A review of R neural network packages (with NNbenchmark): accuracy and ease of use

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Abstract

In the last three decades, neural networks (NN) have evolved from an academic topic to a common scientific computing tool. CRAN currently hosts approximately 80 packages in May 2020 involving neural network modeling, some offering more than one algorithm. However, to our knowledge, there is no comprehensive study which checks the accuracy, the reliability and the ease-of-use of those NN packages.

In this paper, we attempted to test this rather large number of packages against a common set of datasets with different levels of complexity, and to benchmark and rank them with certain metrics.

Restricting our evaluation to regression algorithms applied on the one-hidden layer perceptron and ignoring those for classification or other specialized purposes, there were approximately 60 `package:algorithm` pairs left to test. The criteria used in our benchmark were: (i) the accuracy, i.e. the ability to find the global minima on 13 datasets, measured by the Root Mean Square Error (RMSE) in a limited number of iterations; (ii) the speed of the training algorithm; (iii) the availability of helpful utilities; (iv) and the quality of the documentation.

We have attempted to give a score for each evaluation criterion and to rank each `package:algorithm` pair in a global table. Overall, 15 pairs are considered accurate and reliable and can be recommended for daily usage. Most others should be avoided as they are either less accurate, too slow, too difficult to handle, or have poor or no documentation.

To carry out this work, we developed various codes and templates, as well as the NNbenchmark package used for testing. This material is available at https://akshajverma.com/NNbenchmarkWeb/index.html and https://github.com/pkR-pkR/NNbenchmark, and can be used to verify our work and, we hope, improve both packages and their evaluation. Finally, we provide some hints and features to guide the development of an idealized neural network package for R.

Introduction

The R Project for Statistical Computing by (R Core Team, 2020), as any opensource platform, relies on its contributors to keep it up to date. Neural networks (NN), inspired on the brain's own connections system, are a class of models in the growing field of machine learning for which R has a number of tools. During the last 30 years, neural networks have evolved from an academic topic to a common tool in scientific computing. Previously, neural networks were often considered theoretically instead of pragmatically, partly because the algorithms used were computationally demanding.

As a convenience in the general conversation, the same term is used in a generic manner for different model structures and applications: multilayer perceptron for regression, multilayer perceptron for classification, multilayer perceptron for specialized applications, recurrent neural network for autoregressive time series, convolutional neural networks for dimension reduction and pattern recognition, and even deep neural networks for image or voice recognition. Most of the above types of neural networks can be found in R packages hosted on CRAN but without any warranty about the accuracy or the speed of computation. This is an issue as many slow or poor algorithms are available in the literature and hence poor packages are implemented on CRAN.

A neural network algorithm requires complicated calculations to improve the model

control parameters. As with other optimization problems, the gradient of the chosen cost function that indicates the lack the model's suitability is sought. This lets us improve the model by changing the parameters in the negative gradient direction. Parameters for the model are generally obtained using part of the available data (a training set) and tested on the remaining data. Modern software allows much of this work, including approximation of the gradient, to be carried out without a large effort by the user.

The training process can generally be made more efficient if we can also approximate second derivatives of the cost function, allowing us to use its curvature via the Hessian matrix. There are a large number of approaches, of which quasi-Newton algorithms are perhaps the most common and useful. Within this group, methods based on the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm for updating the (inverse) Hessian approximation provide several well-known examples. In conducting this study, we believed that these second-order algorithms would perform better than first-order methods for fit-in-memory datasets.

Regardless of our belief, we wished to be able to conduct a thorough examination of these training algorithms in R. There are many packages, but barely any information to allow comparison. Our work, reported here, aims to provide a framework for benchmarking neural network packages. We restrict our examination to packages for R, and in this report focus on those that provide neural networks of the perceptron type, that is, one input layer, one normalized layer, one hidden layer with a nonlinear activation function that is usually the hyperbolic tangent $\tanh()$, and one output layer.

Moreover, We restricted our evaluation to one-hidden layer perceptron for regression and ignored those for classification or other specialized purposes. The criteria used in our benchmark were: (i) the accuracy, i.e. the ability to find the global minima on 13 datasets in a limited number of iterations; (ii) the speed of the training algorithm; (iii) the availability of helpful utilities; (iv) and the quality of the documentation.

Neural Networks: the perceptron

Here, we give a short description of the one hidden layer perceptron. As the "layer" term suggests it, some terms come from the representation of graphs whereas some other terms come from the traditional literature on nonlinear models.

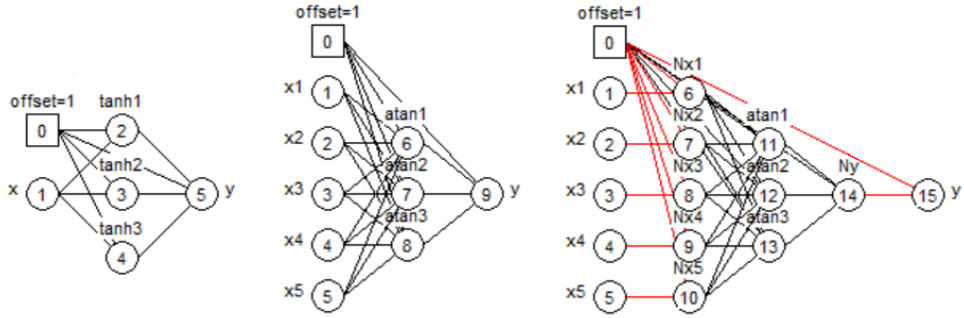
Using the graph description, a one-hidden layer neural network is made of 3 parts: (i) the layer of the input(s), (ii) the hidden layer which consists of independent neurons, each of them performing two operations: a linear combination of the inputs plus an offset, then a nonlinear function applied on this linear combination. (iii) the layer of the output(s) which is a linear combination of the output of the nonlinear functions in the hidden layer.

The nonlinear function used in the hidden layer must have the following four properties: continuous, differentiable, monotonic, bounded. The logistic (invlogit), the hyperbolic tangent (tanh) and the arctangent (atan) functions are the usual candidates. The above description has a simple mathematical equivalence. Let us give two examples.

The model $y = a_1 + a_2 \times \tanh(a_3 + a_4 \times x) + a_5 \times \tanh(a_6 + a_7 \times x) + a_8 \times \tanh(a_9 + a_{10} \times x)$ describes a neural network (Fig. 1a) with one input, three hidden neurons, one output model where x is the input, $\tanh()$ is the activation function, y is the output and $a_1, \ldots, a_{10}$ are the parameters.

The model $y = a_1 + a_2 \times \text{atan}(a_3 + a_4 \times x_1 + a_5 \times x_2 + a_6 \times x_3 + a_7 \times x_4 + a_8 \times x_5) + a_9 \times \text{atan}(a_{10} + a_{11} \times x_1 + a_{12} \times x_2 + a_{13} \times x_3 + a_{14} \times x_4 + a_{15} \times x_5) + a_{16}\text{atan}(a_{17} + a_{18} \times x_1 + a_{19} \times x_2 + a_{20} \times x_3 + a_{21} \times x_4 + a_{22} \times x_5)$ describes a neural network (Fig. 1b) with five inputs, three hidden neurons, one output model where x is the input, $\text{atan}()$ is the activation function, y is the output and $a_1, \ldots, a_{22}$ are the parameters.

In order to get large gradients at the first steps of the training algorithm, it is recommended to use normalized inputs and normalized outputs (Fig. 1c), odd functions like the hyperbolic tangent function or the arctangent function, and small random values to initialize



(a) NN 1-3-1 **(b)** NN 5-3-1 **(c)** NN 5-5N-3-1N-1

Figure 1: Three neural networks

the parameters, for instance extracted from a centered Gaussian $\mathcal{N}(0, 0.1)$ distribution. Such good practices help find good local minima and possibly the global minimum.

The dataset used for the training is assumed to have a number of rows much larger than the number of parameters. While "much larger" is subject to discussion, values of 3 to 5 are generally accepted (in experimental design, some iterative strategies start with a dataset having a number of distinct experiments equal to 1.8 times the number of parameters and then increase the number of experiments to fine tune the model).

It is rather clear from the mathematical formula above that neural networks of perceptron type are nonlinear models and require for their parameter estimation some training algorithms that can handle (highly) nonlinear models. Indeed, the intrinsic and parametric curvatures of such models are usually very high and, with so many parameters, the Jacobian matrix might exhibit some colinearities between its columns and become nearly singular. As a result, appropriate algorithms for such `dataset::model` pairs are rather limited and well-known. They pertain to the class of second-order algorithms such as the BFGS algorithm which is Quasi-Newton in how it updates the approximate inverse Hessian or the Levenberg-Marquardt algorithm which stabilizes the Gauss-Newton search direction at every iteration.

Unfortunately, due to some educative tools on the backpropagation, and an initial literature on the gradient in the early researches and more recently on the "deep neural networks" that manipulate ultra-large models with hundreds or thousands parameters (and sometimes more parameters than examples in the datasets), many papers emphasize the use of first-order gradient algorithms. Therefore, many R packages have implemented such algorithms. In the case of the perceptron, we contend this is an error, and provide evidence to that effect in this paper. We refer interested readers to (Tan and Lim, 2019) for a review of second-order algorithms for neural networks.

Methodology

Convergence and termination

Most of the `package:algorithm` pairs try to minimize the root mean squared error (RMSE) during the training step. Two exceptions are the **brnn** package which minimizes the RMSE plus the sum of the parameters (hence the name Bayesian Regularized Neural Network), and the **qrnn** package which performs quantile regression. For all packages, the datasets were learnt as a whole and without any weighting scheme to favour one part of the datasets. There was no validation subset or test subset as the purpose of our study is just to verify the ability to reach good minima.

When training neural networks, we attempt to tune a set of hyperparameters so that the root mean squared error (RMSE) is minimized. When our method for such adjustment can no longer reduce the RMSE, we say that the given algorithm **terminated**. We consider the

method to have **converged** when termination is not due to some exceptional situation and the final RMSE value is relatively small[1]. In practice, some algorithms require that we stop the optimization process in exceptional situations (e.g., a divide by zero), or a pre-set limit on the number of steps or a maximum elapsed time is reached.

More precisely, second-order algorithms are all set to a maximum of 200 iterations. On the other hand, first-order algorithms were set to several values, depending on how well and how fast they converged: `maxit1storderA=1000` iterations, `maxit1storderB=10000` iterations, and `maxit1storderC=100000` iterations. The full list of the maximum iteration number per `package:algorithm` is given in Table 4 in Appendix D. It can be seen that we were unable to completely harmonize the hyperparameters as an appropriate learning rate differed between packages, despite the algorithm being similarly named.

Performance

We measure **performance** primarily by relative computing time between methods on a particular computing platform. We could also count measures of iterations, function evaluations or similar quantities that indicate the computing effort. We note that differences in machine architecture and in the attached libraries (e.g., BLAS choices for R) will modify our measures. We are putting our tools on a Github repository so that further evaluation can be made by ourselves and others as hardware and software evolves.

The resulting files in our repository were mostly generated by one of us (SM) on a Windows system build 10.0.18362.752 with an i7-8750H CPU, an Intel(R) UHD Graphics 630 and NVIDIA GeForce GTX 1060 chip, and 16 GB of RAM. Tests have also been performed on other platforms: computation times were reasonably similar.

Phase 1 - Preparation of benchmark datasets and selection of packages

Datasets

A non-iterative calculation such as Ordinary Least Squares cannot generally be used to model all the datasets in our evaluation set. Varying levels of difficulty in modeling the different data sets are intended to allow us to further classify different algorithms and the packages that implement them. As we focus on regression analysis, we select only datasets where the response variable is real-valued.

Sonja Surjanovic and Derek Bingham of Simon Fraser University created a useful website from which three of the multivariate datasets were drawn. We note the link, name and difficulty level of the three datasets:

- `http://www.sfu.ca/~ssurjano/fried.html`: `mFriedman`, Friedman's dataset, published in (Friedman, 1991) (average difficulty),
- `http://www.sfu.ca/~ssurjano/detpep10curv.html`: `mDette`, Dette's dataset, published in (Dette and Pepelyshev, 2010) (medium difficulty),
- `http://www.sfu.ca/~ssurjano/ishigami.html`: `mIshigami`, Ishigami's dataset, published in (Ishigami and Homma, 1990) (high difficulty).

The last multivariate dataset, `mRef153`, was used to teach neural networks at ESPCI (The City of Paris Industrial Physics and Chemistry Higher Educational Institution, `https://www.neurones.espci.fr/`) from 2003 to 2013 and is available in the proprietary software Neuro One at `http://www.inmodelia.com/software.html`. This dataset presents some interesting non-linear features.

`uDreyfus1` is a pure neural network which has no error. This can make it difficult for algorithms that assume an error exists. `uDreyfus2` is `uDreyfus1` with errors. Both are

[1]We do not choose the mean absolute error (MAE) for overall ranking nor for convergence testing as there is a lack of consensus in the literature, see e.g. (Willmott and Matsuura, 2005; Chai and Draxler, 2014).

Table 1: Datasets' summary

Dataset	Row nb.	Input nb.	Neuron nb.	Param. nb.
Multivariate				
mDette	500	3	5	26
mFriedman	500	5	5	36
mIshigami	500	3	10	51
mRef153	153	5	3	22
Univariate				
uDmod1	51	1	6	19
uDmod2	51	1	5	16
uDreyfus1	51	1	3	10
uDreyfus2	51	1	3	10
uGauss1	250	1	5	16
uGauss2	250	1	4	13
uGauss3	250	1	4	13
uNeuroOne	51	1	2	7

considered to be of low difficulty and used to teach neural networks at ESPCI from 1991 to 2013. `uDmod1` and `uDmod2` are univariate datasets with few observations but exhibit high nonlinear patterns and prove to be very challenging datasets. The parameters are highly correlated and singular Jacobian matrices often appear.

Three of the univariate datasets were taken from the US National Institute for Standards and Technology (NIST) website: https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml. Namely `uGauss1`, `uGauss2` and `uGauss3` published in (Rust, 1996a,b,c, resp.) created by NIST to assess nonlinear least squares regressions are of low, low and medium difficulty respectively.

The last univariate dataset, `uNeuroOne`, was also used to teach the same course and is now available in the proprietary software Neuro One at http://www.inmodelia.com/software.html. In Table 1, we list some information on each dataset used in the first round of our analysis: the number of neurons and the induced parameter number are available in the last two columns.

To build the final result table, we selected all four multivariate datasets and 4 out of the 8 univariate datasets so that the overall score does not overly weight the univariate datasets. Furthermore the 2019 GSoC code uses all 12 datasets. Our package still allows access to all 12 datasets.

Finally, we also consider a Simon Wood test dataset, named `bWoodN1`, used in (Wood, 2011) for benchmarking generalized additive models. Precisely, we consider a generation of Gaussian random variates Y_i, $i = 1, \ldots, n$ with the mean μ_i defined as

$$\mu_i = 1 + f_0(x_{i,0}) + f_1(x_{i,1}) + f_2(x_{i,2}) + f_3(x_{i,3}) + f_4(x_{i,4}) + f_0(x_{i,5})$$

and standard deviation $\sigma = 1/4$ where f_j are Simon Wood's smooth functions defined in Appendix B, $x_{i,j}$ are uniform variates and $n = 20,000$. `bWoodN1` will only be used in the second round of our analysis when the TOP5 packages will be further analyzed with 5 neurons resulting in 41 parameters.

Whatever the source of the test datasets, there are all available in **NNbenchmark**, so that maintainers or users can perform the analysis.

Packages

Using **RWsearch** (Kiener, 2020), we sought to automate the process of searching for neural network packages. All packages that have "neural network" as a keyword in the package title or in the package description were included. In May 2020, around 80 packages fall into this category. Packages **nlsr**, **minpack.lm**, **caret** were added because the former 2 are important implementations of second-order algorithms while the latter is the first cited meta package in the CRAN task view for machine learning, https://CRAN.R-project.org/view=MachineLearning, as well as a dependency for some of the other packages tested. Restricting to regression analysis left us with 49 `package:algorithm` pairs in 2019 and 60 `package:algorithm` pairs in 2020.

Phase 2 - Review of packages and development of a benchmarking template

Basically, each package was inspected 3 times. Each assessment is described in detail below.

1. The decision to exclude or include

From documentation and example code, we learned that not all packages selected by the automated search fit the scope of our research. Some have no function to generate neural networks. Others were not regression neural networks of the perceptron type or were only intended for very specific purposes. Depending on the package, this could be decided as easily as looking at the DESCRIPTION file or having to go through the process of running some code and seeing the results.

2. Templates for testing accuracy and speed

Benchmarking with the template that was developed in 2019 and encapsulated in the functions of 2020, keeping notes of whether or not the package was easy to use.

As we inspected the packages, we developed a template for benchmarking. The structure of this template (for each package) is as follows:

1. Set up the test environment - loading of packages, setting working directory and options;
2. Summary of tested datasets;
3. Loop over datasets:
    a. setting parameters for a specific dataset,
    b. selecting benchmark options,
    c. training a neural network with a tuned function for each package,
    d. calculation of convergence metrics (RMSE, MAE, WAE)[2],
    e. plot each training over one initial graph, then plot the best result,
    f. add results to the appropriate existing record (*.csv file) and
    g. clear the environment for next loop.
4. Clearing up the environment for the next package. It is optional to print warnings.

To simplify this process, we developed tools in the **NNbenchmark** package, of which the first version was created as part of GSoC 2019. In GSoC 2020, 3 functions encapsulating the template were added that had been made generic with an extensive use of the very helpful `do.call` function from **base** package:

1. In `trainPredict_1mth1data` a neural network is trained on one dataset and then used for predictions, with several utilities. Then the performance of the neural network is exported, plotted and/or summarized.
2. `trainPredict_1data` serves as a wrapper function for `trainPredict_1mth1data` for multiple methods.
3. `trainPredict_1pkg` serves as a wrapper function for `trainPredict_1mth1data` for multiple datasets.

A function for the summary of accuracy and speed, `NNsummary`, was also added. The package repository is `https://github.com/pkR-pkR/NNbenchmark`, with package templates in `https://github.com/pkR-pkR/NNbenchmarkTemplates`.

An example of a call to `trainPredict_1pkg` is given in Appendix C.

3. Ease of use scoring

We define ease-of-use measures to rate NN packages on their user-friendliness. Based on our understanding of what a user may be required to know or do when using a neural network package, we consider: a measure for the availability of appropriate utility functions; a measure for (non-trivial) examples and sufficient documentation (well-written manual,

[2]We measure the quality of our model by RMSE, but the mean absolute error (MAE) and the worst absolute error (WAE) may help distinguish packages with close RMSE values. See Appendix A for definition of convergence metrics.

vignette(s)); and a measure to rate the clarity of the R call to fit a given neural network. Our rating is as follows.

1. Utilities in R to deal with NN - maximum of 1 star
    a. a predict function exists = 0.5 stars
    b. scaling capabilities exist = 0.5 stars
2. Sufficient and reliable documentation - maximum of 2 stars
    a. the existence of useful and relevant example(s)/vignette(s)
        - clear, with regression = 1 star
        - unclear, examples use iris or are for classification only = 0.5 stars
        - no examples = 0 stars
    b. input/output is clearly documented, e.g., what values are expected and returned by a function
        - clear input and output = 1 star
        - only one is clear = 0.5 stars
        - both are not documented = 0 stars
3. User-friendly call to fit a NN
    a. simple one-line call or a single function = 2 stars
    b. multiple-lines call to a single function = 1 star
    c. multiple-lines call to many functions = 0 stars

Hence, to inform users about the usability of packages, the documentation ease-of-use measure ranges from 0 to 3 stars, while the utility and the R call from 0 to 2 stars.

Phase 3 - Collection of and analysis of results

Results collection

Looping over the datasets using each package template, we collected results in the relevant package directories in the templates repository. A large number of runs have been carried out in order to obtain the best result for every package.

Analysis

To rank how well and how fast a package converged, we developed the following method:

1. The results datasets are loaded into the R environment as one large list. The dataset names, `package:algorithm` names and all 10 run numbers, durations, and RMSE are extracted from that list.
2. For the duration score (DUR), the duration is averaged by dataset. 3 criteria for the RMSE score by dataset are calculated:
    a. The minimum value of RMSE for each `package:algorithm` as a measure of their best performance;
    b. The median value of RMSE for each `package:algorithm` as a measure of their average performance, without the influence of outliers;
    c. The spread of the RMSE values for each package which is measured by the difference between the median and the minimum RMSE (d51).
3. Then, the ranks are calculated for every dataset and the results are merged into one wide dataframe.
    a. The duration rank only depends on the duration;
    b. For minimum RMSE values, ties are decided by duration mean, then the RMSE median;

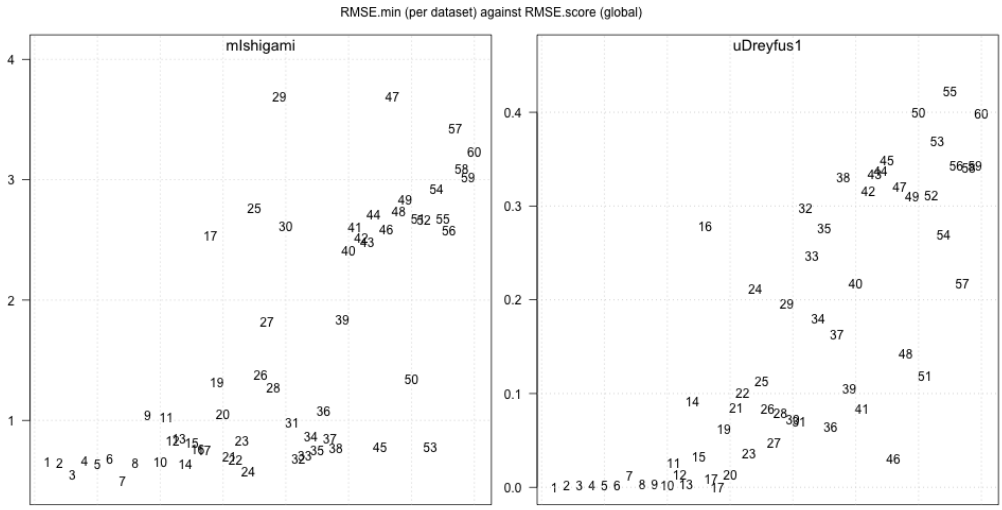


Figure 2: RMSE minimum value per package for `mIshigami` and `uDreyfus1` datasets

c. For median RMSE values, ties are decided by the RMSE minimum, then the duration mean;
d. The d51 rank only depends on itself.

4. A global score for all datasets is found by a sum of the ranks (of duration, minimum RMSE, median RMSE, d51 RMSE) of each `package:algorithm` for each dataset.
5. The final table is the result of ranking by the global minimum RMSE scores for each `package:algorithm`.

Results, discussion and recommendations

Table 2 gives the RMSE and time score per package and per algorithm. The full list of scores is given in Table 5 in Appendix C. We divide our analysis in two groups: packages implementing second-order algorithms and packages implementing first-order algorithms. Figure 2 shows the minimum RMSE value per `package:algorithm` for two datasets `mIshigami` and `uDreyfus1`, whereas Figure 3 displays the average computation time. The number on the x-level refers to the RMSE overall score of the package:algorithm given in Table 2 (last column), e.g., 8 refers to **validann**`:optim(CG)` which is a very slow algorithm.

Both figures show that a good overall score does not necessarily imply a good score on the two datasets under consideration. Furthermore, there is a break between the TOP10 `package:algorithm` and others in terms of RMSE value. Regarding computation time, we observe that some package:algorithms are very slow and poor RMSE, e.g. 41 corresponding to **AMORE**`:BATCHgd`. In the following, we first present the results for second-order algorithms, then low-order algorithms. Finally, we list the reasons for discareded packages.

Second-order algorithms

Of all approaches, the following second-order algorithms generally performed better in terms of convergence despite being limited to one fifth or fewer iterations than the first-order algorithms.

We note that 11 out of 15 of these `package:algorithms` use `optim` from **stats**. 2 of them, **CaDENCE**'s BFGS (Cannon, 2017a) and **validann**'s BFGS and L-BFGS-B (Humphrey, 2017), make the call directly. However, it is not clearly stated in **CaDENCE**'s documentation that optim's BFGS method has been chosen rather than one of the other four methods. Furthermore, the mention of Nelder-Mead in the documentation might suggest that `optim`'s

Table 2: Result from Tested Packages

	Individual rating				Global score	
Package	Util	Doc	Call	Algorithm	Time	**RMSE**
nlsr	*	****	**	41. NashLM	18	**1**
rminer	**	***	**	45. nnet_optim(BFGS)	12	**2**
nnet	*	***	**	42. optim (BFGS)	3	**3**
validann	*	****	**	56. optim(BFGS)	35	**4**
	*	****	**	57. optim(CG)	60	**8**
	*	****	**	58. optim(L-BFGS-B)	36	**15**
	*	****	**	59. optim(Nelder-Mead)	55	**45**
	*	****	**	60. optim(SANN)	20	**55**
MachineShop	*	***	*	32. nnet_optim(BFGS)	6	**5**
traineR	*	**	**	55. nnet_optim(BFGS)	4	**6**
radiant.model	**	**	**	44. nnet_optim(BFGS)	10	**7**
monmlp	**	***	**	34. optimx(BFGS)	26	**9**
	**	***	**	35. optimx(Nelder-Mead)	32	**47**
CaDENCE	**	***	**	12. optim(BFGS)	46	**10**
	**	***	**	14. Rprop	56	**51**
	**	***	**	13. pso_psoptim	54	**54**
h2o	**	**		24. first-order	51	**11**
EnsembleBase	*	*	**	23. nnet_optim(BFGS)	5	**12**
caret	**	***	**	15. avNNet_nnet_optim(BFGS)	17	**13**
brnn	**	****	**	11. Gauss-Newton	8	**14**
qrnn	**	***	**	43. nlm()	28	**16**
RSNNS	**	***	**	51. Rprop	24	**17**
	**	***	**	52. SCG	30	**18**
	**	***	**	53. Std_Backpropagation	22	**27**
	**	***	**	47. BackpropChunk	26	**29**
	**	***	**	48. BackpropMomentum	25	**30**
	**	***	**	49. BackpropWeightDecay	29	**31**
	**	***	**	46. BackpropBatch	43	**49**
	**	***	**	50. Quickprop	45	**57**
automl	*	***	**	8. trainwgrad_adam	50	**18**
	*	***	**	9. trainwgrad_RMSprop	47	**26**
	*	***	**	10. trainwpso	57	**43**
deepnet	*	***	**	20. BP	23	**18**
neuralnet	*	***	**	38. rprop+	19	**21**
	*	***	**	37. rprop-	21	**22**
	*	***	**	40. slr	31	**31**
	*	***	**	39. sag	41	**38**
	*	***	**	36. backprop	37	**50**
keras	**			28. adamax	48	**23**
	**			27. adam	42	**34**
	**			29. nadam	44	**36**
	**			26. adagrad	58	**37**
	**			25. adadelta	59	**40**
	**			31. sgd	48	**44**
	**			30. rmsprop	37	**52**
AMORE	*	***	*	2. ADAPTgdwm	16	**24**
	*	***	*	1. ADAPTgd	9	**35**
	*	***	*	4. BATCHgdwm	40	**39**
	*	***	*	3. BATCHgd	39	**41**
minpack.lm	*	***	**	33. Levenberg-Marquardt	15	**24**
ANN2	**	***	*	6. rmsprop	14	**28**
	**	***	*	5. adam	13	**33**
	**	***	*	7. sgd	11	**42**
deepdive	**	***	**	16. adam	32	**46**
	**	***	**	19. rmsProp	34	**53**
	**	***	**	18. momentum	53	**56**
	**	***	**	17. gradientDescent	52	**58**
snnR	**	**	**	54. SemiSmoothNewton	7	**48**
elmNNRcpp	**	***	**	21. ELM	1	**59**
ELMR	**	***	**	22. ELM	2	**60**

Note: Statistics over 10 runs.

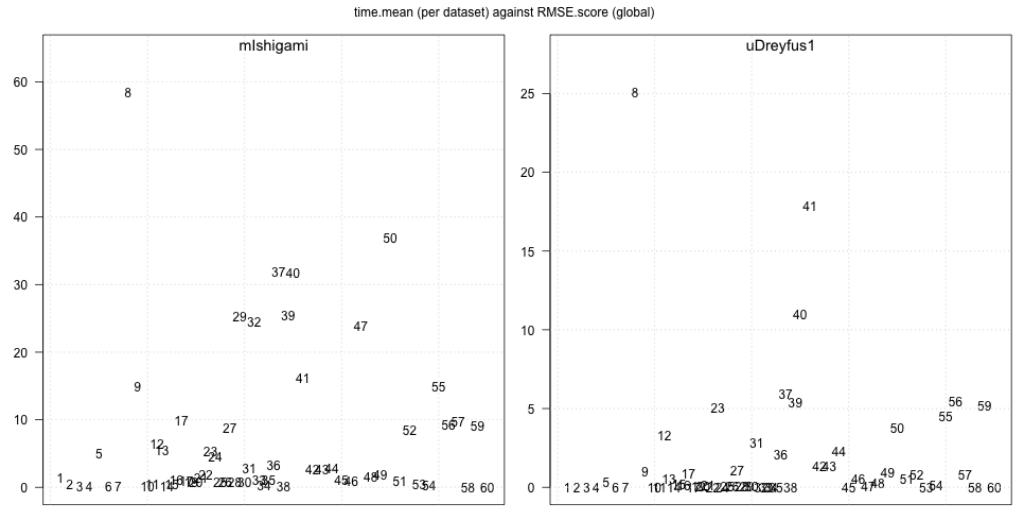


Figure 3: Average time value per package for `mIshigami` and `uDreyfus1`

Nelder-Mead method is used. Speed and variation between results for **CaDENCE** are also not as good as other packages that use `optim`. This could be because **CaDENCE** is intended for probabilistic nonlinear models with a full title of "Conditional Density Estimation Network Construction and Evaluation".

By contrast, **validann** is clearly a package that allows a user to use all optim's algorithms. **validann**::L-BFGS-B ranks mostly lower than **validann**::BFGS, despite the former method being more sophisticated. We believe this is due to our efforts to harmonize parameters, thereby under-utilizing the possibilities of the L-BFGS-B algorithm. Both **CaDENCE** and **validann**'s BFGS are outperformed by **nnet**, especially in terms of speed.

nnet (Ripley, 2020) differs from the two packages above because it uses the C code for BFGS (`vmmin.c`) from `optim` (converted earlier from Pascal) directly instead of calling `optim` from R. This may be what allows it to be faster, but limits the optimization to the single method. **nnet** is only beaten by the Extreme Learning Machine (ELM) algorithms in terms of speed. However, there is a larger variation between results (see the `RMSEd51` in Appendix C) in comparison to **validann**:BFGS. We believe the different default starting values are the cause of this. For instance, **nnet** uses a range of initial random weights of 0.7 while **validann** uses a value of 0.5. In spite of these results, the real reason most authors or users are likely to choose **nnet** is because it is included in the distributed base R and is even mentioned as the very first package in CRAN's task view for machine learning (`https://CRAN.R-project.org/view=MachineLearning`).

Our research found that 6 of the 11 packages tested that use `optim` do so through **nnet**. Moreover, approximately 8 packages for neural networks, though not tested, use **nnet**. The total number of **nnet** dependencies found through a search through the offline database of CRAN with **RWsearch** is 136 packages, although some might be using **nnet** for the multinomial log-linear models, not neural networks.

The packages that use **nnet** for neural networks are often meta packages with a host of other machine learning algorithms. **caret** (Kuhn, 2020), also mentioned in the taskview, boasts 238 methods with 13 different neural network packages, under a deceivingly simple name of "Classification and Regression Training". It has many pre-processing utilities available, as well as other tools.

EnsembleBase (Mahani and Sharabiani, 2016) maybe useful for those who wish to make ensembles and test a grid of parameters although the documentation is rather confusing. **MachineShop** (Smith, 2020) has 51 algorithms, with some additional information about the response variable types in the second vignette, functions for preprocessing and tuning, performance assessment, and presentation of results. **radiant.model** (Nijs, 2020) has an

unalterable maxit of 10000 in the original package. Perhaps the author thought this was reasonable as the algorithm, **nnet**, is quite fast. We changed this to harmonize the parameters. **rminer** (Cortez, 2020) is the only package dependent on **nnet** that ranks above **nnet** at number 2 for minimum RMSE, and even number 1 in some runs. It also ranks number 1 on the other accuracy measures (median RMSE, minimum MAE, minimum WAE) and is only behind **deepdive** and **minpack.lm** in terms of results that are consistent and do not vary (RMSEd51).

The difference is probably from the change of maximum allowable weights in **rminer** to 10000 from 1000 in **nnet**, which is also probably the reason its fits are slower. **traineR** (Rodriguez R., 2019) claims to unify the different methods of creating models between several learning algorithms.

It is worth noting is that **nnet** and **validann** do not have external normalization, which is especially recommended for **validann** . However, some of the packages dependent on **nnet** do have this capability and it is included in the scoring for ease of use. With **NNbenchmark**, this is done through setting `scale = TRUE` in the function `prepare.ZZ`. Note that use of scaling may complicate the application of constraints, so not be worth the effort for some users. Nevertheless, users might want scaling, or at least to have a clear explanation of the method chosen to center the variables. Scaling of both function and parameters is one of the features that **optimx** (Nash and Varadhan, 2020) incorporates, as some optimization algorithms can work significantly better on scaled problems (Nash, 2014).

Of all the packages, only **monmlp** (Cannon, 2017b) calls **optimx**. Since the calls are for BFGS and Nelder-Mead, they could do better to call `optim` directly, though the door is open to other optimization methods in **optimx**. However, the author, Alex J. Cannon who is also the author of **CaDENCE**, has created a package meant to fill a certain niche, namely for multi-layer perceptrons with optional partial monotonicity constraints. GAM-style effect plots are also an interesting feature. Another package by Cannon is **qrnn** (Cannon, 2019) which uses yet another algorithm: `nlm`, a "Newton-type" algorithm, from **stats**. Although it's performance is at the bottom of second-order algorithms, sometimes even being beaten by first-order algorithms, this could also be because of the intended use of the package compared to the tests here. **qrnn** is designed for quantile regression neural networks, with several options. Cannon has included automatic scaling for all 3 of his packages, as is clearly documented.

stats also includes `nls`, for nonlinear least squares, which defaults to an implementation of the second-order algorithm referred to as Gauss-Newton. However, in its documentation, `nls` warns against "zero-residual" or even small residual problems. (Nash, 2014, Section 6.4.1) This was one of the motivations for **nslr** (Nash and Murdoch, 2019). nlsr uses a variant (Nash, 1977) of the Levenberg-Marquardt algorithm versus the plain Gauss-Newton of `nls`, and modifies the relative offset convergence criterion to avoid a zero divide when residuals are small. **minpack.lm** (Elzhov et al., 2016) offers another Marquardt approach. Where **nlsr** is entirely in R, and also allows for symbolic or automatic derivatives (which are not relevant to the present study), **minpack.lm** uses compiled Fortran and C code for some important computations. Its structure is also better adapted to use features already available in `nls` that may be important for some uses.

However, despite the 2 packages ultimately performing well on all runs (capable of being in the top 3 for RMSE and not slow), there are some reasons why users might hesitate to choose them.

First, both require the full formula of the neural network including variables and parameters. Secondly, they require good starting values to achieve the best convergence. Notice that in Table 1, `minpack.lm` does not have a high rank. This is because we removed the random Gaussian start values we had originally used which means the default start values of `minpack.lm` were not appropriate for our datasets. We suspect **nlsr**'s performance on convergence would have similarly dropped if it was possible to use **nlsr** with no user-set starting values and the author's chosen default values were inadequate. `nls` deals with this by suggesting a companion function in **stats**, `selfStart`. Finally, both packages were able to find better minima when the dataset was scaled. With no starting values and no scaling,

`minpack.lm:nlsLM` fails on `uNeuroOne` but performance is better on Friedman & Ishigami datasets. On the other hand, with no start values and no scaling, it fails on everything but `mFriedman`, `mIshigami`, `uDmod2`, and the Dreyfus datasets. Similarly, there is also a notable drop in performance for **nlsr** without scaling on the Gauss datasets and `mRef153`. To conclude, both packages provide algorithms that are capable of doing well on our datasets, but may not be suitable for less experienced users. The vignettes for **nlsr** and earlier book (Nash, 2014) may be useful.

brnn (Rodriguez and Gianola, 2020) is an implementation of the Gauss-Newton algorithm in R that does not rely on `nls` or `nlm` from **stats**. Although it is well-documented and has good speed, **brnn**'s implementation of the Gauss-Newton algorithm still ranks below some of the previously mentioned BFGS and Levenberg-Marquardt tools in terms of its global minimum RMSE. We found 2 reasons that we believe to be the cause of this. First, its model uses one parameter fewer than the other algorithms. Only datasets `uDreyfus1` and `uDreyfus2` which are purely 3 hidden neurons ignore the first term. Second, **brnn** does not minimize the sum of squares of the errors but the sum of squares of the errors plus a penalty on the parameters. In certain circumstances – especially with an almost singular Jacobian matrix as with `mDette`, `mIshigami`, `mRef153`, `uGauss3`, and `uNeuroOne` – this will avoid issues with highly correlated parameters.

The only second-order algorithm which we are unable to recommended from the results of our research is **snnR** (Wang et al., 2017). It ranked among the 10 worst algorithms for minimum RMSE out of all 60 algorithms, but this package, focusing on Sparse Neural Networks for Genomic Selection in Animal Breeding, might prove useful in that perspective.

Lower-order algorithms

Packages with first-order algorithms can be broadly categorized into 2 types: (a) those that allow for one hidden layer (b) those that allow for more than one hidden layer.

A. One hidden layer

The first category is comprised of either packages that also include second-order algorithms previously discussed or packages that use the Extreme Learning Machine algorithm. Only 2 packages include both second-order algorithms and a lower-order algorithm, that is, **monmlp** and **validann**. **monmlp** has one algorithm besides BFGS, that is, **optimx**'s Nelder-Mead. **validann** provides the same algorithm but from `optim`. **validann**'s implementation is slower, as before, but ranks slightly better for minimum RMSE. Both implementations of Nelder-Mead do not rank well in minimum RMSE, around 40 out of 60, with similar ranks for the other criteria. We would also caution users to avoid the other methods in **validann** from `optim`. From Table 1 it may appear that **validann**'s implementation of the Conjugate Gradient (CG) algorithm finds reasonable minima and thus is a good option. It consistently ranked in the top 15 with minimum RMSE. However, it is the slowest algorithm of all 60 algorithms tested. Note, this includes algorithms from packages that call external libraries outside R in Python or Java and packages that use as much as 100,000 iterations. On the other hand, **validann**'s SANN algorithm is relatively worse than other packages as it ranks at number 55 for minimum RMSE although it is in the top one third for speed (rank 20).

Packages that implement the ELMR algorithm are similar to SANN from **validann** in the sense that they are faster but do not converge as well as other package's algorithms. The 2 packages that do so, **elmNNRcpp** (Mouselimis and Gosso, 2020) and **ELMR** (Petrozziello, 2015) are, respectively, number 1 and number 2 in the ranks for time but 59 and 60 (bottom 2) for minimum RMSE. **ELMR** converges slightly worse on all datasets than **elmNNRcpp** but has noticeably worse performance on the Gauss datasets, especially `uGauss1`. Even increasing the number of neurons did not lead to better convergence for those particular datasets.

B. More than one hidden layer

Following the trend of "deep learning", the last 9 packages provide the option for more than one layer with a first-order learning algorithm. Our results show that they are often

either/both slower or worse at converging than the second-order algorithms with the same number of neurons or layers than their counterparts. We recommend choosing better algorithms over more layers for datasets similar to the ones we used.

Choosing more layers often comes at the expense of speed. An example of this is the implementation of the first-order algorithm in **h2o** (LeDell et al., 2020). With the same numbers of neurons it already is quite slow - coming in at 51 out of the 60 algorithms.

With a default hidden layer size of 2, each with 200 neurons, it takes around 10 minutes on `mFriedman` with a minimum RMSE of 0.0022. On the other hand, **nnet** can find a minima of the error function with a minimum RMSE of 0.0088 in less than a second with fewer neurons and only one layer. Thus, despite having a ranking of 11 in minimum RMSE in the final run, beating some of the second-order algorithms, users of **h2o** should be wary of the trade off. Moreover, users might hesitate as it is not actually clear what algorithm is used. The large number of options to choose from seem capable of changing the basic algorithm itself into what is considered a different algorithm by other packages (example: "adaptive_rate: Specify whether to enable the adaptive learning rate (ADADELTA). This option is enabled by default." in link, set to false in latest run). Some users also might not want to setup Java, which is needed, although it is not as painful to setup as some external libraries.

By far, the hardest package to set up which called external libraries was **tensorflow** (Allaire and Tang, 2020) and its derivatives. In the summer of 2019, it took quite some time to figure out how things worked. Then the latest TensorFlow 2.2.0 became available and we hoped to be able to use the Eager Execution provided to avoid the R Session crashing in the summer of 2020. Unfortunately, this led to different problems with the translation between R and Python so we could not use the 2019 code. **tfestimators** (Allaire et al., 2018) also had similar issues and is even less supported. **kerasR** (Arnold, 2017), which provides a consistent interface to Keras, a Python API which provides an easier use interface to TensorFlow, had the same issue. In the end, we tested the algorithms in **keras** (Allaire and Chollet, 2020) with the hope that it would be able to represent the performance of the other packages.

keras has the second-most number of algorithms, a total of 7, with most of them being "adaptive" algorithms. The highest ranking algorithm for minimum RMSE is adamax at 23 and the highest ranking algorithm for speed was rmsprop at 37 (quite slow). However, these results were achieved with a reasonable GPU so users might want to decide on whether to use **keras** based on their own hardware specifications. Other algorithms did not perform well in terms of minimum RMSE and the spread of RMSE represented by RMSEd51. As **keras** also has many options available, including a convolutional layer for CNNs, more experienced users may prefer it. On the other hand, just deciding the learning rate (the default was not appropriate for our datasets) can be a challenge.

The default learning rates in **RSNNS** (Bergmeir, 2019) were more appropriate to use directly. **RSNNS** is an example of a package that directly wraps around an external library, the Stuttgart Neural Network Simulator (SNNS), to provide an easy-to-use interface. This library is rather large with many implementations of neural networks. It contains the biggest number of algorithms tested at a total of 8. Algorithms Rprop and SCG, the best for minimum RMSE, rank at 16 and 17 respectively which is pretty good for a first-order algorithm. Speed for Rprop is better but SCG's results vary less.

Other packages **AMORE** (Limas et al., 2020): Unfortunately, the focus of the paper behind this package, its unique point, is not explained or documented well enough.

An addition of some examples using the TAO option as the error criterion would be helpful for using the TAO-robust learning algorithm, since this type of error measure is most useful for data with outliers. The function for creating a dot file to use with `http://www.graphviz.org` is also interesting. ADAPT algorithms appear to perform better than the BATCH algorithms with the parameters used in this research.

ANN2 (Lammers, 2020): This package's implementation of adam or rmsprop consistently ranked in the top half for minimum RMSE which is not bad for a first-order algorithm. It is not as accurate as second-order algorithms but all its algorithms are quite fast. C++ code

was used to enhance the speed. Functions for autoencoding are included with anomaly detection in mind.

automl (Boulangé, 2020): It would be easier to use the algorithms in this package if they did not rely on the beta parameters and instead had an argument of their own. However, it is nice that there are notes on what parameters have a higher tuning priority. The package is rather slow (highest ranking algorithm for speed is RMSprop at 47) with good enough convergence (highest ranking is adam at 18).

deepdive (Balakrishnan, 2020): All algorithms are very good in terms of little variance between results (see its RMSEd51.score). However, the results on convergence by minimum RMSE score are not as good with the worst being gradientDescent which ranks 3rd from the bottom. There are few exported functions. The novelty of this package is apparently in the `deeptree` and `deepforest` functions it provides.

deepnet (Rong, 2014): This is one of the better performing implementations of the first-order algorithms backpropagation, ranking at 18 for minimum RMSE. It's also relatively fast, ranking at 23 for speed.

neuralnet (Fritsch et al., 2019): Considering that this is the only package that uses 100000 iterations as its maxit parameter (excluding BNN which is not included in the official ranks), it can be considered as not recommended. Nonetheless, the default algorithm, rprop+ and the similar rprop-, managed to rank 20 and 21 respectively, out of 60 algorithms for minimum RMSE. These two also do not do badly in terms of speed. Following, in order, are slr, sag, and traditional backprop as the worst at rank 48 out of 60 for minimum RMSE. Notes on documentation show that is rather difficult to configure this package, and it should probably not be a dependency for other packages that wish to be more certain of the results. For simple datasets, it is less of an issue.

Untested packages

A certain number of packages have been discarded from this study for at least one of the following reasons:

1. For regression but unsuitable for the scope of our research, coded RE in Table 3.
2. For time series, coded TS in Table 2.
3. For classification, coded CL in Table 2.
4. For specific purpose, coded AP in Table 2.
5. For tools to complement NN's by other packages, coded UT in Table 2.
6. Not actually neural networks and other reasons, coded XX in Table 2.

The full list of untested packages is given in Table 2.

Table 3: Review of Discarded Packages

Package	Category	Reason to Discard (File(s) and/or function(s))
appnn	AP	Provide a feed forward neural network to predict the amyloidogenicity propensity of polypeptide sequences (DESCRIPTION file)
autoencoder	AP	Provide a sparse autoencoder, an unsupervised algorithm that learns useful features from the data its given (::autoencode)
BNN	RE*	Use a feed forward neural network to perform regression. It is unclear whether it fits the form of perceptron in the scope. It states that it is intended for variable selection, although how exactly the package would be used to do so is missing. Also the source code is written in C that users of R might not understand. Performance is slowÂ : need 100.000 iterations. (::BNNsel-examples & abstract of paper)
Buddle	CL	Did not include regression in 2019. Unfortunately, the version we tested in 2020 could not be used properly for regression either. See the examples (::TrainBuddle)
cld2	XX	Provide bindings to Google's C++ library CLD2, which detects languages using a NaÃ¯ve Bayesian classifier. CLD3, which does use neural networks, is mentioned in the description (DESCRIPTION file & link to github)
cld3	AP	Bindings to Google's C++ library CLD3, which detects languages using a neural network with an experimental algorithm (DESCRIPTION file)
condmixt	AP	Use neural networks to predict parameters of mixture models (DESCRIPTION file)

Table 3: Review of Discarded Packages *(continued)*

Package	Category	Reason to Discard (File(s) and/or function(s))
DamiaNN	RE	Was designed specificly for training datasets from Numerai, <https://numer.ai/>. We were unable to adapt it to our datasets even after exporting functions from the interactive interface (DESCRIPTION file, help pages)
deep	CL	Seem to implement a perceptron to classify data (implicitly known from choice of iris as example and in source code)
deepNN	RE	Another implementation of deep learning. Its input format of lists of vectors is not standard require users to understand how to use lapply or other functions to convert the format of their data. Univariate datasets can't be used with the functions and we could not manage to adapt it to 2020 code (::train).
DNMF	XX	Help extract features that enforce spatial locality with separability between classes in a discriminant manner (DESCRIPTION file)
evclass	CL	Provide an evidential neural network that outputs Dempster-Shafer mass functions (DESCRIPTION file)
gamlss.add	UT	Allow users to use nnet with a variety of Generalized Additive Models for Location Scale and Shape (::nn). It is not particularly appropriate for all our datasets.
gcForest	XX	Based on an article with "Towards an Alternative to Deep Neural Networks" in its title (DESCRIPTION file)
GMDH	TS	Provide GMDH type neural network algorithms for short term forecasting on a univariate time series (DESCRIPTION file)
GMDH2	CL	Provide GMDH type neural network algorithms for performing binary classification (DESCRIPTION file)
GMDHreg	RE*	Regression using GMDH algorithms. We only managed to tested the COMBI algorithm (the most basic and first in the vignette) on the multivariate datasets. It is strangely slow on the "easy" datasets, mFriedman and mRef153. The convergence is relatively not good considering the ammount of layers (Title in DESCRIPTION file)
gnn	AP	Out of scope: Generative moment matching networks (GMMNs) are introduced for generating quasi-random samples from multivariate models (article abstract)
grnn	RE	Provide an implementation of Specht's General Regression Neural Network in 1991 (DESCRIPTION file). We could not manage to make the functions work on the multivariate datasets. ::guess, the function for predicting, only allows for 1 data at a time. Performance of General Regression Neural Networks can be seen from package yager instead.
hybridEnsemble	RE	Hybrid ensemble of eight different sub-ensembles (DESCRIPTION file)
image.libfacedetection	AP	Face detection with CNNs (DESCRIPTION file)
isingLenzMC	AP	Out of scope: This package provides utilities to simulate one dimensional Ising Model with Metropolis and Glauber Monte Carlo (DESCRIPTION file)
kerasR	RE	See section on keras
leabRa	RE	Provide the local error driven and associative biologically realistic algorithm (Leabra) from O'Reilly 1996. It combines supervised and unsupervised learning, so out of scope (DESCRIPTION file).
learNN	CL	Implement some basic neural networks from \url{http://qua.st/} (DESCRIPTION file). Examples seem to focus on binary classification (::learn_gd, ::learn_bp).
LilRhino	AP	Provide binary neural networks meant for reducing data (DESCRIPTION file), a random forest style collection of neural networks for classification (::Random_Brains), and code for even more purposes. Documentation is satisfyingly clear for a package for applications: a 3 layer network with an adam optimizer, with an explanation of its activation functions (::Binary_Network)
neural	CL	An implementation of "a simple MLP neural network that is suitable for classification tasks" (::mlptrain)
NeuralNetTools	UT	Out of scope: Functions are available for plotting, quantifying variable importance, conducting a sensitivity analysis, and obtaining a simple list of model weights (DESCRIPTION file and Help Pages titles)
NeuralSens	UT	A greater focus on sensitivity, with additional functions (DESCRIPTION file)
NlinTS	TS	A non-linear version of a causality test with feed forward neural networks and a Vector Auto-Regressive Neural Network (VARNN) for non-linear time series analysis models (DESCRIPTION file)
nnetpredint	UT	Out of scope: Computing prediction intervals of neural network models at certain confidence level (DESCRIPTION file)
nnfor	TS	Automatic to fully manual time series modelling with neural networks (DESCRIPTION file)
nnlib2Rcpp	CL	Provide a collection of neural networks, but examples seem to indicate classification and testing our code with the functions provided led to error. Using the RcppClass might be confusing for less experienced R users (::NN-class)
nntrf	AP	Provide useful pre-processing for Machine Learning tasks through data transformation in a non-linear, supervised way with a perceptron (DESCRIPTION file)
onnx	UT	Aims to provide an open source format for neural networks, with definitions of an extensible computation graph model, built-in operators, and standard data types (DESCRIPTION file)

Table 3: Review of Discarded Packages *(continued)*

Package	Category	Reason to Discard (File(s) and/or function(s))
OptimClassifier	UT	Search for the best amount of neurons for binary classifcation neural networks, among other types of binary classifiers (based on how Optim.NN works & DESCRIPTION file)
OSTSC	UT	A tool to solve imbalanced data for univariate time series classification with oversampling using integrated ESPO and ADASYN methods (DESCRIPTION file) thus improving the performance of RNN classifiers (vignette)
passt	AP	This package provides implementation of the Probability Associator Time (PASS-T) model, a memory model based on a simple competitive artificial neural network which imitates human judgment of frequency and duration (DESCRIPTION file)
pnn	CL	This package provides implementation of the Specht algorithm, 1990, for classification with four functions: learn, smooth, perf, and guess (DESCRIPTION file)
polyreg	XX	Polyregression as alternative to NN (DESCRIPTION file)
predictoR	RE	A shiny interface for supervised learning with very minimal documentation. Users may be additionally confused when opening the application only to find that it's default language is Espanol, although this can be changed in the Idioma section. (DESCRIPTION file & ::init_predictor)
ProcData	AP	Provide tools for exploratory process data analysis via functions: reading, process manipulation, action sequence generators, feature extraction and prediction (link + DESCRIPTION file)
quarrint	AP	Out of scope: provide two indexes for interaction prediction between groundwater and quarry extension, one of which is an artificial neural networkÂ ; specified classifier for quarry data (help page - quarrint-package and DESCRIPTION file)
rasclass	CL	Provide neural networks as one of the five supervised classification algorithms for raster images with a design meant to facilitate land-cover analysis (DESCRIPTION file)
rcane	RE	Provide parameter estimation for linear regression, which was not appropriate for the relationships in our data. (DESCRIPTION file)
regressoR	RE	A manual rich version of predictoR
rnn	AP	Implementations of the vanilla Recurrent Neural Network, Long Short-Term Memory (LSTM), and Gated Recurrent Unit (GRU) in native R (DESCRIPTION file)
RTextTools	AP	Out of scope: A machine learning package for automatic text classification (DESCRIPTION file)
ruta	AP	unsupervised neural networks (DESCRIPTION file)
simpleNeural	CL	Neural networks for multi-class or binary classification (DESCRIPTION file)
softmaxreg	CL	Out of scope: Implementation of 'softmax' regression and classification models with multiple layer neural network (DESCRIPTION file)
Sojourn.Data	AP	Stores some neural networks used for Sojourn Accelerometer methods (DESCRIPTION file)
spnn	CL	Out of scopeÂ : Scale invariant version of the original PNN with the added functionality of allowing for smoothing along multiple dimensions while accounting for covariances within the data set (DESCRIPTION file)
studyStrap	AP	Implements multi-study learning algorithms such as merging, the study-specific ensemble the study strap, the covariate-matched study strap, covariate-profile similarity weighting, and stacking weights with single-study learners from caret (DESCRIPTION file)
TeachNet	CL	Provide neural networks with up to 2 hidden layers, 2 different error functions, and a weight decay for 2 class classificationÂ : it is slow. (DESCRIPTION file & ::TeachNet)
tensorflow	RE	See section on keras
tfestimators	RE	See section on keras
trackdem	AP	An artificial neural network can be trained for filtering false positives present in video materials or image sequences (DESCRIPTION file)
TrafficBDE	RE*	Use caret for a grid of parameters for 3 layers combined with neuralnet. Is very slow. Out of scope to test one layer perceptrons. We recommend the author to use other packages and lessen the number of layers. Datasets in Traffic Status Prediction and Urban Places are similar in nature to ours (TrainCR.R, DESCRIPTION file)
tsfgrnn	TS	Out of scope: A general regression neural network (GRNN) is a variant of a Radial Basis Function Network. Allow you to forecast time series using an autoregressive GRNN model (DESCRIPTION file)
yager	RE*	This package provides a neural network that behaves differently from a perceptron. Results indicate that predictions are quite close to the real values, however this comes at the cost of a large number of weights. With less weights or insufficient training data, the performance isn't as great. (::grnn.fit)
yap	CL	Yet another PNN, with a N-level response, where N > 2 (DESCRIPTION file)
zFactor	AP	Computational algorithms to solve equations and find the 'compressibility' factor 'z' of hydrocarbon gases (DESCRIPTION file)

Note: AP=Application, CL=Classification, RE=Regression, RE*=?, TS=Time serie, UT=Utility, XX=Other.

Table 4: Performance on bWoodN1 dataset

Package	Algorithm	RMSE min	RMSE median	RMSE D51	MAE median	WAE median	Time median
MachineShop	32. nnet_optim(BFGS)	3.5467	4.75645	1.20975	3.90085	16.02080	**3.3995**
nlsr	41. NashLM	3.5482	4.70550	1.15730	3.80060	16.56460	**76.7275**
nnet	42. optim (BFGS)	3.5499	4.70570	1.15580	3.80055	16.57275	**3.3805**
rminer	45. nnet_optim(BFGS)	3.3662	3.68795	0.32175	2.95600	15.42995	**11.0725**
validann	56. optim(BFGS)	3.3599	4.49705	1.13715	3.71070	15.89260	**140.7880**

Note: statistics taken over 20 runs; time in seconds.

Further analysis of TOP5 packages

In this subsection, we perform a second round analysis with a larger dataset with a focus on the Top 5 packages given Table 2. That is, we consider packages `nlsr`, `rminer`, `nnet`, `validann` with algorithm BFGS and `MachineShop`. We fit the NN packages on Simon Wood's Gaussian dataset, see `bWoodN1` in dataset description, which contains 20,000 rows with 6 inputs valued in [0,1] for a (single) numeric output. Due to the non-linear functions considered, see Appendix B, the link between the output and each explanatory variable is highly nonlinear which affects deeply the fitting time. Table 4 gives the metric performance over 20 runs of these Top 5 five packages on `bWoodN1`.

We observe that the minimum RMSE (over 20 runs) is very similar for all package, yet `rminer` and `validann` are little bit behind others. The median RMSE and D51 RMSE reveal the very good fits by `rminer`, and it is also true for other metric norms: WAE and MAE. Regarding computation time, the two best in class are `nnet` and `MachineShop`.

Figures in Appendix E 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

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

where $r()$ denotes the round function with two decimal places and $y_i, \hat{y}_i$ stand respectively for the ith observed response and the ith 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.

Conclusion and perspective

??JN: Can we start to put in some major findings? i.e., important positive findings, big negatives?

Positives (no particular order)

1. We are happy to note the existence of neural network packages in R with algorithms that converge well.

- **nnet**, which uses ?? need font choice?? optim's BFGS method, is already often chosen to represent neural networks for packages that are either a collection of independent machine learning algorithms, ensembles, or even applications in a field such as ... ?? need to complete sentence??. JN??: Why is this positive? ==> B: its meant to be part of the above, because nnet's algorithm converged well in our tests, thus the fact that

it is being used by other packages is a plus? See the part about nnet & packages that depend on it in the results
- R users have access to a wide variety of neural network methods, including from libraries of other programming languages and using many different types of algorithms. ?? have we defined hyperparameters?? hyperparameters, and uses

Reproducibility : all our benchmark is reproducible by any user and any package maintainer.

Negatives

- We are disappointed that many of the packages we reviewed had poor documentation.
- It would be helpful if there were more packages with (different) second-order algorithms. A number of the
- We often found it difficult to discover what default starting values were used for model parameters, or

Future work

As the field of neural networks continue to grow, there will always be more algorithms to validate. For current algorithms in R, our research should be extended to encompass more types of neural networks and their data formats (classifier neural networks, recurrent neural networks, and so on). Different rating schemes and different parameters for package functions can also be tried out.

- The dreamed NN package: Recommendation to package authors
- Conclusion

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Appendix

Appendix A

Consider a set of observations y_i and its corresponding predictions $\hat{y}_i$ for $i = 1, \ldots, n$. The three metrics used were:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|,\ RMSE = \frac{1}{n}\sqrt{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2},\ WAE = \frac{1}{n}\max_{i=1,\ldots,n}|y_i - \hat{y}_i|.$$

These values represent the absolute, the squared and the maximum norm of residual vectors.

Appendix B

We define five smooth functions for Simon Wood's test dataset

$$f_0 = 5\sin(2\pi x),\ f_1 = \exp(3x) - 7,$$

$$f_2 = 0.5 \times x^{11}(10(1-x))^6 - 10(10x)^3(1-x)^{10},\ f_3 = 15\exp(-5|x-1/2|) - 6,$$

$$f_4 = 2 - 1_{(x<=1/3)}(6x)^3 - 1_{(x>=2/3)}(6-6x)^3 - 1_{(2/3>x>1/3)}(8 + 2\sin(9(x-1/3)\pi)).$$

Appendix C

An example of our template for the package nnet:

```
library(NNbenchmark)
nrep <- 3
odir <- tempdir()

library(nnet)
nnet.method <- "BFGS"
hyperParams.nnet <- function(...) {
    return (list(iter=200, trace=FALSE))
}
NNtrain.nnet <- function(x, y, dataxy, formula, neur, method, hyperParams, ...) {

    hyper_params <- do.call(hyperParams, list(...))

    NNreg <- nnet::nnet(x, y, size = neur, linout = TRUE,
                        maxit = hyper_params$iter, trace=hyper_params$trace)
    return(NNreg)
}
NNpredict.nnet  <- function(object, x, ...) { predict(object, newdata=x) }
NNclose.nnet    <- function() {  if("package:nnet" %in% search())
                                 detach("package:nnet", unload=TRUE) }
nnet.prepareZZ  <- list(xdmv = "d", ydmv = "v", zdm = "d", scale = TRUE)

res <- trainPredict_1pkg(4, pkgname = "nnet", pkgfun = "nnet", nnet.method,
  prepareZZ.arg = nnet.prepareZZ, nrep = nrep, doplot = TRUE,
  csvfile = FALSE, rdafile = FALSE, odir = odir, echo = FALSE)
```

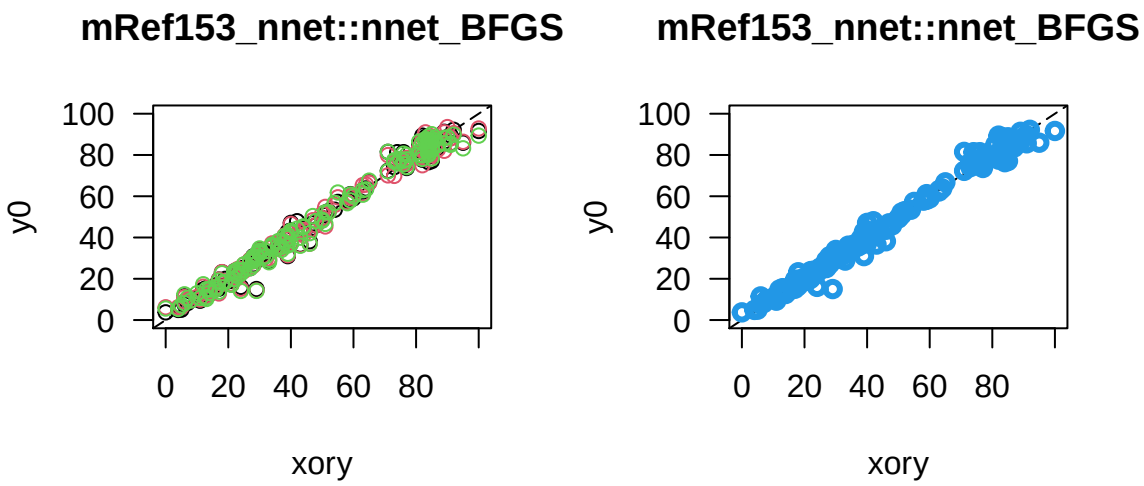

Figure 4: Example of nnet on mRef153

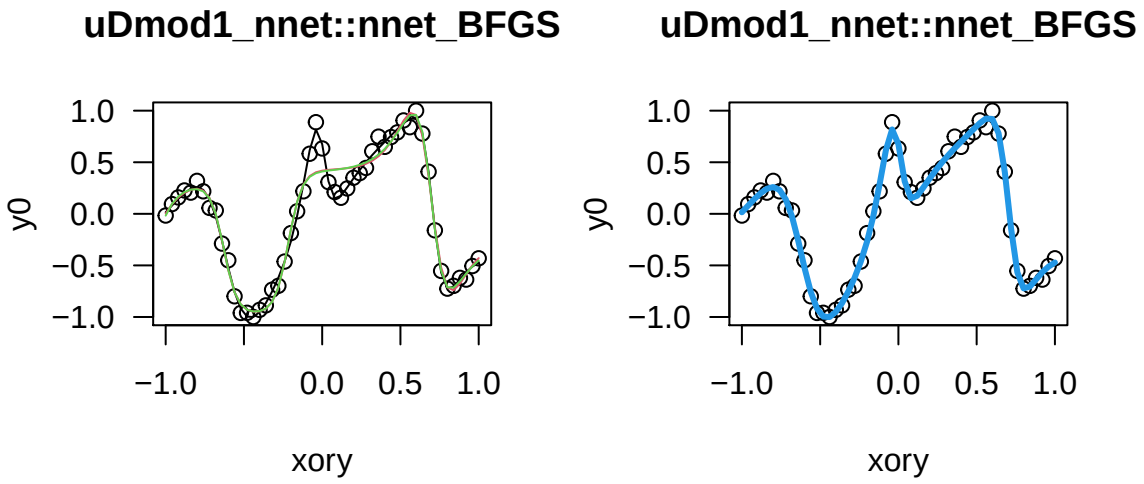

Figure 5: Example of nnet on uDmod1

```
res <- trainPredict_1pkg(5, pkgname = "nnet", pkgfun = "nnet", nnet.method,
  prepareZZ.arg = nnet.prepareZZ, nrep = nrep, doplot = TRUE,
  csvfile = FALSE, rdafile = FALSE, odir = odir, echo = FALSE)
```

Appendix D

Appendix E

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Table 5: All convergence scores per package:algorithm sorted by minimum RMSE

		Input parameter			RMSE Score		Other score	
Package	Algorithm	Input format	Maxit	Learn. rate	median	d51	MAE	WAE
nlsr	41. NashLM	full fmla & data	200	-	3	16	3	6
rminer	45. nnet_optim(BFGS)	fmla & data	200	-	1	6	1	1
nnet	42. optim (BFGS)	x & y	200	-	2	17	2	3
validann	56. optim(BFGS)	x & y	200	-	4	10	4	5
	57. optim(CG)	x & y	1000	-	6	10	5	4
	58. optim(L-BFGS-B)	x & y	200	-	13	30	14	13
	59. optim(Nelder-Mead)	x & y	10000	-	44	45	46	42
	60. optim(SANN)	x & y	1000	-	53	51	56	55
MachineShop	32. nnet_optim(BFGS)	fmla & data	200	-	9	22	9	7
traineR	55. nnet_optim(BFGS)	fmla & data	200	-	5	15	6	2
radiant.model	44. nnet_optim(BFGS)	"y" & data	200	-	8	32	12	10
monmlp	34. optimx(BFGS)	x & y	200	-	10	18	9	11
	35. optimx(Nelder-Mead)	x & y	10000	-	47	45	44	47
CaDENCE	12. optim(BFGS)	x & y	200	-	28	48	21	40
	14. Rprop	x & y	1000	0.01	54	60	52	58
	13. pso_psoptim	x & y	1000	-	56	56	54	56
h2o	24. first-order	"y" & data	10000	0.01	7	7	8	8
EnsembleBase	23. nnet_optim(BFGS)	x & y	200	-	15	34	15	15
caret	15. avNNet_nnet_optim(BFGS)	x & y	200	-	10	21	11	9
brnn	11. Gauss-Newton	x & y	200	-	12	9	13	12
qrnn	43. nlm()	x & y	200	-	14	25	7	36
RSNNS	51. Rprop	x & y	1000	-	23	52	25	28
	52. SCG	x & y	1000	-	17	26	18	19
	53. Std_Backpropagation	x & y	1000	0.1	32	31	31	36
	47. BackpropChunk	x & y	1000	-	34	41	32	34
	48. BackpropMomentum	x & y	1000	-	35	39	35	30
	49. BackpropWeightDecay	x & y	1000	-	30	43	33	31
	46. BackpropBatch	x & y	10000	0.1	48	27	50	48
	50. Quickprop	x & y	10000	-	58	36	58	57
automl	8. trainwgrad_adam	x & y	1000	0.01	20	35	16	20
	9. trainwgrad_RMSprop	x & y	1000	0.01	31	50	29	39
	10. trainwpso	x & y	1000	-	41	49	41	38
deepnet	20. BP	x & y	1000	0.8	18	38	24	17
neuralnet	38. rprop+	fmla & data	100000	-	23	40	23	24
	37. rprop-	fmla & data	100000	-	21	42	21	18
	40. slr	fmla & data	100000	-	39	37	39	46
	39. sag	fmla & data	100000	-	49	59	47	52
	36. backprop	fmla & data	100000	0.001	51	10	49	45
keras	28. adamax	x & y	10000	0.1	18	20	20	16
	27. adam	x & y	10000	0.1	28	44	30	25
	29. nadam	x & y	10000	0.1	39	58	40	41
	26. adagrad	x & y	10000	0.1	43	53	42	35
	25. adadelta	x & y	10000	0.1	35	19	34	33
	31. sgd	x & y	10000	0.1	45	47	45	43
	30. rmsprop	x & y	10000	0.1	55	57	55	54
AMORE	2. ADAPTgdwm	x & y	1000	0.01	22	29	16	26
	1. ADAPTgd	x & y	1000	0.01	25	8	26	21
	4. BATCHgdwm	x & y	10000	0.1	33	14	37	27
	3. BATCHgd	x & y	10000	0.1	38	24	42	31
minpack.lm	33. Levenberg-Marquardt	full fmla & data	200	-	16	5	19	14
ANN2	6. rmsprop	x & y	1000	0.01	25	33	27	23
	5. adam	x & y	1000	0.01	27	27	28	21
	7. sgd	x & y	1000	0.01	37	22	36	29
deepdive	16. adam	x & y	10000	0.4	42	1	38	44
	19. rmsProp	x & y	1000	0.8	46	4	48	50
	18. momentum	x & y	1000	0.8	52	3	53	51
	17. gradientDescent	x & y	10000	0.8	57	2	57	53
snnR	54. SemiSmoothNewton	x & y	200	-	49	13	50	48
elmNNRcpp	21. ELM	x & y	-	-	59	55	59	59
ELMR	22. ELM	fmla & data	-	-	60	53	60	60

Note: TOP5 are nlsr:NashLM, rminer:nnet_optim(BFGS), nnet:optim (BFGS), validann:optim(BFGS), MachineShop:nnet_optim(BFGS).

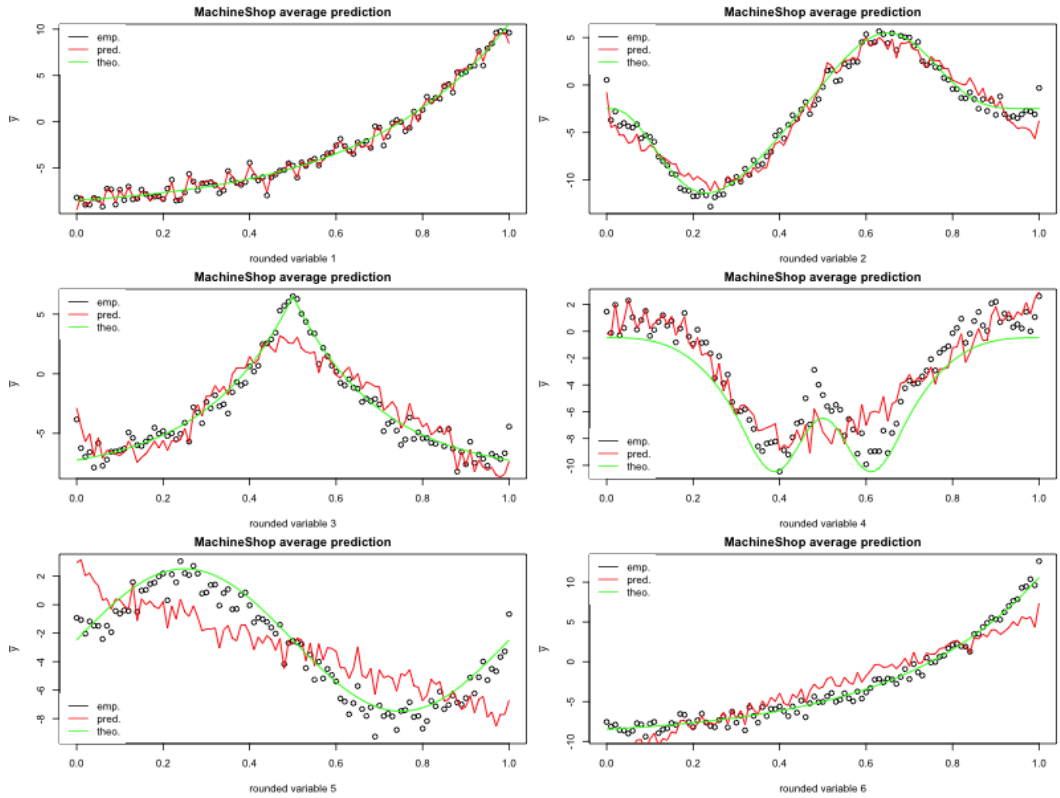

Figure 6: Average predicted mean per explanatory variable for `MachineShop`

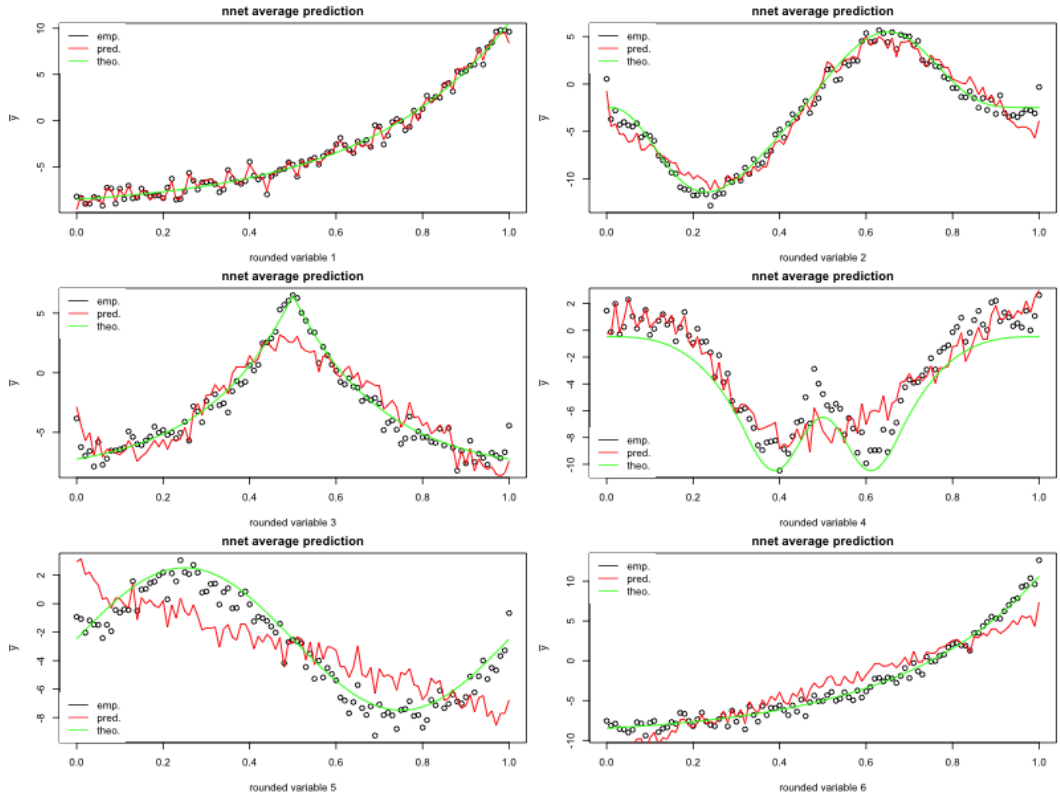

Figure 7: Average predicted mean per explanatory variable for `nnet`

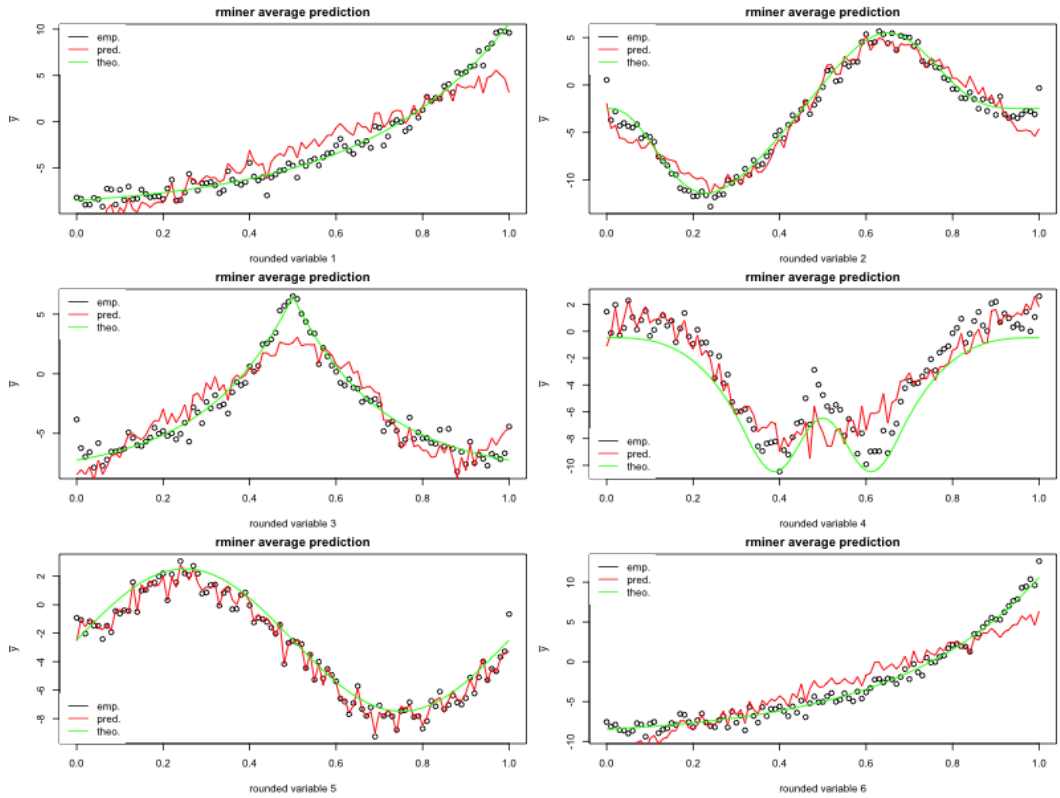

Figure 8: Average predicted mean per explanatory variable for `rminer`

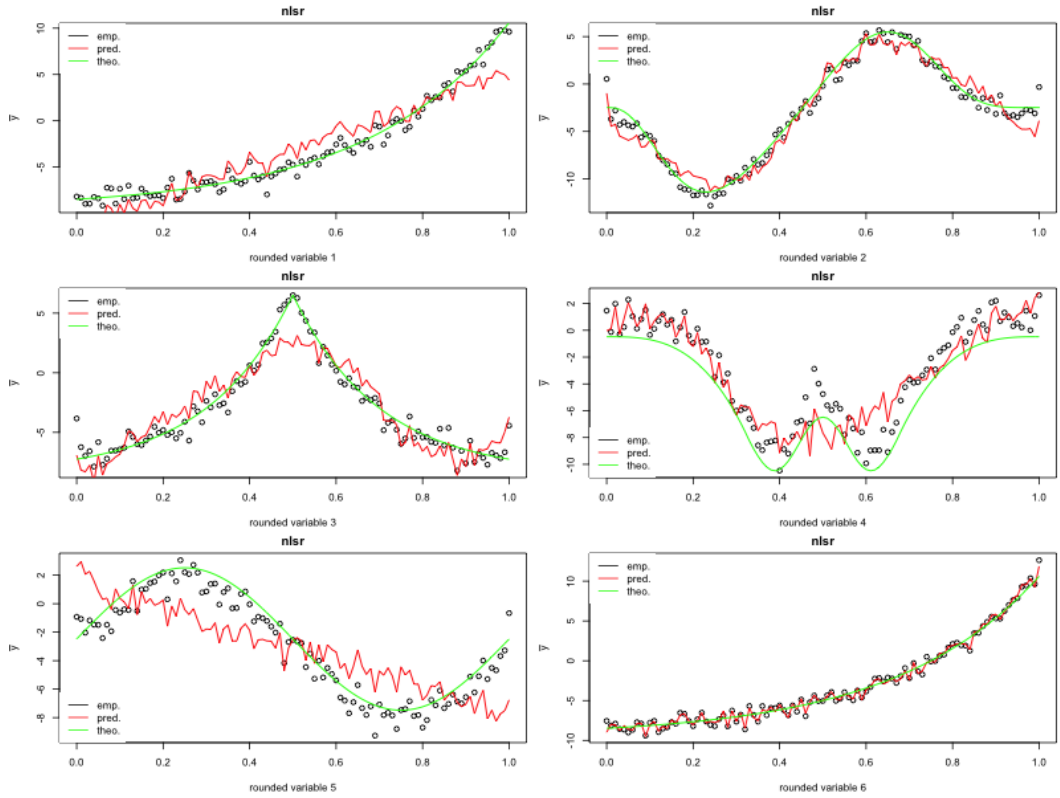

Figure 9: Average predicted mean per explanatory variable for `nlsr`

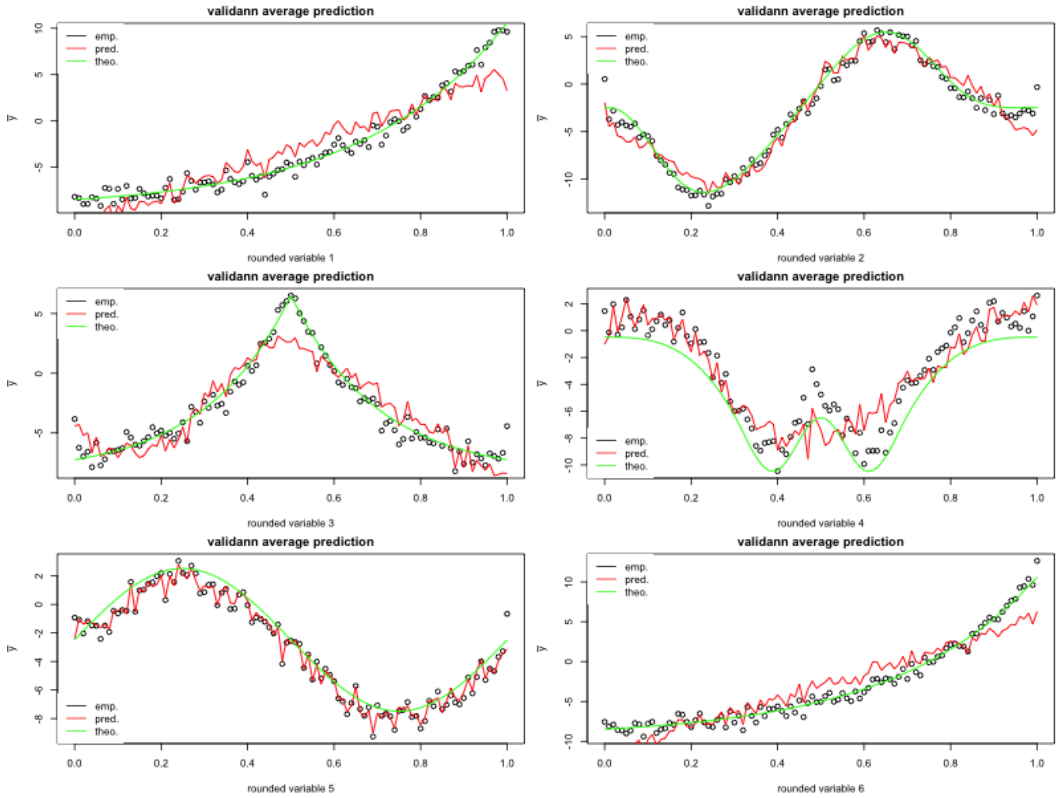

Figure 10: Average predicted mean per explanatory variable for `validann`

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