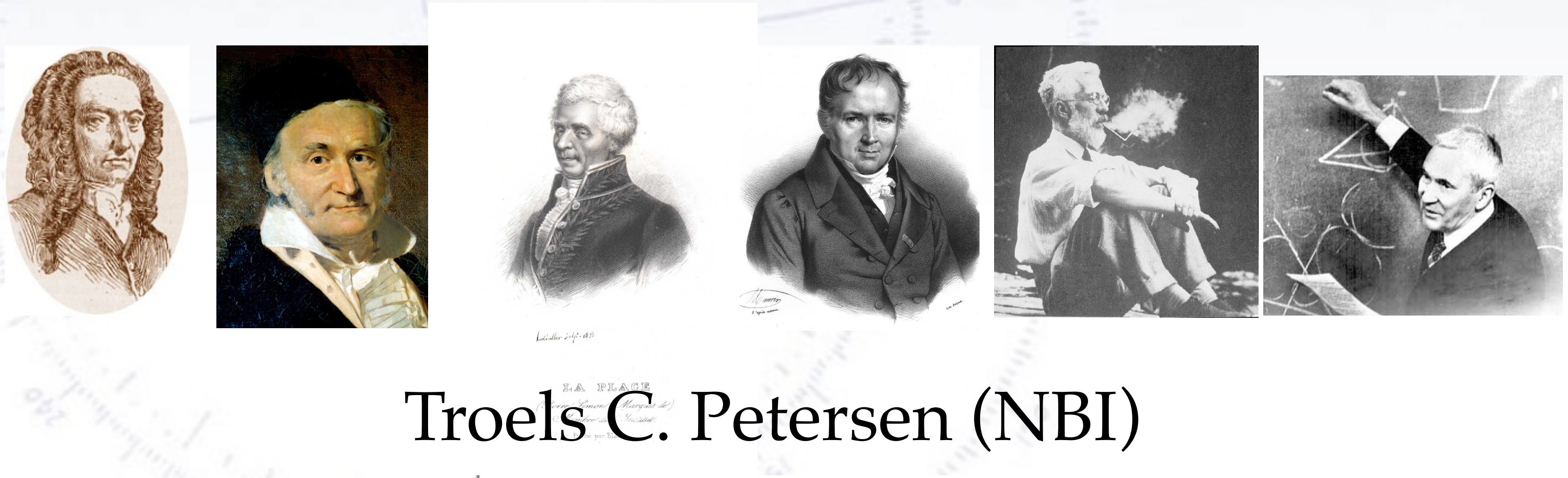
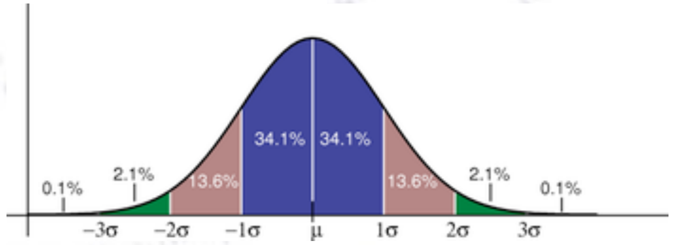
# Big Data Analysis

## Neural Networks & Deep Learning

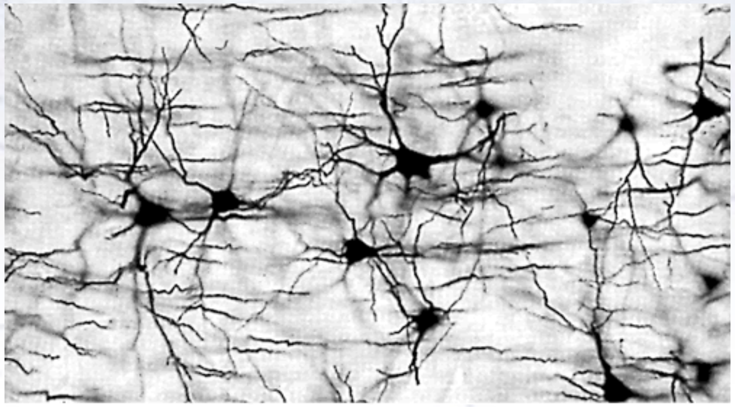


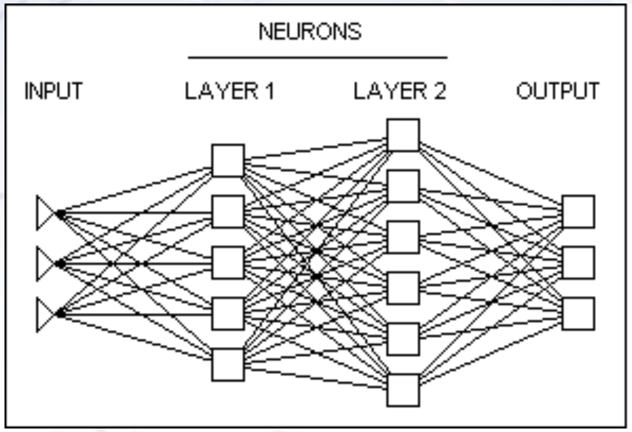
Troels C. Petersen (NBI)



*"Statistics is merely a quantisation of common sense - Machine Learning is a sharpening of it!"*

# Neural Networks (NN)





*In machine learning and related fields, artificial neural networks (ANNs) are computational models inspired by an animal's central nervous systems (in particular the brain) which is capable of* ***machine learning*** *as well as* ***pattern recognition****.*

***Neural networks*** *have been used to solve a wide variety of tasks that are hard to solve using ordinary rule-based programming, including* ***computer vision*** *and* ***speech recognition****.*

[Wikipedia, Introduction to Artificial Neural Network]

# Neural Networks

Neural Networks combine the input variables using a "activation" function s(x) to assign, if the variable indicates signal or background.

The simplest is a single layer perceptron:

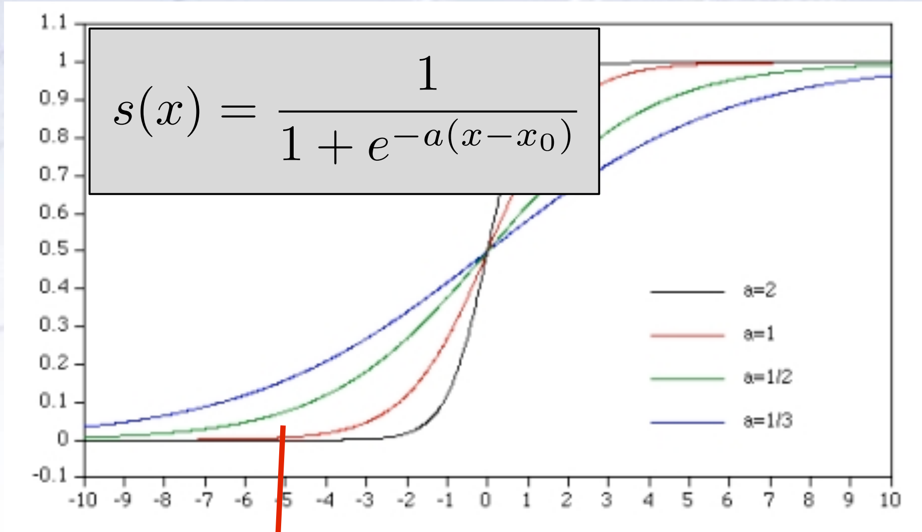
$$t(x) = s\left(a_0 + \sum a_i x_i\right)$$

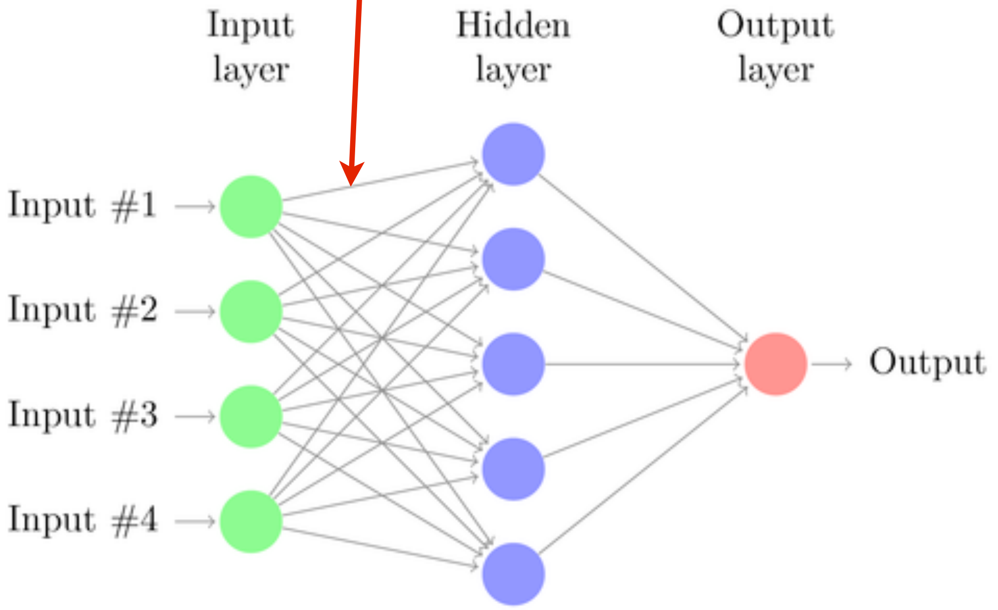
This can be generalised to a multilayer perceptron:

$$t(x) = s\left(a_i + \sum a_i h_i(x)\right)$$

$$h_i(x) = s\left(w_{i0} + \sum w_{ij} x_j\right)$$

Activation function can be any sigmoid function.





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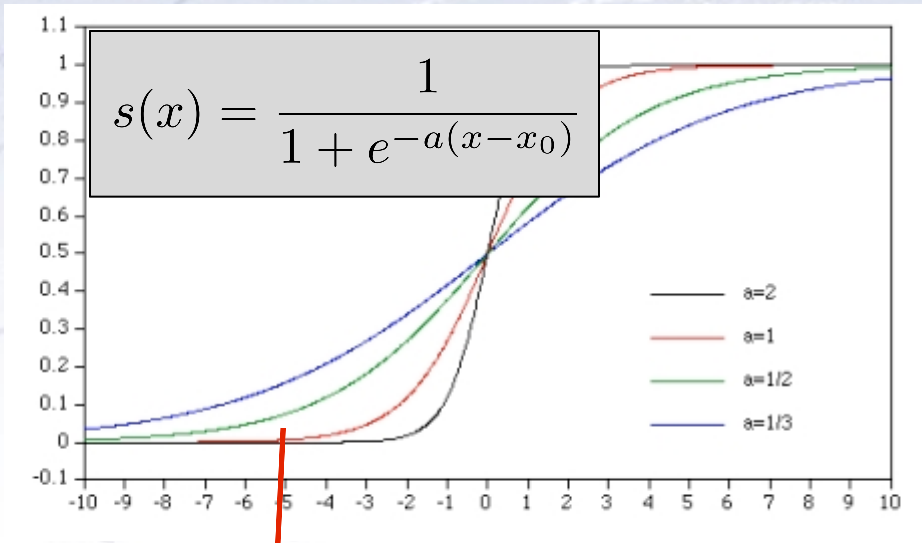
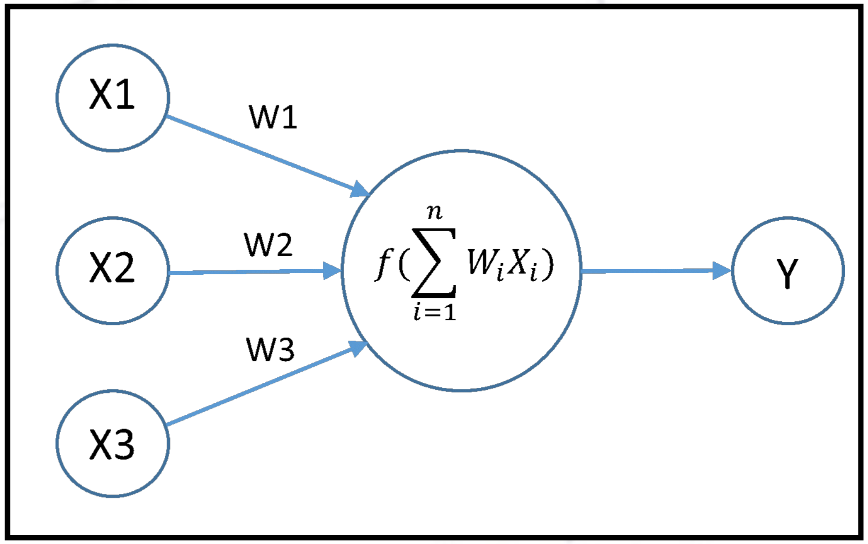
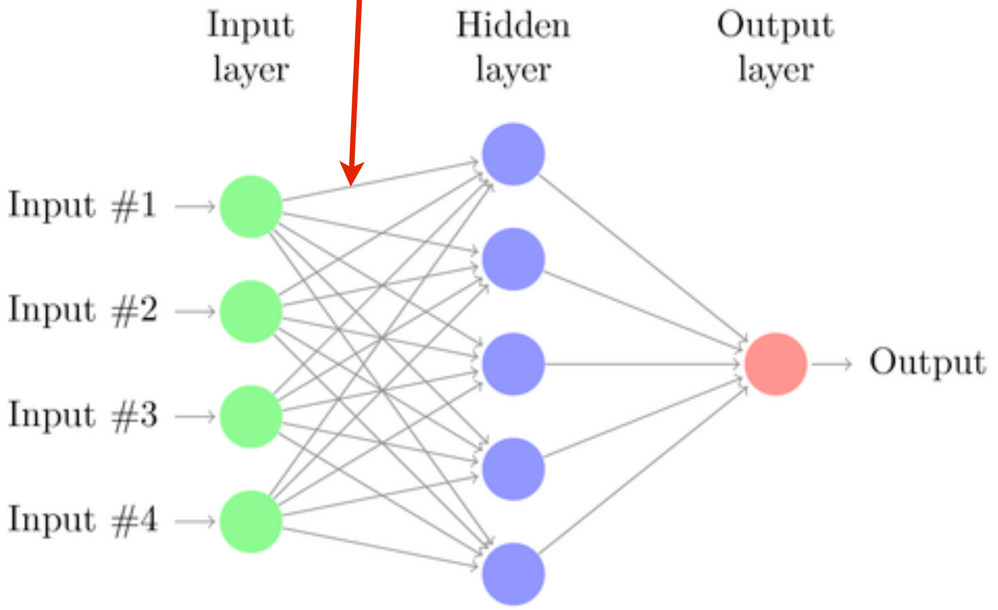


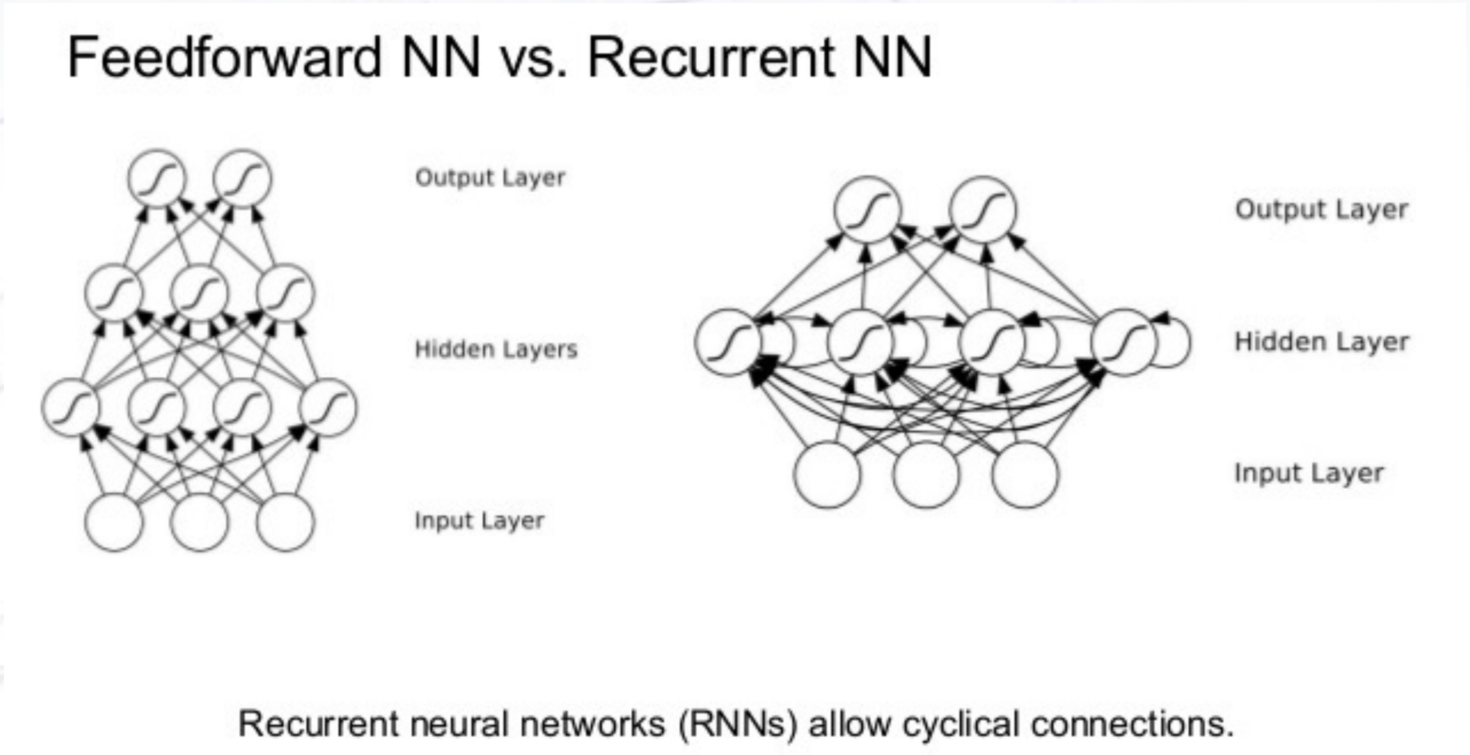




# Recurrent NN

Normally, the information from one layer is fed forward to the next layer in a feedforward Neural Network (NN).

However, it may be of advantage to allow a network to give feedback, which is called a recurrent NN:

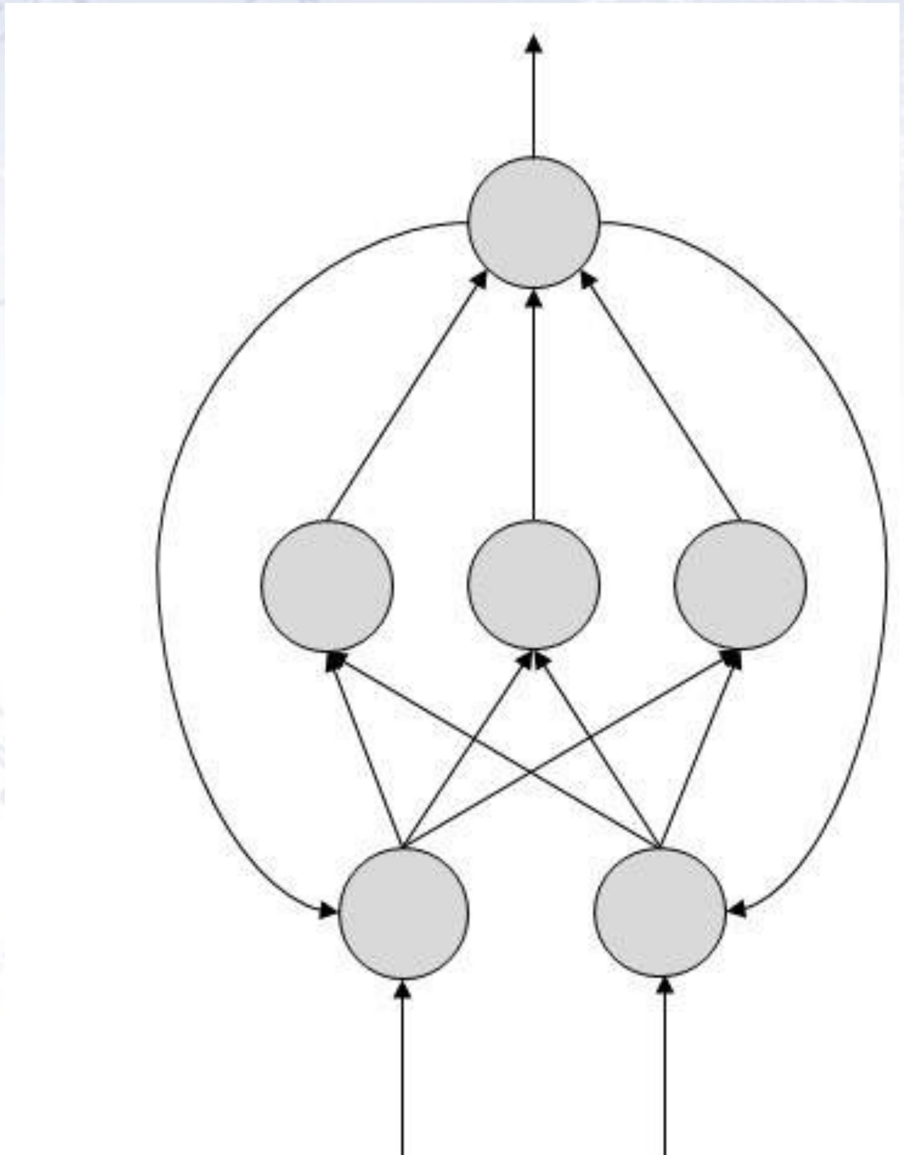

Feedforward NN vs. Recurrent NN
Output Layer
Hidden Layers
Input Layer
Output Layer
Hidden Layer
Input Layer
Recurrent neural networks (RNNs) allow cyclical connections.

# Feedback network

There is nothing that prohibits the use of feedback in the network.

In this way, one can pass information "back" in the network, allowing for input of "more advanced" neurons to earlier neurons.

Note, that it requires skill and knowledge (and time and hard work) to design the network that suits your problem!



# Networks with “memory”

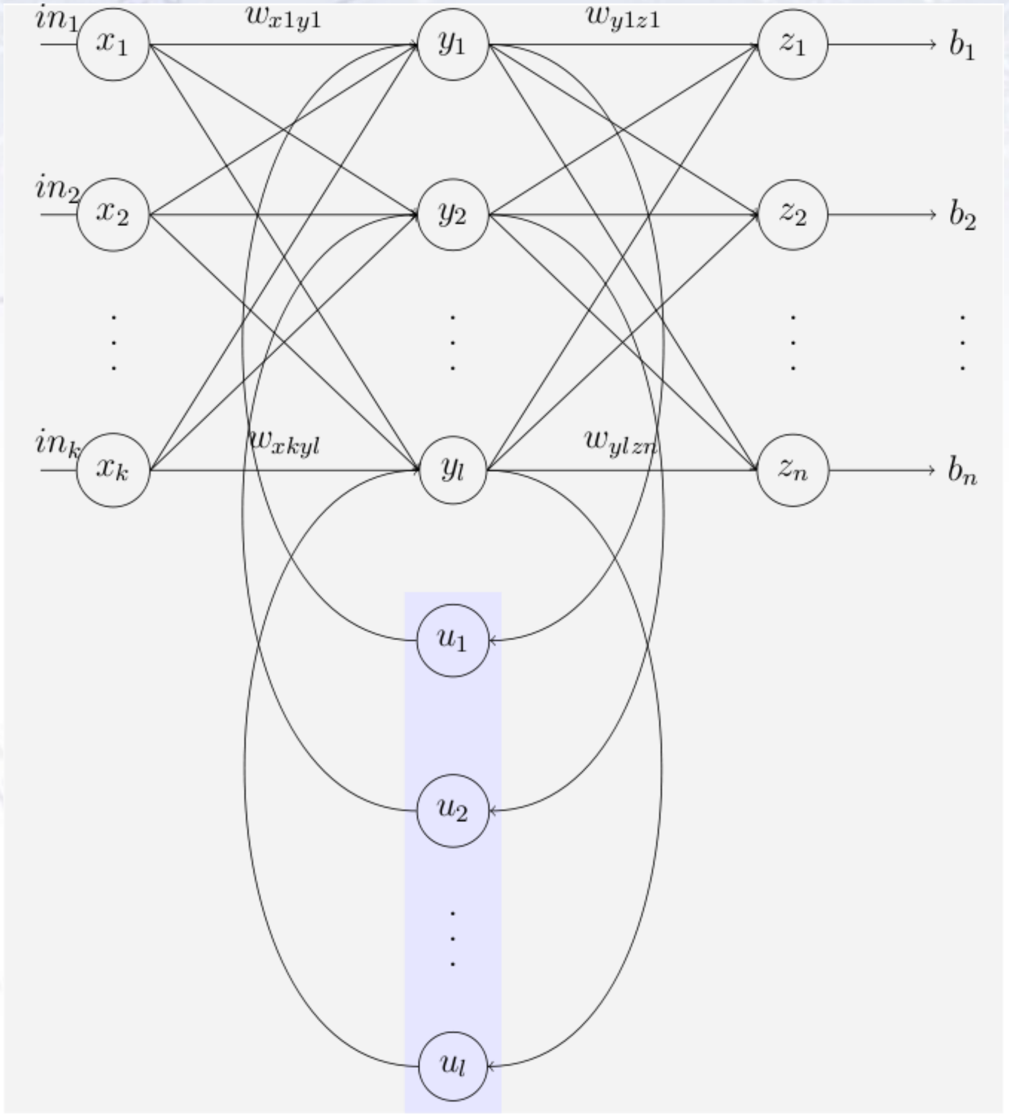
**So-called Long Short-Term Memory (Elman and Jordan) networks**

Allowing for feedback, one can also use this for providing “memory” of the last state(s) of the network.

This can be used for including “context” or “environment” in the network.

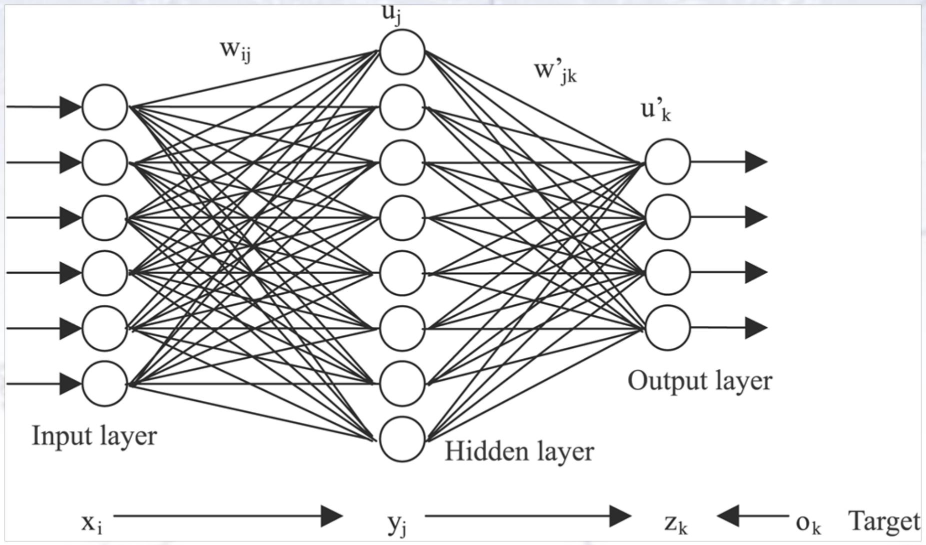
This can be used in case of e.g. a new user regarding adds, a new context regarding translation,

The keyword is Long Short-Term Memory (LSTM), if you want to look for more…



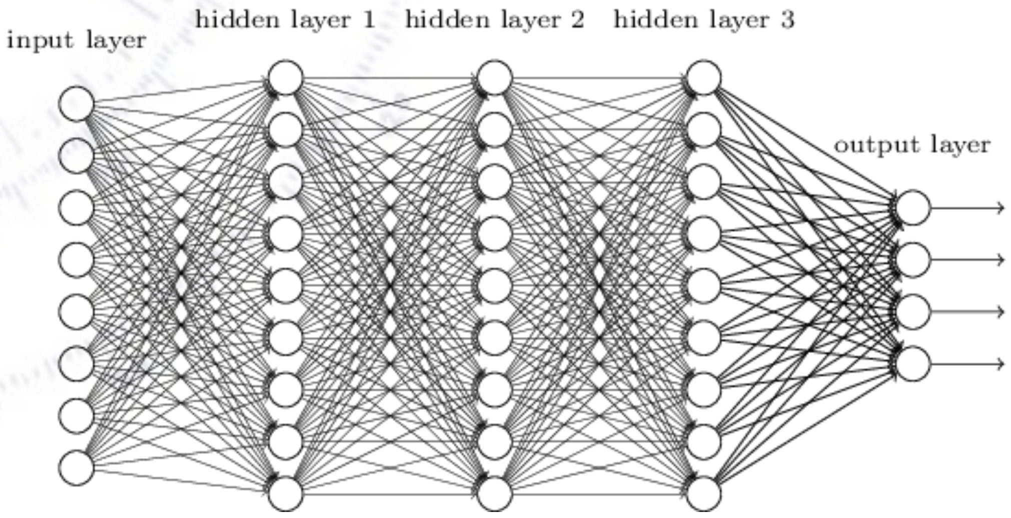
# Deep Neural Networks

Deep Neural Networks (DNN) are simply (much) extended NNs in terms of layers!



Instead of having just one (or few) hidden layers, many such layers are introduced.
This gives the network a chance to produce key features and use them for many different specialised tasks.

Currently, DNNs can have up to millions of neurons and connections, which compares to about the **brain of a worm**.



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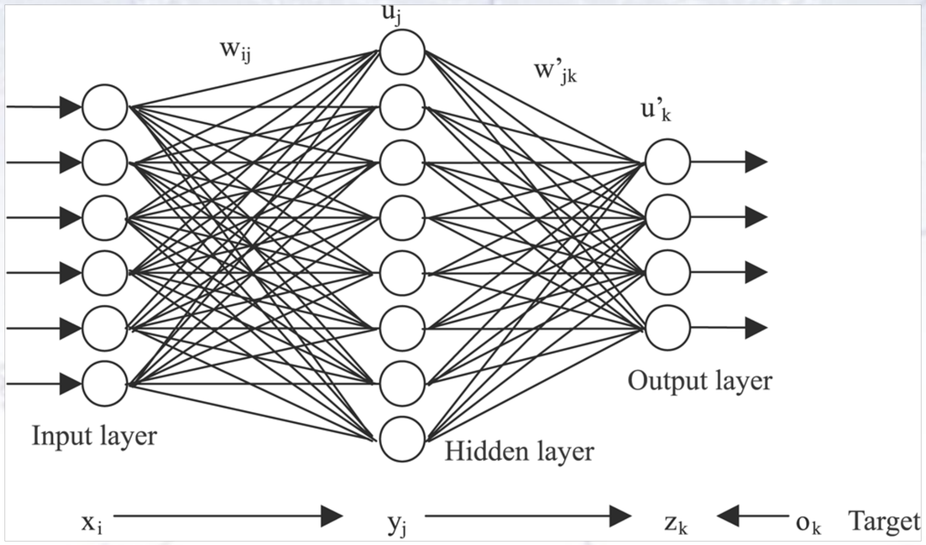

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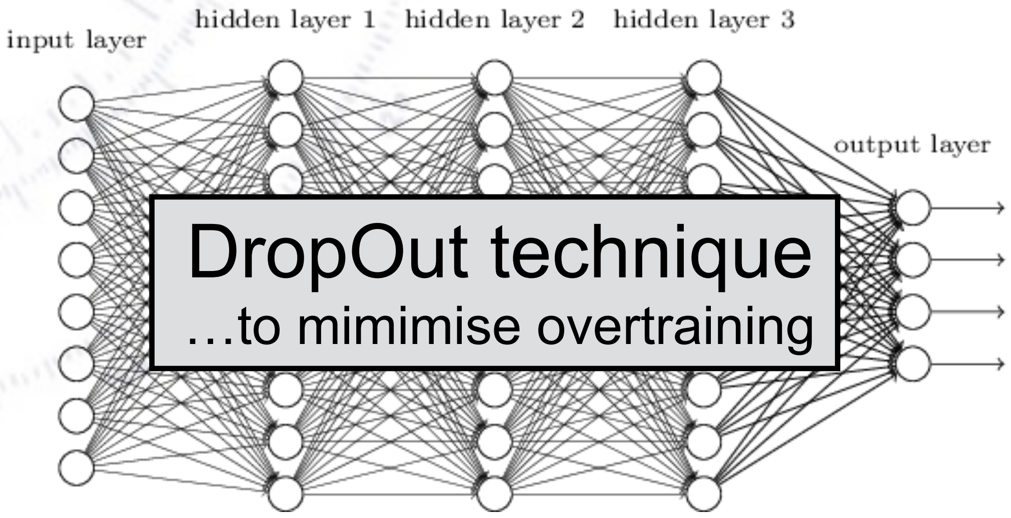
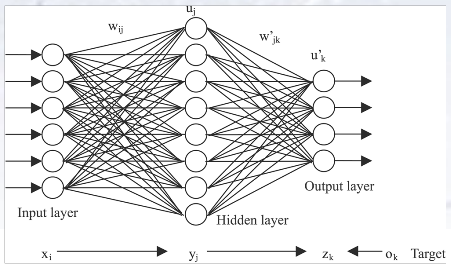
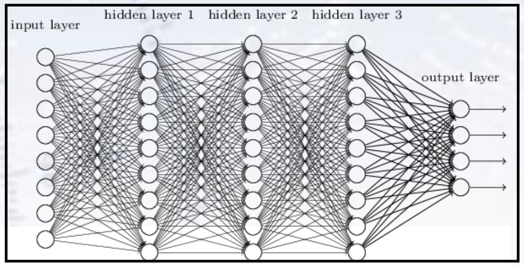


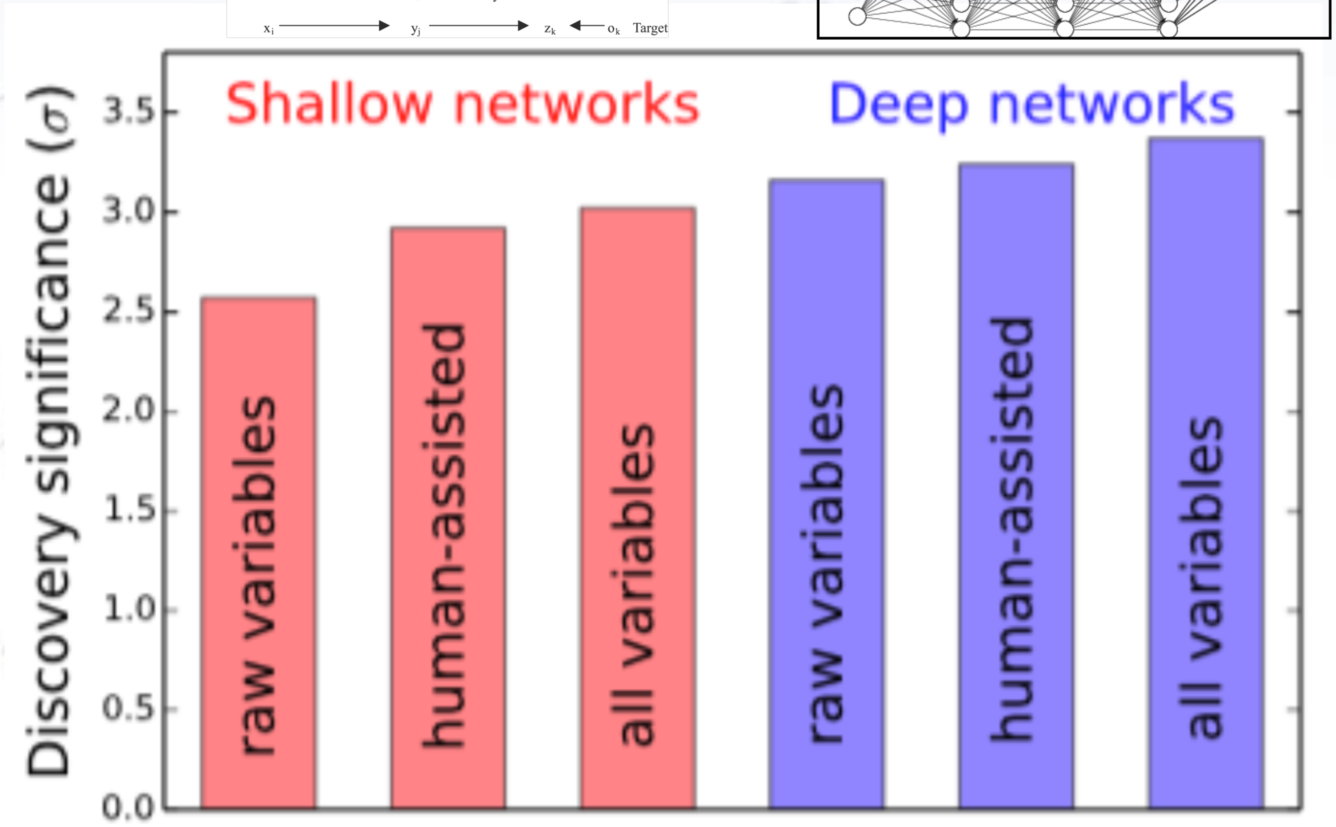
DropOut technique
…to mimimise overtraining

# Deep Neural Networks

Deep Neural Networks likes to get both raw and "assisted" variables:



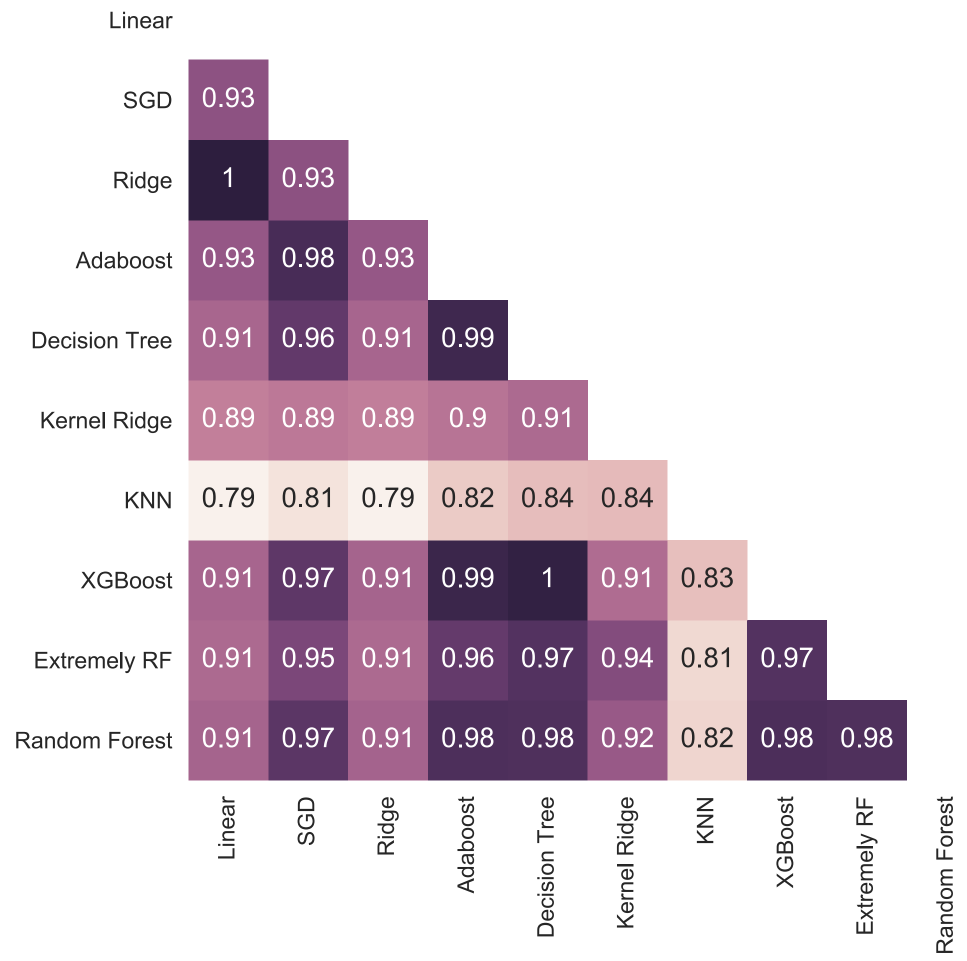




# Different ML answers

The many algorithms each produce an estimate, which are naturally very correlated, with the estimates of the other algorithms. But they are not identical…

Correlation between different models' prediction



| | Linear | SGD | Ridge | Adaboost | Decision Tree | Kernel Ridge | KNN | XGBoost | Extremely RF | Random Forest |
|---|---|---|---|---|---|---|---|---|---|---|
| Linear | | | | | | | | | | |
| SGD | 0.93 | | | | | | | | | |
| Ridge | 1 | 0.93 | | | | | | | | |
| Adaboost | 0.93 | 0.98 | 0.93 | | | | | | | |
| Decision Tree | 0.91 | 0.96 | 0.91 | 0.99 | | | | | | |
| Kernel Ridge | 0.89 | 0.89 | 0.89 | 0.9 | 0.91 | | | | | |
| KNN | 0.79 | 0.81 | 0.79 | 0.82 | 0.84 | 0.84 | | | | |
| XGBoost | 0.91 | 0.97 | 0.91 | 0.99 | 1 | 0.91 | 0.83 | | | |
| Extremely RF | 0.91 | 0.95 | 0.91 | 0.96 | 0.97 | 0.94 | 0.81 | 0.97 | | |
| Random Forest | 0.91 | 0.97 | 0.91 | 0.98 | 0.98 | 0.92 | 0.82 | 0.98 | 0.98 | |

These very high correlations are of course to be expected. But they are mostly driven by values far from the actual price. If these are excluded, we get…

# Different ML answers

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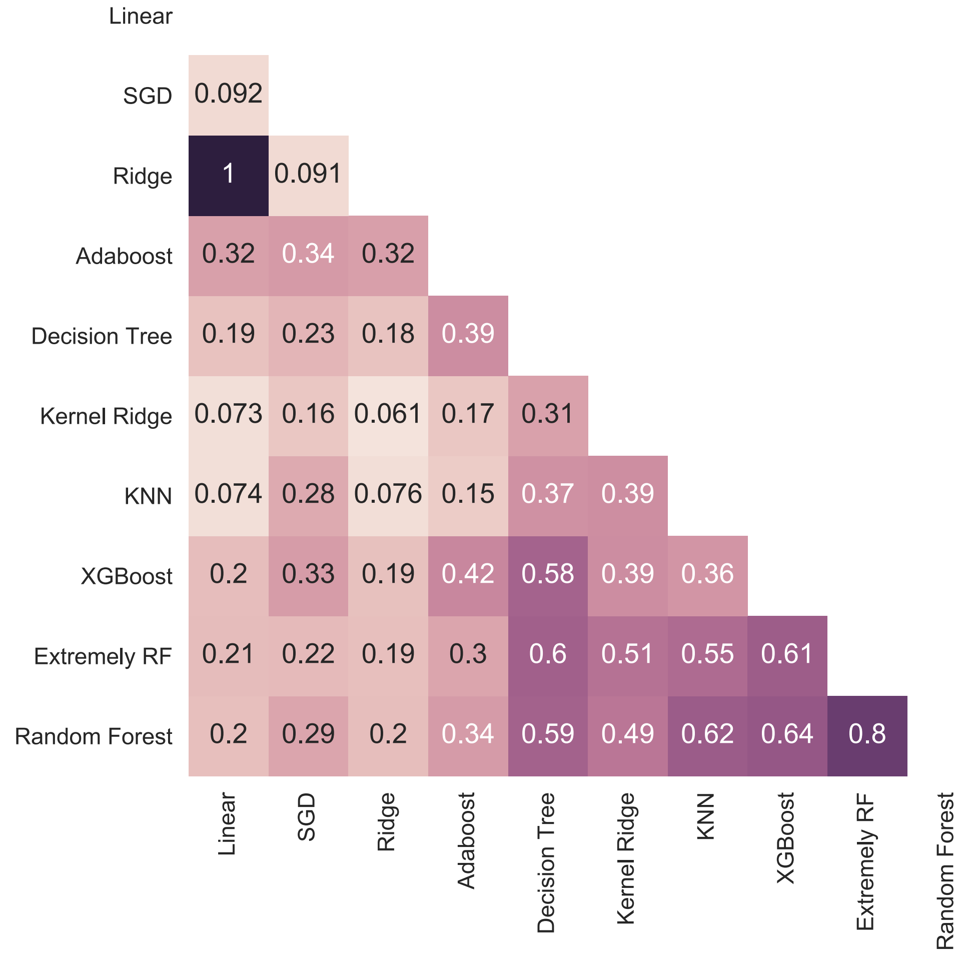
Correlation between different models' prediction within +/- 50%



| | Linear | SGD | Ridge | Adaboost | Decision Tree | Kernel Ridge | KNN | XGBoost | Extremely RF | Random Forest |
|---|---|---|---|---|---|---|---|---|---|---|
| Linear | | | | | | | | | | |
| SGD | 0.092 | | | | | | | | | |
| Ridge | 1 | 0.091 | | | | | | | | |
| Adaboost | 0.32 | 0.34 | 0.32 | | | | | | | |
| Decision Tree | 0.19 | 0.23 | 0.18 | 0.39 | | | | | | |
| Kernel Ridge | 0.073 | 0.16 | 0.061 | 0.17 | 0.31 | | | | | |
| KNN | 0.074 | 0.28 | 0.076 | 0.15 | 0.37 | 0.39 | | | | |
| XGBoost | 0.2 | 0.33 | 0.19 | 0.42 | 0.58 | 0.39 | 0.36 | | | |
| Extremely RF | 0.21 | 0.22 | 0.19 | 0.3 | 0.6 | 0.51 | 0.55 | 0.61 | | |
| Random Forest | 0.2 | 0.29 | 0.2 | 0.34 | 0.59 | 0.49 | 0.62 | 0.64 | 0.8 | |

## So which algorithm to use?

# 179 methods vs. 121 data sets

"Tree learning comes closest to meeting the requirements for serving as an off-the-shelf procedure for data mining", because it:

- is invariant under scaling and various other transformations of feature values,
- is robust to inclusion of irrelevant features,
- produces inspectable models.
- HOWEVER… they are seldom accurate (i.e. most performant)!

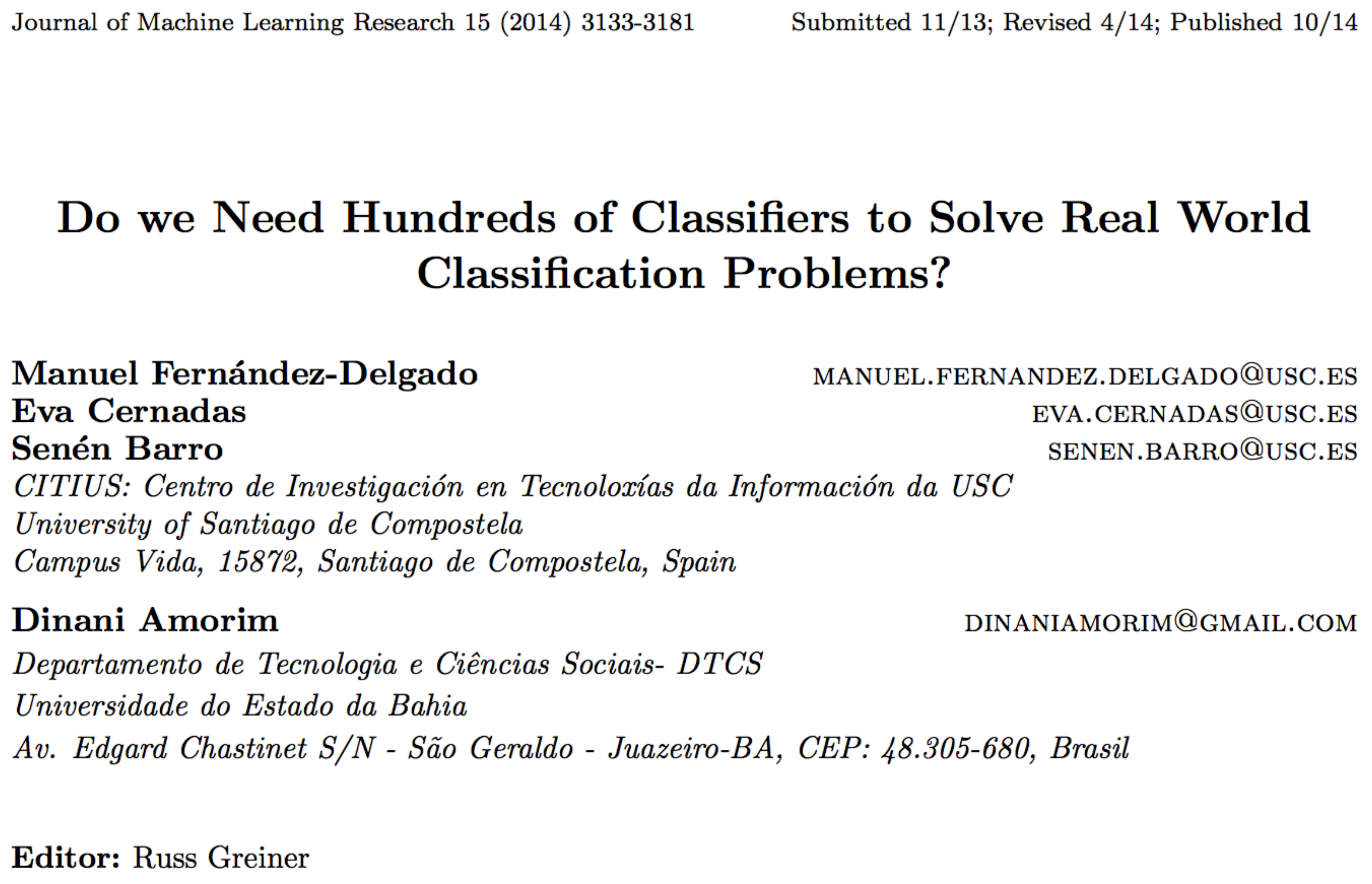
**[Trevor Hastie, Professor of Mathematics & Statistics, Stanford University]**

In a quite interesting paper, four authors investigated the performance of many Machine Learning (ML) methods (179 in total) on a large variety of data sets (121 in total).

The purpose was to see, if there was any general pattern, and if some type of classifiers were more suited for some problems than others.

Their findings were written up in the following paper…

# 179 methods vs. 121 data sets



Journal of Machine Learning Research 15 (2014) 3133-3181 Submitted 11/13; Revised 4/14; Published 10/14

## Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?

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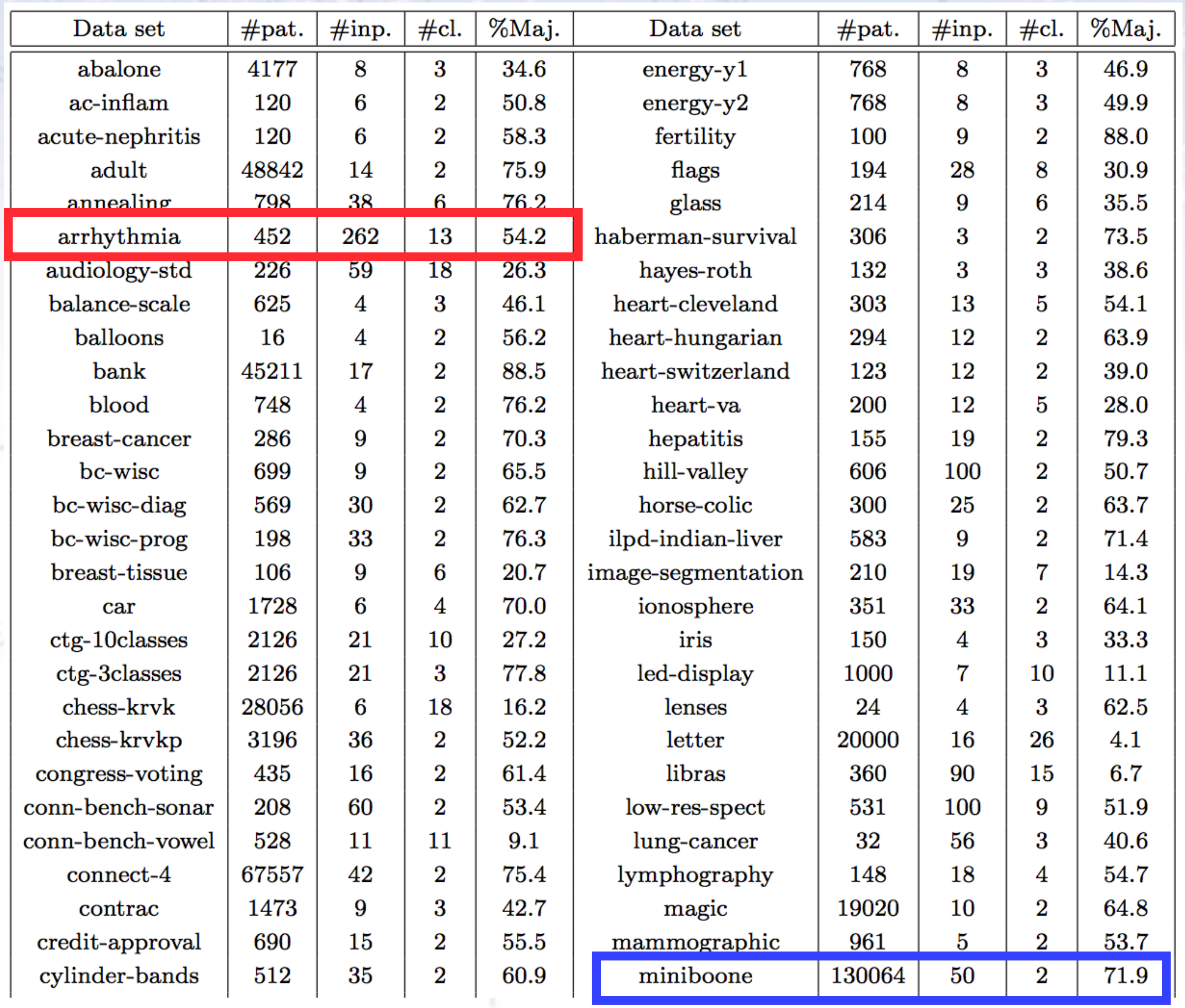
**Editor:** Russ Greiner

# What are the data sets?



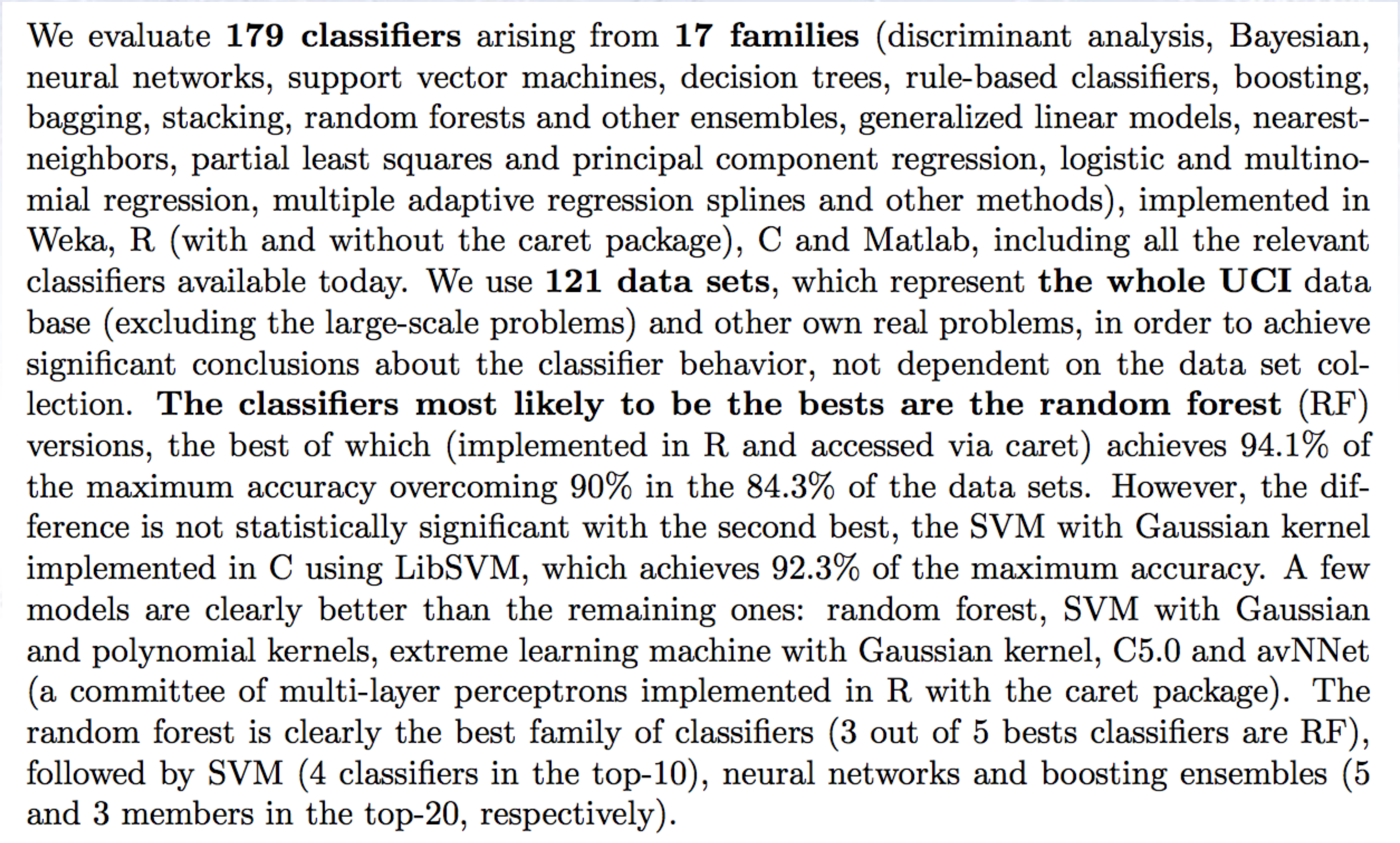
| Data set | #pat. | #inp. | #cl. | %Maj. | Data set | #pat. | #inp. | #cl. | %Maj. |
|---|---|---|---|---|---|---|---|---|---|
| abalone | 4177 | 8 | 3 | 34.6 | energy-y1 | 768 | 8 | 3 | 46.9 |
| ac-inflam | 120 | 6 | 2 | 50.8 | energy-y2 | 768 | 8 | 3 | 49.9 |
| acute-nephritis | 120 | 6 | 2 | 58.3 | fertility | 100 | 9 | 2 | 88.0 |
| adult | 48842 | 14 | 2 | 75.9 | flags | 194 | 28 | 8 | 30.9 |
| annealing | 798 | 38 | 6 | 76.2 | glass | 214 | 9 | 6 | 35.5 |
| arrhythmia | 452 | 262 | 13 | 54.2 | haberman-survival | 306 | 3 | 2 | 73.5 |
| audiology-std | 226 | 59 | 18 | 26.3 | hayes-roth | 132 | 3 | 3 | 38.6 |
| balance-scale | 625 | 4 | 3 | 46.1 | heart-cleveland | 303 | 13 | 5 | 54.1 |
| balloons | 16 | 4 | 2 | 56.2 | heart-hungarian | 294 | 12 | 2 | 63.9 |
| bank | 45211 | 17 | 2 | 88.5 | heart-switzerland | 123 | 12 | 2 | 39.0 |
| blood | 748 | 4 | 2 | 76.2 | heart-va | 200 | 12 | 5 | 28.0 |
| breast-cancer | 286 | 9 | 2 | 70.3 | hepatitis | 155 | 19 | 2 | 79.3 |
| bc-wisc | 699 | 9 | 2 | 65.5 | hill-valley | 606 | 100 | 2 | 50.7 |
| bc-wisc-diag | 569 | 30 | 2 | 62.7 | horse-colic | 300 | 25 | 2 | 63.7 |
| bc-wisc-prog | 198 | 33 | 2 | 76.3 | ilpd-indian-liver | 583 | 9 | 2 | 71.4 |
| breast-tissue | 106 | 9 | 6 | 20.7 | image-segmentation | 210 | 19 | 7 | 14.3 |
| car | 1728 | 6 | 4 | 70.0 | ionosphere | 351 | 33 | 2 | 64.1 |
| ctg-10classes | 2126 | 21 | 10 | 27.2 | iris | 150 | 4 | 3 | 33.3 |
| ctg-3classes | 2126 | 21 | 3 | 77.8 | led-display | 1000 | 7 | 10 | 11.1 |
| chess-krvk | 28056 | 6 | 18 | 16.2 | lenses | 24 | 4 | 3 | 62.5 |
| chess-krvkp | 3196 | 36 | 2 | 52.2 | letter | 20000 | 16 | 26 | 4.1 |
| congress-voting | 435 | 16 | 2 | 61.4 | libras | 360 | 90 | 15 | 6.7 |
| conn-bench-sonar | 208 | 60 | 2 | 53.4 | low-res-spect | 531 | 100 | 9 | 51.9 |
| conn-bench-vowel | 528 | 11 | 11 | 9.1 | lung-cancer | 32 | 56 | 3 | 40.6 |
| connect-4 | 67557 | 42 | 2 | 75.4 | lymphography | 148 | 18 | 4 | 54.7 |
| contrac | 1473 | 9 | 3 | 42.7 | magic | 19020 | 10 | 2 | 64.8 |
| credit-approval | 690 | 15 | 2 | 55.5 | mammographic | 961 | 5 | 2 | 53.7 |
| cylinder-bands | 512 | 35 | 2 | 60.9 | miniboone | 130064 | 50 | 2 | 71.9 |

The data sets are all quite smallish (< 150000 entries), with only 7 / 56 being above 10000 entries!

There are most often between 4-100 input parameters.

The standard problem is to divide into two classes.

# 179 methods vs. 121 data sets



We evaluate **179 classifiers** arising from **17 families** (discriminant analysis, Bayesian, neural networks, support vector machines, decision trees, rule-based classifiers, boosting, bagging, stacking, random forests and other ensembles, generalized linear models, nearest-neighbors, partial least squares and principal component regression, logistic and multinomial regression, multiple adaptive regression splines and other methods), implemented in Weka, R (with and without the caret package), C and Matlab, including all the relevant classifiers available today. We use **121 data sets**, which represent **the whole UCI** data base (excluding the large-scale problems) and other own real problems, in order to achieve significant conclusions about the classifier behavior, not dependent on the data set collection. **The classifiers most likely to be the bests are the random forest** (RF) versions, the best of which (implemented in R and accessed via caret) achieves 94.1% of the maximum accuracy overcoming 90% in the 84.3% of the data sets. However, the difference is not statistically significant with the second best, the SVM with Gaussian kernel implemented in C using LibSVM, which achieves 92.3% of the maximum accuracy. A few models are clearly better than the remaining ones: random forest, SVM with Gaussian and polynomial kernels, extreme learning machine with Gaussian kernel, C5.0 and avNNet (a committee of multi-layer perceptrons implemented in R with the caret package). The random forest is clearly the best family of classifiers (3 out of 5 bests classifiers are RF), followed by SVM (4 classifiers in the top-10), neural networks and boosting ensembles (5 and 3 members in the top-20, respectively).

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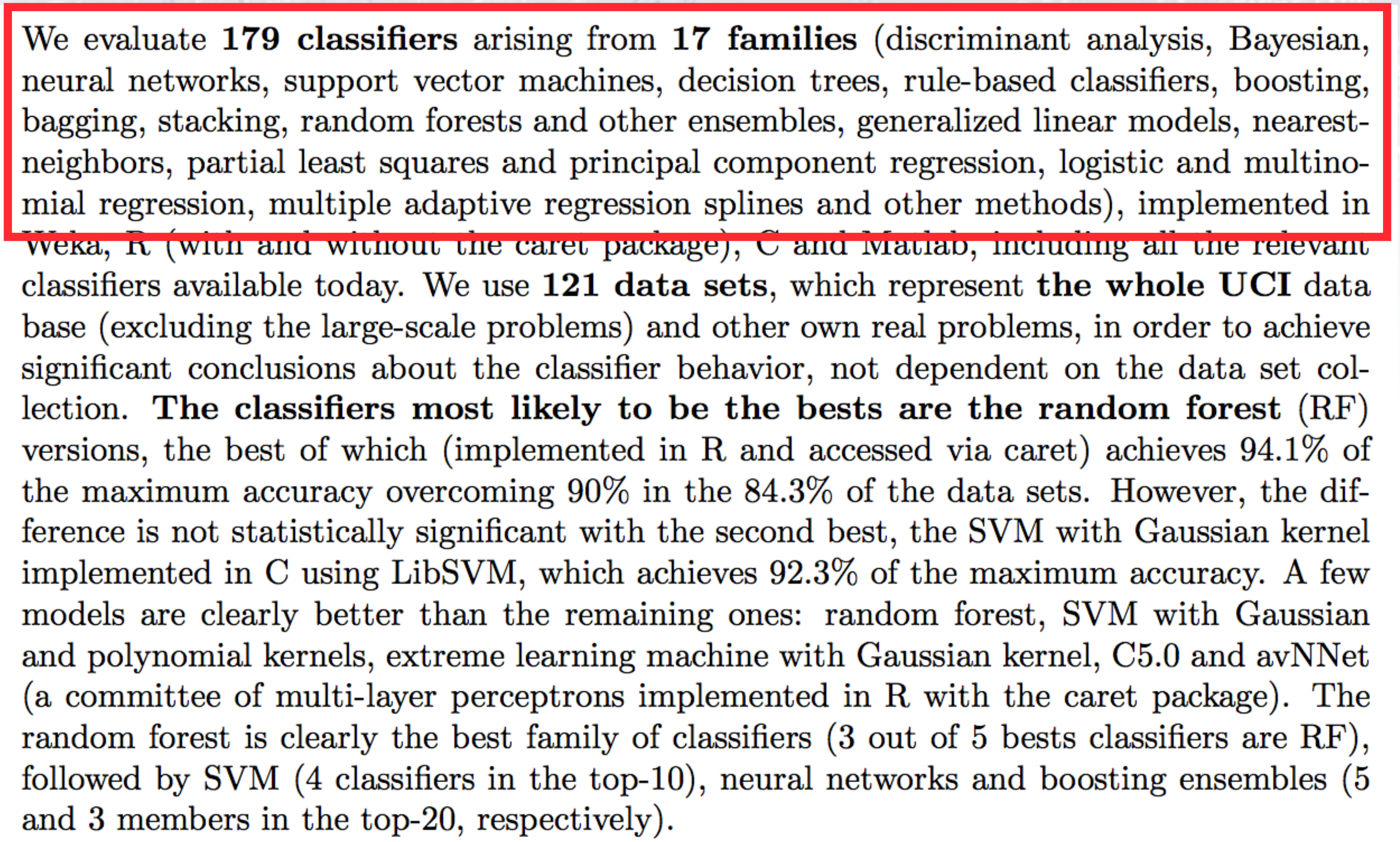

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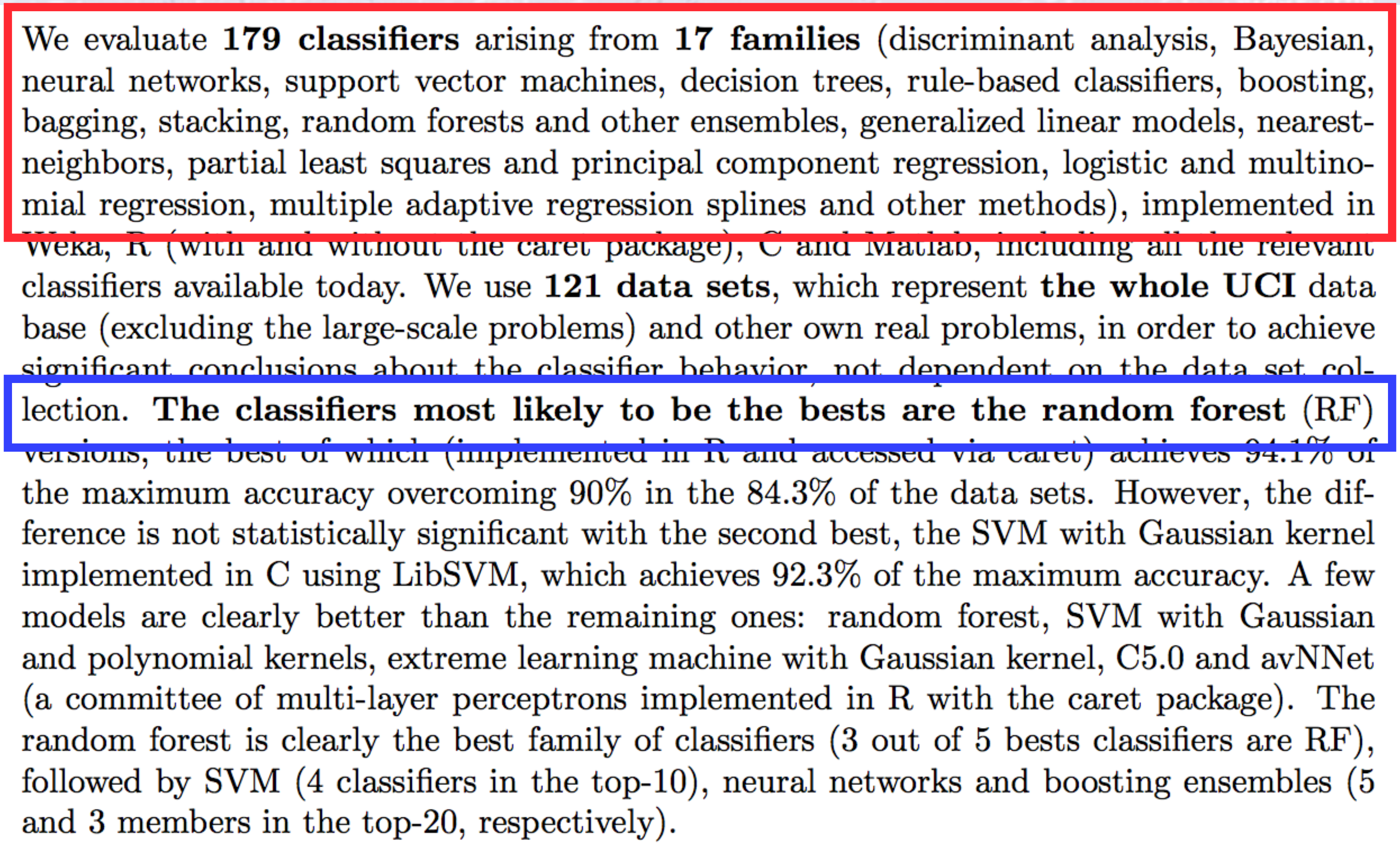

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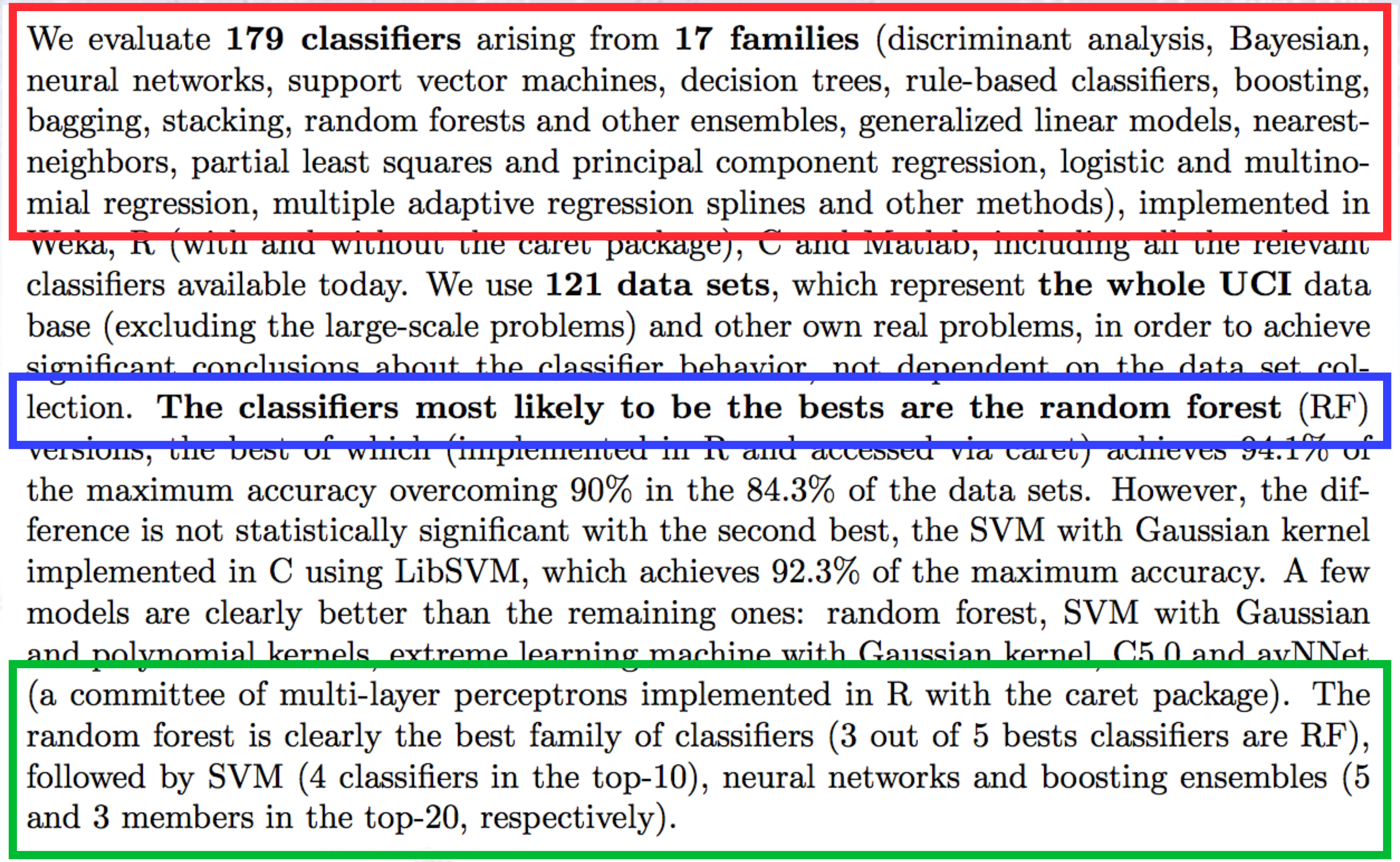

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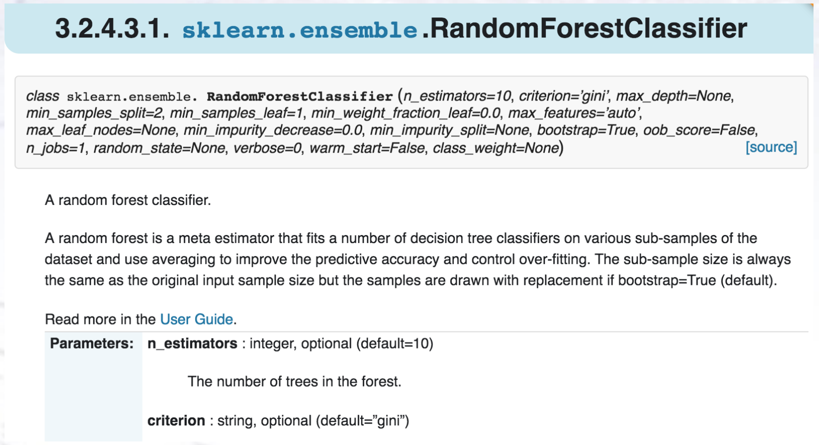
# Random Forests implementations

Given the succes of the RandomForests algorithm, it has naturally been implemented in many languages (the original one being Fortran!!!).

I managed to find it in both Python and R:

Python: scikit-learn package

R: randomForests package



3.2.4.3.1. `sklearn.ensemble`.RandomForestClassifier

*class* `sklearn.ensemble.` **`RandomForestClassifier`** (*n_estimators=10, criterion='gini', max_depth=None, min_samples_split=2, min_samples_leaf=1, min_weight_fraction_leaf=0.0, max_features='auto', max_leaf_nodes=None, min_impurity_decrease=0.0, min_impurity_split=None, bootstrap=True, oob_score=False, n_jobs=1, random_state=None, verbose=0, warm_start=False, class_weight=None*) [source]

A random forest classifier.

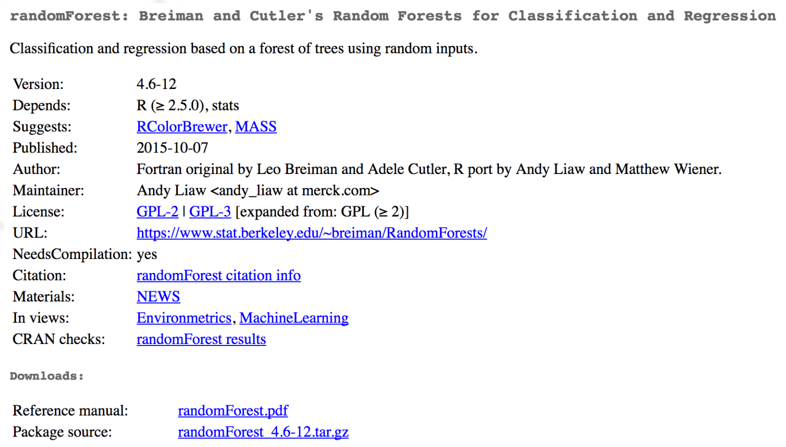
A random forest is a meta estimator that fits a number of decision tree classifiers on various sub-samples of the dataset and use averaging to improve the predictive accuracy and control over-fitting. The sub-sample size is always the same as the original input sample size but the samples are drawn with replacement if bootstrap=True (default).

Read more in the User Guide.

**Parameters:** **n_estimators** : integer, optional (default=10)

The number of trees in the forest.

**criterion** : string, optional (default="gini")



**randomForest: Breiman and Cutler's Random Forests for Classification and Regression**

Classification and regression based on a forest of trees using random inputs.

| | |
|---|---|
| Version: | 4.6-12 |
| Depends: | R (≥ 2.5.0), stats |
| Suggests: | RColorBrewer, MASS |
| Published: | 2015-10-07 |
| Author: | Fortran original by Leo Breiman and Adele Cutler, R port by Andy Liaw and Matthew Wiener. |
| Maintainer: | Andy Liaw <andy_liaw at merck.com> |
| License: | GPL-2 \| GPL-3 [expanded from: GPL (≥ 2)] |
| URL: | https://www.stat.berkeley.edu/~breiman/RandomForests/ |
| NeedsCompilation: | yes |
| Citation: | randomForest citation info |
| Materials: | NEWS |
| In views: | Environmetrics, MachineLearning |
| CRAN checks: | randomForest results |

**Downloads:**

| | |
|---|---|
| Reference manual: | randomForest.pdf |
| Package source: | randomForest_4.6-12.tar.gz |

# The results in more detail…

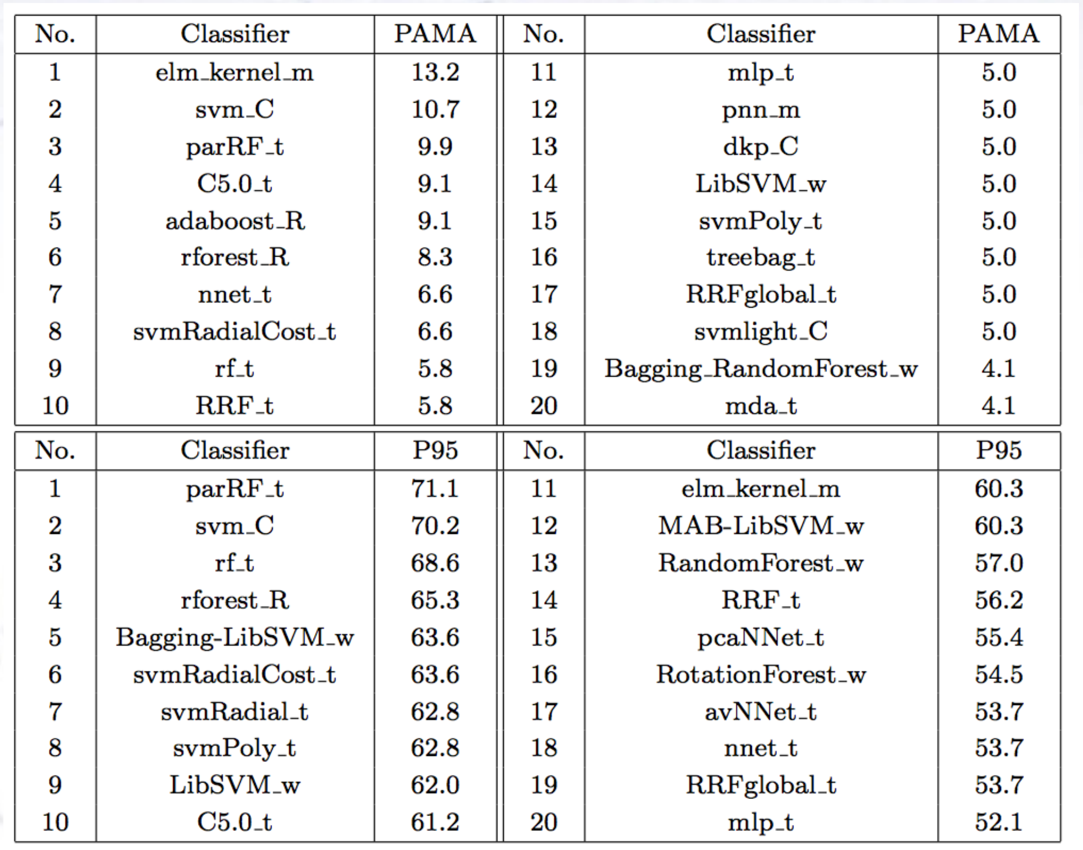
The many good algorithms are ranked according to probability of achieving:

- Maximum Accuracy (PAMA)
- 95% accuracy on all data sets (P95)

As can be seen, the Random Forest (parRF_t) is not the most likely to be the best.
Rather it is the one, which most often is ranked high.

But this just shows, that there is no guarantee that parRF_t is the most powerful method. In fact far from it.

**This is a general problem, which must be considered…**



| No. | Classifier | PAMA | No. | Classifier | PAMA |
|---|---|---|---|---|---|
| 1 | elm_kernel_m | 13.2 | 11 | mlp_t | 5.0 |
| 2 | svm_C | 10.7 | 12 | pnn_m | 5.0 |
| 3 | parRF_t | 9.9 | 13 | dkp_C | 5.0 |
| 4 | C5.0_t | 9.1 | 14 | LibSVM_w | 5.0 |
| 5 | adaboost_R | 9.1 | 15 | svmPoly_t | 5.0 |
| 6 | rforest_R | 8.3 | 16 | treebag_t | 5.0 |
| 7 | nnet_t | 6.6 | 17 | RRFglobal_t | 5.0 |
| 8 | svmRadialCost_t | 6.6 | 18 | svmlight_C | 5.0 |
| 9 | rf_t | 5.8 | 19 | Bagging_RandomForest_w | 4.1 |
| 10 | RRF_t | 5.8 | 20 | mda_t | 4.1 |

| No. | Classifier | P95 | No. | Classifier | P95 |
|---|---|---|---|---|---|
| 1 | parRF_t | 71.1 | 11 | elm_kernel_m | 60.3 |
| 2 | svm_C | 70.2 | 12 | MAB-LibSVM_w | 60.3 |
| 3 | rf_t | 68.6 | 13 | RandomForest_w | 57.0 |
| 4 | rforest_R | 65.3 | 14 | RRF_t | 56.2 |
| 5 | Bagging-LibSVM_w | 63.6 | 15 | pcaNNet_t | 55.4 |
| 6 | svmRadialCost_t | 63.6 | 16 | RotationForest_w | 54.5 |
| 7 | svmRadial_t | 62.8 | 17 | avNNet_t | 53.7 |
| 8 | svmPoly_t | 62.8 | 18 | nnet_t | 53.7 |
| 9 | LibSVM_w | 62.0 | 19 | RRFglobal_t | 53.7 |
| 10 | C5.0_t | 61.2 | 20 | mlp_t | 52.1 |