

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 (www.r-project.org), 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 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 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 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, \dots, a_{10} are the parameters.

The model $y = a_1 + a_2 \times \text{atan}(a_3 + a_4 \times x_1 + a_5 \times x_2 + a_6 \times x_3 + a_7 \times x_4 + a_8 \times x_5) + a_9 \times \text{atan}(a_{10} + a_{11} \times x_1 + a_{12} \times x_2 + a_{13} \times x_3 + a_{14} \times x_4 + a_{15} \times x_5) + a_{16} \times \text{atan}(a_{17} + a_{18} \times x_1 + a_{19} \times x_2 + a_{20} \times x_3 + a_{21} \times x_4 + a_{22} \times x_5)$ 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, \dots, 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 the parameters, for instance extracted from a centered Gaussian $\mathcal{N}(0, 0.1)$ distribution. Such

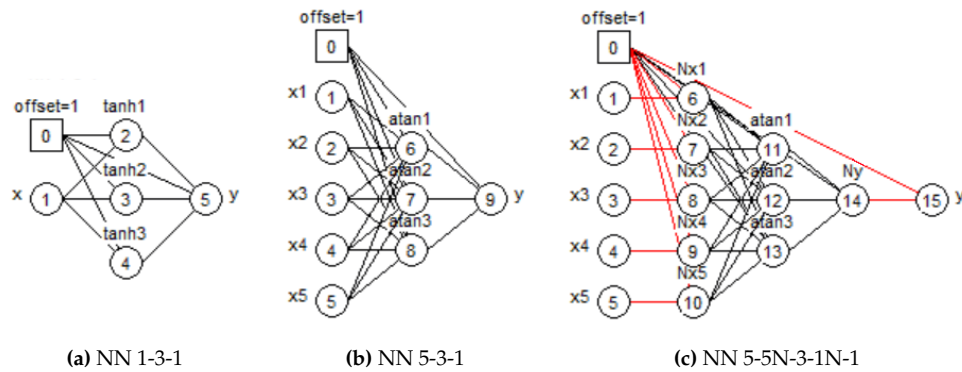


Figure 1: Three neural networks

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 finetune 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 collinearities 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 and 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.

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 small¹. 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 Appendix C. 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.

Phase 1 - Preparation of benchmark datasets

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. 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> (Friedman - average)
- <http://www.sfu.ca/~ssurjano/detpep10curv.html> (Dette - medium)
- <http://www.sfu.ca/~ssurjano/ishigami.html> (Ishigami - high)

The other multivariate dataset, Ref153, was used to teach neural networks at ESPCI from 2003 to 2013 and is available in the software Neuro One at <http://www.inmodelia.com/software.html>

Three of the univariate datasets we used were taken from a website of the US National Institute for Standards and Technology (NIST): https://www.itl.nist.gov/div898/strd/nls/nls_main.shtml. (Gauss1 - low; Gauss2 - low; Gauss3 - average)

Univariate datasets Dmod1, Dmod2 are ...

Dreyfus1 is a pure neural network which has no error. This can make it difficult for algorithms that assume an error exists. Dreyfus2 is Dreyfus1 with errors. Both are considered to be of low difficulty and usually appeared in the first slides when used to teach neural networks at ESPCI from 1991 to 2013 (<https://www.neurones.espci.fr/>)

The last univariate dataset, NeuroOne, was also used to teach the same course and is now available in the software Neuro One.

Finally, we also consider a Simon Wood test dataset, used in (Wood, 2011) for benchmarking generalized additive models. Precisely, we consider a generation of Gaussian random

¹We 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).

variates $Y_i, i = 1, \dots, n$ with the mean μ_i defined as

$$\mu_i = 1 + f_0(x_{i,0}) + f_1(x_{i,1}) + f_2(x_{i,2}) + f_3(x_{i,3}) + f_4(x_{i,4}) + f_5(x_{i,5})$$

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 $n = 20,000$.

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 falls 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's task view for machine learning, <https://CRAN.R-project.org/view=MachineLearning>, as well as the 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

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. Basically, each package was inspected 3 times.

1. The discard/not discard phase: depending on the package, this could be decided as easily as looking at the DESCRIPTION file or having to go through the process of making the code and seeing the results.
2. Benchmarking with 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.

Templates for Testing Accuracy and Speed

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 functions 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, that had been made generic with an extensive use of the incredible `do.call` function, were added:

²We 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.

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>.

3. summarizing or re-reviewing the tested packages utility functions & documentation

Ease of Use Scoring

We define an ease-of-use measure based on what we considered a user would need when using a neural network package for nonlinear regression, namely, utility functions and sufficient documentation.

1. Utilities (1 star)
 - a. a predict function exists
 - b. scaling capabilities exist
2. Sufficient documentation (2 stars)
 - a. the existence of useful example/vignette = (1 star)
 - clear, with regression = 2 points
 - unclear, examples use iris or are for classification only = 1 point
 - no examples = 0 points
 - b. input/output is clearly documented, e.g., what values are expected and returned by a function = (1 star)
 - clear input and output = 2 points
 - only one is clear = 1 point
 - both are not documented = 0 points

The ease-of-use measure ranges from 0 to 3 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.

Analysis

To rank how well a package converged and its speed, 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;
 - 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.

To rank how easy or not a package was to use (TO BE DISCUSSED FURTHER): - Functionality (util): scaling, input, output, trace - Documentation (docs): examples, structure/functions, vignettes

Results

Table 1 gives the RMSE and time score per package and per algorithm. The full list of score is given in Table 2 in Appendix C.

Tables

Discussion and Recommendations

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 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`

Table 1: Result from Tested Packages

Package	Individual score		Algorithm	Global score	
	Util	Doc		Time	RMSE
AMORE	1	3.0	1. ADAPTgd	9	35
	1	3.0	2. ADAPTgdwm	16	24
	1	3.0	3. BATCHgd	39	41
	1	3.0	4. BATCHgdwm	40	39
ANN2	2	3.0	5. adam	13	33
	2	3.0	6. rmsprop	14	28
	2	3.0	7. sgd	11	42
automl	1	3.0	8. trainwgrad_adam	50	18
	1	3.0	9. trainwgrad_RMSprop	47	26
	1	3.0	10. trainwpso	57	43
brnn	2	4.0	11. Gauss-Newton	8	14
CaDENCE	2	3.0	12. optim(BFGS)	46	10
	2	3.0	13. pso_psoptim	54	54
	2	3.0	14. Rprop	56	51
caret	2	3.0	15. avNNet_nnet_optim(BFGS)	17	13
deepdive	2	3.0	16. adam	32	46
	2	3.0	17. gradientDescent	52	58
	2	3.0	18. momentum	53	56
	2	3.0	19. rmsProp	34	53
deepnet	1	3.0	20. BP	23	18
elmNNRcpp	2	3.0	21. ELM	1	59
ELMR	2	3.0	22. ELM	2	60
EnsembleBase	1	1.0	23. nnet_optim(BFGS)	5	12
h2o	2	2.0	24. first-order	51	11
keras	2	0.0	25. adadelata	59	40
	2	0.0	26. adagrad	58	37
	2	0.0	27. adam	42	34
	2	0.0	28. adamax	48	23
	2	0.0	29. nadam	44	36
	2	0.0	30. rmsprop	37	52
	2	0.0	31. sgd	48	44
MachineShop	1	3.0	32. nnet_optim(BFGS)	6	5
minpack.lm	1	3.5	33. Levenberg-Marquardt	15	24
monmlp	2	3.5	34. optimx(BFGS)	26	9
	2	3.5	35. optimx(Nelder-Mead)	32	47
neuralnet	1	3.0	36. backprop	37	50
	1	3.0	37. rprop-	21	22
	1	3.0	38. rprop+	19	21
	1	3.0	39. sag	41	38
	1	3.0	40. slr	31	31
nlsr	1	4.0	41. NashLM	18	1
nnet	1	3.0	42. optim (BFGS)	3	3
qrnn	2	3.0	43. nlm()	28	16
radiant.model	2	2.0	44. nnet_optim(BFGS)	10	7
rminer	2	3.5	45. nnet_optim(BFGS)	12	2
RSNNS	2	3.0	46. BackpropBatch	43	49
	2	3.0	47. BackpropChunk	26	29
	2	3.0	48. BackpropMomentum	25	30
	2	3.0	49. BackpropWeightDecay	29	31
	2	3.0	50. Quickprop	45	57
	2	3.0	51. Rprop	24	17
	2	3.0	52. SCG	30	18
	2	3.0	53. Std_Backpropagation	22	27
snnR	2	2.0	54. SemiSmoothNewton	7	48
traineR	1	2.5	55. nnet_optim(BFGS)	4	6
validann	1	4.0	56. optim(BFGS)	35	4
	1	4.0	57. optim(CG)	60	8
	1	4.0	58. optim(L-BFGS-B)	36	15
	1	4.0	59. optim(Nelder-Mead)	55	45
	1	4.0	60. optim(SANN)	20	55

in Appendix C) in comparison to `validann::BFGS`. We believe the different default JN?? 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 JN?? tested?? that use `optim` do so through `nnet`. Moreover, approximately 8 packages not tested use it. 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 deceptively 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 `deeplive` 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) call `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 its 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 `nlsr` (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`. 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 recommend 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.

First 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 Gauss 1. Even increasing the amount 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 amount 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 the default hidden layer sizes of 2 layers, 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 less 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 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 setup 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 amount of most 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.

AMORE (Limas et al., 2020): It's a shame that the focus of the paper behind this package, it's unique point, is not explained or documented well enough. An addition of some examples using the TAO option as the error criterium would be helpful for using the TAO-robust learning algorithm. Note, this type of error 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's 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 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. 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 aren't that good with the worst being gradientDescent which ranks 3rd from the bottom. Not a lot of exported functions. The novelty of this package is apparently from the "deeptree" and "deepforest" functions it provides.

deepnet (Rong, 2014): 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 bad in terms of speed. After, 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 hard to configure this package, and 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 => TO DO - LIST

1. For regression but unsuitable for the scope of our research
2. For time series
3. For classification
4. For specific purpose
5. For tools to complement NN's by other packages
6. Not actually neural networks
7. Error

```
""{r echo=FALSE, message=FALSE}
```

Following chunk has NOT been executed

```
library(kableExtra)
options(knitr.kable.NA = '')

if(file.exists("../tables/Table2.csv")) {
  Table2 <- read.csv("../tables/Table2.csv", sep = ";")
  Table2 <- Table2[Table2[,3] != "", ]
  Table2 <- Table2[,1:3]
}

colnames(Table2) <- c("Package", "Category", "Reason to Dsicard (Where)")

kableExtra::kable(Table2, booktabs = TRUE, centering = TRUE, longtable = TRUE,
  caption="Review of Discarded Packages") %>%
  kable_styling(font_size=7) %>%
  column_spec(4, width = "10cm")
```

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

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 $i = 1, \dots, n$. The three metrics used were:

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

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

$$\begin{aligned} f_0 &= 5 \sin(2\pi x), f_1 = \exp(3x) - 7f_2 = 0.5x^{11}(10(1-x))^6 - 10(10x)^3(1-x)^{10}, \\ f_3 &= 15 \exp(-5|x - 1/2|) - 6, \\ f_4 &= 2 - 1_{(x <= 1/3)}(6x)^3 - 1_{(x >= 2/3)}(6 - 6x)^3 - 1_{(2/3 > x > 1/3)}(8 + 2 \sin(9(x - 1/3)\pi)). \end{aligned}$$

Appendix C

Appendix D

Appendix E

```
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())
```

Table 2: All convergence scores per package:algorithm

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

Table 3: Review of Ommitted Packages

No	Name (package)	Category	Comment
1	appnn	AP	This package provides a feed forward neural network to predict the amyloidogenicity propensity of polypeptide sequences
2	autoencoder	AP	This package provides a sparse autoencoder, an unsupervised algorithm that learns useful features from the data its given
3	BNN	RE*	This package uses a feed forward neural network to perform regression as provided in the examples, however, it is unclear whether it fits the form of perceptron that is the scope of our research. Moreover, it states that it is intended for variable selection. Although how exactly the package would be used to do so isn't accessible in the package, especially considering the source code is based on .c code that users of R might not understand. It's performance is slow, which may have to do with the 100.000 iterations it needs, although quite accurate for simple datasets.
4	Buddle	RE**	(errors)
5	cld2	00	
6	cld3	AP	
7	condmixt	AP	
8	deep	CL	
9	DALEX2	00	removed keyword, included in 2019
10	DamiaNN	RE**	(errors) exported functions, still doesn't work
11	DChaos	??	removed keyword for some reason, need to check out!
12	deepNN	RE**	(errors) I/O weird, ragged vector array
13	DNMF	AP	
14	evclass	CL	
15	gamlss.add	RE	there is some code but dist not appropriate
16	gcForest	00	
17	GMDH	TS	
18	GMDH2	CL	
19	GMDHreg	RE*	
20	grnn	RE**	
21	hybridEnsemble	??	
22	isingLenzMC	AP	
23	leabRa	??	
24	learNN	??	
25	LilRhino	AP	
26	neural	CL	
27	NeuralNetTools	UT	tools for neural networks
28	NeuralSens	UT	tools for neural networks
29	NlinTS	TS	Time Series
30	nnetpredint	UT	confidence intervals for NN
31	nnfor	TS	Times Series, uses neuralnet
32	nntrf	UT	
33	onnx		provides an open source format
34	OptimClassifier		choose classifier parameters, nnet
35	OSTSC		solving oversampling classification
36	passt		
36	pnn		Probabilistic
37	polyreg		polyregression as alternative to NN
38	predictoR		shiny interface, neuralnet
39	ProcData		
40	QuantumOps		classifies MNIST, Schuld (2018), removed keyword, in 2019
41	quarrint		specified classifier for quarry data
42	rasclass		classifier for raster images, nnet?
43	rcane		
44	regressoR		a manual rich version of predictoR
45	rnn		Recurrent
46	RTextTools		
47	ruta		
48	simpleNeural		
49	softmaxreg		
50	Sojourn.Data		sojourn Accelerometer methods, nnet?
51	spnn		classifier, probabilistic
52	studyStrap		
53	TeachNet		classifier, selfbuilt, slow
54	tensorflow		
55	tfestimators		
56	trackdem		classifier for particle tracking
57	TrafficBDE	RE*	
58	tsfgrnn		
59	yap		
60	yager	RE*	
61	zFactor	AP	'compressibility' of hydrocarbon gas

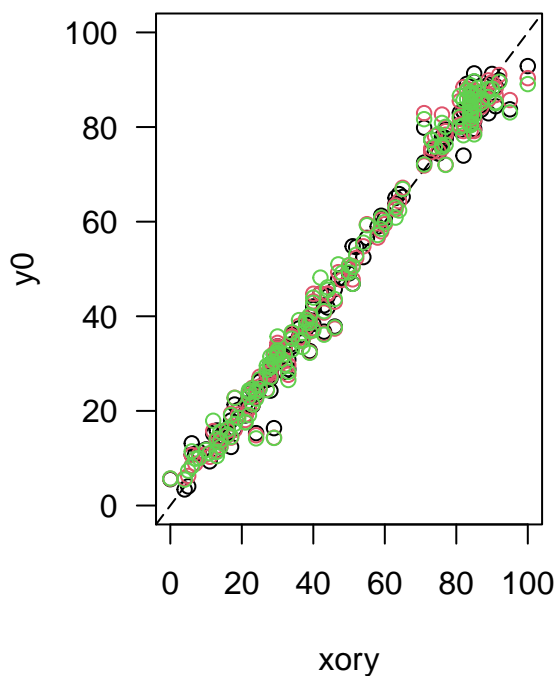
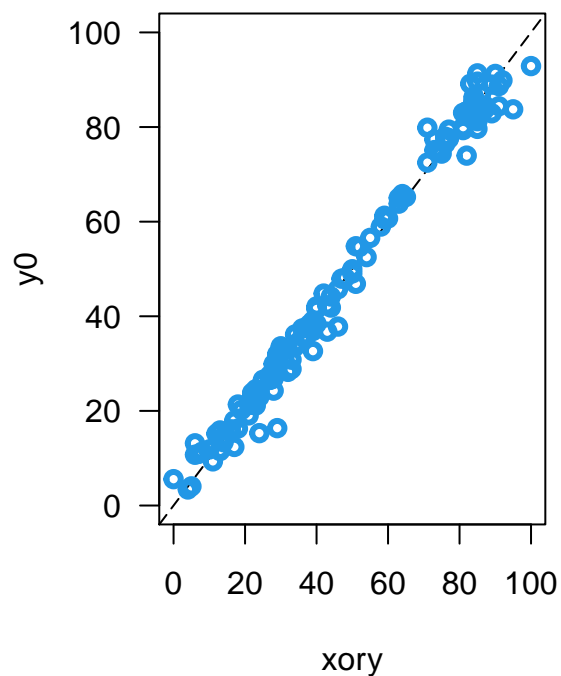
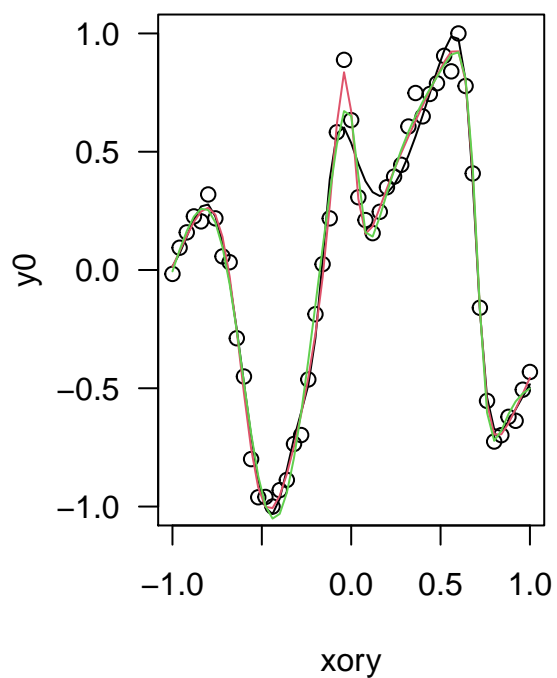
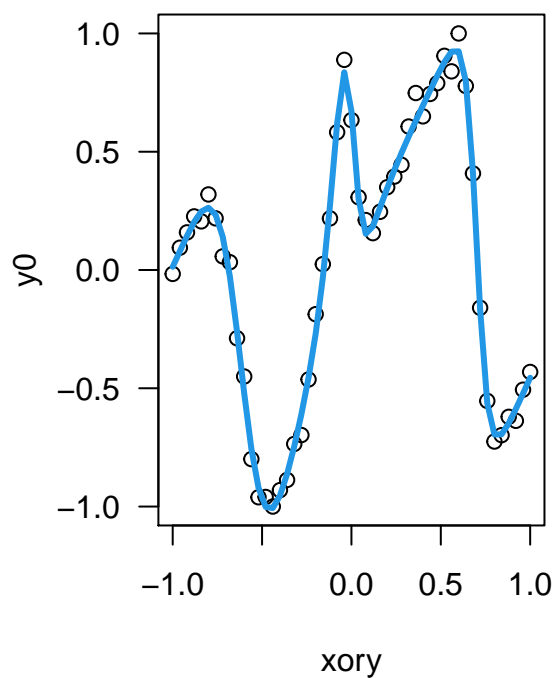
```

detach("package:nnet", unload=TRUE) }
nnet.prepareZZ <- list(xdmv = "d", ydmv = "v", zdm = "d", scale = TRUE)

res <- trainPredict_1pkg(4:5, pkgname = "nnet", pkgfun = "nnet", nnet.method,
  prepareZZ.arg = nnet.prepareZZ, nrep = nrep, doplot = TRUE,

```

```
csvfile = FALSE, rdafile = FALSE, odir = odir, echo = FALSE)
```

mRef153_nnet::nnet_BFGS**mRef153_nnet::nnet_BFGS****uDmod1_nnet::nnet_BFGS****uDmod1_nnet::nnet_BFGS**

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