Random Forests Destructured: Introduction, Overview, Possibilities

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Abstract

This report a rather new machine learning algorithm called "Random Forests", its qualities, use, problems, and a small number of improvements that have been tried. Random forests are getting a lot of attention outside of psychology, and it would be nice to encourage their application within psychology too. However, it is important to keep in mind that random forests are relatively unstudied. This hasn't hindered a number of people to suggest improvements. This paper tries to give the reader a practical understanding of the method, which hopefully leads to a better application random forests.

Keywords: ensemble methods, introduction, random forests

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Introduction

Motivation

Psychology has become a science, thus psychological research has to follow the *scientific method*, according to which positive proof is an impossibility unless we have complete knowledge, and could eliminate all alternative theories. However, we won't ever have complete knowledge, therefore scientific isn't about proofs, but probabilities. Research works under the assumption that if we disprove just enough alternative theories, we can eventually tell which theory is probably true. So, the scientific method really is nothing but the use of countless attempts to disprove alternative theories, until only a single such theory remains.

Since there is an unweildly number of theories to disprove, and every researcher likes to see the result of his work during his lifetime, a more speedy method is usually employed, although this comes with a caveat. The speedier method has the researcher pit his favored theory against the null hypothesis, a fancy word for chance. This is way more efficient than comparing the thousands of theories that researchers have come up with, and continue to come up with. The caveat, commonly called confirmation bias, is that the result only has significance in the experimental set-up being tested. In the greater scale of things, i.e. reality, the results might well be completely bogus. Nonetheless, most of the subjects being studied are sufficiently constant or change predictably enough to allow researchers to generalize from the results of an experiment

to the world at large, and likely remain correct. This likelihood depends on the size of the effects measured in the experiment, the number of experimental subjects, and on the properties of the statistical methods involved. In psychological research, where large effects are rare and experiments usually study only a handful of psychology students, it is vital to use good statistical methods, because that is the only parameter remaining for the researcher to tweak in his favour.

Recently, researchers in psychology began to turn to a new breed of statistical methods, in hope of ever better results. This new breed of statistical methods is called *machine learning*.

In this paper, I aim to introduce the reader to *random forests*, which are just one family of algorithms. I intend to do this in a way that gives every reader a chance to understand this method without prior knowledge. I also intend to present the reader with some context around random forests, in hope that they will benefit from a more big-picture view.

In the next sections I introduce the reader to machine learning, the differences between the traditional statistical and this new machine learning approach, random forests in particular, and finally delve into some improvements to random forests that have been suggested in the literature.

Machine Learning

In order to understand random forests, it might be useful to set the stage by briefly discussing machine learning in general. Machine Learning is both a part of predictive statistics and the artificial intelligence branch of computer science.

Predictive statistics is the sub-field of statistics that is concerned with making predictions based on past observations. It's probably most widely known method is *linear regression* (Wikipedia, 2013k) that associates two variables y and x in such a way that they describe a straight line: $y = \alpha * x + \beta$. Predictive statistics is widely used in psychology because it allows the researcher to look at the unobservable by making assumptions of the form $reaction = mind * stimulus + variation$. This is the standard

approach in personality questionaires.

Artificial intelligence is a field commonly associated with the computer sciences, where it began with the advent of higher-order programming languages based on mathematical foundations around the *1960s* (Wikipedia, 2013j). Its aim is to give computers human-like capabilites, so that they can assist us by combining intelligence, with flawless logic and super-human knowledge. It includes things like *logic programming* (Wikipedia, 2013l), *expert systems* (Wikipedia, 2013f), *databases* (Wikipedia, 2013d) and *neural networks* (Wikipedia, 2013b), that all represent some form of storing and querying knowledge. Unfortunately, early computers back then didn't have the speed and memory required to push the envelope far enough, and the field was deemed dead. Only the rather recent coexistance of powerful computers and massive amounts of stored data, sometimes called *big data*, revived artificial intelligence as an important field of research.

Machine learning is that part of artificial intelligence that is concerned with the computer's learning of facts about the world. These facts can then be stored and subsequently queried later on. As such machine learning is concerned with making statements based on past observations, and, is therefore, close to predictive statistics (Wikipedia, 2013m).

The Machine Learning Life Cycle

This section discusses the difference between machine learning and traditional statistical methods. Terminology. The following section heavily relies on information found in Wikipedia, as well as what I learned in statistics lectures in the past years. A good introductory article is (Wikipedia, 2013m).

Traditionally, the statistical methods used in psychology take a model of how the world works, and a set of data, and return one of two things. They either return a probability of how likely an improvement in prediction can be observed at random, or how likely a difference in measurement can be observed at random.

Regression methods try to derive the values of one variable from the other

variables in the dataset using a formula the researcher specifies. They then compare the actual values and the prediction my the model with different inputs, and calculate how probable an improvement in this comparison is to show up due to random variations (Wikipedia, 2013q).

Analysis of variance methods partition the dataset according to all but one variable. They then calculate the probability with which the variation in the one variable among the groups could be due to random variations in the dataset (Wikipedia, 2013a).

The probabilities the methods output are what statisticians call the significance. Statisticians usually define a target significance level, e.g. 5%, and compare it to the output of their statistical calculations. If the calculated probability is less than the targeted significance level the measured effects are said to he significant at the chosen significance level. For example, a result that is significant at 5%, we know that it is less likely to show up at random than in 5% of all experiments.

The most striking difference between traditional statistical methods and machine learning methods is that the researcher can't specify his model of how the world works, other than through the selection of a machine learning algorithm. Because of this, machine learning algorithms are sometimes described as *black boxes*, meaning that the user can only see what's going into the algorithm, and what is coming out. This is unlike the statistical methods, where the researcher supplies a formula, because in machine learning, algorithms derive the model on their own. This is what the learning in machine learning means. The second difference is what the algorithms return. Since machine learning algorithms represent the model, what they output is not a percentage, i.e. significance, but the model itself. In short, machine learning provides the researcher with a generic model that adapts to the world. The prediction of such a model can then be calculated for data for which the values of the output variable are known, but that hasn't been included in the learning phase, to calculate the significance. The problem with this flexibility is, that one cannot really tell what the model looks like, that is, the model is not in a human-readable form. As will be pointed out later, decision trees, the

underlying mechanism in random forests, are quite easily understandable, but random forests consist of dozens to thousands of such trees, so that a human can hardly tell what they mean. Therefore, it is very important to find ways to condense this complexity into something that can be more easily interpreted. The variable importance measure of random forests, which will be introduced later, is one such way.

Classification

The *classification problem* is the problem of classifying new data based on a set of example data, but without the explicit set of rules that guided the classification of the example data. Unlike in *regression*, the result here is one of many given classes and not a numeric value. One might describe classification as regression with discreet output values. Output variables are commonly called *classes*, while input variables are commonly called *features* independent of the type of problem.

Regression

A short discussion of regression, the why and how, and the difference between classical regression and regression in machine learning. Terminology. Classification with continuous classes.

Randomness

Many machine learning algorithms consume random numbers in different places. While computer generated random numbers are not truly random, they still cause the outcome of the algorithm to change slightly between different executions, due to the fact that they are customarily initialized with the current time at the start of the program. These changes might unnerve a novice, but don't change the outcome of the algorithm significantly. Still, for publication purposes it can make sense to set and publish the random number generator's *seed*, i.e. the value the generator is being initialized with. However, doing so during the experiment is a serious mistake. Indeed, it is good practice to run the analysis multiple times to ensure that these random variations don't change the outcome.

Random Forests

Introduction

This part of the paper discusses random forests. "Random forests are a combination of tree predictors such that each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest" (Breiman, 2001). Leo Breiman developed random forests with Adele Cutler, building on work by Ho, Amit, Geman, and Dietterich (Wikipedia, 2013p).

Although the name random forests is usually taken to refer to the random forests as defined by (Breiman, 2001), the large number of variants that have been derived from the original forests, e.g. Forest-rk (Bernard, Heutte, & Adam, 2008), RFW (Maudes, Rodríguez, García-Osorio, & García-Pedrajas, 2012), DRF (Bernard, Adam, & Heutte, 2012), Fuzzy random forests (Bonissone, Cadenas, Garrido, & Dıaz-Valladares, 2008), Rotation forest (Rodriguez, Kuncheva, & Alonso, 2006), random forests that are more random (Geurts, Ernst, & Wehenkel, 2006), (Liu, Ting, & Fan, 2005), (Cutler & Zhao, 2001), and various other improvements, e.g. by (Banfield, Hall, Bowyer, & Kegelmeyer, 2007), (Robnik-Šikonja, 2004), (Strobl, Malley, & Tutz, 2009), (G. Zhang & Lu, 2012), make it so that it is better to think of random forests as being a framework instead of being a single method (Wikipedia, 2013p). To understand this framework, it is best to look at the different aspects of random forests, first in a top-down view, and later part by part. The top-down view is strictly based on (Breiman, 2001), while the part by part discussion will also go into tweaking random forests.

Random forests is an ensemble learning method where the ensemble consists of decision trees. Every decision tree is constructed on a sample of the input dataset, that is selected using bootstrapping with replacement from the original dataset and equally large. Every node split in the decision tree is an optimal two-way split selected from a random subset of all input variables. The number of randomly selected variables for each split is commonly called `mtry`. If the number of input variables is small, additional input variables can be derived as linear combinations of input variables. The decision trees are grown maximally without pruning, and new trees are generated until the

ensemble of decision trees reaches its target size, usually called `ntree`. Random forests features error estimates using out-of-bag data. Out-of-bag data are the records in the dataset that were not selected during the bootstrap aggregation, and make up approximately one third of the dataset. Random forests also features variable importance measures, which are calculated by reclassifying the out-of-bag data, but randomizing the variable under consideration. The variable importance of the randomized variable is the increase of misclassifications.

The the reference implementation of random forests is written in Fortran, but a package for the statistical software framework R (R Core Team, 2012), is called `randomForest` (Liaw & Wiener, 2002) exists. An alternative within the R framework, which includes improvements to correct a bias in variable importance measures is available under the name `party` (Strobl, Boulesteix, Kneib, Augustin, & Zeileis, 2008). A third implementation using Java is available in the WEKA machine learning suite (Hall et al., 2009). For illustration purposes I include a source code example and the corresponding output taken from (Strobl et al., 2008):

```
> load("dat_smoking.rda")
> library("party")
> myctree <- ctree(intention_to_smoke ~ ., data = dat_smoking)
> class(dat_smoking$intention_to_smoke)
> plot(myctree)
```

The use case for random forests is quite wide. Random forests has been used in applications from psychology and computational biology as is outlined in (Strobl et al., 2009), to customer churn prediction (Xie, Li, Ngai, & Ying, 2009), to software testing (Guo, Ma, Cukic, & Singh, 2004) and internet security (J. Zhang & Zulkernine, 2005). The reasons why random forests is such a widely used method, are its prediction accuracy, which is comparable to other state-of-the-art machine learning algorithms like Adaboost (Breiman, 2001), its ability to handle “small n large p” datasets (Strobl et al., 2009), its practical built in error estimates, and its variable importance measures. The last of which, random forests’ variable importance measures, might be its most useful

feature. Many domains don't require accurate predictions as much as a model that can be understood by humans. While ensemble methods are unsuitably complex, random forests' variable importance measures can be used to select variables for use in simpler models, e.g. generalized linear models, logit and probit models, which are more easily interpreted (Strobl et al., 2009).

Ensemble Learning Methods

As mentioned above, random forests build on quite a rich collection of previous work, most of which also concerns ensemble learning methods. In fact, random forests can be seen as a composition of elements from different other ensemble learning methods, e.g. random subspaces (Ho, 1998) and bagging (Breiman, 1996). Although detailed knowledge of these methods is not a requirement to understand random forests, it is important to understand what ensemble learning is. Again, this paper will first give an abstract definition and then look at examples in detail.

Ensemble learning is a supervised learning algorithm: its task is to take an example of input and output data, and find a hypothesis that connects the two. This hypothesis can then be used to predict the output data that corresponds to new input data. In theory this problem can be solved by a construct called Bayes optimal classifier, which considers every possible hypothesis, but, which unfortunately can't be implemented except for trivial problems. However, the principle that the combination of possible hypotheses becomes a stronger hypothesis, because it can represent more functions that every component hypothesis could, holds. In short, ensemble methods rely on the principle that the ensemble is more than the sum of its parts. The usual wording of this is, that ensemble learning turns a set of *weak classifiers* into one *strong classifier*. Weak also stands for unstable, meaning that the underlying classifier is susceptible to even small variations in the input data. Ensemble learning methods can be called meta algorithm, because they rely on other simpler classifier algorithms, and it is theoretically possible to create an ensemble learner for any supervised learning algorithm. (Wikipedia, 2013e) (Polikar, 2009)

Bagging. The ensemble learning algorithm that most prominently underlies random forests is bagging. Bagging stands for bootstrap aggregation. Bootstrapping is a term that was used to describe "[...] the process by which lumberjacks hoist themselves up trees [...]" (Wikipedia, 2013c). In statistics it refers to the process of deriving additional samples by resampling the original sample, essentially simulating drawing additional samples from the population. Bootstrap aggregation is an ensemble learning algorithm, which trains each of its underlying weak classifiers on a different set of input data created by bootstrapping. It is another algorithm developed by Leo Breiman (Breiman, 1996).

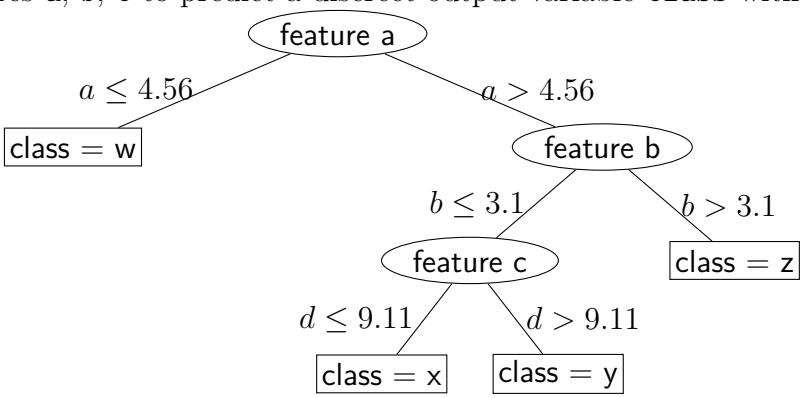
Bagging is typically uses bootstrapping with replacement, which leads the inclusion of on average two thirds of the original sample in the derived sample. Random forests uses the remaining third as out-of-bag data (Breiman, 2001).

Boosting. Boosting is an ensemble method, where every weak classifiers gets to train on the original sample, but the sample is improved with importance weights. These weights are different for every weak classifier. They are lower for records in the dataset that are correctly predicted by the classifiers already in the ensemble, and higher for records that classified wrongly. In short, boosting focuses on eliminating one classification error after another all data is classified correctly, or a targeted ensemble size is reached. This behavior makes boosting algorithms very fast learners, but susceptible to errors in the dataset (Long & Servedio, 2010). Boosting isn't used in random forests as introduced by (Breiman, 2001), but there are variants who do, e.g. dynamic random forests (Bernard et al., 2012). Adaboost (Freund & Schapire, 1995) is probably the most popular boosting algorithm, and the algorithm random forests in most commonly compared to in terms of performance, e.g. (Breiman, 2001), (Banfield et al., 2007) and (Rodriguez et al., 2006).

A large study (Banfield et al., 2007) compared eight ensemble of decision tree classifiers on 57 publicly available datasets and concluded "[...] that boosting, random forests and randomized trees are statistically significantly better than bagging."

Decision Trees

The underlying algorithm of random forests is the decision tree classifier, which is either a regression tree, or a classification tree. The difference between the two types of trees is the type of output produced. Classifications trees work with discreet output values, while regression trees output a continuous numeric value. For classification the most commonly chosen output value among an ensemble of decision trees is assumed to be the right prediction. For regression purposes the output of the ensemble is calculated by averaging the outcomes the single trees. As the name indicates, a decision tree is a tree data structure, i.e. a set of nodes that are connected in a forward manner allowing branching, but not cross links and circles. Decision trees usually are binary trees, meaning that each node either has two child nodes, or is a leaf node. Each node represents a decision criterion, each edge a criterion match or mismatch, and each leaf node an outcome of the represented decision tree. Tree data structures are typically drawn from top to bottom. For example, the following decision tree takes three numeric features `a`, `b`, `c` to predict a discreet output variable `class` with four possible values.



The decision trees used by random forests are constructed by randomly selecting a certain number of input variables as configured by the parameter `mtry` for each node. The algorithm then selects the best threshold among these input variables as the node's criterion. This process is repeated for every child node until a node is reached which only matches records in the dataset with the same output value. This node becomes a leaf node. This is described as growing a tree maximally. This ensures that each decision tree has a high strength, meaning no decision tree outputs wrong predictions for the subsets of data it matches. (Breiman, 2001)

As a component classifier to an ensemble learning algorithm, every decision tree should be different from the other decision trees in the ensemble, i.e. the decision trees should be unstable, to cover a wide range of possible interactions between the input data, i.e. hypotheses. This is commonly described as the trees being uncorrelated. Tree strength and inter-tree correlation are what the prediction accuracy of random forests depends on. (Breiman, 2001)

The procedure by which decision trees are grown is modified by some variants of random forests. PERT (Cutler & Zhao, 2001) for example doesn't perform a search for the best split on a random selection of input variables, but selects variable and threshold at random, while RFW (Maudes et al., 2012) searches all variables but attaches random weights to them, and DRF (Bernard et al., 2012) influences the decision tree creation by a procedure inspired by boosting. Other variants, e.g. (Van Essen, Macaraeg, Gokhale, & Prenger, 2012), change this procedure to grow smaller or more balanced trees, to meet performance or hardware requirements.

Random Forests

As has been described in the sections on ensemble learning and decision trees, random forests build up ensembles of decision trees. This process depends on two parameters: the ensemble size, commonly called `ntree`, and the randomization parameter `mtry`. Actually, random forests depend on another parameter, the state of a random number generator, but being random, it doesn't and usually shouldn't be specified. The following is an exemplary implementation of random forest following the original version by (Breiman, 2001).

`TODO: Implementation of Random Forests`

Parameters. The two parameters random forests depends on, are problematic, in that users set them according to one recommendation or another, or just use the default setting, which again can differ from implementation to implementation. Furthermore, not every dataset is best learned by random forests using the same setting. This lack of a standard way to determine the parameter values makes it hard to

compare the accuracy of different methods. The comparative study by (Banfield et al., 2007) gives a nice overview over the datasets used in previous publications, among which are (Breiman, 2001) and (Dietterich, 2000), that each used ensemble sizes of 50-200, and applied the algorithms being compared to 18-27 datasets. In each case the authors concluded that their method was superior to the other methods in the study. However, the more recent study by (Banfield et al., 2007) found "no stat. sig. improvement over bagging in 38 of 57 data sets" when ensemble sizes of up to 1000 trees where used. The study also concludes that bagging with an ensemble size of 1000 and random forests with the randomization parameter set to the binary logarithm of the number of input variables were the best methods. The study by (Banfield et al., 2007) also suggests a mechanism to determine the best size of the ensemble automatically. Methodologically, this would be a welcome improvement, because it takes away one way researchers can fiddle with the outcome of their calculations, and because it would ensure better results due to the usually larger ensemble sizes. In defense of older studies, like those by (Breiman, 2001) and (Dietterich, 2000), one has to consider that the average computer back then weren't as powerful. (Breiman, 2001) mentions run times for random forests of 4 minutes and 3 hours for Adaboost when building ensembles of size 100, while I can execute all examples in (Strobl et al., 2009) in well under 30 seconds.

The second parameter of random forests is the randomization parameter `mtry` which controls how many variables are being selected randomly at each decision tree node to search for an optimal split. If `mtry` is set to 1, random forests acts like a linear combination of the input variables. If `mtry` is set to the number of variables, random forest becomes bagging as proposed by (Breiman, 1996). Common choices for `mtry` are 1, 2, and other small values in older studies, e.g. (Breiman, 2001), and the square root of n, or the binary logarithm of n, with n being the number of input variables, becoming increasingly popular in newer literature, e.g. (Strobl et al., 2009). As mentioned above, using the binary logarithm of the number of input variables is indeed the best choice for most datasets (Banfield et al., 2007). However, depending on the dataset and the ensemble size, `mtry` needs to be chosen differently. For example in studies of genetics,

where the dataset often includes many irrelevant input variables in addition to the dataset being a “small n large p case”, it is necessary to use a larger value for `mtry`, else some variables might never be used in the ensemble at all (Strobl et al., 2009). It might be interesting to consider choosing `mtry` automatically, and two obvious suggestions for that would be to choose a random `mtry` value for every decision tree being grown, or to use a function of the number of input variables satisfying some statistical distribution criterion. According to (Bernard et al., 2008) a greedy search or choosing one of the values discussed above is the usual approach in the literature. The same paper shows, that this doesn’t have to be the case, by demonstrating a "push-button" method that automatically derives a suitable value for `mtry` and "is at least as statistically significant as the original".

Out-of-bag Data. Because random forests is based on bagging and uses bootstrapped samples, each tree has a set of approximately one third of the original dataset that has not been used to grow the tree. This set can be used to test the prediction accuracy of each tree, and the prediction accuracy of all trees can then be averaged to give an error estimation of the entire random forest. This out-of-bag error estimation is more precise than the standard error estimate, which is using all of the dataset (Strobl et al., 2009). This said, one should not forget that out-of-bag data isn’t the same thing as a genuine test dataset. Depending on the size of the dataset, and the ensemble size, the downsides of bootstrapping might shine through, and lead to an underestimation of the prediction accuracy.

Variable Importance. As has been mentioned above, random forests have a built in variable importance measure, which is calculated, by permutating the input variable in the out-of-bag data of every tree, and calculating a new error estimate. The difference between the out-of-bag error estimates with and without randomly permutated input variable is the variable importance. The more important a variable is, the more drastically the prediction error increases when the variable is being randomized. The variable is sometimes scaled, i.e. z-standardized, but because it strongly depends on the parameter of random forests, it’s not possible to compare these

variable importances across studies, hence there is little use in doing so (Strobl et al., 2009).

The idea behind this way of calculating variable importances is, that one would like to compare a prediction model with and without a particular input variable to measure the variable's impact. Obviously, one can't ignore all trees that incorporate a variable, because each tree incorporates multiple input variables, and their impact on the prediction would be modified too. By randomly permutating the values of an input variable, the variable's characteristics don't change, but the connection to the output variable is broken. However, according to (Strobl, Boulesteix, Zeileis, & Hothorn, 2007) the variable importance might still depend on which variable is being measured, because this variable importance measure is biased towards variables with many categories and variables with many missing values. Numeric variable usually have as many different values as there are records in the dataset, meaning that their importance measure is greatly biased due to the large number of "categories". Fortunately, this can be fixed, but "Only when subsamples drawn without replacement, instead of bootstrap samples, in combination with unbiased split selection criteria, are used in constructing the forest, can the resulting permutation importance be interpreted reliably" (Strobl et al., 2007), although correlated input variables still are problematic. The R package party includes two functions, `ctree` and `cforest`, that are not affected by this bias, due to yet another variable importance termed "conditional variable importance" (Strobl et al., 2008). Correlated variables can be problematic, because trees that include a pair of correlated input variables are less affected by the random permutation of one of them. Conditional variable importance considers these correlations. However, (Grömping, 2009) argues, that this can't be avoided as long as `mtry` is smaller than the number of input variables, and that considering all input variables, i.e. bagging, "might already go a long way" towards remedying the problem, although due to the "large p small n case", "unbiased estimation of all coefficients is impossible" in any case.

Another problem that the variable importance measure can be affected by, is that some variables might not be well represented in a random forest. This can be due to a

small setting for `mtry` and or `ntree` in the presence of many irrelevant input variables, as often is the case in genetics datasets, or if variables show perfect higher order effects, i.e. interaction effects, but no main effects. The latter is called the XOR problem. It is important to note, that random forests with a different split selection algorithm don't have to be affected by this, e.g. PERT (Cutler & Zhao, 2001).

Last but no least, both (Strobl et al., 2009) and (Grömping, 2009) see one of the advantages of random forests in their variable importance measure. (Grömping, 2009) compares linear variable importance measures with the one built into random forests, and finds that the latter are heavily dependent on the mtry parameter. The larger `mtry` is, the better the importance estimates become. Variable importance measures are used to select input variables for a simpler model, e.g. a generalized liner model, which is more interpretable than a forest of decision trees (Strobl et al., 2009). Variable importance measures are also the probably only simple way to "shed some light into the black box of random forests" (Grömping, 2009). A alternative, but rather naive way to estimate variable importance is to count the occurance of a variable over all trees (Strobl et al., 2009). Other imaginable ways to estimate variable importance would be to use algorithms that analyze the structure of each decision tree. Another interesting point to make, is that random perturbation of an input variable could in theory be used as part of many other models, including but not limited to generalized linear models.

The way variable selection based on the variable importance measure is being done, is by finding variables whose randomization led to an improvement in prediction accuracy. These improvements are just random effects, and function as an indicator for which variable importances are within the random fluctuations, and which are true indicators for important variables.

Regression. Random forest can not only be used for classification, but also for regression. To produce the numeric output values necessary in regression, the vote on the most popular output class in the forest is replaced by an average calculation over all tree outputs. One problem with regression using random forests is that more decision trees end up covering the middle of the range of values of an output variable. This

means, that the prediction accuracy is good in the middle of the range of values, but the predictions for extremer values become more and more inaccurate (G. Zhang & Lu, 2012). The same paper also suggests five ways to estimate and reduce this bias.

Overfitting. Overfitting (Wikipedia, 2013n) is the situation where an algorithm learns the example dataset well enough to not only reproduce the underlying rules, but to also reproduce the random errors in the dataset. This is also called *generalization error*, since the algorithm generalizes errors in the data by deriving rules for them. Random forests grow optimal decision trees, meaning they try to represent their bootstrapped sample perfectly. Except for the case where different records in the sample have the same values in their input variables, but different values in their output variable, this leads to decision trees which represent the sample perfectly, including all errors. The advantage of ensemble learning is that by combining decision trees for different samples, and constructed using different random split selections, this errors are canceled out. However, this also means that there is an upper bound on how accurate random forests can become depending on the noise present in the dataset. Of course, this only applies if the trees in an ensemble are reasonably diverse, i.e. uncorrelated (Breiman, 2001). An analysis by (Liu et al., 2005) showed that the generalization error is at its lowest when the tree ensemble is maximally diverse, and that bootstrapping tends to limit tree diversity.

Different variants of random forests try to grow random forests on data that is less prone to noise. FRF stands for *Fuzzy random forests*, and is a method described by (Bonissone et al., 2008). FRF use what are called Fuzzy Sets to represent the data in the dataset, and build their decision trees on top. The advantages of this approach are that the resulting FRF are more immune to noise, and (Cadenas, Garrido, Martínez, & Bonissone, 2012) extend this framework to handle missing data too. Another attempt to construct random forests on higher quality data are rotation forests by (Rodriguez et al., 2006), which use principal component analysis, or PCA, to find derived input variables that separate the input dimensions better. Although linear combinations of input dimensions aren't the same thing as noise, since the dataset is of a limited size,

the decision trees might well fail to tease out the interactions between all pairs of input variables, which will end up looking like noise. Because better input dimensions lead to better splits, and to more uncorrelated random variable selections, rotation forests are more accurate than random forests (Rodriguez et al., 2006).

Optimality Criterion. Random forests construct the underlying decision trees by selecting the best split at each node from a number of randomly selected variables. To compare the different possible splits, an optimality criterion gets calculated for each split. The most commonly used criterion is the Gini index. The gini index is "a measure of statistical dispersion developed by the Italian statistician and sociologist Corrado Gini" (Wikipedia, 2013i). As has been mentioned in the section on variable importance, the fact that the Gini index is biased towards variables with many different values is problematic. Another common optimality criterion is entropy, although it suffers from the same bias towards variables with many different values. The point of using an optimality criterion in the first place is, to grow trees using an impurity reduction algorithm, i.e. to select the split which returns the least dispersed subsets is selected recursively at each node.

A huge disadvantage of using an optimality criterion is the computational cost one has to pay. Trees who use random splits are much faster to grow, e.g. PERT ensembles are claimed to be two orders of magnitude faster than the classical random forests (Cutler & Zhao, 2001).

In Search of the Super-Forest

Alternative: PERT. PERT, a variant in the random forests framework was developed by (Cutler & Zhao, 2001). The nice thing about PERT, is that its strong reliance on randomness gives it a simple structure that is easier to describe and implement than the classical random forests by (Breiman, 2001). In fact, PERT is simple enough that its algorithm is completely described in the following quote from (Cutler & Zhao, 2001):

> The perfect random tree ensemble, PERT, is so named because the

> PERT base learner is a random tree classifier that fits the training data perfectly. The PERT base learner is constructed by first placing all data points in the root node. At each step of the tree construction, each nonterminal node is split by randomly choosing two data points from the node until these two belong to different classes. Let $x = (x_1, ..., x_p)$ and $z = (z_1, ..., z_p)$. If this is not possible, all the data points in the node must be from the same class and the node is terminal. Now, randomly choose a feature on which to split, say feature j, and split at $\alpha x_j + (1 - \alpha)z_j$, where α is generated from a uniform(0,1) distribution.
>
> Ties are taken care of by repeating the procedure until a definitive split is obtained. If no such split is found after 10 tries, the node is declared to be terminal (so in this case, the tree would not perfectly fit the data). To form an ensemble, PERT base learners can be combined by simply fitting many PERT base learners to the entire training set and voting these classifiers. Alternatively, PERT base learners can be combined by bagging (Breiman, 1996). In this case, the PERT base learner is fit to many bootstrap samples from the training data and these classifiers are combined by voting.

On the one hand, bagging is not required, because PERT doesn't depend on randomness introduced through bootstrapping. On the other hand, bagging is necessary if one requires out-of-bag error estimates or variable importance measures. As (Liu et al., 2005) has indicated, using bootstrapping might lead to less diverse trees, thus it should not be used unless one requires these features.

The advantage of PERT over random forests is speed. (Cutler & Zhao, 2001) compares the different runtimes of classical random forests construction as described in (Breiman, 2001), and PERT, and finds the latter to be faster by two orders of magnitude, while providing similar accuracy in prediction. Of course, there are other advantages too: The absence of a variable selection criterion means that PERT doesn't suffer from the bias introduced by it, thus, variable importance estimates are less affected. An instance where the use of a selection criterion is especially problematic is

the XOR problem mentioned above in the section on variable importance. Since PERT forests don't depend on an optimality criterion to select its splits, it has the advantage of being able to deal with perfect interaction effects. A disadvantage might be that PERT is even more difficult to interpret than the classical random forests, but since this is rarely tried, it probably doesn't matter much in practice. It is important to mention that PERT can only be used for classification, since its base learner fits the training data perfectly, applying PERT to regression would "drastically overfit the data" (Cutler & Zhao, 2001).

PERT isn't the only random forest variant that emphasizes randomness in its algorithm for growing trees. (Geurts et al., 2006) suggested what they call extremely randomized trees. Despite their name, extremely randomized trees are actually closer to the trees of random forests by (Breiman, 2001) than PERT. Extremely randomized trees allow to configure the randomness of the constructed decision trees through an additional parameter in order to adapt the random forest algorithm to the problem domain of the dataset.

Alternative: Fuzzy random forests. Fuzzy random forests by (Bonissone et al., 2008) use input variables encoded as fuzzy sets. Fuzzy sets (Wikipedia, 2013h) model membership by a value between one and zero, while fuzzy logic (Wikipedia, 2013g) allows to reason using fuzzy data: For example, a day with a temperature of 45 degrees Celsius is to 100hot day, and to 0belong to the label cold day by 40The advantage of using fuzzy sets is the added flexibility of representing uncertainty. (Cadenas et al., 2012) extended fuzzy random forests to handle missing data, thus making fuzzy random forests even better at representing real world data.

Rotation. Rotation forests use principle component analysis to transform the dataset before creating the ensemble of decision trees. "Principal component analysis (PCA) is a mathematical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components." (Wikipedia, 2013o) Rotation forests have been suggested by (Rodriguez et al., 2006). Rotation forests are created by

calculating a principal component analysis on a bootstrapped sample of the data for every tree. The input variables are split into subsets, and random values of the output variable are removed for the principal component analysis, which means that another parameter for the size of the input variable subsets is required. Rotation forests significantly outperform random forests, bagging, and boosting on many datasets (Rodriguez et al., 2006).

The transformation of the input data leads to less correlation between trees, and to improved prediction accuracy, which (Rodriguez et al., 2006) demonstrate with the help of diversity-error diagrams.

Method

Selection of Papers

I started my research on *random forests* by reading the introductory paper suggested by my supervisor titled *An introduction to recursive partitioning: Rationale, application and characteristics of classification and regression trees, bagging and random forests* (Strobl et al., 2009). I then searched the research databases *PsychARTICLES* and *PsychINFO* querying for *random forest* and limiting my results to the last two years. I only considered papers that focus on *random forests* and dismissed every paper where *random forests* are merely used as a research method. I also used *Google Scholar* to look for more technical publications outside the field of psychology. I searched for combinations of *random forest*, *comparison*, *analysis*, and *ensemble*. I also included keywords seen in interesting titles, like *fuzzy*, *perfect*, *full*, *balanced*, *extremely*, and *rotation*. I also queried for some of the referenced publications while I read the found material, but only included (Strobl et al., 2008), because it was referenced multiple times, and co-authored by this paper's supervisor.

The final criteria for inclusion were the online availability of a freely downloadable PDF-file, which thanks to *Google Scholar* often turned out to be no problem at all, and my decision on the topic of this report.

A lot of the information in the fields of computer science, artificial intelligence,

machine learning, databases, and especially programming I acquired through different means in the last ten years. As I couldn't remember the original sources, I can only include the pages on Wikipedia, which I used to refresh my memories.

Aim and Structure of the Paper

Possible options for this topic were the presentation of exemplary uses of random forests, the discussion of strengths and weaknesses, and any of the more specialized variants. During my research I had the impression, that there were serious differences in the understanding of random forests among researchers, and even among designers of improved variants. A study comparing different decision tree ensemble techniques also confirmed this expression by saying that many of the commonly used methods of comparison weren't robust enough for use with random forests (Banfield et al., 2007).

Because of this fuzziness, I decided on a different focus, and to write a very broad - big picture - introduction to random forests.

Conclusion

State of the art? Well... They are not yet properly understood, and many comparisons and lots of the advantages might be accidential. Strong dependance on parameters, with no rationally pleasing way to set them.

The End

Bye.

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