0.0863	0.0703	0.0442	0.3640	9.226
	14. Rprop	0.0850	0.1295	0.0445	0.0858	0.5842	22.516
	13. psoptim	0.0950	0.1148	0.0198	0.0739	0.4058	12.056
h2o	24. first-order	0.0225	0.0261	0.0036	0.0204	0.0902	6.046
EnsembleBase	23. default	0.0245	0.0262	0.0017	0.0181	0.1321	0.092
caret	15. default	0.0123	0.0197	0.0074	0.0162	0.0727	0.288
brnn	11. Gauss-Newton	0.0046	0.0052	0.0006	0.0043	0.0154	0.238
qrnn	43. default	0.0105	0.0296	0.0191	0.0190	0.1330	0.578
RSNNS	51. Rprop	0.0307	0.0452	0.0145	0.0374	0.1660	0.706
	52. SCG	0.0202	0.0218	0.0016	0.0170	0.0747	1.140
	53. Backpropagation	0.0420	0.0900	0.0480	0.0761	0.2168	0.694
	47. BackpropChunk	0.0541	0.0657	0.0116	0.0532	0.2284	0.732
	48. BackpropMomentum	0.0558	0.0789	0.0231	0.0582	0.2590	0.706
	49. BackpropWeightDecay	0.0429	0.0595	0.0166	0.0488	0.1832	0.726
	46. BackpropBatch	0.0434	0.0851	0.0417	0.0754	0.2084	6.886
	50. Quickprop	0.1664	0.1722	0.0058	0.1384	0.5541	7.502
automl	8. adam	0.0277	0.0323	0.0046	0.0250	0.1346	9.568
	9. RMSprop	0.0397	0.0504	0.0107	0.0399	0.2019	8.550
	10. trainwpso	0.1029	0.1228	0.0199	0.0976	0.3922	14.836
deepnet	20. BP	0.0396	0.0967	0.0571	0.0838	0.2139	0.664
neuralnet	38. rprop+	0.0102	0.0106	0.0004	0.0083	0.0356	5.862
	37. rprop-	0.0095	0.0110	0.0015	0.0085	0.0412	5.058
	40. slr	0.0690	0.2348	0.1658	0.1880	0.6346	12.928
	39. sag	0.0806	0.2348	0.1542	0.1880	0.6346	13.202
	36. backprop	0.2348	0.2348	0.0000	0.1880	0.6346	14.676
keras	28. adamax	0.0326	0.0395	0.0069	0.0319	0.1140	4.326
	27. adam	0.0636	0.0774	0.0138	0.0612	0.2686	2.160
	29. nadam	0.0732	0.0992	0.0260	0.0817	0.3144	2.482
	26. adagrad	0.0296	0.0842	0.0546	0.0747	0.2012	14.836
	25. adadelta	0.0257	0.0267	0.0010	0.0211	0.0948	29.424
	31. sgd	0.0365	0.0527	0.0162	0.0403	0.1922	4.136
	30. rmsprop	0.1010	0.1147	0.0137	0.0860	0.3822	2.240
AMORE	2. ADAPTgdwm	0.0439	0.0450	0.0011	0.0321	0.1788	0.178
	1. ADAPTgd	0.0264	0.0296	0.0032	0.0235	0.1101	0.128
	4. BATCHgdwm	0.0173	0.0176	0.0003	0.0138	0.0586	1.882
	3. BATCHgd	0.0177	0.0816	0.0639	0.0748	0.1692	1.876
minpack.lm	33. default	0.1269	0.1269	0.0000	0.1009	0.3714	0.380
ANN2	6. rmsprop	0.0250	0.0314	0.0064	0.0251	0.0945	0.226
	5. adam	0.0183	0.0201	0.0018	0.0166	0.0579	0.234
	7. sgd	0.0178	0.0185	0.0007	0.0147	0.0603	0.222
deepdive	16. adam	0.0875	0.0875	0.0000	0.0764	0.2699	0.768
	19. rmsProp	0.1287	0.1287	0.0000	0.0990	0.4133	0.772
	18. momentum	0.1363	0.1363	0.0000	0.1061	0.4860	7.848
	17. gradientDescent	0.1474	0.1474	0.0000	0.1154	0.4581	7.642
snnR	54. default	0.0457	0.0839	0.0382	0.0747	0.2113	0.102
elmNNRepp	21. extremeML	0.1516	0.1734	0.0218	0.1379	0.5055	0.000
ELMR	22. extremeML	0.1677	0.1924	0.0247	0.1538	0.5716	0.008

Note: Statistics over 10 runs.

1.3 Result for dataset mIshigami

Table 3: Result for mIshigami

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.6602	2.2311	1.5709	1.8053	5.7864	1.470
rminer	45. default	0.6490	0.6668	0.0178	0.5016	3.0019	0.446
nnet	42. default	0.5462	0.6959	0.1497	0.5147	3.0034	0.152
validann	56. BFGS	0.6342	0.7284	0.0942	0.5216	3.3533	5.086
	57. CG	0.6427	0.7212	0.0785	0.5352	3.3323	58.524
	58. L-BFGS-B	0.8502	1.1103	0.2601	0.8812	3.5016	5.418
	59. Nelder-Mead	2.6029	2.6812	0.0783	2.2886	7.2908	16.114
	60. SANN	2.9199	2.9986	0.0787	2.4922	10.0706	0.270
MachineShop	32. default	0.6685	2.1956	1.5271	1.7857	5.3089	0.152
traineR	55. default	0.6846	0.7400	0.0554	0.5453	3.2851	0.152
radiant.model	44. default	0.4934	0.7868	0.2934	0.5896	3.1250	0.172
monmlp	34. BFGS	0.8185	0.9739	0.1554	0.7577	3.6164	0.460
	35. Nelder-Mead	2.7368	2.8463	0.1095	2.3257	8.7509	1.600
CaDENCE	12. optim	1.0465	1.6993	0.6528	0.8815	5.3208	14.912
	14. Rprop	1.3422	2.3133	0.9711	1.3927	8.8022	36.926
	13. psoptim	2.6775	2.7432	0.0657	2.3281	8.8488	14.936
h2o	24. first-order	0.8347	0.8467	0.0120	0.6295	3.6234	6.462
EnsembleBase	23. default	0.6342	0.8141	0.1799	0.5735	3.9523	0.132
caret	15. default	1.0310	1.6339	0.6029	1.3615	4.7983	0.418
brnn	11. Gauss-Newton	0.6588	0.6635	0.0047	0.5100	2.9395	0.204
qrnn	43. default	0.7656	0.7907	0.0251	0.4951	4.0838	1.122
RSNNS	51. Rprop	1.3146	2.3451	1.0305	1.8953	6.5010	0.840
	52. SCG	0.6980	0.7363	0.0383	0.5439	3.0529	1.456
	53. Backpropagation	2.7659	2.8040	0.0381	2.1912	11.0805	0.814
	47. BackpropChunk	1.3784	2.6226	1.2442	2.0664	8.9928	0.816
	48. BackpropMomentum	2.6138	2.6595	0.0457	2.1268	10.0368	0.822
	49. BackpropWeightDecay	1.2711	2.0728	0.8017	1.5275	7.9148	0.854
	46. BackpropBatch	2.6668	2.6742	0.0074	2.3004	7.1688	8.542
	50. Quickprop	3.4245	3.5389	0.1144	2.8752	13.1137	9.656
automl	8. adam	0.7511	0.7995	0.0484	0.6120	2.9212	9.932
	9. RMSprop	1.8225	2.5662	0.7437	2.1749	6.0520	8.882
	10. trainwpso	1.8381	2.4317	0.5936	1.9867	7.8872	25.376
deepnet	20. BP	1.0536	1.4687	0.4151	1.0190	6.8677	0.770
neuralnet	38. rprop+	0.5788	0.6650	0.0862	0.5052	2.7746	4.596
	37. rprop-	0.6728	0.7126	0.0398	0.5316	2.8674	1.954
	40. slr	0.6816	3.6898	3.0082	2.9776	13.1137	24.586
	39. sag	3.6898	3.6898	0.0000	2.9776	13.1137	25.218
	36. backprop	3.6898	3.6898	0.0000	2.9776	13.1137	23.958
keras	28. adamax	0.8307	0.8615	0.0308	0.6388	3.6379	5.302
	27. adam	0.9777	1.0728	0.0951	0.7886	4.0357	2.796
	29. nadam	1.0800	2.7592	1.6792	2.3587	8.0273	3.264
	26. adagrad	0.8522	2.5746	1.7224	2.1958	6.9534	31.856
	25. adadelta	2.4074	2.6007	0.1933	2.2281	6.9184	31.676
	31. sgd	2.7076	2.7302	0.0226	2.3252	7.5362	2.788
	30. rmsprop	2.8335	3.0118	0.1783	2.4550	9.4367	1.924
AMORE	2. ADAPTgdwm	0.8636	0.9950	0.1314	0.7280	3.8394	0.330
	1. ADAPTgd	0.7690	0.8135	0.0445	0.6083	2.9968	0.222
	4. BATCHgdwm	2.4805	2.5259	0.0454	2.1518	6.4536	2.678
	3. BATCHgd	2.5215	2.5544	0.0329	2.1768	6.3018	2.624
minpack.lm	33. default	2.5379	2.5379	0.0000	2.0524	7.6035	0.940
ANN2	6. rmsprop	0.7045	0.8590	0.1545	0.6409	2.9940	1.048
	5. adam	0.7560	0.8062	0.0502	0.6130	3.5492	1.058
	7. sgd	0.7787	0.9097	0.1310	0.6798	3.8085	1.048
deepdive	16. adam	2.5913	2.5913	0.0000	2.0819	10.0604	0.902
	19. rmsProp	2.6728	2.6728	0.0000	2.3060	7.1452	0.892
	18. momentum	2.5791	2.5791	0.0000	2.0107	8.7569	9.220
	17. gradientDescent	3.0218	3.0218	0.0000	2.4940	10.2360	9.062
snnR	54. default	0.7757	0.8621	0.0864	0.6030	3.4730	0.430
elmNNRepp	21. extremeML	3.0949	3.2590	0.1641	2.6511	11.3823	0.000
ELMR	22. extremeML	3.2348	3.2840	0.0492	2.6674	12.0160	0.008

Note: Statistics over 10 runs.

1.4 Result for dataset mRef153

Table 4: Result for mRef153

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.6602	2.2311	1.5709	1.8053	5.7864	1.470
rminer	45. default	0.6490	0.6668	0.0178	0.5016	3.0019	0.446
nnet	42. default	0.5462	0.6959	0.1497	0.5147	3.0034	0.152
validann	56. BFGS	0.6342	0.7284	0.0942	0.5216	3.3533	5.086
	57. CG	0.6427	0.7212	0.0785	0.5352	3.3323	58.524
	58. L-BFGS-B	0.8502	1.1103	0.2601	0.8812	3.5016	5.418
	59. Nelder-Mead	2.6029	2.6812	0.0783	2.2886	7.2908	16.114
	60. SANN	2.9199	2.9986	0.0787	2.4922	10.0706	0.270
MachineShop	32. default	0.6685	2.1956	1.5271	1.7857	5.3089	0.152
traineR	55. default	0.6846	0.7400	0.0554	0.5453	3.2851	0.152
radiant.model	44. default	0.4934	0.7868	0.2934	0.5896	3.1250	0.172
monmlp	34. BFGS	0.8185	0.9739	0.1554	0.7577	3.6164	0.460
	35. Nelder-Mead	2.7368	2.8463	0.1095	2.3257	8.7509	1.600
CaDENCE	12. optim	1.0465	1.6993	0.6528	0.8815	5.3208	14.912
	14. Rprop	1.3422	2.3133	0.9711	1.3927	8.8022	36.926
	13. psoptim	2.6775	2.7432	0.0657	2.3281	8.8488	14.936
h2o	24. first-order	0.8347	0.8467	0.0120	0.6295	3.6234	6.462
EnsembleBase	23. default	0.6342	0.8141	0.1799	0.5735	3.9523	0.132
caret	15. default	1.0310	1.6339	0.6029	1.3615	4.7983	0.418
brnn	11. Gauss-Newton	0.6588	0.6635	0.0047	0.5100	2.9395	0.204
qrnn	43. default	0.7656	0.7907	0.0251	0.4951	4.0838	1.122
RSNNS	51. Rprop	1.3146	2.3451	1.0305	1.8953	6.5010	0.840
	52. SCG	0.6980	0.7363	0.0383	0.5439	3.0529	1.456
	53. Backpropagation	2.7659	2.8040	0.0381	2.1912	11.0805	0.814
	47. BackpropChunk	1.3784	2.6226	1.2442	2.0664	8.9928	0.816
	48. BackpropMomentum	2.6138	2.6595	0.0457	2.1268	10.0368	0.822
	49. BackpropWeightDecay	1.2711	2.0728	0.8017	1.5275	7.9148	0.854
	46. BackpropBatch	2.6668	2.6742	0.0074	2.3004	7.1688	8.542
	50. Quickprop	3.4245	3.5389	0.1144	2.8752	13.1137	9.656
automl	8. adam	0.7511	0.7995	0.0484	0.6120	2.9212	9.932
	9. RMSprop	1.8225	2.5662	0.7437	2.1749	6.0520	8.882
	10. trainwpso	1.8381	2.4317	0.5936	1.9867	7.8872	25.376
deepnet	20. BP	1.0536	1.4687	0.4151	1.0190	6.8677	0.770
neuralnet	38. rprop+	0.5788	0.6650	0.0862	0.5052	2.7746	4.596
	37. rprop-	0.6728	0.7126	0.0398	0.5316	2.8674	1.954
	40. slr	0.6816	3.6898	3.0082	2.9776	13.1137	24.586
	39. sag	3.6898	3.6898	0.0000	2.9776	13.1137	25.218
	36. backprop	3.6898	3.6898	0.0000	2.9776	13.1137	23.958
keras	28. adamax	0.8307	0.8615	0.0308	0.6388	3.6379	5.302
	27. adam	0.9777	1.0728	0.0951	0.7886	4.0357	2.796
	29. nadam	1.0800	2.7592	1.6792	2.3587	8.0273	3.264
	26. adagrad	0.8522	2.5746	1.7224	2.1958	6.9534	31.856
	25. adadelta	2.4074	2.6007	0.1933	2.2281	6.9184	31.676
	31. sgd	2.7076	2.7302	0.0226	2.3252	7.5362	2.788
	30. rmsprop	2.8335	3.0118	0.1783	2.4550	9.4367	1.924
AMORE	2. ADAPTgdwm	0.8636	0.9950	0.1314	0.7280	3.8394	0.330
	1. ADAPTgd	0.7690	0.8135	0.0445	0.6083	2.9968	0.222
	4. BATCHgdwm	2.4805	2.5259	0.0454	2.1518	6.4536	2.678
	3. BATCHgd	2.5215	2.5544	0.0329	2.1768	6.3018	2.624
minpack.lm	33. default	2.5379	2.5379	0.0000	2.0524	7.6035	0.940
ANN2	6. rmsprop	0.7045	0.8590	0.1545	0.6409	2.9940	1.048
	5. adam	0.7560	0.8062	0.0502	0.6130	3.5492	1.058
	7. sgd	0.7787	0.9097	0.1310	0.6798	3.8085	1.048
deepdive	16. adam	2.5913	2.5913	0.0000	2.0819	10.0604	0.902
	19. rmsProp	2.6728	2.6728	0.0000	2.3060	7.1452	0.892
	18. momentum	2.5791	2.5791	0.0000	2.0107	8.7569	9.220
	17. gradientDescent	3.0218	3.0218	0.0000	2.4940	10.2360	9.062
snnR	54. default	0.7757	0.8621	0.0864	0.6030	3.4730	0.430
elmNNRepp	21. extremeML	3.0949	3.2590	0.1641	2.6511	11.3823	0.000
ELMR	22. extremeML	3.2348	3.2840	0.0492	2.6674	12.0160	0.008

Note: Statistics over 10 runs.

1.5 Result for dataset uDmod1

Table 5: Result for uDmod1

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.0433	0.0433	0.0000	0.0349	0.1063	0.088
rminer	45. default	0.0449	0.0495	0.0046	0.0418	0.1258	0.030
nnet	42. default	0.0437	0.0865	0.0428	0.0636	0.3435	0.008
validann	56. BFGS	0.0435	0.0725	0.0290	0.0540	0.1810	0.790
	57. CG	0.0506	0.0679	0.0173	0.0544	0.1577	29.066
	58. L-BFGS-B	0.0489	0.1090	0.0601	0.0759	0.4093	0.880
	59. Nelder-Mead	0.1034	0.1810	0.0776	0.1538	0.4017	28.208
	60. SANN	0.2296	0.3046	0.0750	0.2441	0.6614	0.128
MachineShop	32. default	0.0442	0.0456	0.0014	0.0365	0.1181	0.012
traineR	55. default	0.0410	0.0470	0.0060	0.0393	0.1293	0.004
radiant.model	44. default	0.0800	0.1088	0.0288	0.0817	0.3346	0.026
monmlp	34. BFGS	0.0919	0.0983	0.0064	0.0750	0.3693	0.208
	35. Nelder-Mead	0.1381	0.2639	0.1258	0.2153	0.6177	0.428
CaDENCE	12. optim	0.0564	0.2112	0.1548	0.1061	0.6888	2.442
	14. Rprop	0.2005	0.4116	0.2111	0.3162	0.8665	6.654
	13. psoptim	0.3096	0.3190	0.0094	0.2672	0.7427	5.378
h2o	24. first-order	0.0480	0.0494	0.0014	0.0402	0.1185	3.346
EnsembleBase	23. default	0.0733	0.1033	0.0300	0.0759	0.4193	0.004
caret	15. default	0.0535	0.0948	0.0413	0.0602	0.3176	0.030
brnn	11. Gauss-Newton	0.0451	0.5884	0.5433	0.5069	1.0104	0.010
qrnn	43. default	0.1162	0.1349	0.0187	0.0830	0.6014	0.230
RSNNS	51. Rprop	0.1232	0.1401	0.0169	0.1048	0.4453	0.090
	52. SCG	0.0970	0.1118	0.0148	0.0916	0.4280	0.140
	53. Backpropagation	0.1215	0.2226	0.1011	0.1736	0.5618	0.094
	47. BackpropChunk	0.1298	0.1448	0.0150	0.1073	0.5245	0.140
	48. BackpropMomentum	0.1445	0.1647	0.0202	0.1252	0.5800	0.088
	49. BackpropWeightDecay	0.1314	0.1656	0.0342	0.1218	0.5395	0.090
	46. BackpropBatch	0.2568	0.3344	0.0776	0.2870	0.7691	0.874
	50. Quickprop	0.5775	0.5884	0.0109	0.5068	1.0104	0.938
automl	8. adam	0.0596	0.1157	0.0561	0.0741	0.5060	1.262
	9. RMSprop	0.1052	0.1595	0.0543	0.1323	0.3299	1.128
	10. trainwpso	0.2424	0.2517	0.0093	0.1929	0.6461	6.964
deepnet	20. BP	0.0582	0.1173	0.0591	0.0845	0.3896	0.094
neuralnet	38. rprop+	0.1086	0.1639	0.0553	0.1319	0.5153	0.042
	37. rprop-	0.1634	0.1750	0.0116	0.1370	0.5212	0.030
	40. slr	0.0839	0.1213	0.0374	0.0922	0.3196	0.100
	39. sag	0.0583	0.1315	0.0732	0.1061	0.3669	1.430
	36. backprop	0.1521	0.1699	0.0178	0.1280	0.5924	0.490
keras	28. adamax	0.0883	0.2240	0.1357	0.1782	0.5854	4.566
	27. adam	0.1376	0.1811	0.0435	0.1461	0.4721	2.576
	29. nadam	0.1786	0.2607	0.0821	0.2055	0.6971	2.242
	26. adagrad	0.2252	0.3529	0.1277	0.3037	0.8099	8.322
	25. adadelta	0.2314	0.2333	0.0019	0.1843	0.5698	23.966
	31. sgd	0.2044	0.3548	0.1504	0.2992	0.8224	2.644
	30. rmsprop	0.2375	0.3800	0.1425	0.2964	0.8503	1.326
AMORE	2. ADAPTgdwm	0.2197	0.2765	0.0568	0.2204	0.6575	0.054
	1. ADAPTgd	0.3082	0.3271	0.0189	0.2829	0.7263	0.036
	4. BATCHgdwm	0.3265	0.3274	0.0009	0.2853	0.7289	1.804
	3. BATCHgd	0.2023	0.2922	0.0899	0.2393	0.6802	1.780
minpack.lm	33. default	0.0445	0.0445	0.0000	0.0362	0.1153	0.038
ANN2	6. rmsprop	0.2345	0.2495	0.0150	0.1926	0.6040	0.016
	5. adam	0.2198	0.2274	0.0076	0.1806	0.5242	0.012
	7. sgd	0.2581	0.3342	0.0761	0.2899	0.6824	0.014
deepdive	16. adam	0.1178	0.1178	0.0000	0.0797	0.4868	0.568
	19. rmsProp	0.1728	0.1728	0.0000	0.1257	0.4478	0.584
	18. momentum	0.3320	0.3320	0.0000	0.2891	0.7441	5.524
	17. gradientDescent	0.3353	0.3353	0.0000	0.2912	0.7067	5.340
snnR	54. default	0.2927	0.2927	0.0000	0.2512	0.6561	0.040
elmNNRepp	21. extremeML	0.3320	0.3623	0.0303	0.3038	0.8727	0.000
ELMR	22. extremeML	0.3003	0.3082	0.0079	0.2529	0.7867	0.000

Note: Statistics over 10 runs.

1.6 Result for dataset uDmod2

Table 6: Result for uDmod2

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.0427	0.0427	0.0000	0.0333	0.1058	0.036
rminer	45. default	0.0405	0.0579	0.0174	0.0479	0.1065	0.016
nnet	42. default	0.0602	0.0615	0.0013	0.0489	0.1408	0.008
validann	56. BFGS	0.0405	0.0437	0.0032	0.0342	0.1131	0.676
	57. CG	0.0536	0.0610	0.0074	0.0476	0.1415	31.616
	58. L-BFGS-B	0.0691	0.0778	0.0087	0.0617	0.2019	0.784
	59. Nelder-Mead	0.0633	0.1987	0.1354	0.1673	0.4305	30.686
	60. SANN	0.2274	0.2546	0.0272	0.1990	0.5099	0.148
MachineShop	32. default	0.0406	0.0494	0.0088	0.0374	0.1288	0.012
traineR	55. default	0.0505	0.0649	0.0144	0.0529	0.1392	0.016
radiant.model	44. default	0.0647	0.0771	0.0124	0.0602	0.2202	0.022
monmlp	34. BFGS	0.0522	0.0796	0.0274	0.0625	0.2280	0.210
	35. Nelder-Mead	0.1342	0.1780	0.0438	0.1371	0.4534	0.370
CaDENCE	12. optim	0.0688	0.0805	0.0117	0.0582	0.2385	2.310
	14. Rprop	0.1820	0.2615	0.0795	0.2061	0.6887	5.784
	13. psoptim	0.2114	0.3238	0.1124	0.2711	0.6808	5.052
h2o	24. first-order	0.0474	0.0482	0.0008	0.0394	0.1126	3.342
EnsembleBase	23. default	0.0618	0.0638	0.0020	0.0504	0.1716	0.006
caret	15. default	0.0512	0.0558	0.0046	0.0454	0.1561	0.024
brnn	11. Gauss-Newton	0.0435	0.0673	0.0238	0.0522	0.1838	0.020
qrnn	43. default	0.0511	0.0821	0.0310	0.0598	0.2411	0.214
RSNNS	51. Rprop	0.0447	0.0959	0.0512	0.0717	0.2622	0.090
	52. SCG	0.0555	0.0788	0.0233	0.0618	0.2070	0.132
	53. Backpropagation	0.0788	0.1292	0.0504	0.0999	0.3342	0.086
	47. BackpropChunk	0.0829	0.0892	0.0063	0.0732	0.2035	0.090
	48. BackpropMomentum	0.0752	0.0964	0.0212	0.0786	0.2134	0.092
	49. BackpropWeightDecay	0.0799	0.0888	0.0089	0.0704	0.2063	0.094
	46. BackpropBatch	0.2601	0.2736	0.0135	0.2371	0.6099	0.870
	50. Quickprop	0.2570	0.4804	0.2234	0.4177	1.0187	0.906
automl	8. adam	0.0511	0.0867	0.0356	0.0707	0.1976	1.260
	9. RMSprop	0.1245	0.2296	0.1051	0.1669	0.5276	1.104
	10. trainwpso	0.2032	0.2573	0.0541	0.2232	0.5240	10.432
deepnet	20. BP	0.0563	0.0608	0.0045	0.0490	0.1446	0.092
neuralnet	38. rprop+	0.1077	0.1207	0.0130	0.0926	0.2648	0.036
	37. rprop-	0.0955	0.1186	0.0231	0.0920	0.2812	0.062
	40. slr	0.0840	0.1039	0.0199	0.0866	0.2554	0.092
	39. sag	0.0811	0.1160	0.0349	0.0943	0.2960	0.950
	36. backprop	0.1091	0.1355	0.0264	0.1084	0.3411	0.372
keras	28. adamax	0.1082	0.1728	0.0646	0.1393	0.3885	3.696
	27. adam	0.0963	0.1767	0.0804	0.1397	0.4913	2.338
	29. nadam	0.1201	0.1884	0.0683	0.1486	0.5214	2.460
	26. adagrad	0.1597	0.1792	0.0195	0.1379	0.4143	13.616
	25. adadelta	0.1746	0.1792	0.0046	0.1379	0.4116	26.680
	31. sgd	0.2431	0.3056	0.0625	0.2606	0.6923	1.868
	30. rmsprop	0.1629	0.2166	0.0537	0.1697	0.5175	1.744
AMORE	2. ADAPTgdwm	0.1145	0.1924	0.0779	0.1573	0.4195	0.034
	1. ADAPTgd	0.2579	0.2632	0.0053	0.2333	0.5307	0.022
	4. BATCHgdwm	0.1585	0.2621	0.1036	0.2341	0.4898	1.650
	3. BATCHgd	0.2228	0.2644	0.0416	0.2347	0.4989	1.650
minpack.lm	33. default	0.0427	0.0427	0.0000	0.0333	0.1058	0.024
ANN2	6. rmsprop	0.1831	0.2585	0.0754	0.2227	0.5514	0.012
	5. adam	0.1702	0.2126	0.0424	0.1747	0.4630	0.014
	7. sgd	0.2518	0.2732	0.0214	0.2401	0.5272	0.012
deepdive	16. adam	0.3189	0.3189	0.0000	0.2113	0.7209	0.572
	19. rmsProp	0.2252	0.2252	0.0000	0.1580	0.5513	0.558
	18. momentum	0.2656	0.2656	0.0000	0.2355	0.5269	5.460
	17. gradientDescent	0.2699	0.2699	0.0000	0.2369	0.5509	5.326
snnR	54. default	0.2585	0.2984	0.0399	0.2556	0.6651	0.020
elmNNRepp	21. extremeML	0.2589	0.2648	0.0059	0.2308	0.5419	0.000
ELMR	22. extremeML	0.2613	0.2735	0.0122	0.2358	0.5366	0.000

Note: Statistics over 10 runs.

1.7 Result for dataset uDreyfus1

Table 7: Result for uDreyfus1

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.0000	0.0000	0.0000	0.0000	0.0001	0.014
rminer	45. default	0.0020	0.0023	0.0003	0.0018	0.0057	0.012
nnet	42. default	0.0026	0.0716	0.0690	0.0449	0.2254	0.004
validann	56. BFGS	0.0022	0.0023	0.0001	0.0019	0.0070	0.350
	57. CG	0.0035	0.0076	0.0041	0.0061	0.0205	25.106
	58. L-BFGS-B	0.0038	0.0084	0.0046	0.0066	0.0207	0.512
	59. Nelder-Mead	0.0833	0.1951	0.1118	0.1633	0.3615	17.878
	60. SANN	0.2692	0.3271	0.0579	0.2707	0.6914	0.142
MachineShop	32. default	0.0023	0.0034	0.0011	0.0028	0.0102	0.010
traineR	55. default	0.0019	0.0022	0.0003	0.0019	0.0076	0.000
radiant.model	44. default	0.0121	0.0682	0.0561	0.0555	0.1546	0.022
monmlp	34. BFGS	0.0323	0.0541	0.0218	0.0434	0.1524	0.190
	35. Nelder-Mead	0.1425	0.2017	0.0592	0.1653	0.4572	0.270
CaDENCE	12. optim	0.0032	0.6701	0.6669	0.3727	1.9004	1.030
	14. Rprop	0.3995	1.1290	0.7295	0.8219	2.2557	3.762
	13. psoptim	0.4218	0.5720	0.1502	0.3001	1.6829	4.512
h2o	24. first-order	0.0131	0.0146	0.0015	0.0112	0.0432	3.334
EnsembleBase	23. default	0.0922	0.1151	0.0229	0.0834	0.3335	0.002
caret	15. default	0.0262	0.0359	0.0097	0.0282	0.1115	0.018
brnn	11. Gauss-Newton	0.0026	0.0034	0.0008	0.0029	0.0115	0.000
qrnn	43. default	0.2781	0.2841	0.0060	0.1815	0.9095	0.128
RSNNS	51. Rprop	0.0617	0.0689	0.0072	0.0484	0.2211	0.080
	52. SCG	0.0851	0.1018	0.0167	0.0848	0.2408	0.122
	53. Backpropagation	0.1127	0.1190	0.0063	0.1000	0.2547	0.078
	47. BackpropChunk	0.0838	0.1275	0.0437	0.0822	0.3313	0.088
	48. BackpropMomentum	0.0719	0.0795	0.0076	0.0606	0.2070	0.080
	49. BackpropWeightDecay	0.0797	0.0849	0.0052	0.0657	0.2541	0.090
	46. BackpropBatch	0.3120	0.3387	0.0267	0.2647	0.7662	0.812
	50. Quickprop	0.2177	0.2408	0.0231	0.2084	0.5154	0.822
automl	8. adam	0.0087	0.0725	0.0638	0.0481	0.2070	0.906
	9. RMSprop	0.0479	0.0727	0.0248	0.0498	0.2335	1.114
	10. trainwpso	0.1052	0.1154	0.0102	0.0854	0.3281	5.358
deepnet	20. BP	0.0139	0.0704	0.0565	0.0451	0.2219	0.084
neuralnet	38. rprop+	0.2119	0.3475	0.1356	0.2662	0.7910	0.004
	37. rprop-	0.1014	0.2856	0.1842	0.2227	0.7157	0.008
	40. slr	0.2981	0.3450	0.0469	0.2730	0.7821	0.012
	39. sag	0.1963	0.3371	0.1408	0.2652	0.7510	0.048
	36. backprop	0.3201	0.3503	0.0302	0.2743	0.7831	0.040
keras	28. adamax	0.0365	0.0487	0.0122	0.0404	0.1489	5.074
	27. adam	0.0706	0.0897	0.0191	0.0690	0.2075	2.808
	29. nadam	0.0648	0.1550	0.0902	0.1179	0.3970	2.082
	26. adagrad	0.1630	0.3528	0.1898	0.2697	0.8045	5.918
	25. adadelta	0.2178	0.3498	0.1320	0.2655	0.8040	10.958
	31. sgd	0.3373	0.3450	0.0077	0.2698	0.7744	2.312
	30. rmsprop	0.3101	0.3622	0.0521	0.2798	0.9265	0.942
AMORE	2. ADAPTgdwm	0.1804	0.2112	0.0308	0.1476	0.4856	0.030
	1. ADAPTgd	0.3308	0.3475	0.0167	0.2718	0.7716	0.020
	4. BATCHgdwm	0.3346	0.3370	0.0024	0.2785	0.7142	1.376
	3. BATCHgd	0.3160	0.3346	0.0186	0.2740	0.7087	1.382
minpack.lm	33. default	0.0000	0.0000	0.0000	0.0000	0.0001	0.000
ANN2	6. rmsprop	0.2467	0.3428	0.0961	0.2715	0.7616	0.006
	5. adam	0.2762	0.3201	0.0439	0.2542	0.7372	0.006
	7. sgd	0.3493	0.3546	0.0053	0.2689	0.8481	0.008
deepdive	16. adam	0.0304	0.0304	0.0000	0.0265	0.0644	0.564
	19. rmsProp	0.1184	0.1184	0.0000	0.0878	0.3446	0.566
	18. momentum	0.3429	0.3429	0.0000	0.2801	0.7341	5.460
	17. gradientDescent	0.3429	0.3429	0.0000	0.2801	0.7346	5.162
snnR	54. default	0.3691	0.3691	0.0000	0.2756	0.8531	0.006
elmNNRepp	21. extremeML	0.3407	0.4066	0.0659	0.2973	1.0342	0.000
ELMR	22. extremeML	0.3987	0.4505	0.0518	0.3027	1.1845	0.000

Note: Statistics over 10 runs.

1.8 Result for dataset uDreyfus2

Table 8: Result for uDreyfus2

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlr	41. default	0.0906	0.0906	0.0000	0.0723	0.2197	0.064
rminer	45. default	0.0906	0.0906	0.0000	0.0724	0.2202	0.018
nnet	42. default	0.0906	0.0906	0.0000	0.0725	0.2202	0.000
validann	56. BFGS	0.0906	0.0906	0.0000	0.0724	0.2200	0.442
	57. CG	0.0910	0.0913	0.0003	0.0730	0.2244	26.808
	58. L-BFGS-B	0.0907	0.1123	0.0216	0.0897	0.2733	0.504
	59. Nelder-Mead	0.1300	0.1604	0.0304	0.1224	0.4798	16.024
	60. SANN	0.2712	0.2972	0.0260	0.2354	0.7465	0.152
MachineShop	32. default	0.0906	0.1415	0.0509	0.1045	0.4507	0.012
traineR	55. default	0.0906	0.1123	0.0217	0.0901	0.2736	0.004
radiant.model	44. default	0.0907	0.0917	0.0010	0.0732	0.2275	0.026
monmlp	34. BFGS	0.0917	0.0951	0.0034	0.0746	0.2363	0.210
	35. Nelder-Mead	0.1762	0.2448	0.0686	0.1940	0.6268	0.248
CaDENCE	12. optim	0.0924	0.3856	0.2932	0.2560	1.1222	1.046
	14. Rprop	0.1684	0.2586	0.0902	0.1963	0.7853	4.272
	13. psoptim	0.3210	0.3814	0.0604	0.2825	1.0638	4.500
h2o	24. first-order	0.0926	0.0933	0.0007	0.0740	0.2242	3.356
EnsembleBase	23. default	0.1196	0.1272	0.0076	0.1022	0.3102	0.008
caret	15. default	0.0926	0.1039	0.0113	0.0811	0.2375	0.022
brnn	11. Gauss-Newton	0.0913	0.0913	0.0000	0.0730	0.2241	0.000
qrnn	43. default	0.1601	0.2693	0.1092	0.1983	0.6891	0.170
RSNNS	51. Rprop	0.1145	0.1252	0.0107	0.1009	0.3338	0.082
	52. SCG	0.1238	0.2542	0.1304	0.1876	0.7205	0.114
	53. Backpropagation	0.1298	0.1325	0.0027	0.1025	0.3352	0.080
	47. BackpropChunk	0.1199	0.1689	0.0490	0.1245	0.5094	0.084
	48. BackpropMomentum	0.1209	0.1297	0.0088	0.1042	0.3327	0.086
	49. BackpropWeightDecay	0.1186	0.1214	0.0028	0.0950	0.2751	0.082
	46. BackpropBatch	0.3063	0.3491	0.0428	0.2736	0.8922	0.820
	50. Quickprop	0.2122	0.2993	0.0871	0.2338	0.8131	0.826
automl	8. adam	0.0933	0.1579	0.0646	0.1212	0.4579	1.244
	9. RMSprop	0.1179	0.1615	0.0436	0.1223	0.4550	1.096
	10. trainwpso	0.1180	0.1616	0.0436	0.1233	0.4403	5.164
deepnet	20. BP	0.0928	0.1049	0.0121	0.0824	0.2577	0.080
neuralnet	38. rprop+	0.2846	0.3562	0.0716	0.2762	0.8861	0.008
	37. rprop-	0.1632	0.3537	0.1905	0.2756	0.9038	0.014
	40. slr	0.3374	0.3435	0.0061	0.2714	0.9130	0.012
	39. sag	0.1663	0.2521	0.0858	0.1997	0.7213	0.098
	36. backprop	0.3205	0.3655	0.0450	0.2776	0.9575	0.042
keras	28. adamax	0.1118	0.1154	0.0036	0.0935	0.3048	4.740
	27. adam	0.1105	0.1345	0.0240	0.1062	0.3156	2.354
	29. nadam	0.1341	0.1957	0.0616	0.1530	0.5132	2.366
	26. adagrad	0.1847	0.1979	0.0132	0.1420	0.6153	14.992
	25. adadelta	0.3605	0.3726	0.0121	0.2763	0.9935	7.248
	31. sgd	0.3523	0.3548	0.0025	0.2760	0.9224	2.546
	30. rmsprop	0.2221	0.3598	0.1377	0.2805	0.8788	1.096
AMORE	2. ADAPTgdwm	0.1675	0.2519	0.0844	0.1964	0.6689	0.030
	1. ADAPTgd	0.3555	0.3612	0.0057	0.2824	0.9010	0.020
	4. BATCHgdwm	0.2097	0.3405	0.1308	0.2704	0.8640	1.380
	3. BATCHgd	0.1778	0.2708	0.0930	0.2148	0.6304	1.378
minpack.lm	33. default	0.0906	0.0906	0.0000	0.0723	0.2197	0.022
ANN2	6. rmsprop	0.2338	0.2845	0.0507	0.2093	0.8061	0.014
	5. adam	0.3222	0.3836	0.0614	0.2918	0.8958	0.010
	7. sgd	0.3581	0.3717	0.0136	0.2806	0.9555	0.008
deepdive	16. adam	0.1149	0.1149	0.0000	0.0907	0.2749	0.566
	19. rmsProp	0.1625	0.1625	0.0000	0.1232	0.4839	0.552
	18. momentum	0.3570	0.3570	0.0000	0.2907	0.8468	5.390
	17. gradientDescent	0.3570	0.3570	0.0000	0.2905	0.8478	5.222
snnR	54. default	0.3837	0.3837	0.0000	0.2773	1.0352	0.012
elmNNRepp	21. extremeML	0.4534	0.6226	0.1692	0.5077	1.4031	0.000
ELMR	22. extremeML	0.4554	0.5844	0.1290	0.4293	1.3727	0.002

Note: Statistics over 10 runs.

1.9 Result for dataset uGauss1

Table 9: Result for uGauss1

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	2.2321	2.6129	0.3808	2.0484	8.2482	0.156
rminer	45. default	2.2452	2.2628	0.0176	1.7485	7.3946	0.084
nnet	42. default	2.2380	2.2557	0.0177	1.7541	7.3381	0.032
validann	56. BFGS	2.2606	2.3192	0.0586	1.8215	7.5409	0.932
	57. CG	2.3620	2.3962	0.0342	1.9105	8.2206	41.996
	58. L-BFGS-B	2.7065	3.4311	0.7246	2.6492	9.8990	1.060
	59. Nelder-Mead	9.2009	11.1644	1.9635	9.1979	26.4353	42.914
	60. SANN	12.6829	15.2562	2.5733	12.8000	37.0901	0.204
MachineShop	32. default	2.2521	2.2681	0.0160	1.7734	7.5718	0.034
traineR	55. default	2.2431	2.3022	0.0591	1.7999	7.5122	0.038
radiant.model	44. default	2.3275	6.3010	3.9735	5.1479	17.4222	0.054
monmlp	34. BFGS	2.7246	5.7229	2.9983	4.8218	14.7964	0.226
	35. Nelder-Mead	12.1868	12.7777	0.5909	9.8127	35.0537	0.574
CaDENCE	12. optim	2.3392	2.4124	0.0732	1.9079	7.6898	2.906
	14. Rprop	17.7666	25.2780	7.5114	17.3441	56.1202	9.070
	13. psoptim	25.3213	29.0788	3.7575	22.9938	64.9998	6.144
h2o	24. first-order	2.2985	2.3587	0.0602	1.8349	7.6990	4.372
EnsembleBase	23. default	2.5261	2.6857	0.1596	2.0641	8.3968	0.038
caret	15. default	2.3241	2.6365	0.3124	2.0948	7.8111	0.108
brnn	11. Gauss-Newton	2.2434	2.4366	0.1932	1.8814	8.7824	0.042
qrnn	43. default	2.7155	2.7208	0.0053	2.0888	8.1916	0.158
RSNNS	51. Rprop	2.9859	10.3291	7.3432	7.2486	33.1339	0.320
	52. SCG	2.7001	4.7483	2.0482	3.6042	16.9268	0.558
	53. Backpropagation	3.0594	3.2011	0.1417	2.5444	9.0758	0.370
	47. BackpropChunk	2.9425	2.9820	0.0395	2.4160	10.5110	0.368
	48. BackpropMomentum	2.8791	2.9074	0.0283	2.2991	9.6946	0.334
	49. BackpropWeightDecay	2.8682	3.0805	0.2123	2.3657	8.8148	0.372
	46. BackpropBatch	14.5624	19.9070	5.3446	16.5809	52.1745	3.478
	50. Quickprop	23.6323	24.1323	0.5000	20.1405	57.6774	3.696
automl	8. adam	4.4523	4.9986	0.5463	3.8522	18.0133	4.982
	9. RMSprop	4.9906	5.2304	0.2398	4.1778	17.4681	4.482
	10. trainwpso	9.8111	13.4226	3.6115	9.5187	39.8505	8.586
deepnet	20. BP	3.4191	4.2839	0.8648	3.5260	11.8002	0.304
neuralnet	38. rprop+	2.9603	3.7997	0.8394	2.8334	14.1152	0.298
	37. rprop-	2.6198	3.8778	1.2580	2.9818	13.8198	0.308
	40. slr	2.8881	4.3263	1.4382	3.1765	14.4615	0.440
	39. sag	2.2972	41.6253	39.3281	36.1679	91.5205	7.138
	36. backprop	2.9109	3.4962	0.5853	2.6743	11.9971	0.622
keras	28. adamax	2.5783	3.1920	0.6137	2.5827	8.6394	6.082
	27. adam	2.8614	3.0075	0.1461	2.3994	8.8657	3.620
	29. nadam	5.2915	12.2499	6.9584	9.8464	27.3131	3.166
	26. adagrad	6.5047	6.7324	0.2277	5.3578	20.2040	52.480
	25. adadelta	4.4960	5.1564	0.6604	3.8748	16.8817	73.920
	31. sgd	3.4196	3.9121	0.4925	3.1018	14.8772	13.988
	30. rmsprop	6.6698	13.1877	6.5179	10.5806	32.3150	2.552
AMORE	2. ADAPTgdwm	14.8661	28.9286	14.0625	15.0901	75.7312	0.084
	1. ADAPTgd	12.5180	28.6849	16.1669	23.0898	63.3445	0.050
	4. BATCHgdwm	12.0720	12.5131	0.4411	10.6879	26.8772	1.724
	3. BATCHgd	12.0830	12.6864	0.6034	10.8841	27.5733	1.694
minpack.lm	33. default	2.2329	2.2329	0.0000	1.7383	6.9429	0.068
ANN2	6. rmsprop	5.5210	8.5210	3.0000	7.0532	20.1249	0.076
	5. adam	2.7029	9.5851	6.8822	7.9902	22.2599	0.080
	7. sgd	11.0994	11.9128	0.8134	10.0259	25.8843	0.080
deepdive	16. adam	20.5179	20.5179	0.0000	16.5474	47.6354	0.634
	19. rmsProp	23.5833	23.5833	0.0000	19.1113	57.9958	0.658
	18. momentum	16.2557	16.2557	0.0000	13.0878	49.2409	6.236
	17. gradientDescent	23.6597	23.6597	0.0000	19.1988	57.7174	6.084
snnR	54. default	11.6175	11.6175	0.0000	9.5749	25.9147	0.038
elmNNRepp	21. extremeML	17.0430	18.7830	1.7400	15.4373	50.7429	0.000
ELMR	22. extremeML	37.3986	490.0535	452.6549	426.0995	1516.4503	0.010

Note: Statistics over 10 runs.

1.10 Result for dataset uGauss2

Table 10: Result for uGauss2

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	2.3327	2.9754	0.6427	2.3838	9.0619	0.118
rminer	45. default	2.3604	2.3690	0.0086	1.8630	7.5477	0.082
nnet	42. default	2.3625	3.0894	0.7269	2.4567	9.4881	0.026
validann	56. BFGS	2.3571	2.3654	0.0083	1.8640	7.5013	0.792
	57. CG	3.5928	6.3016	2.7088	4.7543	17.8412	34.308
	58. L-BFGS-B	3.0632	4.0776	1.0144	3.1853	13.2715	0.840
	59. Nelder-Mead	6.7221	7.5819	0.8598	5.9618	22.5839	29.606
	60. SANN	9.9162	14.2730	4.3568	11.6041	32.1496	0.204
MachineShop	32. default	2.5986	3.1210	0.5224	2.4847	9.3644	0.024
traineR	55. default	2.3713	2.6020	0.2307	2.0822	8.0308	0.018
radiant.model	44. default	2.5784	4.5795	2.0011	3.7498	11.3454	0.056
monmlp	34. BFGS	3.0438	4.6769	1.6331	3.6151	13.7834	0.224
	35. Nelder-Mead	8.2728	9.5898	1.3170	6.7817	30.1673	0.412
CaDENCE	12. optim	2.4041	3.1503	0.7462	2.3988	10.7996	2.320
	14. Rprop	11.7899	17.6638	5.8739	12.7742	39.4495	5.810
	13. psoptim	11.1566	15.4210	4.2644	12.0091	37.0326	5.752
h2o	24. first-order	2.8574	3.4454	0.5880	2.7928	11.6466	4.394
EnsembleBase	23. default	2.7901	3.8821	1.0920	3.0341	11.9878	0.030
caret	15. default	2.4240	3.2653	0.8413	2.6499	9.8629	0.086
brnn	11. Gauss-Newton	2.3781	3.5508	1.1727	2.9377	10.2283	0.048
qrnn	43. default	2.6571	3.7782	1.1211	2.6654	16.0998	0.248
RSNNS	51. Rprop	3.5732	6.3892	2.8160	4.6858	19.1326	0.316
	52. SCG	6.2398	6.4892	0.2494	4.8401	20.2438	0.556
	53. Backpropagation	3.4215	4.8320	1.4105	3.8106	15.2518	0.318
	47. BackpropChunk	3.2955	4.7181	1.4226	3.6073	15.4886	0.332
	48. BackpropMomentum	3.3532	4.8150	1.4618	3.7195	15.6644	0.352
	49. BackpropWeightDecay	4.5703	6.7390	2.1687	5.5508	19.8255	0.320
	46. BackpropBatch	12.1638	14.7088	2.5450	11.5655	30.3793	3.266
	50. Quickprop	24.5455	25.0662	0.5207	19.9234	51.7595	3.522
automl	8. adam	8.1454	8.6420	0.4966	6.1349	30.0687	4.952
	9. RMSprop	3.9723	8.4113	4.4390	5.6794	30.3739	4.436
	10. trainwpso	6.1384	8.6501	2.5117	6.2805	24.3330	8.702
deepnet	20. BP	3.4032	6.4830	3.0798	4.8425	17.3581	0.320
neuralnet	38. rprop+	3.6133	8.6404	5.0271	6.1594	25.2448	0.064
	37. rprop-	3.5904	4.4020	0.8116	3.4777	14.1560	0.080
	40. slr	3.5678	3.7435	0.1757	2.7163	14.9299	0.190
	39. sag	3.3723	8.6390	5.2667	6.1167	24.7388	1.916
	36. backprop	4.2479	4.3983	0.1504	3.4494	12.7619	0.866
keras	28. adamax	3.8559	4.2292	0.3733	3.3180	12.7852	6.844
	27. adam	3.9732	6.7909	2.8177	5.1083	18.9390	3.046
	29. nadam	4.2819	7.1607	2.8788	5.6164	19.4085	3.374
	26. adagrad	5.0447	8.8810	3.8363	6.5481	25.2992	31.862
	25. adadelta	3.8515	3.8918	0.0403	2.8916	15.2710	51.048
	31. sgd	5.1907	8.8123	3.6216	6.4800	24.8510	9.784
	30. rmsprop	8.1016	10.2651	2.1635	7.5917	28.4689	2.276
AMORE	2. ADAPTgdwm	4.3864	10.4646	6.0782	6.6054	38.5720	0.068
	1. ADAPTgd	7.4794	8.1969	0.7175	6.0059	23.9130	0.054
	4. BATCHgdwm	9.2190	9.4697	0.2507	6.9325	27.9676	1.578
	3. BATCHgd	9.1582	9.7638	0.6056	7.1783	28.5231	1.552
minpack.lm	33. default	2.9795	2.9795	0.0000	2.3890	9.0540	0.050
ANN2	6. rmsprop	3.5637	4.2355	0.6718	3.2536	15.9291	0.100
	5. adam	3.7310	4.0836	0.3526	3.2330	12.0798	0.086
	7. sgd	7.4578	8.3914	0.9336	6.3470	25.3806	0.078
deepdive	16. adam	16.8843	16.8843	0.0000	11.6361	46.6218	0.618
	19. rmsProp	18.3426	18.3426	0.0000	12.6957	49.5614	0.620
	18. momentum	28.8104	28.8104	0.0000	25.1756	67.8020	6.176
	17. gradientDescent	28.8118	28.8118	0.0000	25.1770	67.7823	5.934
snnR	54. default	8.8419	9.4678	0.6259	6.9147	30.1105	0.044
elmNNRepp	21. extremeML	20.3911	23.5586	3.1675	20.1337	51.5475	0.000
ELMR	22. extremeML	27.8077	31.2976	3.4899	25.2946	82.5683	0.014

Note: Statistics over 10 runs.

1.11 Result for dataset uGauss3

Table 11: Result for uGauss3

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlr	41. default	2.2991	2.8185	0.5194	2.2078	7.5077	0.110
rminer	45. default	2.3033	2.3232	0.0199	1.8528	7.0323	0.062
nnet	42. default	2.3554	3.1706	0.8152	2.5057	9.8058	0.020
validann	56. BFGS	2.3046	2.8185	0.5139	2.2078	7.5077	0.744
	57. CG	2.4990	3.5798	1.0808	2.7264	11.3586	37.490
	58. L-BFGS-B	2.5172	3.5450	1.0278	2.7137	10.7114	0.870
	59. Nelder-Mead	4.9577	5.3229	0.3652	4.3142	15.0154	30.822
	60. SANN	6.9649	10.8474	3.8825	8.3651	26.5278	0.210
MachineShop	32. default	2.3086	3.1576	0.8490	2.4940	9.7409	0.034
traineR	55. default	2.2976	2.8669	0.5693	2.2422	7.9607	0.020
radiant.model	44. default	2.6848	3.4127	0.7279	2.7026	10.5356	0.046
monmlp	34. BFGS	2.9135	3.5782	0.6647	2.8497	10.8707	0.220
	35. Nelder-Mead	5.8001	7.3161	1.5160	5.7523	20.8098	0.424
CaDENCE	12. optim	2.4116	2.8622	0.4506	2.2233	7.8710	2.334
	14. Rprop	9.1862	21.8896	12.7034	15.2197	62.4249	5.790
	13. psoptim	10.8502	14.8615	4.0113	11.6021	34.5796	5.746
h2o	24. first-order	2.9525	3.2931	0.3406	2.5635	9.9032	4.706
EnsembleBase	23. default	2.3829	3.1571	0.7742	2.4537	9.9903	0.036
caret	15. default	2.4976	3.1181	0.6205	2.3743	9.6517	0.080
brnn	11. Gauss-Newton	2.8273	3.1966	0.3693	2.5109	10.0153	0.026
qrnn	43. default	2.7773	3.9015	1.1242	2.8959	13.2058	0.208
RSNNS	51. Rprop	2.9609	8.8744	5.9135	6.0200	30.1870	0.352
	52. SCG	3.3416	3.7196	0.3780	2.9009	11.2479	0.538
	53. Backpropagation	3.0294	3.2409	0.2115	2.6432	9.4181	0.316
	47. BackpropChunk	2.9280	3.8323	0.9043	3.0061	11.0342	0.320
	48. BackpropMomentum	2.9271	3.2533	0.3262	2.6246	8.8194	0.320
	49. BackpropWeightDecay	2.8723	3.0215	0.1492	2.3931	8.5837	0.360
	46. BackpropBatch	6.7104	9.7422	3.0318	7.6756	23.2263	3.274
	50. Quickprop	27.8595	28.8119	0.9524	22.8776	59.8157	3.518
automl	8. adam	3.1214	3.4986	0.3772	2.7250	9.7689	4.984
	9. RMSprop	3.5555	3.7519	0.1964	3.0224	11.8905	4.398
	10. trainwpso	4.8318	6.6613	1.8295	4.7306	20.0899	6.586
deepnet	20. BP	3.5001	3.7035	0.2034	2.9180	12.1143	0.300
neuralnet	38. rprop+	2.5491	3.6200	1.0709	2.8585	10.5212	0.066
	37. rprop-	2.6706	3.6253	0.9547	2.8533	9.9037	0.036
	40. slr	2.8318	3.7840	0.9522	3.0024	10.4000	0.102
	39. sag	2.7247	3.8181	1.0934	2.8290	11.6167	1.016
	36. backprop	3.8802	4.2928	0.4126	3.4361	11.4729	0.302
keras	28. adamax	2.5583	2.9976	0.4393	2.3357	9.7110	5.008
	27. adam	3.2791	4.0840	0.8049	3.1478	11.9057	2.296
	29. nadam	3.2682	3.4600	0.1918	2.8802	9.8016	2.708
	26. adagrad	3.4760	4.8342	1.3582	3.7910	14.2616	13.448
	25. adadelta	3.9293	4.3921	0.4628	3.3906	13.1185	19.964
	31. sgd	4.8610	5.1138	0.2528	3.9761	15.1244	5.274
	30. rmsprop	5.4568	6.4457	0.9889	5.4036	15.4436	1.890
AMORE	2. ADAPTgdwm	4.4658	5.1079	0.6421	3.6709	20.0320	0.080
	1. ADAPTgd	4.7958	4.8043	0.0085	3.9113	12.5672	0.046
	4. BATCHgdwm	5.0868	5.2355	0.1487	4.1127	14.7918	1.566
	3. BATCHgd	5.0863	5.2682	0.1819	4.1337	14.8772	1.556
minpack.lm	33. default	3.1472	3.1472	0.0000	2.4837	9.7293	0.040
ANN2	6. rmsprop	2.9727	3.2852	0.3125	2.5929	9.6420	0.082
	5. adam	3.1354	3.6437	0.5083	2.8900	10.5979	0.082
	7. sgd	4.8318	4.8821	0.0503	3.8567	14.4928	0.080
deepdive	16. adam	10.0466	10.0466	0.0000	7.3484	31.6838	0.624
	19. rmsProp	20.7977	20.7977	0.0000	15.4531	49.0396	0.622
	18. momentum	32.2413	32.2413	0.0000	27.7055	70.2077	6.146
	17. gradientDescent	32.2441	32.2441	0.0000	27.7063	70.1972	5.946
snnR	54. default	5.2818	5.2818	0.0000	4.0957	15.6475	0.032
elmNNRepp	21. extremeML	8.4445	19.1869	10.7424	16.8753	35.7678	0.000
ELMR	22. extremeML	31.0706	41.2586	10.1880	33.0051	112.2972	0.010

Note: Statistics over 10 runs.

1.12 Result for dataset uNeuroOne

Table 12: Result for uNeuroOne

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
nlsr	41. default	0.2830	0.2830	0.0000	0.2313	0.5675	0.008
rminer	45. default	0.2830	0.2830	0.0000	0.2313	0.5675	0.004
nnet	42. default	0.2830	0.2830	0.0000	0.2313	0.5675	0.000
validann	56. BFGS	0.2830	0.2830	0.0000	0.2313	0.5675	0.104
	57. CG	0.2830	0.2830	0.0000	0.2313	0.5675	23.762
	58. L-BFGS-B	0.2830	0.2830	0.0000	0.2313	0.5675	0.222
	59. Nelder-Mead	0.3256	0.3341	0.0085	0.2793	0.8397	9.006
	60. SANN	0.3084	0.3344	0.0260	0.2773	0.6937	0.168
MachineShop	32. default	0.2830	0.2830	0.0000	0.2313	0.5675	0.010
traineR	55. default	0.2830	0.2830	0.0000	0.2313	0.5675	0.000
radiant.model	44. default	0.2830	0.2830	0.0000	0.2313	0.5677	0.010
monmlp	34. BFGS	0.2831	0.2834	0.0003	0.2312	0.5810	0.194
	35. Nelder-Mead	0.3020	0.3266	0.0246	0.2601	0.6451	0.224
CaDENCE	12. optim	0.2831	0.2831	0.0000	0.2310	0.5816	0.298
	14. Rprop	0.3054	0.3248	0.0194	0.2626	0.7872	2.786
	13. psoptim	0.5523	0.7577	0.2054	0.5800	1.9676	4.244
h2o	24. first-order	0.2831	0.2832	0.0001	0.2331	0.5539	3.344
EnsembleBase	23. default	0.2826	0.2831	0.0005	0.2326	0.5543	0.012
caret	15. default	0.2904	0.2946	0.0042	0.2437	0.6434	0.010
brnn	11. Gauss-Newton	0.3523	0.3523	0.0000	0.2848	0.8271	0.008
qrnn	43. default	0.2939	0.2939	0.0000	0.2258	0.7231	0.094
RSNNS	51. Rprop	0.2830	0.3141	0.0311	0.2531	0.7252	0.076
	52. SCG	0.2855	0.6216	0.3361	0.5100	1.4782	0.104
	53. Backpropagation	0.2834	0.3135	0.0301	0.2457	0.7675	0.082
	47. BackpropChunk	0.2912	0.6365	0.3453	0.5156	1.6363	0.074
	48. BackpropMomentum	0.2968	0.3315	0.0347	0.2742	0.7631	0.074
	49. BackpropWeightDecay	0.3096	0.6423	0.3327	0.5179	1.6618	0.082
	46. BackpropBatch	0.6867	0.6888	0.0021	0.5629	1.6534	0.788
	50. Quickprop	0.5304	0.5304	0.0000	0.4235	1.2829	0.764
automl	8. adam	0.2844	0.2895	0.0051	0.2378	0.6469	1.214
	9. RMSprop	0.2842	0.2888	0.0046	0.2403	0.6528	1.090
	10. trainwpso	0.2847	0.2878	0.0031	0.2350	0.5413	4.896
deepnet	20. BP	0.2830	0.2830	0.0000	0.2314	0.5653	0.084
neuralnet	38. rprop+	0.2848	0.3165	0.0317	0.2586	0.6196	0.000
	37. rprop-	0.2864	0.2935	0.0071	0.2480	0.6059	0.010
	40. slr	0.2923	0.3203	0.0280	0.2607	0.8073	0.052
	39. sag	0.2893	0.3212	0.0319	0.2638	0.6316	0.056
	36. backprop	0.2898	0.2926	0.0028	0.2423	0.5889	0.152
keras	28. adamax	0.2841	0.2864	0.0023	0.2366	0.5789	2.502
	27. adam	0.2869	0.2875	0.0006	0.2340	0.5886	1.320
	29. nadam	0.2855	0.2896	0.0041	0.2437	0.6055	1.518
	26. adagrad	0.2893	0.2936	0.0043	0.2429	0.5637	13.868
	25. adadelta	0.2871	0.2879	0.0008	0.2377	0.5887	19.378
	31. sgd	0.2901	0.2922	0.0021	0.2410	0.5769	3.468
	30. rmsprop	0.3042	0.3629	0.0587	0.3049	0.7486	1.108
AMORE	2. ADAPTgdwm	0.2854	0.2854	0.0000	0.2285	0.6436	0.028
	1. ADAPTgd	0.2958	0.2965	0.0007	0.2451	0.6433	0.020
	4. BATCHgdwm	0.2924	0.2933	0.0009	0.2419	0.6303	1.240
	3. BATCHgd	0.2931	0.2935	0.0004	0.2421	0.6309	1.232
minpack.lm	33. default	1.2720	1.2720	0.0000	1.1104	2.5150	0.004
ANN2	6. rmsprop	0.2904	0.2912	0.0008	0.2376	0.6015	0.008
	5. adam	0.3082	0.3485	0.0403	0.2776	0.7493	0.008
	7. sgd	0.3069	0.3088	0.0019	0.2535	0.6226	0.010
deepdive	16. adam	0.2946	0.2946	0.0000	0.2459	0.5582	0.562
	19. rmsProp	0.3161	0.3161	0.0000	0.2695	0.5981	0.552
	18. momentum	0.3544	0.3544	0.0000	0.3001	0.6152	5.348
	17. gradientDescent	0.3666	0.3666	0.0000	0.3105	0.6748	5.160
snnR	54. default	0.6793	0.6793	0.0000	0.5564	1.6288	0.004
elmNNRepp	21. extremeML	0.8650	0.9526	0.0876	0.7905	2.2943	0.000
ELMR	22. extremeML	0.9735	1.0466	0.0731	0.8640	2.4817	0.000

Note: Statistics over 10 runs.

1.13 Score probabilities

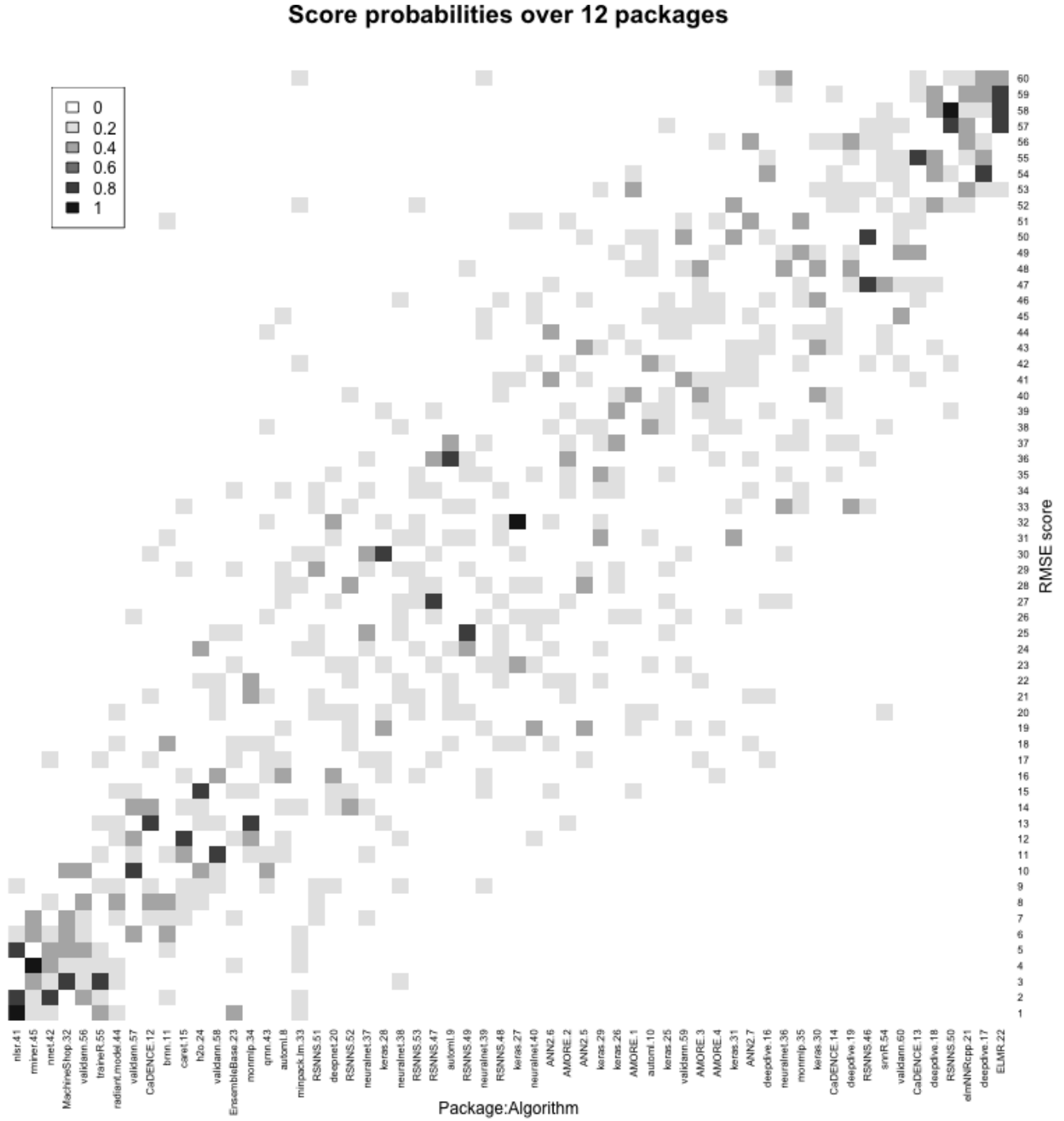


Figure 1: Score probabilities of package:algorithm

2 Additionnal materials on the large dataset bWoodN1

2.1 Summary statistics for non top-5 packages

The table provides the summary statistics of the best run of NN packages over two runs on the large dataset bWoodN1.

Table 13: Result for bWoodN1

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time mean
CaDENCE	12. optim	3.3667	4.60750	1.24080	3.78875	16.57340	228.5210
h2o	24. first-order	4.5704	4.64945	0.07905	3.76315	17.46895	127.9933
monmlp	34. BFGS	4.5442	4.70060	0.15640	3.80100	15.31885	8.6500
	35. Nelder-Mead	5.8579	6.51625	0.65835	5.25615	27.00875	36.3201
radiant.model	44. default	10.9572	10.95720	0.00000	8.76850	42.61880	0.0036
traineR	55. default	3.5488	4.57530	1.02650	3.72975	15.38630	3.2575

Note: Statistics over 10 runs.

2.2 Graphics for top-5 packages

Figures below provides some insights where a package performs reasonably well with respect to one explanatory variable and where the fit misses the correct behavior of an explanatory variable. It displays the average response per rounded explanatory variable for the predicted, the empirical and the theoretical values. That is, the empirical value and the predicted value for the j th explanatory variable are respectively computed at x-value x as

$$\bar{y}_j^{emp}(x) = \frac{1}{n_x} \sum_{i=1}^n y_i 1_{r(x_{i,j})=x}, \quad \bar{y}_j^{pred}(x) = \frac{1}{n_x} \sum_{i=1}^n \hat{y}_i 1_{r(x_{i,j})=x}, \quad n_x = \sum_{i=1}^n 1_{r(x_{i,j})=x},$$

where $r()$ denotes the round function with two decimal places and y_i, \hat{y}_i stand respectively for the i th observed response and the i th predicted response. For instance, **MachineShop**, **nnet**, **nlsr** do not correctly capture the sinusoidal aspect of explanatory variable x_5 on the expected response, whereas **rminer**, **validann** miss the increasing non-linear trend of explanatory variable x_1 on the expected response.

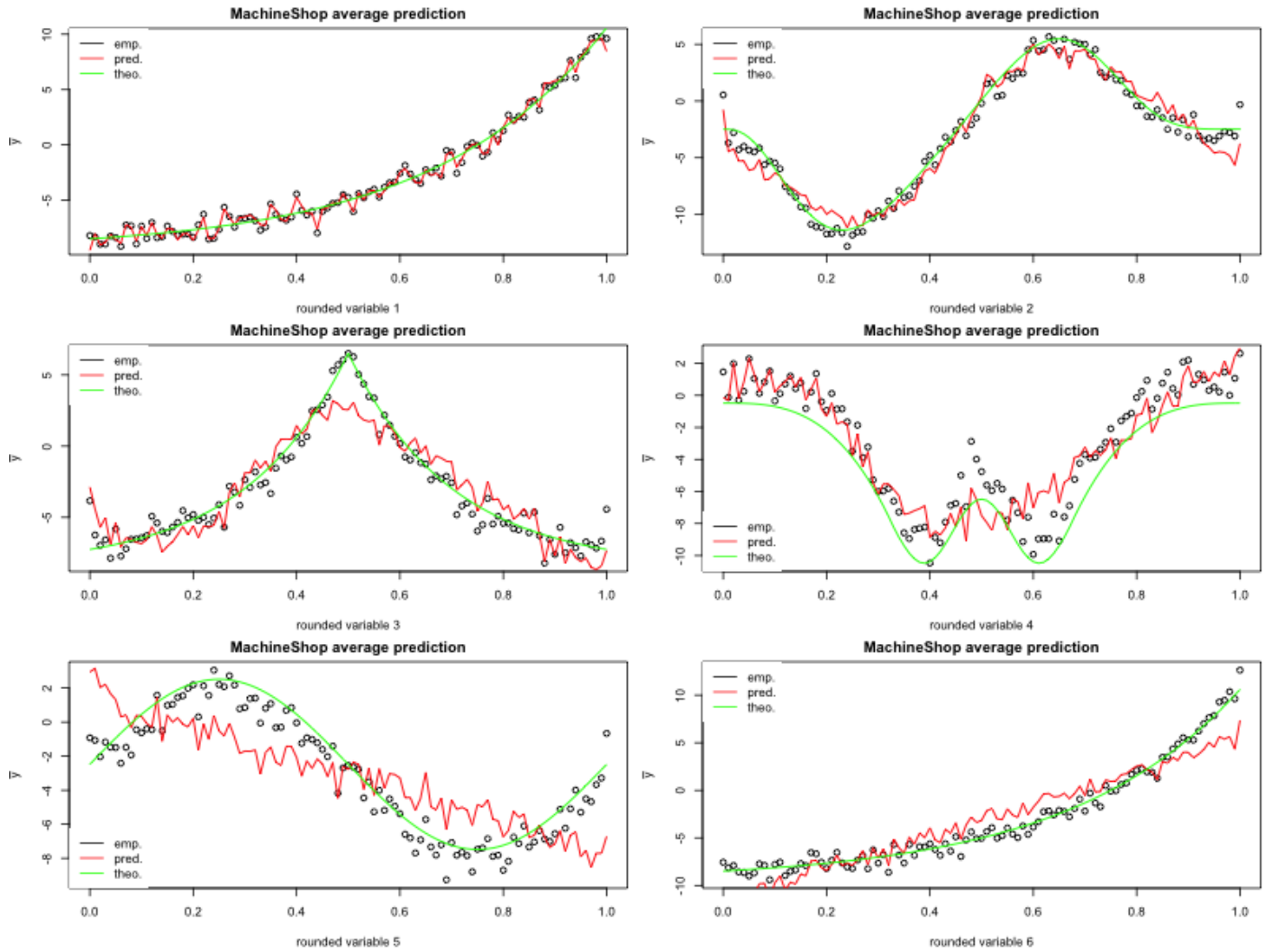


Figure 2: Average predicted mean per explanatory variable for MachineShop

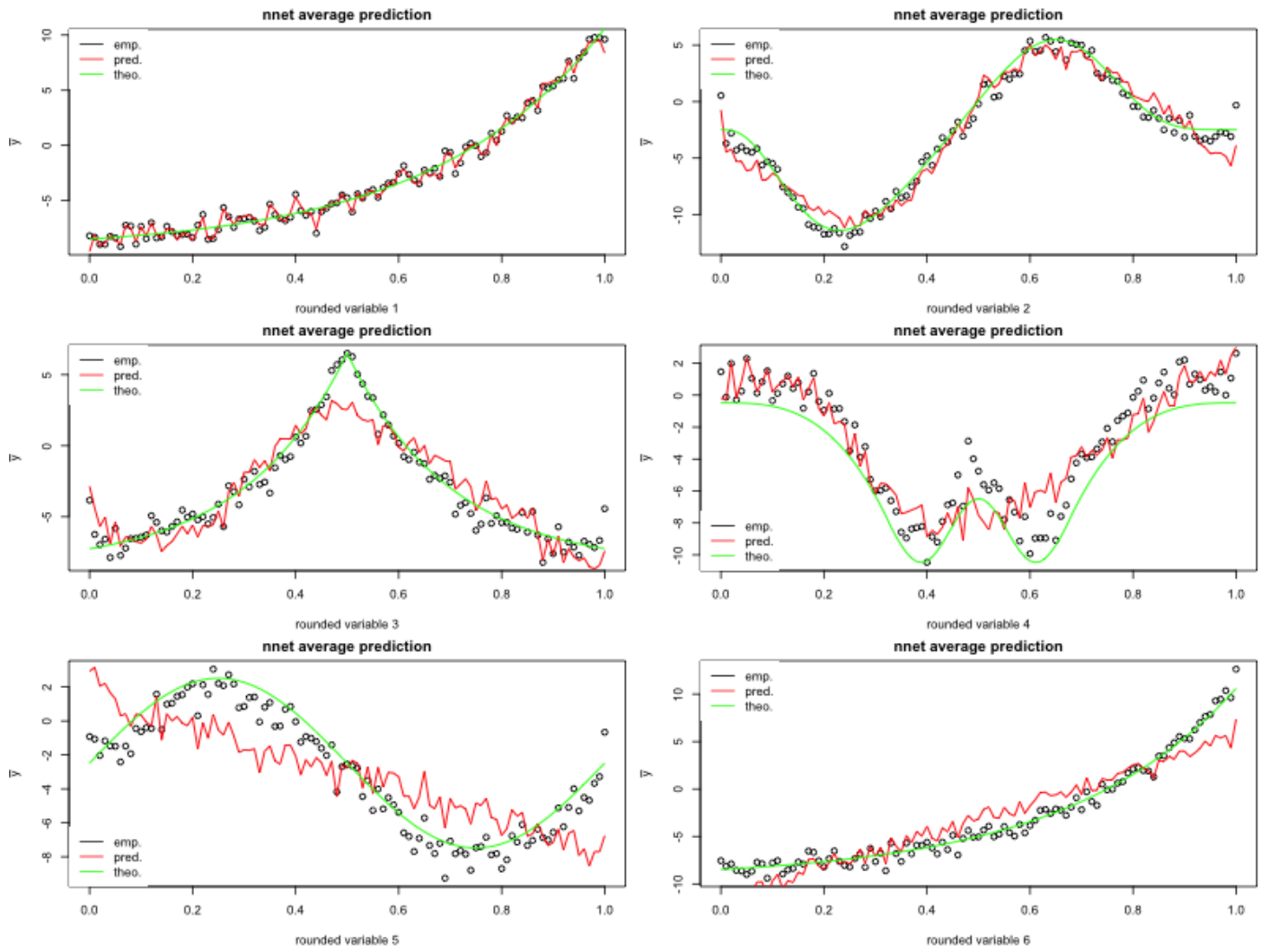


Figure 3: Average predicted mean per explanatory variable for `nnet`

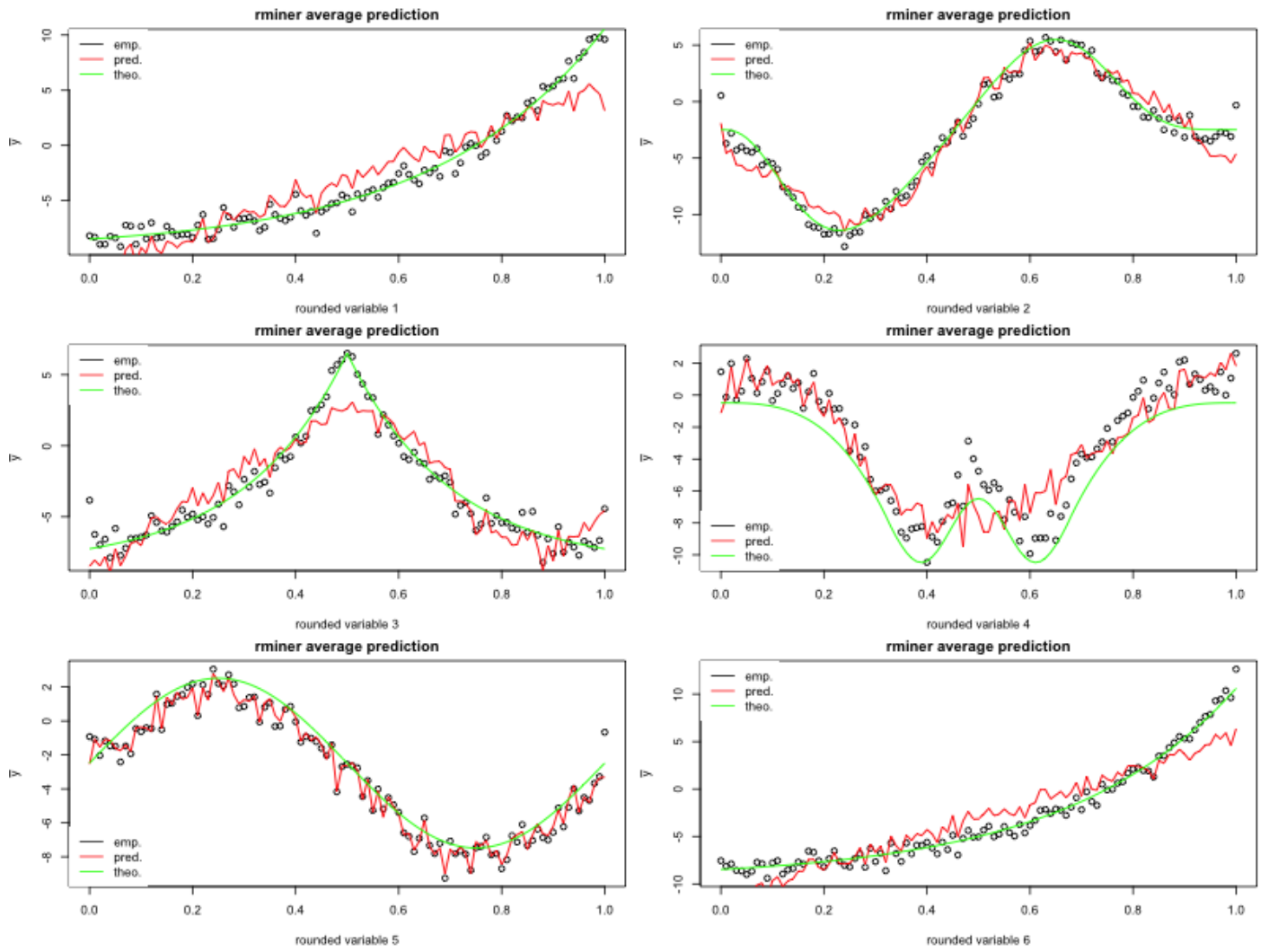


Figure 4: Average predicted mean per explanatory variable for `rminer`

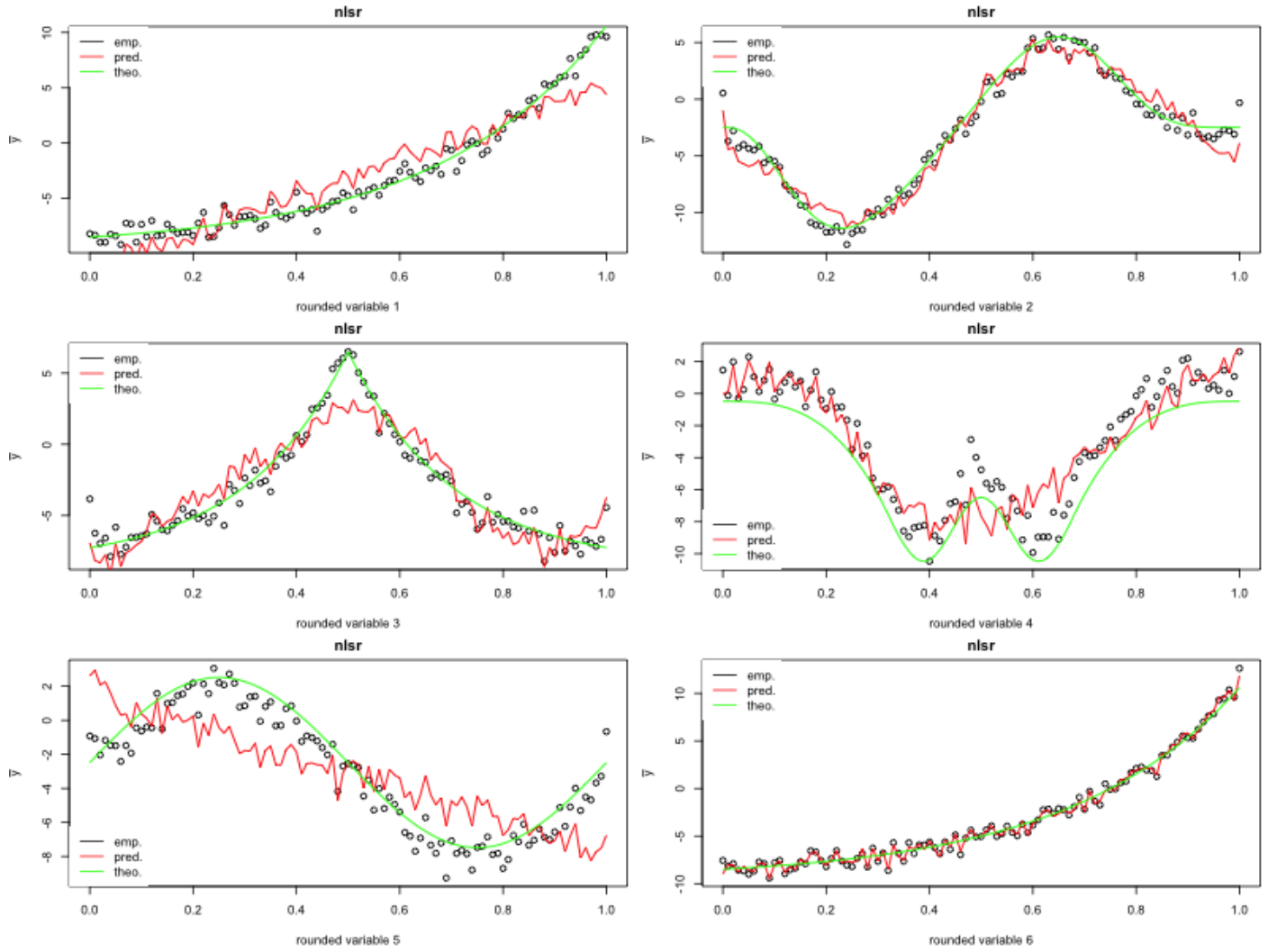


Figure 5: Average predicted mean per explanatory variable for `nlsr`

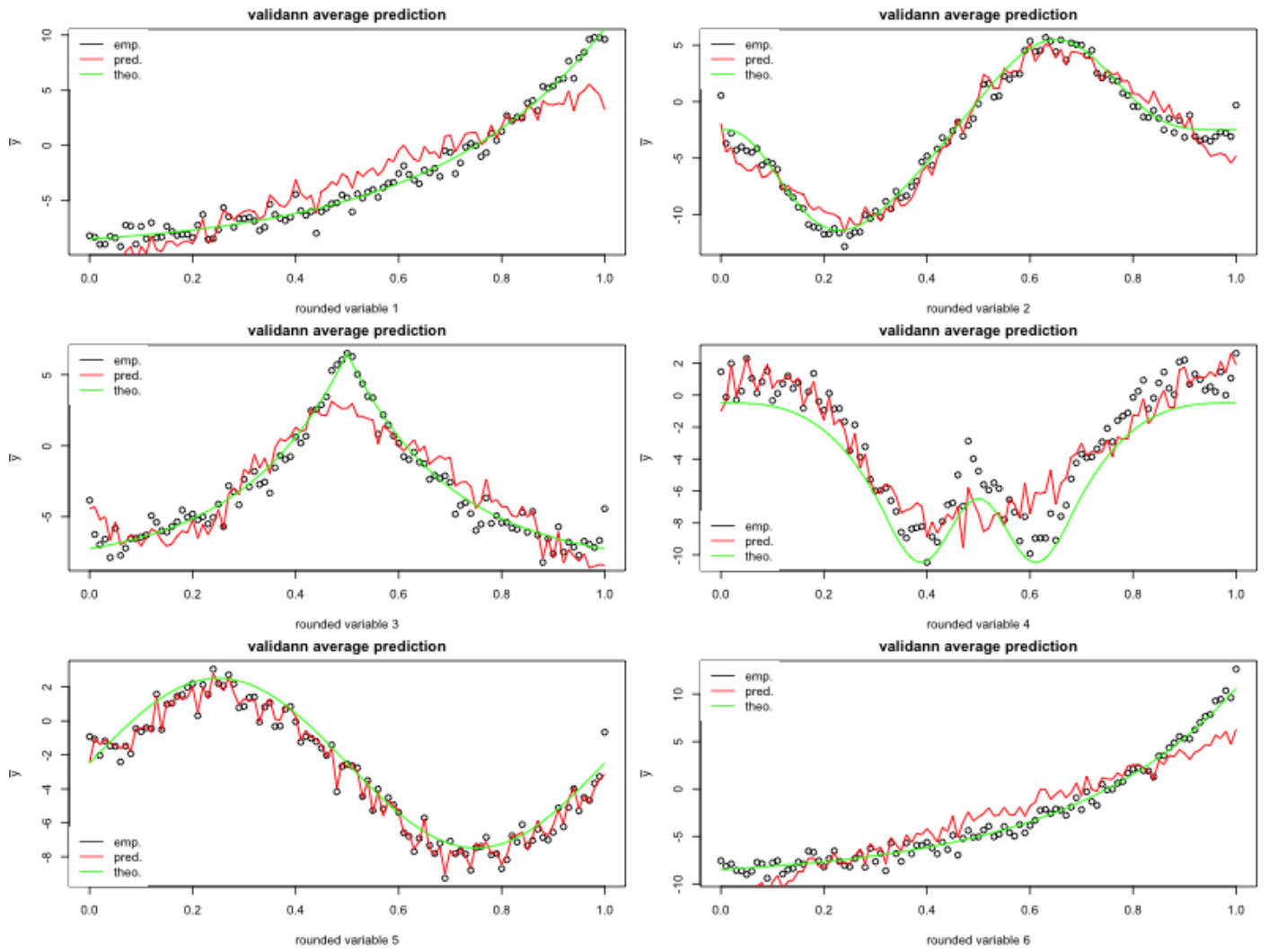


Figure 6: Average predicted mean per explanatory variable for validann