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

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Abstract

(SB) There are many R packages whose purpose is neural network modeling. With support of the Google Summer of Code (GSoC) initiative for R, two of the authors were supported, mentored by the other authors, to attempt to benchmark and report on as many ofthese packages as possible. This article presents the overall purpose of the study and the research problems investigated, the basic design of the study, the major findings or trends found as a result of our analysism a brief summary of our interpretations and conclusions. These have been encapsulated in the NNbenchmark package.

(PK) For the last 30 years, neural networks have evolved from an academic topic (exploratory field of research in the academic community) to a common word in scientific computing. Following this trend, CRAN has been accepting and hosts many packages that claim to provide neural network modeling. Our latest count in May 2020 is 70 (?) packages. This is fine but how accurate and reliable are these packages? Can we trust all them? Are there packages that perfom better and are easier to use than other packages? Are there packages better suited to beginners and other packages better suited to experts? Do these packages provide the (full set of) features that can be found in some older respected (trusted) proprietary software?

This paper is, to our knowledge, the first attempt to test this vast amount of packages on (with/against) a few datasets of (with) different levels of complexity, from simple to difficult (hard) to train, benchmark them with a certain metrics, and finally rank them. The evaluation was conducted by the first two authors during summers 2019 and 2020, as students enrolled in the Google Summer of Code program, with templates prepared by the last two authors. Due to time constraints, we restricted our evaluation to regression algorithms and ignore algorithms for classification and exotic purpose. This left us with 49 (in 2019, 60 in 2020?) pairs packages::algorithms. The criteria used in our benchmark are: (i) the accuracy, i.e. the ability to find the global minima on 13 datasets, measured by the Root Mean Square Error (RMSE), (ii) the speed of the training algorithm, (iii) the ease of use, (iv) the quality of the documentation.

All packages::algorithms were given a score for each criterion and ranked in a global table. Overall, 12/15 packages::algorithms are considered accurate and reliable and can be recommended for a daily use. 45 packages should be avoided as they are not accurate, takes too much time, are difficult to handle or have poor or even no documentation.

Our package called NNbenchmark, the templates and the code used to test each package::algorithm are available on Github at the address github.com/ and can be used by the package authors to verify their metrics and eventually improve their package. Finally, we provide some hints and features of a dreamed neural network package that could serve as a guidance for developing the next generation of R neural network packages.

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 are a class of models, based on the brain's own connections system, in the growing field of machine learning for which R has a number of tools. Previously, neural networks could be considered more theory than practise, partly because the algorithms used are computationally demanding.

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 of suitability of the model 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 our available data (a training set) and tested on the remaining data. Modern software allows the much of this work, including approximation of the gradient, to be carried out without a large effort by the the user.

This process can generally be made more efficient if we also can 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) ideas for updating the Hessian approximation (or its inverse) provide several well-known examples. In conducting this study, we believed that these second-order algorithms would perform better than first-order methods.

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 tanh(), and one output output layer.

Methodology

??JN: ******************************

In working on material below, I think we need to provide some explanation of goals - What does "convergence" mean in our context? - What do we mean by RMSE, other measures? Should define here for later use. - What do we mean by "performance"? Other goals?

Our research process was divided into 3 phases.

Phase 1 - Preparation

Datasets => NEED TO BE FINISHED

All the datasets used are nonlinear. ??JN. what do we mean by nonlinear – it has several different uses?? Linear data sets are more simple and can even be solved with OLS (Ordinary Least Squares) regression.

?? Do we mean?

All the datasets we use are nonlinear in that they cannot be modelled using a non-iterative calculation such as Ordinary Least Squares. In this study, we wish to test the ability of neural networks to model systems that are beyond the scope of linear regression. Varying levels of difficulty in modelling 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 taken from . . .

Three of the univariate datasets we used were taken from a webside 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 from . . .

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. NeuroOne from . . .
Wood . . .

Packages

Using **RWsearch** (Kiener, 2020) we sought all were able to automate the process. All packages that have "neural network" as a keyword in the package title or in the package description were included.

The following is a list of packages we included in this study, with brief descriptions.

1. **AMORE** (Limas et al., 2020),
2. **ANN2** (Lammers, 2020),
3. **appnn** (Família et al., 2015),
4. **autoencoder** (Dubossarsky and Tyshetskiy, 2015),
5. **automl** (Boulangé, 2020),
6. **BNN** (Jia, 2018),
7. **brnn** (Rodriguez and Gianola, 2020),
8. **Buddle** (Kim, 2020),
9. **CaDENCE** (Cannon, 2017a),
10. **cld2** (Ooms, 2018),
11. **cld3** (Ooms, 2020),
12. **condmixt** (Carreau, 2020),
13. **DamiaNN** (Siniakowicz, 2016),
14. **deep** (Mayer, 2019),
15. **deepdive** (Balakrishnan, 2020),
16. **deepnet** (Rong, 2014),
17. **deepNN** (Taylor, 2020),
18. **DNMF** (Jia and Zhang, 2015),
19. **elmNNRcpp** (Mouselimis and Gosso, 2018),
20. **ELMR** (Petrozziello, 2015),
21. **EnsembleBase** (Mahani and Sharabiani, 2016),
22. **evclass** (Denoeux, 2017),
23. **gamlss.add** (Stasinopoulos et al., 2020),
24. **gcForest** (Jing, 2018),
25. **GMDH** (Dag and Yozgatligil, 2016),
26. **GMDH2** (Dag et al., 2019),
27. **GMDHreg** (Tilve, 2019),
28. **gnn** (Hofert and Prasad, 2020),
29. **grnn** (Chasset, 2013a),
30. **h2o** (LeDell et al., 2020),
31. **hybridEnsemble** (Ballings et al., 2015),
32. **isingLenzMC** (Suzen, 2016),
33. **keras** (Allaire and Chollet, 2019),
34. **kerasR** (Arnold, 2017),
35. **leabRa** (Titz, 2017),
36. **learNN** (Quast, 2015),
37. **LilRhino** (Barton, 2019),
38. **minpack.lm** (Elzhov et al., 2016),
39. **MachineShop** (Smith, 2020),

40. **monmlp** (Cannon, 2017b),
41. **neural** (Nagy, 2014),
42. **neuralnet** (Fritsch et al., 2019),
43. **NeuralNetTools** (Beck, 2018),
44. **NeuralSens** (Portela González et al., 2020),
45. **NlinTS** (Hmamouche, 2020),
46. **nlsr** (Nash and Murdoch, 2019),
47. **nnet** (Ripley, 2020),
48. **nnetpredint** (Ding, 2015),
49. **nnfor** (Kourentzes, 2019),
50. **nntrf** (Aler and Valls, 2020),
51. **nnli2bRcpp** (Nikolaidis, 2020),
52. **onnx** (Tang and ONNX Authors, 2018),
53. **OptimClassifier** (Perez-Martin et al., 2020),
54. **OSTSC** (Dixon et al., 2017),
55. **pnn** (Chasset, 2013b),
56. **polyreg** (Matloff et al., 2020),
57. **predictoR** (with contributions from Diego Jimenez A. and D., 2019),
58. **qrnn** (Cannon, 2019),
59. **QuantumOps** (Resch, 2020),
60. **quarrint** (Barthelemy et al., 2016),
61. **radiant.model** (Nijs, 2020),
62. **rasclass** (Wiesmann and Quinn, 2016),
63. **rcane** (Suresh et al., 2018),
64. **regressoR** (Rodriguez R., 2019),
65. **rminer** (Cortez, 2020),
66. **rnn** (Quast and Fichou, 2019),
67. **RSNNS** (Bergmeir, 2019),
68. **ruta** (Charte et al., 2019),
69. **simpleNeural** (Dernoncourt, 2020),
70. **snnR** (Wang et al., 2017),
71. **softmaxreg** (Ding, 2016),
72. **Sojourn.Data** (Hibbing and Lyden, 2019),
73. **spnn** (Ebrahimi, 2020),
74. **TeachNet** (Steinbuss, 2018),
75. **tensorflow** (Allaire and Tang, 2019),
76. **tfestimators** (Allaire et al., 2018),
77. **trackdem** (Bruijning et al., 2020),
78. **TrafficBDE** (Chatzopoulou et al., 2018),
79. **tsensembler** (Cerqueira et al., 2017),
80. **validann** (Humphrey, 2017),
81. **zFactor** (Reyes, 2019).

In contrast, we consider the following packages to be ill-suited to our investigations, and include a brief description of each with a reason why we have excluded it.

?? packages here.

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. They are simply meta-packages. Others were not regression neural networks of the perceptron type or were only intended for very specific purposes.

Template => TO REVISE AFTER 2020 CODE

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 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 RMSE and MAE (??definition, reference) (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; and
(4) Clearing up the environment for the next package. (5) 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 the 2019 GSoC activity and later refined in the 2020 initiative. The package repository is `https://github.com/pkR-pkR/NNbenchmark`, with package templates in `https://github.com/pkR-pkR/NNbenchmarkTemplates`).

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 tempplates repository.

Analysis

To rank the 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
6. In addition to the previous metrics, two other convergence metrics have been considered: the Mean Absolute Error (MAE) and the Worst Absolute Error (WAE), see Appendix. The ranking on those two metrics may help distinguish packages with close RMSE values. However, we do not choose the MAE for overall ranking as there

is no consensus in the literature, see e.g. (Willmott and Matsuura, 2005; Chai and Draxler, 2014).

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

Tables (NOTE: FINAL MEASURE FOR CONVERGENCE - RMSE RANKS? OR A COMBINATION OF OTHER MEASURES? As in Christophe's recent email: L1 MAE(), L2 RMSE(), Linfinity (WAE)) –> see Appendix

(ALSO: THE FOLLOWING IS SIMPLY ALPHABETIC LIST FOR ALL TESTED, I WILL DIVIDE THE TABLE INTO 4: 2nd ORDER always recommended, 1st ORDER recommended, 1st ORDER not recommended, untested packages)

Table X: Ratings

No	Name (package::algorithm)	RMSE	DUR	UTIL	DOCS	OVERALL
1	**AMORE**::train.ADAPTgd					
	AMORE::train.ADAPTgdwm					
	AMORE::train.BATCHgd					
	AMORE::train.BATCHgdwm					
2	**automl**					
3	**ANN2**::neuralnetwork.sgd					
	ANN2::neuralnetwork.adam					
	ANN2::neuralnetwork.rmsprop					
4	**brnn**					
5	**CaDENCE**					
6	**deepnet**::gradientdescent					
7	**elmNNRcpp**					
8	**ELMR**					
9	**h2o**::deeplearning					
10	**keras**					
11	**kerasformula**					
12	**kerasR**					
13	**minpack.lm**::nlsLM					
14	**MachineShop**::fit.NNetModel()					
15	**monmlp**::fit.BFGS					
	monmlp::fit.Nelder-Mead					
16	**neural**::mlptrain					
17	**neuralnet**::backprop					
	neuralnet::rprop+					
	neuralnet::rprop-					
	neuralnet::sag					
	neuralnet::slr					
18	**nlsr**::nlxb					
19	**nnet**::nnet.BFGS					
20	**qrnn**::qrnn.fit					
21	**radiant.model**::radiant.model					
22	**rcane**::rlm					
23	**rminer**::fit					
24	**RSNNS**::BackpropBatch					
	RSNNS::BackpropChunk					
	RSNNS::BackpropMomentum					
	RSNNS::BackpropWeightDecay					
	RSNNS::Quickprop					
	RSNNS::Rprop					
	RSNNS::SCG					
	RSNNS::Std-Backpropagation					
25	**ruta**					
26	**simpleNeural**::sN.MLPtrain					
27	**snnR**					
28	**softmaxreg**					
29	**tensorflow**::AdadeltaOptmizer					
	tensorflow::AdagradOptmizer					
	tensorflow::AdamOptmizer					
	tensorflow::FtrlOptmizer					
	tensorflow::GradientDescent					
	tensorflow::MomentumOptmizer					
30	**tfestimators**					
31	**tsensembler**					
32	**validann**::Nelder-Mead					
	validann::BFGS					
	validann::CG					
	validann::L-BFGS-B					
	validann::SANN					
	validann::Brent					

(THE FOLLOWING IS JUST AN ALPHABETICALLY ORDERED LIST OF CURRENTLY UNTESTED PACKAGES)

Table 2: Review of Ommitted Packages

No	Name (package)	Category	Comment
1	**appnn**	-	
2	**autoencoder**	-	
3	**BNN**	-	
4	**Buddle**	-	
5	**cld2**	-	
6	**cld3**	-	
7	**condmixt**	-	
8	**DALEX2**	-	
9	**DamiaNN**	-	
10	**DChaos**	-	
11	**deepNN**	-	
12	**DNMF**	-	
13	**EnsembleBase**	-	
14	**evclass**	-	
15	**gamlss.add**	-	
16	**gcForest**	-	
17	**GMDH**	-	
18	**GMDH2**	-	
19	**GMDHreg**	-	
20	**grnn**	-	
21	**hybridEnsemble**	-	
22	**isingLenzMC**	-	
23	**leabRa**	-	
24	**learNN**	-	
25	**LilRhino**	-	
26	**NeuralNetTools**	-	tools for neural networks
27	**NeuralSens**	-	tools for neural networks
28	**NlinTS**	NA	Time Series
29	**nnetpredint**	-	confidence intervals for NN
30	**nnfor**	NA	Times Series, uses neuralnet
31	**onnx**	-	provides an open source format
32	**OptimClassifier**	NA	choose classifier parameters, nnet
33	**OSTSC**	-	solving oversampling classification
34	**pnn**	NA	Probabilistic
35	**polyreg**	-	polyregression ALT to NN
36	**predictoR**	NA	shiny interface, neuralnet
37	**QuantumOps**	NA	classifies MNIST, Schuld (2018)
38	**quarrint**	NA	specified classifier for quarry data
39	**rasclass**	NA	classifier for raster images, nnet?
40	**regressoR**	NA	a manual rich version of predictoR
41	**rnn**	NA	Recurrent
42	**Sojourn.Data**	NA	sojourn Accelerometer methods, nnet?
43	**spnn**	NA	classifier, probabilistic
44	**TeachNet**	NA	classifier, selfbuilt, slow
45	**trackdem**	NA	classifier for particle tracking
46	**TrafficBDE**	NA	specific reg, predicting traffic
47	**zFactor**	NA	'compressibility' of hydrocarbon gas

Discussion and Recommandations

A. Recommended: 2nd order algorithms Out of all the algorithms, these second algorithms generally performed better in terms of convergence despite being set to a much lower number of iterations, 200, than the first-order algorithms. Moreover, they performed better in terms of speed. The best in this class were. **minpack.lm** and. **nlsr**, tied at rank number 1. The Levenberg-Marquardt (LM) algorithm used is fast and converges well. stats::nls() is used. However, these packages require a handwritten formula that may not be ideal for certain situations. A more popular package for neural networks is nnet. This might be because it is part of base R. It implements the BFGS algorithm with stats::optim().

Ranked directly after are some packages that depend on nnet or use the same functions. They differ in how well they decide initial parameters. rminer (rank 4), MachineShop (rank 5), and radiant.model (rank 7) use nnet. Note, radiant.model has its iterations set to 10000, which originally made it slower yet converge better. We used a modified version of the package. At rank 6 is validann's BFGS algorithm using stats::optim(). Its use of optim's L-BFGS-B ranked at number 9 with CaDENCE's use of optim's BFGS.. **monmlp**, from the same author as CaDENCE (Alex Cannon), uses the package. **optimx**'s BFGS (Nash and Varadhan, 2020).

Alex Cannon also implemented a quantile regression neural network in qrnn with stats::nlm(). It requires more iterations and is not as fast compared to the other second-order algorithms. However, it is a valuable implementation of quantile regression. Last but not least is **brnn**'s Gauss Newton algorithm which ranks at number 8. brnn is easy to use but does not converge as well due to a hidden constraint: a missing first parameter. Furthermore, brnn's algorithm minimizes the sum of squared errors and a penalty on parameters instead of just the sum of squared errors. This may prevent parameters to get highly correlated, especially with an almost degenerated Jacobian matrix.

B. Recommended: 1st order algorithms validann optim CG RSNNS SCG h2o back-propagation RSNNS Rprop ANN2 adam CaDENCE Rprop -SLOW deepnet BP AMORE ADAPTgdwm AMORE ADAPTgd ANN2 sgd automl trainwgrad ANN2 rmsprop RSNNS BackpropChunk RSNNS BackWeightDecay RSNNS Std_Backpropagation RSNNS Backprop-Momentum automl trainwpso validann optim NelderMead snnR Semi Smooth Newton RSNNS BackpropBatch validann optim SANN monmlp optimx Nelder Mead

C. Not recommended: 1st order algorithms <- DISCUSS CUTOFF By package ELMR, elmNNRcpp - fast ELM algorithms. Unfortunately, can't finetune, does not converge well. neuralnet: a large ammount of iterations, slow, erratic failures tensorflow: NOT EASY TO USE, subsequently keras, tfestimators, ruta ... user needs to understand the language However, advanced users might be able to highly specify a neural network to their needs (customization?)

By algorithm: neuralnet rprop+ neuralnet rprop- neuralnet slr - once ranked well with 100000 iterations AMORE BATCHgd CaDENCE pso psoptim - need to reconfigure? elmN-NRcpp - fast, no iterations RSNNS Quickprop (?) AMORE BATCHgdwm tensorflow Mo-mentumOptimizer tensorflow AdamOptimizer ELMR - fast, no iterations tensorflow Gra-dientDescentOptimizer keras rmsprop keras adagrad keras sgd keras adadelta tensorflow AdagradOptimizer keras adam tensorflow FtrlOptimizer neuralnetwork sag tensorflow AdadeltaOptimizer neuralnet backprop - note, might not actually reflect standings, some-how from template to template the learning rate disappeared. Will fix this in future runs

D. Untested => TO DO - LIST

Conclusion => TO DO AFTER 2020 CODE

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

Future work

As the alogrithms for neural networks continue to grow, there will always be more 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.

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- The dreamed NN package: Recommandation to package authors
- Conclusion
- Acknowledgments

For the acknowledgements, maybe : « » + later some aknowledgements to the referees. How do we proceed?

Appendix

Considered a set of observations y_i and its corresponding predictions $\hat{y}_i$ for $i = 1, \ldots, n$. The three considered metrics are

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

That is, there are the absolute, the squared and the maximum norm of residual vectors.

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