Introduction to classification and regression trees, random forests and model-based recursive partitioning in R

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Ensemble methods (bagging, random forests)

have become a popular and widely used tool in many scientific fields, e.g., in genetics and bioinformatics, because they are applicable in high dimensional problems with complex interactions

(cf.,e.g., Furlanello et al., 2003, Gunther et al., 2003, Svetnik et al., 2003, Cummings and Myers, 2004, Cummings and Segal, 2004, Guha and Jurs, 2003, Lunetta et al., 2004, Segal et al., 2004, Arun and Langmead, 2006, Bureau et al., 2005, Huang et al., 2005, Shih, 2005, Diaz-Uriarte and de Andrés, 2006, Qi et al., 2006, Ward et al., 2006)

Problems of CART (and single trees in general)

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  - different kinds of instability: two trees may look very different, but identify very similar subgroups and generate very similar predictions for new observations

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II. instability to small changes in the training sample

- small changes in the training sample $\Rightarrow$ different splitting variable and value selected for a node $\Rightarrow$ different tree from there on
  - different kinds of instability: two trees may look very different, but identify very similar subgroups and generate very similar predictions for new observations
  - extent of instability depends on characteristics of the data (e.g., signal/noise ratio, correlations between predictor variables)

Solution I: Evaluating stability

- Draw random samples from the training data and refit tree
- Assess stability of variables and values selected for splitting
- Philipp et al. (2016): Stability assessment of tree-based learners
- Implemented in function `stabletree` in package `stablelearner`

Solution II: Ensembling trees

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- grow a large number of trees on modified versions of the data (e.g., random samples, ...)
- generate predictions through averaging over or majority voting of the trees
- E.g., bagging (Breiman, 1996a, 1998), random forests (Breiman, 2001), boosted tree ensembles (e.g., Breiman, 1997)

Ensemble learning

Motivation:

Can we improve the accuracy of a set of simple trees (weak learners) by combining them into an ensemble (a strong learner)?

Yes, we can!

- A weak learner is a method that does better than random guessing
- The predictive accuracy of the ensemble is better than any of its constituent members
- Can be applied to other learners than trees
- Works best for unstable methods

Decorrelating trees I: Bagging

take bootstrap samples from the original data

average over trees

bootstrap aggregating
(alternatively, we may use subsample aggregating)

Bootstrap sampling

from the original sample of size N draw a bootstrap sample of size N with replacement

$\Rightarrow$ some observations appear twice or more, some not at all

Bootstrap sampling

Bootstrap sampling

probability for one observation <u>not</u> to be drawn in one draw

$$1 - \frac{1}{n}$$

probability for one observation <u>not</u> to be drawn in any one of the n bootstrap draws

$$\lim_{n \to \infty} \left(1 - \frac{1}{n}\right)^n = e^{-1} \approx 0.368 = 1 - 0.632$$

$\Rightarrow$ approx. 63.2% of all observations are in the bootstrap sample

$\Rightarrow$ approx. 36.8% of all observations are "out of bag"

Bagging

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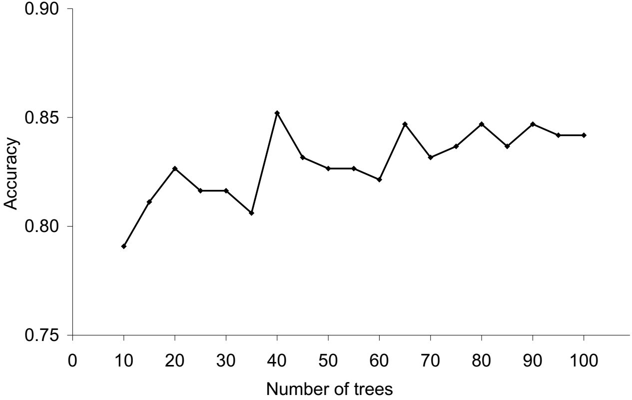
$\Rightarrow$ averaging increases prediction accuracy (Breiman, 1996a, 1998)

Bagging

prediction accuracy increases with the number of trees

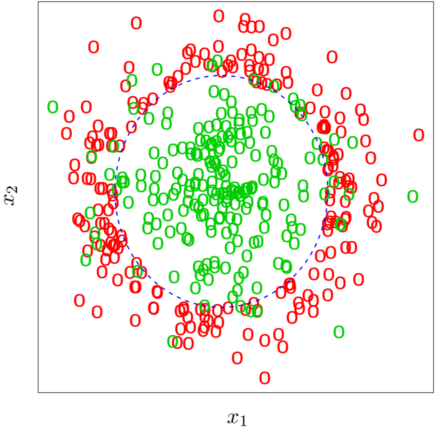


Bagging

decision boundaries are smoothed

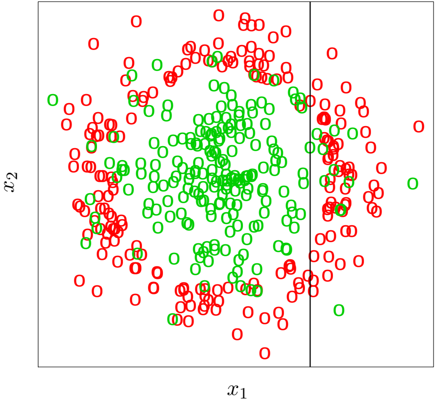
(thanks to Ji Zhu, University of Michigan, for the following graphical illustration)

Example: Nested Spheres

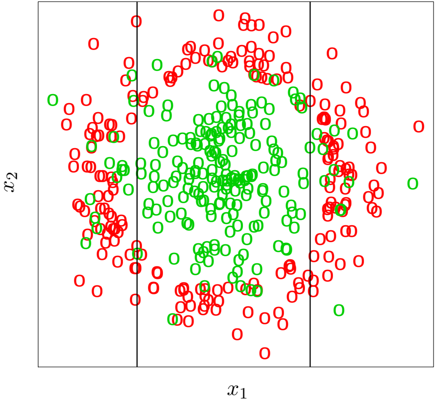


- Green class: two independent standard normal inputs X_1, X_2
- Red class: conditioned on $X_1^2 + X_2^2 \geq 4.6$

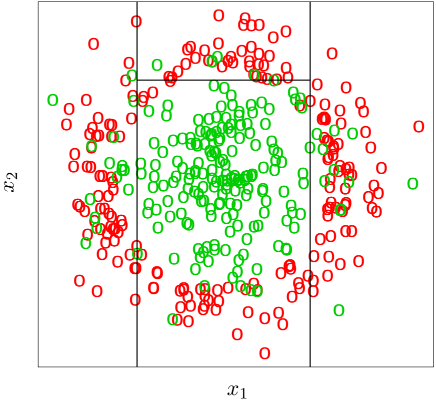
Classification Tree in Action: 1



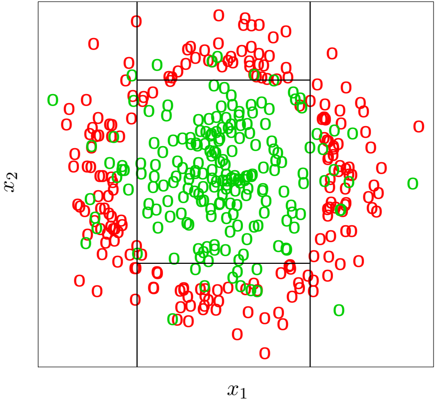
Classification Tree in Action: 2



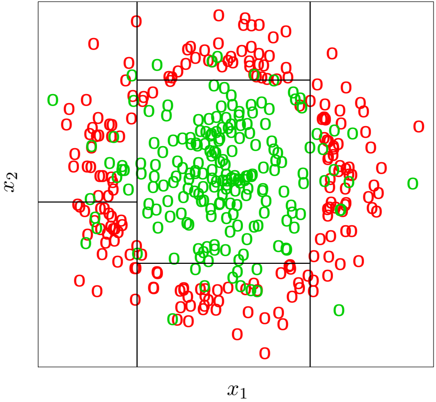
Classification Tree in Action: 3



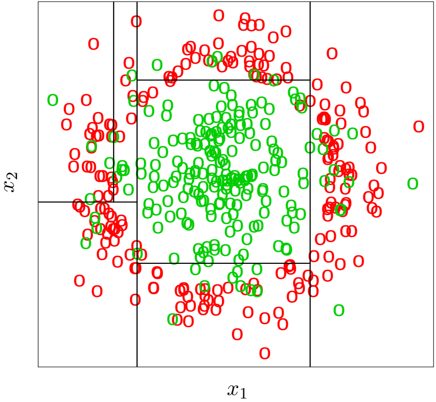
Classification Tree in Action: 4



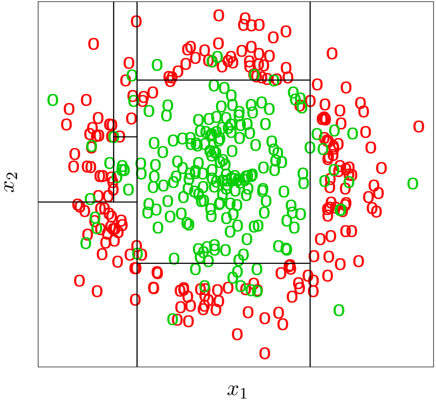
Classification Tree in Action: 5



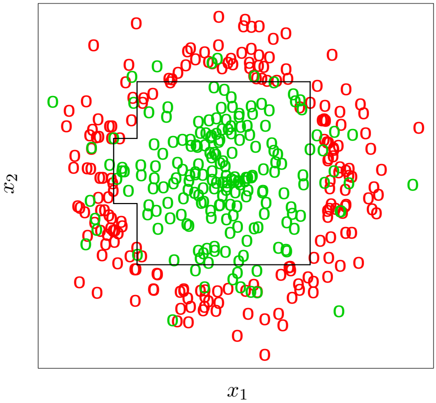
Classification Tree in Action: 6



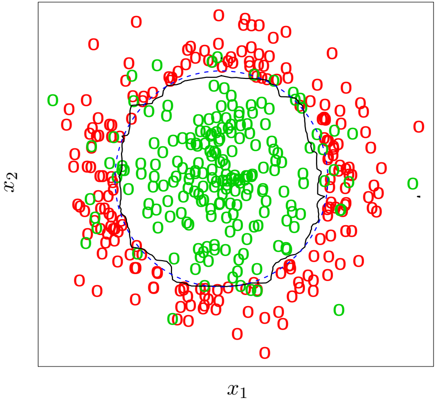
Classification Tree in Action: 7



Decision Boundary: Tree



Decision Boundary: Bagging



Bagging averages many trees, and produces more flexible decision boundaries.

Decorrelating trees II: Random forests

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$\Rightarrow$ individual trees look even more different

$\Rightarrow$ prediction accuracy is even higher (Breiman, 2001)

Advanced reading

- why bagging works: Bühlmann and Yu (2002)
  bagging smoothes hard decisions $\Rightarrow$ reduces variance
  (ugly asymptotics for trees as base learners)
- why random forests work: Lin and Jeon (2006)
  random forests can be viewed as adaptively weighted k-NN
  with terminal node size determining size of neighborhood

Bagging and random forests - tuning parameters

- number of trees
  argument `ntree` (default: 500)
  - more is better (does not negatively affect predictive accuracy) especially with many potential predictor variables
- number of randomly preselected predictors for each split
  argument `mtry` (usually $\sqrt{p}$ for classification, for smaller number of predictor variables sometimes $p/3$ is suggested, in `cforest` default: 5)
  - `mtry` $= p$ is bagging
  - different values for `mtry` can affect performance and estimates of variable importance

Random forests - tuning parameters

- tree depth
  - in bagging and random forests trees are usually grown large without pruning
  - only the minimum number of observations per node is fixed
  - results of Lin and Jeon (2006) indicate that the depth / number of observations per node do affect performance
- sampling size and method: for bootstrap sampling (default: N) and subsampling (default: $.632 \cdot N$)
  - subsampling gives better estimates of variable importance, see below

Decorrelating trees III: Boosting

main idea: fit trees on modified versions of the outcome variable Y

- can be used in addition to random sampling of rows and columns of X
- boosting is performed sequentially (in bagging and random forests, trees can be fit simultaneously)

Boosting

- At each stage $1 \leq m \leq M$ we have an imperfect model $F_(m-1)$
- we aim to improve the model with an estimator h_m, such that $F_m(X) = F_{m-1}(X) + h(X)$ provides a better model
  - How to find $h(X)$?
  - the perfect model would be $F_m(X) = F_{m-1}(X) + h(X) = y$
  - or, equivalently, $h(X) = y - F_{m-1}(X)$
- Therefore, we fit the model (the tree) at stage m to the residual $(y - F_{m-1}(X))$ instead of y
- Generally, a learning rate $0 < \nu < 1$ is applied in updating the ensemble:
  - $F_m(X) = F_{m-1}(X) + \nu \cdot h_m(X)$

Boosting

Requires more parameter tuning than bagging and random forests.

In noisy data, bagging and random forests are often more robust than boosting (Kotsiantis, 2011, e.g.,).

In R: function `gbm()` from package `gbm`

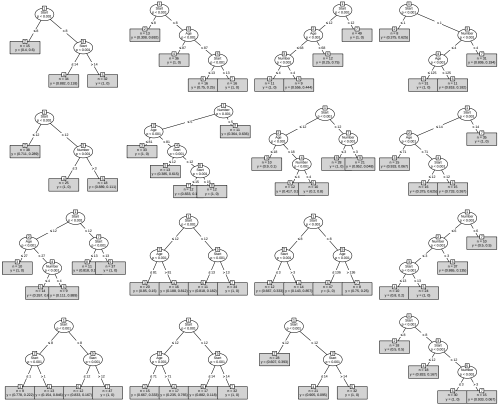
Boosting - tuning parameters

- `n.trees =`
  Increasing the number of trees may overfit the data with boosting. Optimal number of trees depends on learning rate and best determined by k-fold CV.
- `interaction.depth =`
  Typically, 4 through 8 terminal nodes work well, results are fairly insensitive to the exact choice (e.g., Hastie et al., 2009).
- `shrinkage =`
  a.k.a. learning rate ν. Typically, small values (e.g., $.001 \leq \nu < .01$) perform well (e.g., Efron et al., 2004, Bühlmann and Yu, 2003). Like number of trees, best determined by CV.

Note: list is non-exhaustive.

Interpretation

interpretation of predictor variables?



Measuring variable importance

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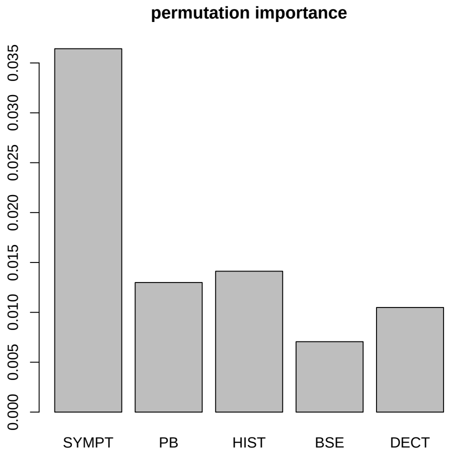
- permutation importance
  mean decrease in classification accuracy after permuting X_j over all trees
  - informative variables produce a systematic decrease in accuracy when permuted
  - uninformative variables produce a random decrease or increase in accuracy when permuted

Measuring variable importance



Measuring variable importance

Problems:

- Gini importance
  biased estimation of Gini gain in each tree $\Rightarrow$ Gini importance is biased in favor of continuous variables and variables with many categories

Strobl et al. (2007)

Measuring variable importance

Problems:

- Gini importance
  biased estimation of Gini gain in each tree $\Rightarrow$ Gini importance is biased in favor of continuous variables and variables with many categories
- permutation importance
  even if individual trees are unbiased, as in function `cforest`
  - bootstrap sampling affects variance of variable importance
  - variable importance of variables with many categories may be over/underestimated

  $\Rightarrow$ subsampling without replacement is used by default

Strobl et al. (2007)

Conditional permutation importance

spurious correlation between shoe size and reading skills in school-children

```
> mycf <- cforest(score ~ ., data = readingSkills,
+                     control = cforest_unbiased(mtry = 2))
> varimp(mycf)
nativeSpeaker           age      shoeSize
     12.62926      74.89542      20.01108
> varimp(mycf, conditional = TRUE)
nativeSpeaker           age      shoeSize
    11.808192     46.995336      2.092454
```

Strobl et al. (2008)

Measuring variable importance

Choice of hyperparameters:

- results are more stable when `ntree` is high
- results can vary for different `mtry`, especially in the case of correlated predictors
- subsampling size down to $.5 \cdot N$ (Buja and Stuetzle, 2006)

Random forests and bagging

pros	cons

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nonparametric approach	heuristic
easy to grasp	

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applicable to predictors of different types	selection can be biased

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Random forests and bagging - continued

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immune to outliers in predictors	

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Random forests and bagging - continued

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variable scales irrelevant	
few hyperparameters work well “off-the-shelve”	
variable importance	merely descriptive importance can be biased

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out of bag error estimates	

Random forests and bagging

each tree is grown on a training (bootstrap or sub-) sample

each tree brings its own test (out of bag; OOB) sample

$\Rightarrow$ OOB error estimates are not overly optimistic (e.g., Breiman, 1996b)

Highly recommended

- Friedman, J., Hastie, T., & Tibshirani, R. (2009). *The elements of statistical learning.* Second edition. Springer, Berlin.
  - Especially chapters 1, 2, 9, 10, 15
  - Yay, free! http://statweb.stanford.edu/~tibs/ElemStatLearn/download.html
- James, G., Witten, D., Hastie, T., & Tibshirani, R. (2013). *An introduction to statistical learning*. New York: Springer.
  - More introductory version of Friedman et al. (2009)
  - Yay, free! http://www-bcf.usc.edu/~gareth/ISL/getbook.html
- Strobl, C., Malley, J., & Tutz, G. (2009). An introduction to recursive partitioning: rationale, application, and characteristics of classification and regression trees, bagging, and random forests. *Psychological Methods, 14*(4), 323.
  - Note of first author: please do not interpret negative importances as a measure of statistical significance

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