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

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| 1 | Additionnal | materials | on small | /medium-size | datasets for | r all | packages |
|---|-------------|-----------|----------|--------------|--------------|-------|----------|
|---|-------------|-----------|----------|--------------|--------------|-------|----------|

1.1 Result for dataset mDette

Table 1: Result for mDette

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mean |
|---------------|---------------------------------------|--------------------|-----------------|-----------------|-----------------|----------------------|------------------|
| nlsr | 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 |
| | 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 |
| validann | 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 14. Rprop | 0.3277 4.6664 | 2.5664 5.7488 | 2.2387 1.0824 | 1.2936 3.4794 | 17.3208 31.0108 | 7.072 17.178 |
| Cadence | 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 |
| | 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 47. BackpropChunk | 0.4789 0.5892 | 0.5588 0.7126 | 0.0799 0.1234 | 0.4219 0.5252 | 2.0582 2.8993 | 0.638 0.702 |
| RSNNS | 48. BackpropMomentum | 0.6547 | 0.7744 | 0.1234 0.1197 | 0.5909 | 3.1612 | 0.702 |
| | 49. BackpropWeightDecay | | 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 |
| | 8. adam | 0.4255 | 0.6160 | 0.1905 | 0.4710 | 3.2585 | 9.584 |
| automl | 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 |
| | 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 |
| neuralnet | 40. slr | 0.5494 | 0.5688 | 0.0194 | 0.4293 | 2.4012 | 6.914 |
| | 39. sag 36. backprop | $2.1196 \\ 8.1656$ | 8.1656 8.1656 | 6.0460 0.0000 | 6.5262 6.5262 | 36.2385 36.2385 | 12.916 14.200 |
| | 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 |
| keras | 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 |
| | 2. ADAPTgdwm | 0.3972 | 0.4012 | 0.0040 | 0.3084 | 1.7312 | 0.184 |
| AMORE | 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 5. adam | 1.9463 1.7980 | 2.0761 2.0396 | 0.1298 0.2416 | 1.5240 1.5178 | $12.6858 \\ 11.5812$ | $0.206 \\ 0.218$ |
| AIVIV2 | 5. adam 7. sgd | 1.7980 | 2.0396 | 0.2416 0.8020 | 1.4953 | 8.6218 | 0.218 0.204 |
| | 16. adam | 3.0971 | 3.0971 | 0.0000 | 2.0640 | 18.6373 | 0.738 |
| doonding | 19. rmsProp | 2.7205 | 2.7205 | 0.0000 | 1.8705 | 16.1780 | 0.758 |
| deepdive | 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 |
| elmNNRcpp | 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 |
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| 1.2 | Result for dataset mFriedman |
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Table 2: Result for mFriedman

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|---------------------------|----------------------------|-----------------|--------------------|-----------------|------------------|-----------------|------------------|
| 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 |
| | 56. BFGS | 0.0096 | 0.0688 | 0.0592 | 0.0500 | 0.1513 | 2.500 |
| | 57. CG | 0.0163 | 0.0088 | 0.0021 | 0.0300 | 0.1515 | 25.592 |
| validann | 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 |
| ${ m traineR}$ | 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 |
| CoDENCE | 12. optim | 0.0160 | 0.0863 | 0.0703 | 0.0442 | 0.3640 | 9.226 |
| CaDENCE | 14. Rprop 13. psoptim | 0.0850 0.0950 | 0.1295 0.1148 | 0.0445 0.0198 | 0.0858 0.0739 | 0.5842 0.4058 | 22.516 12.056 |
| h2o | 24. first-order | 0.0930 | 0.0261 | 0.0198 | 0.0739 | 0.4038 | 6.046 |
| EnsembleBase | 23. default | 0.0225 | 0.0261 | 0.0036 | 0.0204 | 0.0902 | 0.092 |
| caret | 15. default | 0.0243 | 0.0202 | 0.0074 | 0.0161 | 0.1321 | 0.092 |
| brnn | 11. Gauss-Newton | 0.0123 | 0.0052 | 0.0074 | 0.0102 | 0.0121 | 0.238 |
| qrnn | 43. default | 0.0040 | 0.0032 | 0.0191 | 0.0043 | 0.0134 | 0.238 |
| 41111 | 51. Rprop | 0.0307 | 0.0452 | 0.0191 | 0.0190 | 0.1660 | 0.706 |
| | 52. SCG | 0.0202 | 0.0432 | 0.00145 | 0.0170 | 0.0747 | 1.140 |
| | 53. Backpropagation | 0.0420 | 0.0900 | 0.0480 | 0.0761 | 0.2168 | 0.694 |
| DONING | 47. BackpropChunk | 0.0541 | 0.0657 | 0.0116 | 0.0532 | 0.2284 | 0.732 |
| RSNNS | 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 |
| | 8. adam | 0.0277 | 0.0323 | 0.0046 | 0.0250 | 0.1346 | 9.568 |
| automl | 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 |
| | 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 |
| neuralnet | 40. slr | 0.0690 | 0.2348 | 0.1658 | 0.1880 | 0.6346 | 12.928 |
| | 39. sag 36. backprop | 0.0806 0.2348 | 0.2348 0.2348 | 0.1542 0.0000 | 0.1880 0.1880 | 0.6346 0.6346 | 13.202 14.676 |
| | | | | | | | |
| | 28. adamax 27. adam | 0.0326 0.0636 | $0.0395 \\ 0.0774$ | 0.0069 0.0138 | 0.0319 0.0612 | 0.1140 0.2686 | 4.326 2.160 |
| | 29. nadam | 0.0732 | 0.0992 | 0.0260 | 0.0817 | 0.3144 | 2.482 |
| keras | 26. adagrad | 0.0296 | 0.0842 | 0.0200 | 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 |
| | 2. ADAPTgdwm | 0.0439 | 0.0450 | 0.0011 | 0.0321 | 0.1788 | 0.178 |
| AMORE | 1. ADAPTgd | 0.0264 | 0.0296 | 0.0032 | 0.0235 | 0.1101 | 0.128 |
| | 4. BATCHgdwm 3. BATCHgd | 0.0173 0.0177 | 0.0176 0.0816 | 0.0003 0.0639 | 0.0138 0.0748 | 0.0586 0.1692 | 1.882 1.876 |
| minpack.lm | 33. default | 0.1269 | 0.1269 | 0.0000 | 0.1009 | 0.1032 | 0.380 |
| | 6. rmsprop | 0.0250 | 0.0314 | 0.0064 | 0.1003 | 0.0945 | 0.226 |
| ANN2 | 5. adam | 0.0230 | 0.0314 | 0.0004 | 0.0166 | 0.0579 | 0.220 |
| | 7. sgd | 0.0178 | 0.0185 | 0.0007 | 0.0147 | 0.0603 | 0.222 |
| | 16. adam | 0.0875 | 0.0875 | 0.0000 | 0.0764 | 0.2699 | 0.768 |
| deepdive | 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 |
| | | 0.0457 | 0.0839 | 0.0382 | 0.0747 | 0.2113 | 0.102 |
| snnR | 54. default | 0.0457 | | | | | |
| snnR elmNNRcpp ELMR | 54. default 21. extremeML | 0.0457 | 0.1734 | 0.0218 | 0.1379 | 0.5055 | 0.000 |

| 1.3 | Result for dataset mIshigami |
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Table 3: Result for mIshigami

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|-------------------|---------------------------------|-----------------|--------------------|-----------------|-----------------|------------------|------------------|
| 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 |
| | 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 |
| validann | 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 |
| Machine Shop | 32. default | 0.6685 | 2.1956 | 1.5271 | 1.7857 | 5.3089 | 0.152 |
| ${ m traineR}$ | 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 35. Nelder-Mead | 0.8185 2.7368 | 0.9739 2.8463 | 0.1554 0.1095 | 0.7577 2.3257 | 3.6164 8.7509 | $0.460 \\ 1.600$ |
| | 12. optim | 1.0465 | 1.6993 | 0.6528 | 0.8815 | 5.3208 | 14.912 |
| CaDENCE | 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 |
| h 2 o | 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 |
| | 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 |
| RSNNS | 47. BackpropChunk | 1.3784 | 2.6226 | 1.2442 | 2.0664 | 8.9928 | 0.816 |
| 10511115 | 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 50. Quickprop | 2.6668 3.4245 | 2.6742 3.5389 | 0.0074 0.1144 | 2.3004 2.8752 | 7.1688 13.1137 | 8.542 9.656 |
| | 8. adam | 0.7511 | 0.7995 | 0.0484 | 0.6120 | 2.9212 | 9.932 |
| automl | 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 |
| | 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 |
| neuralnet | 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 |
| | 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 |
| luama a | 29. nadam | 1.0800 | 2.7592 | 1.6792 | 2.3587 | 8.0273 | 3.264 |
| keras | 26. adagrad 25. adadelta | 0.8522 2.4074 | 2.5746 2.6007 | 1.7224 0.1933 | 2.1958 2.2281 | 6.9534 6.9184 | 31.856 31.676 |
| | 31. sgd | 2.7076 | 2.7302 | 0.1933 | 2.3252 | 7.5362 | 2.788 |
| | 30. rmsprop | 2.8335 | 3.0118 | 0.0220 | 2.4550 | 9.4367 | 1.924 |
| | 2. ADAPTgdwm | 0.8636 | 0.9950 | 0.1314 | 0.7280 | 3.8394 | 0.330 |
| AMORE | 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 5. adam | 0.7045 0.7560 | $0.8590 \\ 0.8062$ | 0.1545 0.0502 | 0.6409 0.6130 | 2.9940 3.5492 | 1.048 1.058 |
| | 7. sgd | 0.7587 | 0.9097 | 0.0302 | 0.6798 | 3.8085 | 1.038 |
| | 16. adam | 2.5913 | 2.5913 | 0.0000 | 2.0819 | 10.0604 | 0.902 |
| doondire | 19. rmsProp | 2.6728 | 2.6728 | 0.0000 | 2.3060 | 7.1452 | 0.892 |
| deepdive | 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 |
| | 54. default | 0.7757 | 0.8621 | 0.0864 | 0.6030 | 3.4730 | 0.430 |
| snnR | | | | | | | |
| snnR elmNNRcpp | 21. extremeML | 3.0949 | 3.2590 | 0.1641 | 2.6511 | 11.3823 | 0.000 |

| 1.4 | Result | for | ${\bf dataset}$ | mRef153 | |
|-----|--------|-----|-----------------|---------|--|
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Table 4: Result for mRef153

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|---------------|--|------------------|------------------|-----------------|-----------------|-------------------|------------------|
| 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 |
| | 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 |
| validann | 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 35. Nelder-Mead | 0.8185 2.7368 | 0.9739 2.8463 | 0.1554 0.1095 | 0.7577 2.3257 | 3.6164 8.7509 | 0.460 1.600 |
| | | | | | | | |
| CaDENCE | 12. optim 14. Rprop | 1.0465 1.3422 | 1.6993 2.3133 | 0.6528 0.9711 | 0.8815 1.3927 | 5.3208 8.8022 | 14.912 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 |
| | 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 |
| RSNNS | 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 50. Quickprop | 2.6668 3.4245 | 2.6742 3.5389 | 0.0074 0.1144 | 2.3004 2.8752 | 7.1688 13.1137 | 8.542 9.656 |
| | 8. adam | 0.7511 | 0.7995 | 0.0484 | 0.6120 | 2.9212 | 9.932 |
| automl | 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 |
| | 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 |
| neuralnet | 40. slr | 0.6816 | 3.6898 | 3.0082 | 2.9776 | 13.1137 | 24.586 |
| | 39. sag 36. backprop | 3.6898 3.6898 | 3.6898 3.6898 | 0.0000 0.0000 | 2.9776 2.9776 | 13.1137 13.1137 | 25.218 23.958 |
| | 28. adamax | | | | | | |
| | 28. adamax 27. adam | 0.8307 0.9777 | 0.8615 1.0728 | 0.0308 0.0951 | 0.6388 0.7886 | 3.6379 4.0357 | 5.302 2.796 |
| | 29. nadam | 1.0800 | 2.7592 | 1.6792 | 2.3587 | 8.0273 | 3.264 |
| keras | 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 |
| | 2. ADAPTgdwm | 0.8636 | 0.9950 | 0.1314 | 0.7280 | 3.8394 | 0.330 |
| AMORE | 1. ADAPTgd | 0.7690 | 0.8135 | 0.0445 | 0.6083 | 2.9968 | 0.222 |
| | 4. BATCHgdwm 3. BATCHgd | 2.4805 2.5215 | 2.5259 2.5544 | 0.0454 0.0329 | 2.1518 2.1768 | 6.4536 6.3018 | 2.678 2.624 |
| minpack.lm | 33. default | 2.5379 | 2.5379 | 0.0000 | 2.0524 | 7.6035 | 0.940 |
| <u> </u> | 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 |
| ANN2 | 7. sgd | 0.7787 | 0.9097 | 0.1310 | 0.6798 | 3.8085 | 1.048 |
| ANN2 | 16. adam | 2.5913 | 2.5913 | 0.0000 | 2.0819 | 10.0604 | 0.902 |
| ANN2 | | 2 6720 | 2.6728 | 0.0000 | 2.3060 | 7.1452 | 0.892 |
| | 19. rmsProp | 2.6728 | | | | 0.7500 | 9.220 |
| | 19. rmsProp 18. momentum | 2.5791 | 2.5791 | 0.0000 | 2.0107 2.4940 | 8.7569 10.2360 | |
| deepdive | 19. rmsProp 18. momentum 17. gradientDescent | 2.5791 3.0218 | 2.5791 3.0218 | 0.0000 | 2.4940 | 10.2360 | 9.062 |
| | 19. rmsProp 18. momentum | 2.5791 | 2.5791 | | | | |

| 1.5 | \mathbf{Result} | for | ${\bf dataset}$ | 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 |
| | | | | | | | |
| | 56. BFGS 57. CG | 0.0435 0.0506 | 0.0725 0.0679 | 0.0290 0.0173 | 0.0540 0.0544 | 0.1810 0.1577 | 0.790 29.066 |
| validann | 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 |
| | 12. optim | 0.0564 | 0.2112 | 0.1548 | 0.1061 | 0.6888 | 2.442 |
| CaDENCE | 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 |
| | 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 |
| RSNNS | 47. BackpropChunk 48. BackpropMomentum | 0.1298 0.1445 | 0.1448 0.1647 | 0.0150 0.0202 | 0.1073 0.1252 | 0.5245 0.5800 | $0.140 \\ 0.088$ |
| | 49. BackpropWeightDecay | 0.1314 | 0.1656 | 0.0202 | 0.1232 | 0.5395 | 0.088 |
| | 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 |
| | 8. adam | 0.0596 | 0.1157 | 0.0561 | 0.0741 | 0.5060 | 1.262 |
| automl | 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 |
| | 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 |
| neuralnet | 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 |
| | 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 |
| l.o.o.o | 29. nadam | 0.1786 | 0.2607 | 0.0821 | 0.2055 | 0.6971 | 2.242 |
| keras | 26. adagrad 25. adadelta | 0.2252 0.2314 | 0.3529 0.2333 | 0.1277 0.0019 | 0.3037 0.1843 | 0.8099 0.5698 | 8.322 23.966 |
| | 31. sgd | 0.2314 0.2044 | 0.2333 | 0.0019 0.1504 | 0.1843 | 0.5698 0.8224 | 23.966 |
| | 31. sga 30. rmsprop | 0.2044 0.2375 | 0.3800 | 0.1504 0.1425 | 0.2964 | 0.8224 0.8503 | $\frac{2.644}{1.326}$ |
| | 2. ADAPTgdwm | 0.2197 | 0.2765 | 0.0568 | 0.2204 | 0.6575 | 0.054 |
| AMORE | 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 5. adam | 0.2345 0.2198 | 0.2495 | 0.0150 0.0076 | 0.1926 | 0.6040 0.5242 | $0.016 \\ 0.012$ |
| AININZ | 5. adam 7. sgd | 0.2198 0.2581 | 0.2274 0.3342 | 0.0076 | 0.1806 0.2899 | 0.5242 0.6824 | 0.012 0.014 |
| | 16. adam | 0.1178 | 0.1178 | 0.0000 | 0.0797 | 0.4868 | 0.568 |
| deepdive | 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 |
| deepaive | 17. gradientDescent | 0.3353 | 0.3353 | 0.0000 | 0.2912 | 0.7067 | 5.340 |
| deepuive | | | | | | | |
| snnR | 54. default | 0.2927 | 0.2927 | 0.0000 | 0.2512 | 0.6561 | 0.040 |
| | 54. default 21. extremeML | 0.2927 0.3320 | 0.2927 0.3623 | 0.0000 | 0.2512 0.3038 | 0.6561 0.8727 | 0.040 |

| 1.6 | \mathbf{Result} | $ \mathbf{for} $ | ${\bf dataset}$ | uDmod2 | |
|-----|-------------------|------------------|-----------------|--------|--|
| | | | | | |

Table 6: Result for uDmod2

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|------------------|--|--------------------------------------|--------------------------------------|----------------------------|----------------------------|----------------------------|-------------------------|
| 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 |
| | 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 |
| validann | 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 14. Rprop | 0.0688 0.1820 | $0.0805 \\ 0.2615$ | 0.0117 0.0795 | 0.0582 0.2061 | 0.2385 0.6887 | 2.310 5.784 |
| Cadence | 13. psoptim | 0.1820 | 0.3238 | 0.0793 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 | 0.021 |
| qrnn | 43. default | 0.0511 | 0.0821 | 0.0310 | 0.0522 | 0.2411 | 0.214 |
| 4 | 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 |
| RSNNS | 47. BackpropChunk | 0.0829 | 0.0892 | 0.0063 | 0.0732 | 0.2035 | 0.090 |
| ICSIVIVS | 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 50. Quickprop | 0.2601 0.2570 | 0.2736 0.4804 | 0.0135 0.2234 | 0.2371 0.4177 | 0.6099 1.0187 | 0.870 0.906 |
| | 8. adam | 0.0511 | 0.0867 | 0.0356 | 0.0707 | 0.1976 | 1.260 |
| automl | 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 |
| | 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 |
| neuralnet | 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 |
| | 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 |
| keras | 29. nadam 26. adagrad | 0.1201 0.1597 | 0.1884 0.1792 | 0.0683 0.0195 | 0.1486 0.1379 | 0.5214 0.4143 | 2.460 13.616 |
| nor as | 25. adadelta | 0.1746 | 0.1792 0.1792 | 0.0193 | 0.1379 | 0.4143 | 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 |
| | 2. ADAPTgdwm | 0.1145 | 0.1924 | 0.0779 | 0.1573 | 0.4195 | 0.034 |
| AMORE | 1. ADAPTgd | 0.2579 | 0.2632 | 0.0053 | 0.2333 | 0.5307 | 0.022 |
| | 4. BATCHgdwm 3. BATCHgd | 0.1585 0.2228 | $0.2621 \\ 0.2644$ | 0.1036 0.0416 | 0.2341 0.2347 | 0.4898 0.4989 | 1.650 1.650 |
| minpack.lm | 33. default | 0.0427 | 0.0427 | 0.0000 | 0.0333 | 0.1058 | 0.024 |
| | 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 |
| - | o. adam | | 0.2732 | 0.0214 | 0.2401 | 0.5272 | 0.012 |
| | 7. sgd | 0.2518 | | | | | |
| | 7. sgd 16. adam | 0.3189 | 0.3189 | 0.0000 | 0.2113 | 0.7209 | 0.572 |
| ANN2 | 7. sgd 16. adam 19. rmsProp | 0.3189 0.2252 | 0.3189 0.2252 | 0.0000 | 0.1580 | 0.5513 | 0.558 |
| ANN2 | 7. sgd 16. adam 19. rmsProp 18. momentum | 0.3189 0.2252 0.2656 | 0.3189 0.2252 0.2656 | 0.0000 0.0000 | $0.1580 \\ 0.2355$ | 0.5513 0.5269 | $0.558 \\ 5.460$ |
| ANN2 deepdive | 7. sgd 16. adam 19. rmsProp 18. momentum 17. gradientDescent | 0.3189 0.2252 0.2656 0.2699 | 0.3189 0.2252 0.2656 0.2699 | 0.0000 0.0000 0.0000 | 0.1580 0.2355 0.2369 | 0.5513 0.5269 0.5509 | 0.558 5.460 5.326 |
| ANN2 | 7. sgd 16. adam 19. rmsProp 18. momentum | 0.3189 0.2252 0.2656 | 0.3189 0.2252 0.2656 | 0.0000 0.0000 | $0.1580 \\ 0.2355$ | 0.5513 0.5269 | $0.558 \\ 5.460$ |

Result for dataset uDreyfus1

1.7

Table 7: Result for uDreyfus1 $\,$

| Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|----------------------------------|--|--|---|--|--|--|
| 41. default | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0001 | 0.014 |
| 45. default | 0.0020 | 0.0023 | 0.0003 | 0.0018 | 0.0057 | 0.012 |
| 42. default | 0.0026 | 0.0716 | 0.0690 | 0.0449 | 0.2254 | 0.004 |
| 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 |
| 32. default | 0.0023 | 0.0034 | 0.0011 | 0.0028 | 0.0102 | 0.010 |
| 55. default | 0.0019 | 0.0022 | 0.0003 | 0.0019 | 0.0076 | 0.000 |
| 44. default | 0.0121 | 0.0682 | 0.0561 | 0.0555 | 0.1546 | 0.022 |
| 34. BFGS | 0.0323 | 0.0541 | 0.0218 | 0.0434 | 0.1524 | $0.190 \\ 0.270$ |
| | | | | | | |
| - | | | | | | 1.030 3.762 |
| | | | | | | 4.512 |
| | | | | | | 3.334 |
| 23. default | 0.0922 | 0.1151 | 0.0229 | 0.0834 | 0.3335 | 0.002 |
| 15. default | 0.0262 | 0.0359 | 0.0097 | 0.0282 | | 0.018 |
| 11. Gauss-Newton | | | 0.0008 | 0.0029 | | 0.000 |
| 43. default | 0.2781 | 0.2841 | 0.0060 | 0.1815 | 0.9095 | 0.128 |
| | | | | | | 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 0.822 |
| · · · | | | | | | 0.906 |
| | | | | | | 1.114 |
| 10. trainwpso | 0.1052 | 0.1154 | 0.0102 | 0.0854 | 0.3281 | 5.358 |
| 20. BP | 0.0139 | 0.0704 | 0.0565 | 0.0451 | 0.2219 | 0.084 |
| 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 |
| 28. adamax | 0.0365 | 0.0487 | 0.0122 | 0.0404 | 0.1489 | 5.074 |
| | | | | | | 2.808 |
| | | | | | | 2.082 5.918 |
| | | | | | | 5.918 10.958 |
| | | | | | | 2.312 |
| 30. rmsprop | 0.3101 | 0.3622 | 0.0521 | 0.2798 | 0.9265 | 0.942 |
| 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 |
| 3 | | | | | | 1.376 1.382 |
| | | | | | | 0.000 |
| | | | | | | 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 |
| 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 17. gradientDescent | 0.3429 0.3429 | 0.3429 0.3429 | 0.0000 0.0000 | 0.2801 0.2801 | 0.7341 0.7346 | 5.460 5.162 |
| TIL BLUGGERED COCCIE | 0.0423 | 0.0423 | 0.0000 | 0.2001 | 0.1940 | 0.102 |
| 54 default | 0.3601 | 0.3601 | 0.0000 | 0.2756 | 0.8531 | 0.006 |
| 54. default 21. extremeML | 0.3691 | 0.3691 0.4066 | 0.0000 | 0.2756 | 0.8531 1.0342 | 0.006 |
| | 41. default 45. default 42. default 56. BFGS 57. CG 58. L-BFGS-B 59. Nelder-Mead 60. SANN 32. default 55. default 44. default 34. BFGS 35. Nelder-Mead 12. optim 14. Rprop 13. psoptim 24. first-order 23. default 15. default 11. Gauss-Newton 43. default 51. Rprop 52. SCG 53. Backpropagation 47. BackpropChunk 48. BackpropMomentum 49. BackpropWeightDecay 46. BackpropBatch 50. Quickprop 8. adam 9. RMSprop 10. trainwpso 20. BP 38. rprop+ 37. rprop- 40. slr 39. sag 36. backprop 28. adamax 27. adam 29. nadam 29. nadam 29. nadam 26. adagrad 25. adadelta 31. sgd 30. rmsprop 2. ADAPTgdwm 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam 7. sgd | 41. default 0.0000 45. default 0.0020 42. default 0.0026 56. BFGS 0.0022 57. CG 0.0035 58. L-BFGS-B 0.0038 59. Nelder-Mead 0.0833 60. SANN 0.2692 32. default 0.0019 44. default 0.0019 44. default 0.0121 34. BFGS 0.0323 35. Nelder-Mead 0.1425 12. optim 0.0032 14. Rprop 0.3995 13. psoptim 0.4218 24. first-order 0.0131 23. default 0.0922 15. default 0.0922 15. default 0.0922 16. adam 0.0026 43. default 0.2781 51. Rprop 0.0617 52. SCG 0.0851 53. Backpropagation 0.1127 47. BackpropChunk 0.0838 48. BackpropMomentum 0.0719 49. BackpropWeightDecay 0.0797 46. BackpropWeightDecay 0.0719 49. BackpropWeightDecay 0.0719 49. BackpropBatch 0.3120 50. Quickprop 0.2177 8. adam 0.0087 9. RMSprop 0.0479 10. trainwpso 0.1052 20. BP 0.0139 38. rprop+ 0.2119 37. rprop- 0.1014 40. slr 0.2981 39. sag 0.1963 36. backprop 0.3201 28. adamax 0.0365 27. adam 0.0706 29. nadam 0.0648 29. nadam 0.0706 29. nadam 0.0648 26. adagrad 0.1630 27. adam 0.0706 29. nadam 0.0648 40. BATCHgdwm 0.3316 31. sgd 0.3373 30. rmsprop 0.3101 2. ADAPTgd 0.3306 3. BATCHgdwm 0.3366 3. BATCHgdwm 0.3366 3. BATCHgdwm 0.3366 3. BATCHgdwm 0.3366 3. BATCHgd 0.33160 3. default 0.0000 6. rmsprop 0.2467 5. adam 0.2762 7. sgd 0.3493 | 41. default 0.0000 0.0000 45. default 0.0020 0.0023 42. default 0.0026 0.0716 56. BFGS 0.0022 0.0023 57. CG 0.0035 0.0076 58. L-BFGS-B 0.0038 0.0084 59. Nelder-Mead 0.0833 0.1951 60. SANN 0.2692 0.3271 32. default 0.0023 0.0034 55. default 0.0019 0.0022 44. default 0.011 0.0682 34. BFGS 0.0323 0.0541 35. Nelder-Mead 0.1425 0.2017 12. optim 0.0032 0.6701 14. Rprop 0.3995 1.1290 13. psoptim 0.4218 0.5720 24. first-order 0.0131 0.0146 23. default 0.0922 0.1151 15. default 0.0922 0.1151 15. default 0.0262 0.0359 11. Gauss-Newton 0.0026 0.0034 43. default 0.2781 0.2841 51. Rprop 0.0617 0.0689 52. SCG 0.0851 0.1018 53. Backpropagation 0.1127 0.1190 47. BackpropChunk 0.0838 0.1275 48. BackpropMomentum 0.0719 0.0795 49. BackpropWeightDecay 0.0797 0.0849 46. BackpropBatch 0.3120 0.3387 50. Quickprop 0.2177 0.2408 8. adam 0.0087 0.0725 9. RMSprop 0.0479 0.0727 10. trainwpso 0.1052 0.1154 20. BP 0.0139 0.0704 38. prop+ 0.1014 0.2856 40. slr 0.2981 0.3450 39. sag 0.1963 0.3371 36. backprop 0.3201 0.3307 28. adamx 0.0065 0.0487 27. adam 0.0706 0.0897 29. nadam 0.0648 0.1550 20. ADAPTgd 0.3308 0.3475 31. sgd 0.3370 3.346 31. sgd 0.3370 3.346 33. default 0.0000 0.0000 6. rmsprop 0.2467 0.3428 4. BATCHgd 0.3160 0.3346 4. BATCHgd 0.3160 0.3346 4. BATCHgd 0.3160 0.3346 | 41. default 0.0000 0.0000 0.0000 45. default 0.0020 0.0023 0.0003 42. default 0.0026 0.0716 0.0690 56. BFGS 0.0022 0.0023 0.0001 57. CG 0.0035 0.0076 0.0041 58. L-BFGS-B 0.0038 0.0084 0.0046 59. Nelder-Mead 0.0833 0.1951 0.1118 60. SANN 0.2692 0.3271 0.0579 32. default 0.0019 0.0022 0.0003 44. default 0.0019 0.0022 0.0003 44. default 0.0121 0.0682 0.0561 34. BFGS 0.0323 0.0541 0.0218 35. Nelder-Mead 0.1425 0.2017 0.0599 12. optim 0.0032 0.6701 0.6669 14. Rprop 0.3995 1.1290 0.7295 13. psoptim 0.4218 0.5720 0.1502 24. first-order 0.0131 0.0146 0.0015 23. default 0.0022 0.1151 0.0229 15. default 0.0022 0.1151 0.0229 16. default 0.0026 0.0359 0.0097 11. Gauss-Newton 0.0026 0.0034 0.0008 43. default 0.0262 0.0359 0.0097 15. Rprop 0.0617 0.0689 0.0072 15. Rprop 0.0617 0.0689 0.0072 15. SCG 0.0851 0.1108 0.0167 15. BackpropOhmentum 0.0719 0.0795 0.0076 15. BackpropOhmentum 0.0719 0.0795 0.0076 15. BackpropOhmentum 0.0719 0.0795 0.0076 16. BackpropOhmentum 0.0719 0.0727 0.0484 17. BackpropOhmentum 0.0719 0.0777 0.0498 0.0027 18. BackpropOhmentum 0.0719 0.0777 0.0498 0.0027 19. RMSprop 0.0479 0.0727 0.0488 19. RMSprop 0.0479 0.0727 0.0488 19. RMSprop 0.0479 0.0727 0.0489 10. trainwpso 0.1052 0.1150 0.0038 10. trainwpso 0.1052 0.1154 0.0016 10. trainwpso 0.1052 0.1154 0.0027 11. trainwpso 0.1052 0.1154 0.0027 12. adam 0.0068 0.0337 0.0302 0.0303 0.0302 0.0303 0.0302 0.0303 0.0302 0.0303 0.0303 0.0302 0.0303 0.0302 0.0303 0.0302 0.0303 0.0302 0.0303 0.0303 0.0302 0.0303 0.0303 0.0302 0.0303 0.0302 0.0303 0.0303 0.0302 0.0303 0.0303 0.0303 0.0302 0.0303 0 | 41. default 0.0000 0.0000 0.0000 0.0000 45. default 0.0020 0.0023 0.0003 0.0018 42. default 0.0026 0.0716 0.0690 0.0419 56. BFGS 0.0022 0.0023 0.0001 0.0019 57. CG 0.0035 0.0076 0.0041 0.0061 58. L-BFCS-B 0.0038 0.0084 0.0046 0.0066 58. L-BFCS-B 0.0038 0.0084 0.0046 0.0066 59. Nelder-Mead 0.0833 0.1951 0.1118 0.1633 60. SANN 0.2692 0.3271 0.0579 0.2707 32. default 0.0023 0.0034 0.0011 0.0028 55. default 0.0019 0.0022 0.0003 0.0019 44. default 0.0121 0.0682 0.0561 0.0555 45. Healt 0.0121 0.0682 0.0561 0.0555 45. Nelder-Mead 0.1425 0.2017 0.0592 0.1653 15. Nelder-Mead 0.1425 0.2017 0.0592 0.1653 17. Order 0.0032 0.0701 0.6669 0.3727 14. Rprop 0.0395 0.1200 0.7295 0.8219 13. psoptim 0.4218 0.5720 0.1502 0.3001 24. first-order 0.0131 0.0146 0.0015 0.0112 23. default 0.0922 0.1151 0.0229 0.0834 15. default 0.0922 0.1151 0.0229 0.0834 15. default 0.0922 0.1151 0.0229 0.0834 15. default 0.0262 0.0359 0.0007 0.0282 11. Gauss-Newton 0.026 0.0334 0.0000 0.0025 11. Gauss-Newton 0.026 0.0334 0.0000 0.0025 15. Rprop 0.0617 0.0689 0.0072 0.0484 25. SCG 0.0851 0.1018 0.0167 0.0848 25. SCG 0.0851 0.1018 0.0167 0.0848 26. Backpropagation 0.1127 0.1190 0.063 0.1007 47. BackpropChunk 0.0838 0.1275 0.0437 0.0822 48. BackpropBatch 0.1127 0.1190 0.0663 0.10076 0.0666 49. BackpropWeightDecay 0.0797 0.0849 0.0052 0.0657 49. BackpropWeightDecay 0.0797 0.0849 0.0052 0.0657 40. BackpropWeightDecay 0.0797 0.0849 0.0052 0.0657 40. BackpropBatch 0.3120 0.3375 0.0438 0.0489 9. RMSprop 0.0479 0.0727 0.0248 0.0498 9. RMSprop 0.0479 0.0727 0.0248 0.0494 9. RMSprop 0.0479 0.0727 0.0248 0.0494 9. RMSprop 0.0479 0.0727 0.0248 0.0498 9. RMSprop 0.0409 0.050 | 41. default 0.0000 0.0000 0.0000 0.0000 0.0001 45. default 0.0002 0.0023 0.0003 0.0018 0.0057 42. default 0.00026 0.0716 0.0009 0.0449 0.2254 42. default 0.00026 0.0716 0.0009 0.0449 0.2254 43. default 0.00026 0.0023 0.0001 0.0019 0.0070 57. CG 0.0035 0.0076 0.0041 0.0061 0.0020 58. L-BFGS-B 0.0038 0.0084 0.0046 0.0066 0.0027 59. Nelder-Mead 0.0833 0.1951 0.1118 0.1633 0.3615 60. SANN 0.2692 0.3271 0.0579 0.2707 0.6614 43. default 0.0019 0.0022 0.0003 0.0019 0.0076 44. default 0.0019 0.0022 0.0003 0.0019 0.0076 44. default 0.0121 0.00682 0.00561 0.0555 0.1546 34. BFGS 0.0323 0.0641 0.0218 0.0553 0.1546 34. BFGS 0.0323 0.0641 0.0218 0.0553 0.1546 34. BFGS 0.0323 0.0641 0.0218 0.0553 0.4572 12. optim 0.0032 0.6701 0.6669 0.3727 1.9004 14. Rprop 0.3905 1.1200 0.7205 0.8219 2.2557 13. paoptim 0.4218 0.5720 0.1502 0.3001 1.6829 24. first-order 0.0131 0.0146 0.0015 0.0112 0.0432 25. default 0.0692 0.1151 0.0229 0.3341 0.3335 15. default 0.0692 0.1151 0.0229 0.3341 0.3335 15. default 0.0692 0.0355 0.0007 0.0282 0.1151 16. Guss-Newton 0.0026 0.0334 0.0008 0.0029 0.0115 24. first-order 0.0131 0.0146 0.0015 0.0112 0.0432 25. default 0.0692 0.1151 0.0229 0.0344 0.3335 15. default 0.0692 0.0355 0.0007 0.0282 0.1151 16. Guss-Newton 0.0026 0.0334 0.0008 0.0029 0.0115 24. Rprop 0.0017 0.0689 0.0072 0.0484 0.2211 25. SCG 0.0051 0.0007 0.0084 0.0029 0.0115 26. SCG 0.0051 0.0007 0.0089 0.0029 0.0155 27. SCG 0.0051 0.0007 0.0089 0.0029 0.0155 28. Adam 0.0008 0.0079 0.0484 0.2211 29. SCG 0.0051 0.0007 0.0048 0.0009 0.0051 20. SANNO 0.0068 0.0072 0.0484 0.2211 20. SCG 0.0051 0.0007 0.0008 0.0007 0.0008 0.0009 20. SANNO 0.0009 0.0009 0.0009 0.0009 20. SANNO 0. |

Result for dataset uDreyfus2

1.8

Table 8: Result for uDreyfus2

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mear |
|-------------------|----------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|------------------------|
| nlsr | 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 |
| | 56. BFGS | 0.0906 | 0.0906 | 0.0000 | 0.0724 | 0.2200 | 0.442 |
| | 57. CG | 0.0900 | 0.0913 | 0.0003 | 0.0724 | 0.2244 | 26.808 |
| validann | 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 |
| Cadence | 14. Rprop 13. psoptim | 0.1684 0.3210 | 0.2586 0.3814 | 0.0902 0.0604 | 0.1963 0.2825 | 0.7853 1.0638 | 4.272 4.500 |
| h2o | 24. first-order | 0.0926 | 0.0933 | 0.0007 | 0.2323 | 0.2242 | 3.356 |
| EnsembleBase | 23. default | 0.0920 | 0.1272 | 0.0007 | 0.1022 | 0.2242 | 0.008 |
| caret | 15. default | 0.0926 | 0.1272 | 0.0070 | 0.1022 | 0.3102 | 0.008 |
| brnn | 11. Gauss-Newton | 0.0920 | 0.1039 | 0.00113 | 0.0811 | 0.2241 | 0.022 |
| qrnn | 43. default | 0.1601 | 0.2693 | 0.1092 | 0.1983 | 0.6891 | 0.170 |
| | 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 |
| Daning | 47. BackpropChunk | 0.1199 | 0.1689 | 0.0490 | 0.1245 | 0.5094 | 0.084 |
| RSNNS | 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 |
| | 8. adam | 0.0933 | 0.1579 | 0.0646 | 0.1212 | 0.4579 | 1.244 |
| automl | 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 |
| | 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 |
| neuralnet | 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 |
| | 28. adamax 27. adam | 0.1118 0.1105 | 0.1154 0.1345 | 0.0036 0.0240 | 0.0935 0.1062 | 0.3048 0.3156 | 4.740 2.354 |
| | 29. nadam | 0.1103 | 0.1945 0.1957 | 0.0240 | 0.1530 | 0.5130 | 2.366 |
| keras | 26. adagrad | 0.1341 0.1847 | 0.1957 | 0.0010 | 0.1330 0.1420 | 0.6153 | $\frac{2.300}{14.992}$ |
| | 25. adadelta | 0.3605 | 0.3726 | 0.0132 | 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 |
| | 2. ADAPTgdwm | 0.1675 | 0.2519 | 0.0844 | 0.1964 | 0.6689 | 0.030 |
| AMORE | 1. ADAPTgd 4. BATCHgdwm | 0.3555 0.2097 | 0.3612 0.3405 | 0.0057 | 0.2824 0.2704 | 0.9010 | 0.020 1.380 |
| | 3. BATCHgdwm | 0.2097 | 0.3405 | 0.1308 0.0930 | 0.2704 | 0.8640 0.6304 | 1.380 1.378 |
| minpack.lm | 33. default | 0.0906 | 0.0906 | 0.0000 | 0.0723 | 0.2197 | 0.022 |
| | 6. rmsprop | 0.2338 | 0.2845 | 0.0507 | 0.2093 | 0.8061 | 0.014 |
| ANN2 | 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 |
| | 16. adam | 0.1149 | 0.1149 | 0.0000 | 0.0907 | 0.2749 | 0.566 |
| deepdive | 19. rmsProp | 0.1625 | 0.1625 | 0.0000 | 0.1232 | 0.4839 | 0.552 |
| asopaive | 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 |
| $_{ m elmNNRcpp}$ | 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 |

Result for dataset uGauss1

1.9

Table 9: Result for uGauss1

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|-----------------|--|--|--------------------------------|------------------------------|-------------------------------|---------------------------------|-------------------------|
| 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 |
| | | 2.2606 | | 0.0586 | | | |
| | 56. BFGS 57. CG | 2.2606 | 2.3192 2.3962 | 0.0342 | 1.8215 1.9105 | 7.5409 8.2206 | 0.932 41.996 |
| validann | 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 35. Nelder-Mead | $\begin{array}{c} 2.7246 \\ 12.1868 \end{array}$ | $5.7229 \\ 12.7777$ | 2.9983 0.5909 | 4.8218 9.8127 | $\frac{14.7964}{35.0537}$ | $0.226 \\ 0.574$ |
| | 12. optim | 2.3392 | 2.4124 | 0.0732 | 1.9079 | 7.6898 | 2.906 |
| CaDENCE | 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 |
| | 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 |
| RSNNS | 47. BackpropChunk 48. BackpropMomentum | 2.9425 2.8791 | 2.9820 2.9074 | 0.0395 0.0283 | 2.4160 2.2991 | 10.5110 9.6946 | 0.368 0.334 |
| | 49. BackpropWeightDecay | 2.8682 | 3.0805 | 0.0283 | 2.3657 | 8.8148 | 0.334 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 |
| | 8. adam | 4.4523 | 4.9986 | 0.5463 | 3.8522 | 18.0133 | 4.982 |
| automl | 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 |
| | 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 |
| neuralnet | 40. slr | 2.8881 | 4.3263 | 1.4382 | 3.1765 | 14.4615 | 0.440 |
| | 39. sag 36. backprop | 2.2972 2.9109 | 41.6253 3.4962 | 39.3281 0.5853 | 36.1679 2.6743 | 91.5205 11.9971 | 7.138 0.622 |
| | | | | | | | |
| | 28. adamax 27. adam | 2.5783 2.8614 | 3.1920 3.0075 | 0.6137 0.1461 | 2.5827 2.3994 | 8.6394 8.8657 | 6.082 3.620 |
| | 29. nadam | 5.2915 | 12.2499 | 6.9584 | 9.8464 | 27.3131 | 3.166 |
| keras | 26. adagrad | 6.5047 | 6.7324 | 0.9384 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 |
| | 2. ADAPTgdwm | 14.8661 | 28.9286 | 14.0625 | 15.0901 | 75.7312 | 0.084 |
| AMORE | 1. ADAPTgd | 12.5180 | 28.6849 | 16.1669 | 23.0898 | 63.3445 | 0.050 |
| | 4. BATCHgdwm 3. BATCHgd | 12.0720 12.0830 | 12.5131 12.6864 | 0.4411 0.6034 | $10.6879 \\ 10.8841$ | $26.8772 \\ 27.5733$ | 1.724 1.694 |
| minpack.lm | 33. default | 2.2329 | 2.2329 | 0.0004 | 1.7383 | 6.9429 | 0.068 |
| paoniiii | 6. rmsprop | 5.5210 | 8.5210 | 3.0000 | 7.0532 | 20.1249 | 0.076 |
| ANN2 | 5. adam | 2.7029 | 9.5851 | 6.8822 | 7.9902 | 22.2599 | 0.070 |
| | 7. sgd | 11.0994 | 11.9128 | 0.8134 | 10.0259 | 25.8843 | 0.080 |
| | 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 |
| deepdive | 18. momentum | 16.2557 | 16.2557 | 0.0000 | 13.0878 | 49.2409 | 6.236 |
| deepdive | 17. gradientDescent | 23.6597 | 23.6597 | 0.0000 | 19.1988 | 57.7174 | 6.084 |
| | | 2 | | | | | |
| snnR | 54. default | 11.6175 | 11.6175 | 0.0000 | 9.5749 | 25.9147 | 0.038 |
| | | 11.6175 17.0430 37.3986 | 11.6175 18.7830 490.0535 | 0.0000 1.7400 452.6549 | 9.5749 15.4373 426.0995 | 25.9147 50.7429 1516.4503 | 0.038 0.000 0.010 |

Table 10: Result for uGauss2

| Do also mo | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|----------------|----------------------------------|--------------------|-------------------------|-----------------|-------------------|-------------------|----------------|
| Package | 41. default | | | | | | |
| nlsr | | 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 |
| | 56. BFGS 57. CG | 2.3571 3.5928 | 2.3654 6.3016 | 0.0083 2.7088 | 1.8640 4.7543 | 7.5013 17.8412 | 0.792 34.308 |
| validann | 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 |
| ${ m traineR}$ | 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 14. Rprop | 2.4041 11.7899 | 3.1503 17.6638 | 0.7462 5.8739 | 2.3988 12.7742 | 10.7996 39.4495 | 2.320 5.810 |
| Cadence | 13. psoptim | 11.1566 | 15.4210 | 4.2644 | 12.7742 | 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 |
| <u> </u> | 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 |
| DONING | 47. BackpropChunk | 3.2955 | 4.7181 | 1.4226 | 3.6073 | 15.4886 | 0.332 |
| RSNNS | 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 |
| _ | 8. adam | 8.1454 | 8.6420 | 0.4966 | 6.1349 | 30.0687 | 4.952 |
| automl | 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 |
| | 38. rprop+ | 3.6133 3.5904 | 8.6404 4.4020 | 5.0271 | 6.1594 3.4777 | 25.2448 | 0.064 0.080 |
| neuralnet | 37. rprop- 40. slr | 3.5678 | $\frac{4.4020}{3.7435}$ | 0.8116 0.1757 | 2.7163 | 14.1560 14.9299 | 0.080 |
| neur amet | 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 |
| | 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 |
| keras | 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 |
| | 2. ADAPTgdwm | 4.3864 | 10.4646 | 6.0782 | 6.6054 | 38.5720 | 0.068 |
| AMORE | 1. ADAPTgd | 7.4794 | 8.1969 | 0.7175 | 6.0059 | 23.9130 | 0.054 |
| | 4. BATCHgdwm 3. BATCHgd | 9.2190 9.1582 | 9.4697 9.7638 | 0.2507 0.6056 | 6.9325 7.1783 | 27.9676 28.5231 | 1.578 1.552 |
| minpack.lm | 33. default | 2.9795 | 2.9795 | 0.0000 | 2.3890 | 9.0540 | 0.050 |
| | 6. rmsprop | 3.5637 | 4.2355 | 0.6718 | 3.2536 | 15.9291 | 0.100 |
| ANN2 | 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 |
| | 16. adam | 16.8843 | 16.8843 | 0.0000 | 11.6361 | 46.6218 | 0.618 |
| deepdive | 19. rmsProp | 18.3426 | 18.3426 | 0.0000 | 12.6957 | 49.5614 | 0.620 |
| = | 18. momentum 17. gradientDescent | 28.8104 28.8118 | 28.8104 28.8118 | 0.0000 0.0000 | 25.1756 25.1770 | 67.8020 67.7823 | 6.176 5.934 |
| snnR | 54. default | 8.8419 | 9.4678 | 0.6259 | 6.9147 | 30.1105 | 0.044 |
| elmNNRcpp | 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 |

| 1.11 | Result | for | ${\bf dataset}$ | uGauss3 | |
|------|--------|-----|-----------------|---------|--|
| | | | | | |

Table 11: Result for uGauss3

| | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|--------------------------------|--|--|--|--|---|--|--|
| nlsr | 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 |
| | 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 |
| validann | 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 |
| Machine Shop | 32. default | 2.3086 | 3.1576 | 0.8490 | 2.4940 | 9.7409 | 0.034 |
| $_{ m traineR}$ | 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 |
| manmin | 34. BFGS | 2.9135 | 3.5782 | 0.6647 | 2.8497 | 10.8707 | 0.220 |
| monmlp | 35. Nelder-Mead | 5.8001 | 7.3161 | 1.5160 | 5.7523 | 20.8098 | 0.424 |
| | 12. optim | 2.4116 | 2.8622 | 0.4506 | 2.2233 | 7.8710 | 2.334 |
| CaDENCE | 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 |
| h 2 o | 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 |
| | 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 |
| RSNNS | 47. BackpropChunk | 2.9280 | 3.8323 | 0.9043 | 3.0061 | 11.0342 | 0.320 |
| COTTIO | 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 50. Quickprop | 6.7104 27.8595 | 9.7422 28.8119 | 3.0318 0.9524 | 7.6756 22.8776 | 23.2263 59.8157 | 3.274 3.518 |
| | 8. adam | 3.1214 | 3.4986 | 0.3772 | 2.7250 | 9.7689 | 4.984 |
| automl | 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 |
| | 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 |
| neuralnet | 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 |
| | 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 |
| keras | 26. adagrad | 3.4760 | 4.8342 | 1.3582 | 3.7910 | 14.2616 | 13.448 |
| | 25. adadelta 31. sgd | 3.9293 4.8610 | 4.3921 5.1138 | 0.4628 0.2528 | 3.3906 3.9761 | 13.1185 15.1244 | 19.964 5.274 |
| | 30. rmsprop | 5.4568 | 6.4457 | 0.2328 | 5.4036 | 15.1244 | 1.890 |
| | | | F 1070 | 0.6421 | 3.6709 | 20.0320 | 0.080 |
| | 2. ADAPTgdwm | 4.4658 | 5.1079 | | | 12.5672 | 0.046 |
| AMORE | 1. ADAPTgd | 4.4658 4.7958 | 4.8043 | 0.0085 | 3.9113 | 12.3072 | 0.046 |
| AMORE | 1. ADAPTgd 4. BATCHgdwm | 4.7958 5.0868 | 4.8043 5.2355 | $0.0085 \\ 0.1487$ | 4.1127 | 14.7918 | 1.566 |
| | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd | 4.7958 5.0868 5.0863 | 4.8043 5.2355 5.2682 | 0.0085 0.1487 0.1819 | 4.1127 4.1337 | 14.7918 14.8772 | 1.566 1.556 |
| | 1. ADAPTgd 4. BATCHgdwm | 4.7958 5.0868 | 4.8043 5.2355 | $0.0085 \\ 0.1487$ | 4.1127 | 14.7918 | 1.566 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop | 4.7958 5.0868 5.0863 3.1472 2.9727 | 4.8043 5.2355 5.2682 3.1472 3.2852 | 0.0085 0.1487 0.1819 0.0000 0.3125 | 4.1127 4.1337 2.4837 2.5929 | 14.7918 14.8772 9.7293 9.6420 | 1.566 1.556 0.040 0.082 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 | 4.1127 4.1337 2.4837 2.5929 2.8900 | 14.7918 14.8772 9.7293 9.6420 10.5979 | 1.566 1.556 0.040 0.082 0.082 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 | 1.566 1.556 0.040 0.082 0.082 0.082 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 10.0466 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 10.0466 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 7.3484 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 31.6838 | 1.566 1.556 0.040 0.082 0.082 0.080 0.624 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam 19. rmsProp | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 10.0466 20.7977 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 10.0466 20.7977 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 0.0000 0.0000 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 7.3484 15.4531 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 31.6838 49.0396 | 1.566 1.556 0.040 0.082 0.082 0.080 0.624 0.622 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam 19. rmsProp 18. momentum | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 10.0466 20.7977 32.2413 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 10.0466 20.7977 32.2413 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 0.0000 0.0000 0.0000 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 7.3484 15.4531 27.7055 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 31.6838 49.0396 70.2077 | 1.566 1.556 0.040 0.082 0.082 0.080 0.624 0.622 6.146 |
| AMORE minpack.lm ANN2 deepdive | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam 19. rmsProp 18. momentum 17. gradientDescent | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 10.0466 20.7977 32.2413 32.2441 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 10.0466 20.7977 32.2413 32.2441 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 0.0000 0.0000 0.0000 0.0000 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 7.3484 15.4531 27.7055 27.7063 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 31.6838 49.0396 70.2077 70.1972 | 1.566 1.556 0.040 0.082 0.082 0.080 0.624 0.622 6.146 5.946 |
| minpack.lm | 1. ADAPTgd 4. BATCHgdwm 3. BATCHgd 33. default 6. rmsprop 5. adam 7. sgd 16. adam 19. rmsProp 18. momentum | 4.7958 5.0868 5.0863 3.1472 2.9727 3.1354 4.8318 10.0466 20.7977 32.2413 | 4.8043 5.2355 5.2682 3.1472 3.2852 3.6437 4.8821 10.0466 20.7977 32.2413 | 0.0085 0.1487 0.1819 0.0000 0.3125 0.5083 0.0503 0.0000 0.0000 0.0000 | 4.1127 4.1337 2.4837 2.5929 2.8900 3.8567 7.3484 15.4531 27.7055 | 14.7918 14.8772 9.7293 9.6420 10.5979 14.4928 31.6838 49.0396 70.2077 | 1.566 1.556 0.040 0.082 0.082 0.080 0.624 0.622 6.146 |

| 1.12 | Result | for | ${\bf dataset}$ | uNeuroOne | |
|------|--------|-----|-----------------|-----------|--|
| | | | | | |

Table 12: Result for uNeuroOne

| Package | Algorithm | RMSE min | RMSE median | RMSE D51 | MAE median | WAE median | Time mea |
|--------------------------|---------------------------------|-----------------|-----------------|-----------------|-----------------|-----------------|----------------|
| 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 |
| | 56. BFGS | 0.2830 | 0.2830 | 0.0000 | 0.2313 | 0.5675 | 0.104 |
| validann | 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 |
| Machine Shop | 32. default | 0.2830 | 0.2830 | 0.0000 | 0.2313 | 0.5675 | 0.010 |
| $\operatorname{traineR}$ | 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 50. Quickprop | 0.6867 0.5304 | 0.6888 0.5304 | 0.0021 0.0000 | 0.5629 0.4235 | 1.6534 1.2829 | 0.788 0.764 |
| automl | 8. adam | 0.2844 | 0.2895 | 0.0051 | 0.2378 | 0.6469 | 1.214 |
| | 9. RMSprop | 0.2842 | 0.2888 | 0.0031 | 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 |
| | 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 |
| neuralnet | 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 |
| | 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 |
| keras | 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 30. rmsprop | 0.2901 0.3042 | 0.2922 0.3629 | 0.0021 0.0587 | 0.2410 0.3049 | 0.5769 0.7486 | 3.468 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 |
| AWURE | 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 |
| | 6. rmsprop | 0.2904 | 0.2912 | 0.0008 | 0.2376 | 0.6015 | 0.008 |
| ANN2 | 5. adam | 0.3082 | 0.3485 | 0.0403 | 0.2776 | 0.7493 | 0.008 |
| deepdive | 7. sgd | 0.3069 | 0.3088 | 0.0019 | 0.2535 | 0.6226 | 0.010 |
| | 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 |
| | - 4 1 0 1: | 0.6793 | 0.6793 | 0.0000 | 0.5564 | 1.6288 | 0.004 |
| snnR | 54. default | 0.0793 | 0.0.00 | | | | |
| snnR elmNNRcpp | 54. default 21. extremeML | 0.8650 | 0.9526 | 0.0876 | 0.7905 | 2.2943 | 0.000 |

| 1.13 Score | probabilities |
|------------|---------------|
|------------|---------------|

Score probabilities over 12 packages

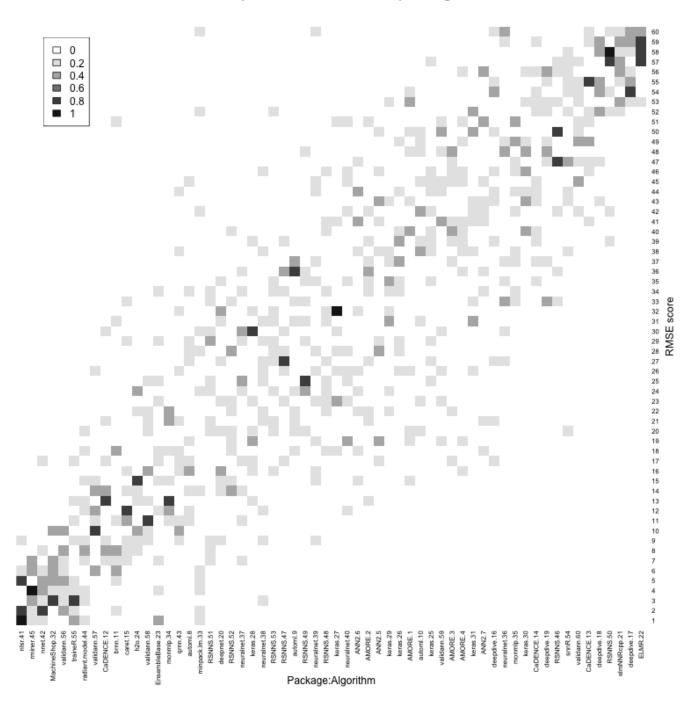


Figure 1: Score probabilities of package:algorithm

2 Additionnal materials on the large dataset bWoodN1 for TOP-10 packages

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; time in seconds.

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 jth explanatory variable are respectively computed at x-value x as

$$\bar{y}_{j}^{emp}(x) = \frac{1}{n_{x}} \sum_{i=1}^{n} y_{i} 1_{r(x_{i,j})=x}, \ \bar{y}_{j}^{pred}(x) = \frac{1}{n_{x}} \sum_{i=1}^{n} \hat{y}_{i} 1_{r(x_{i,j})=x}, \ n_{x} = \sum_{i=1}^{n} 1_{r(x_{i,j})=x},$$

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.

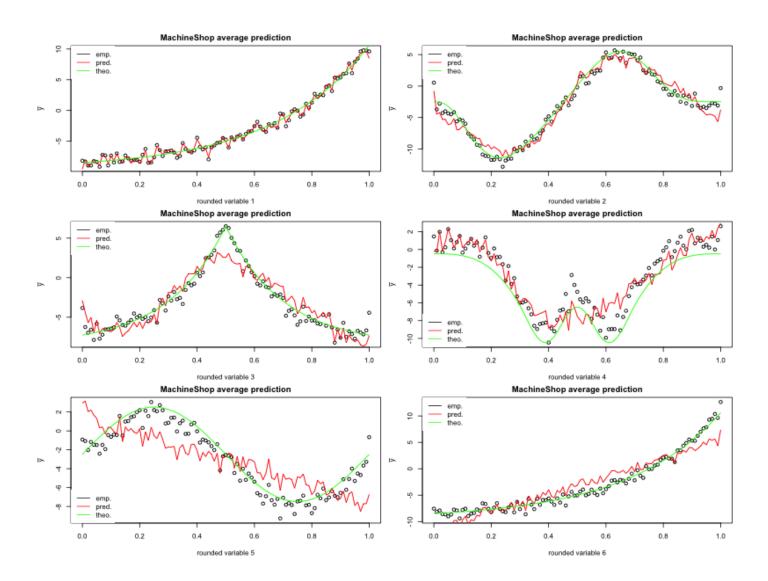


Figure 2: Average predicted mean per explanatory variable for MachineShop

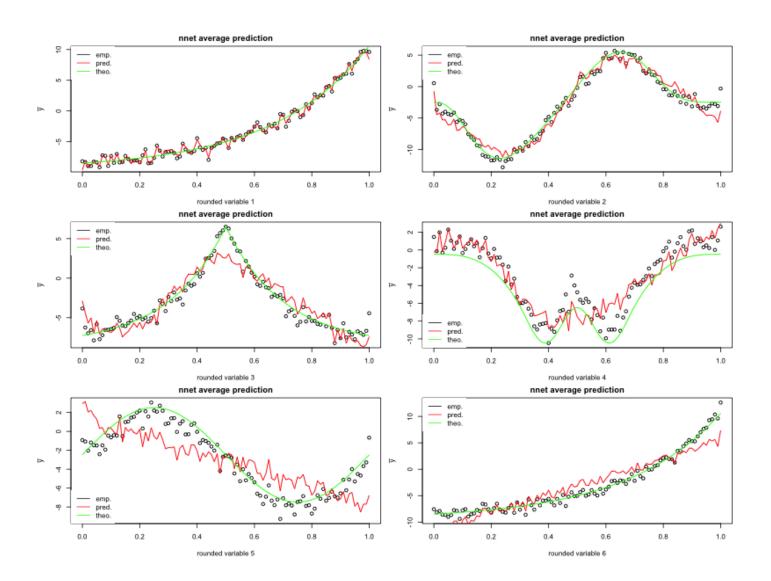


Figure 3: Average predicted mean per explanatory variable for nnet

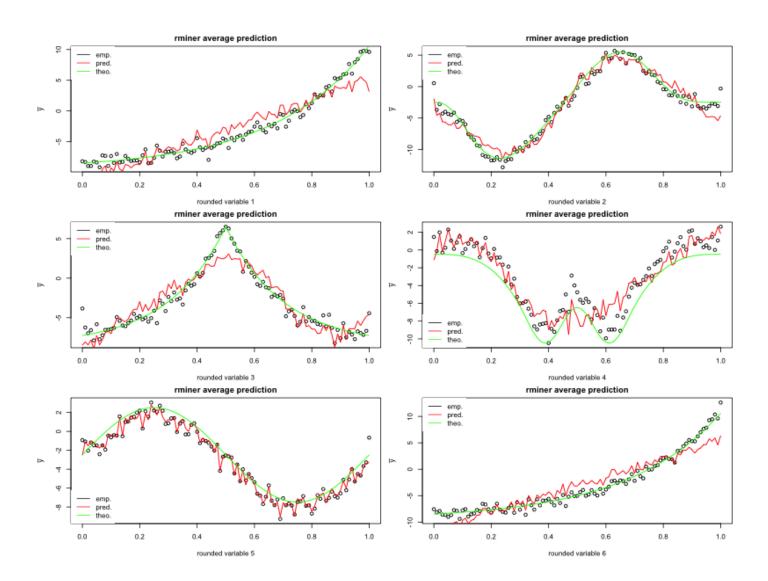


Figure 4: Average predicted mean per explanatory variable for rminer

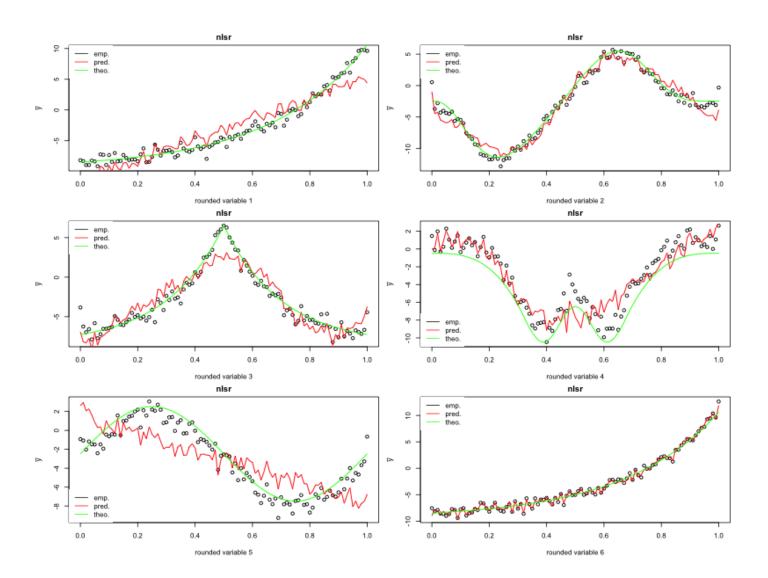


Figure 5: Average predicted mean per explanatory variable for ${\tt nlsr}$

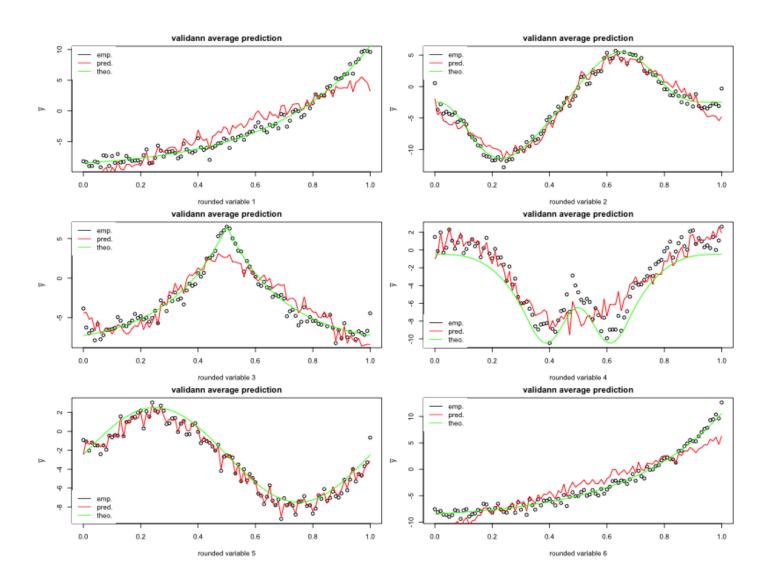


Figure 6: Average predicted mean per explanatory variable for validann