Random forests: The first-choice method for every data analysis?

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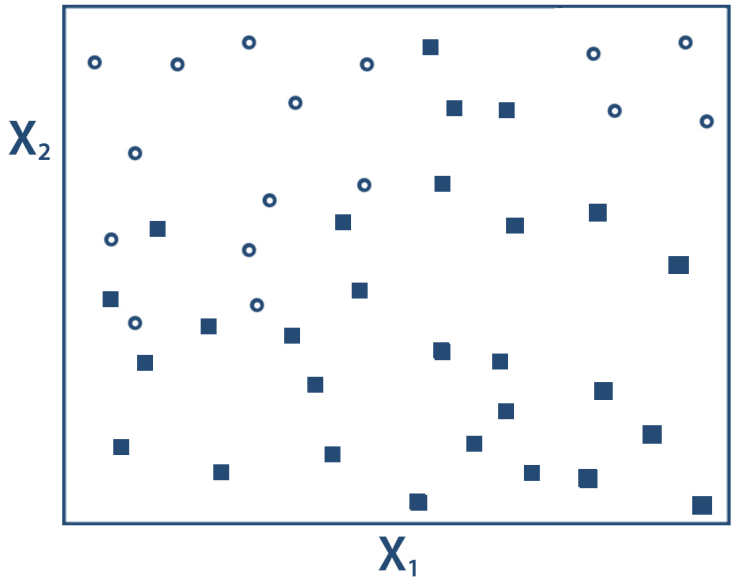
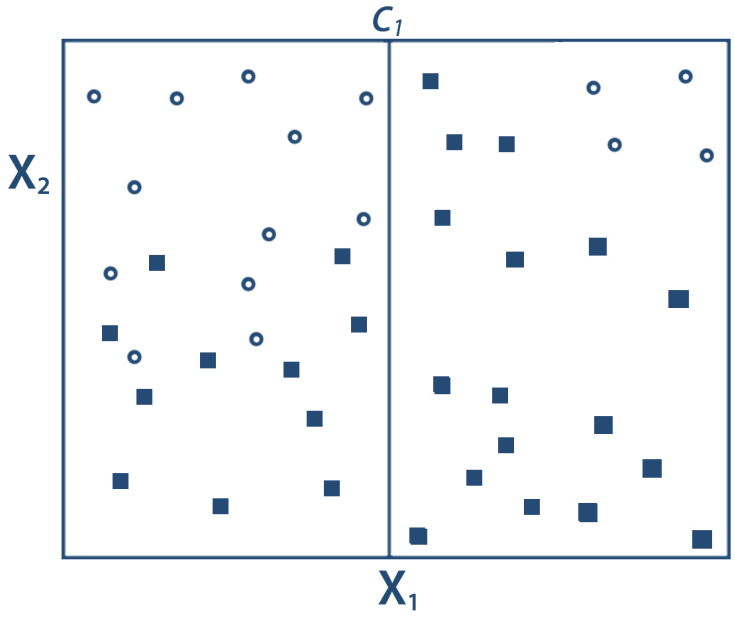
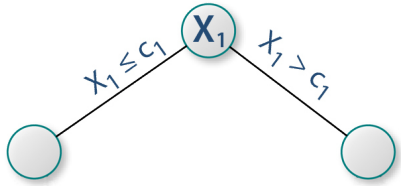
Outline

Random forests



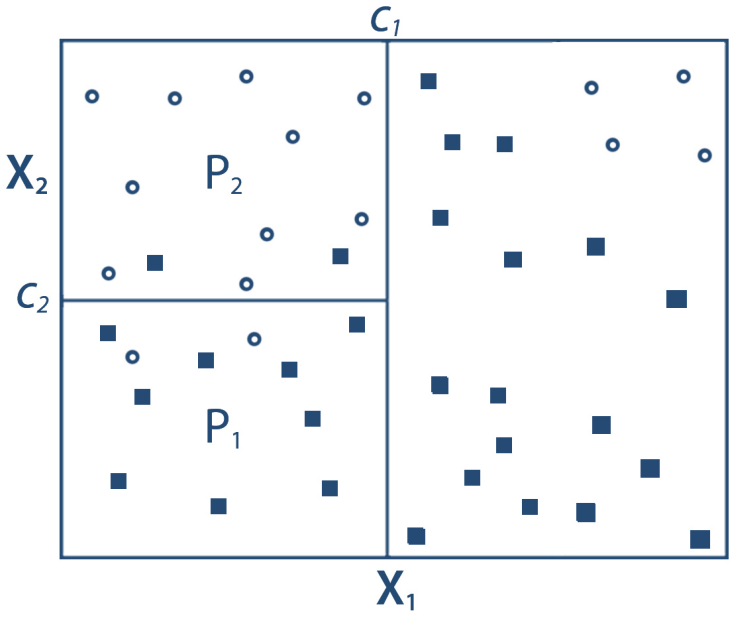
Random forests

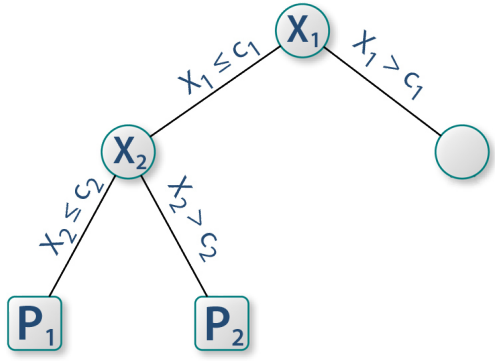




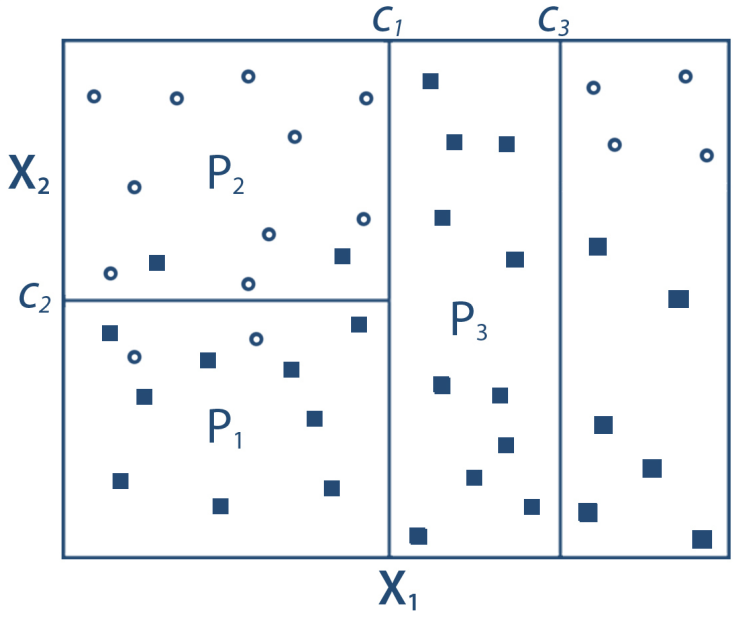
Breiman 2001 Mach Learn 45:5

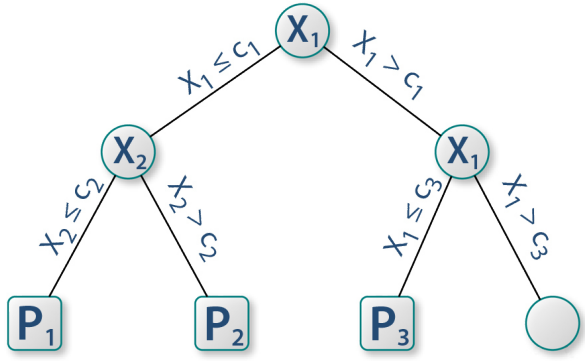
Random forests





Random forests





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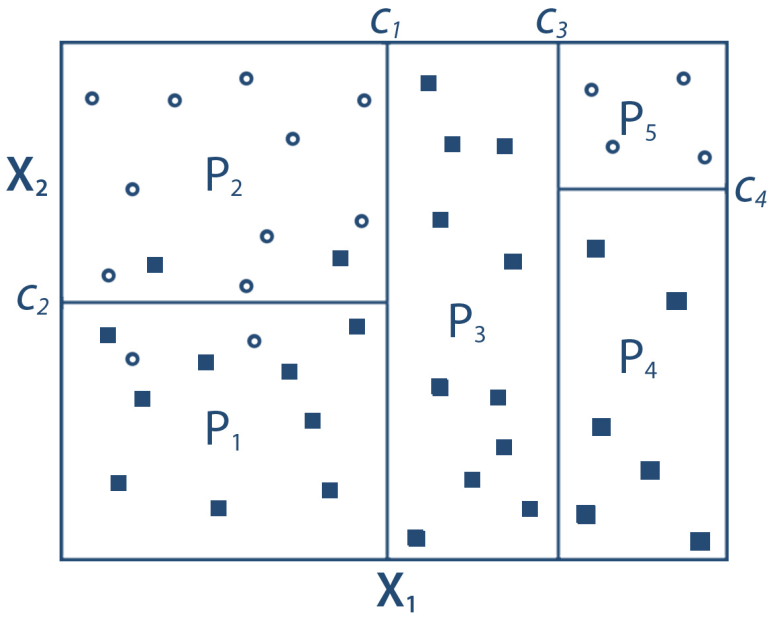

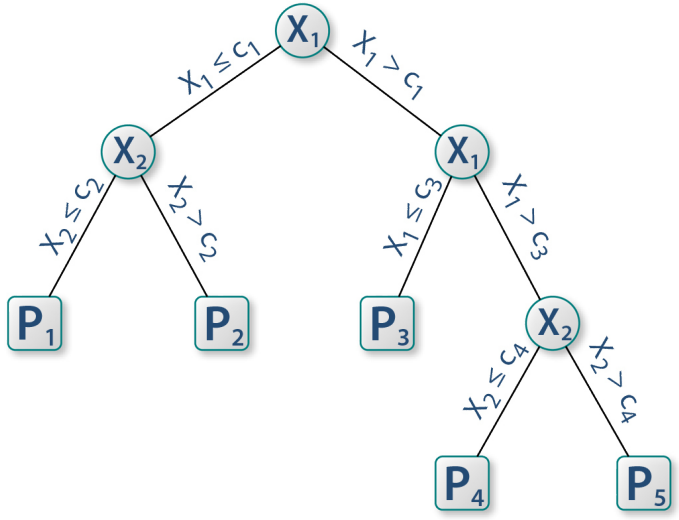

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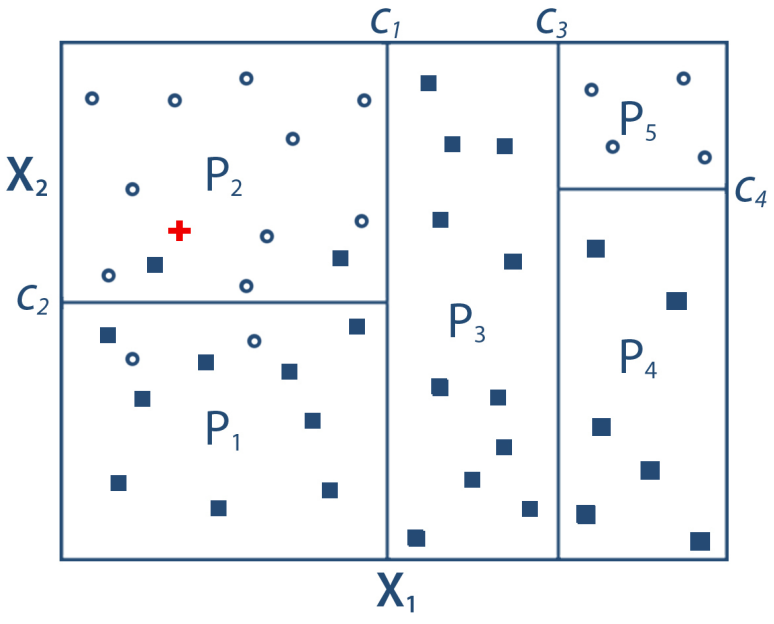

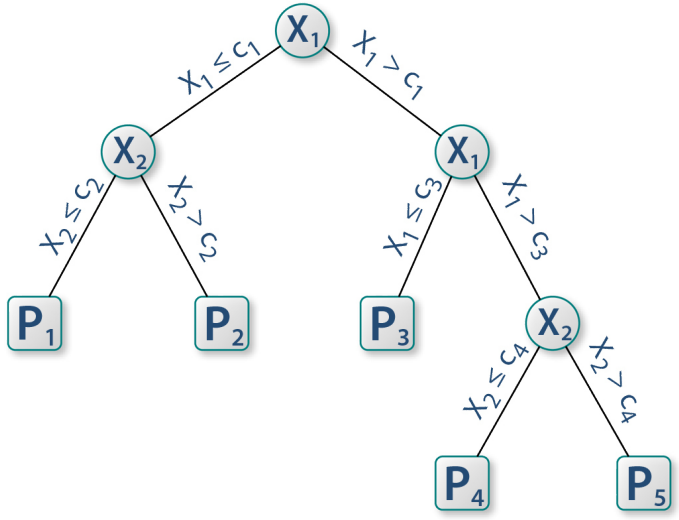

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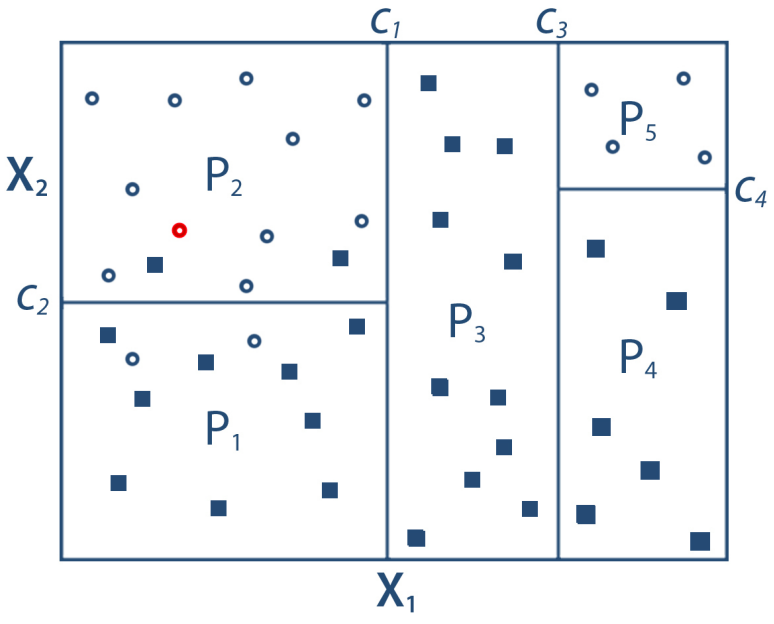

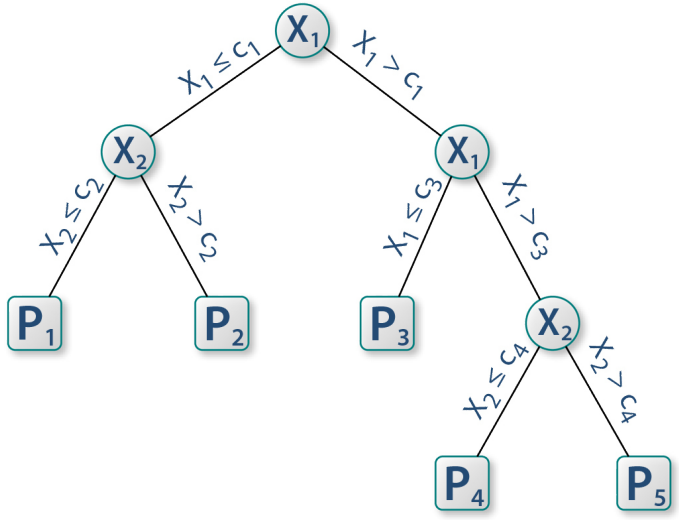

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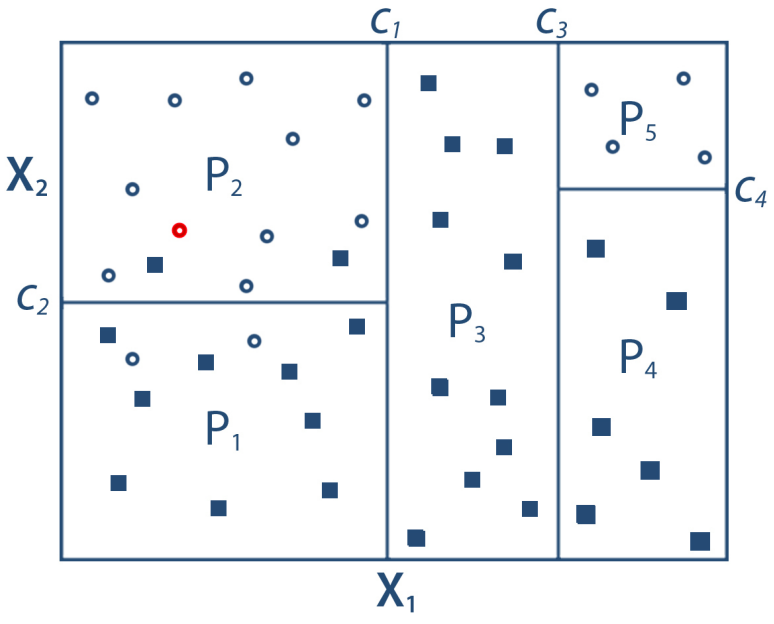

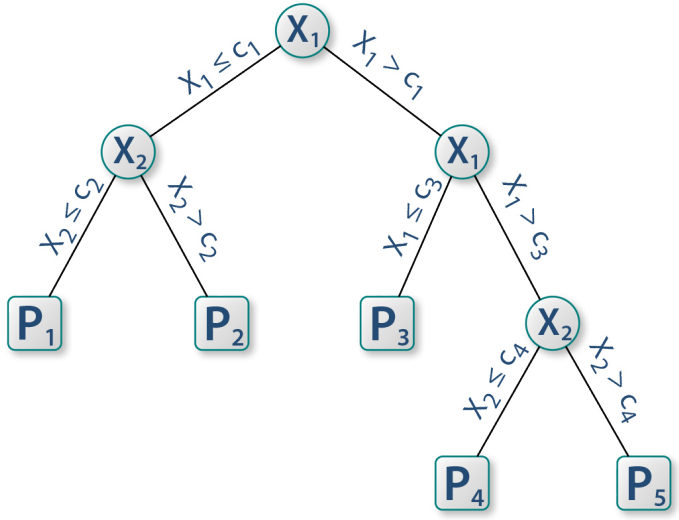

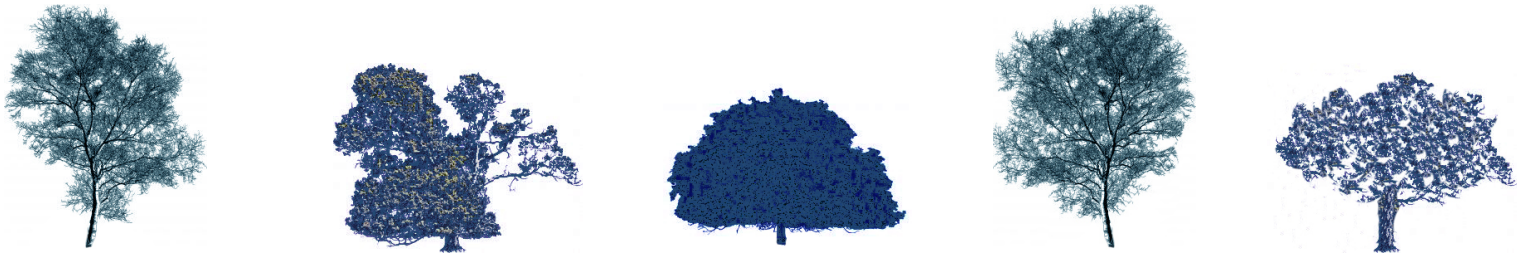

Breiman 2001 Mach Learn 45:5

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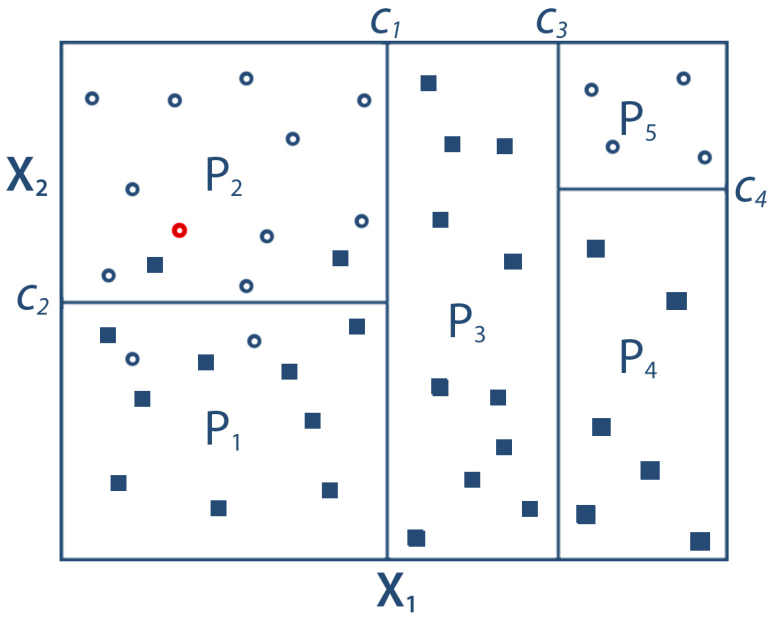
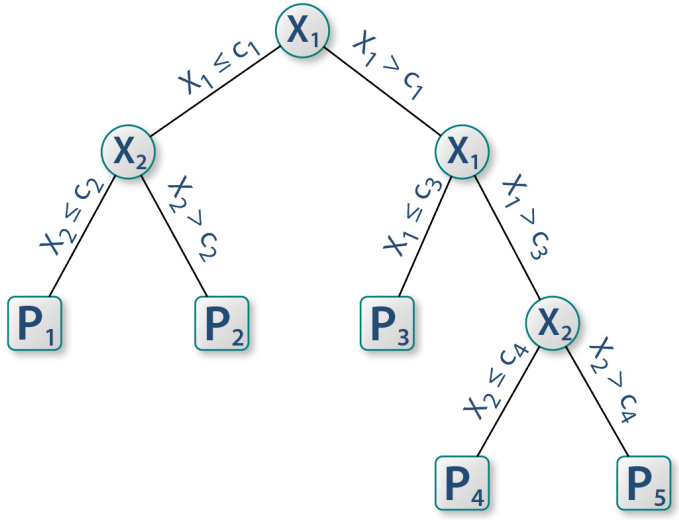
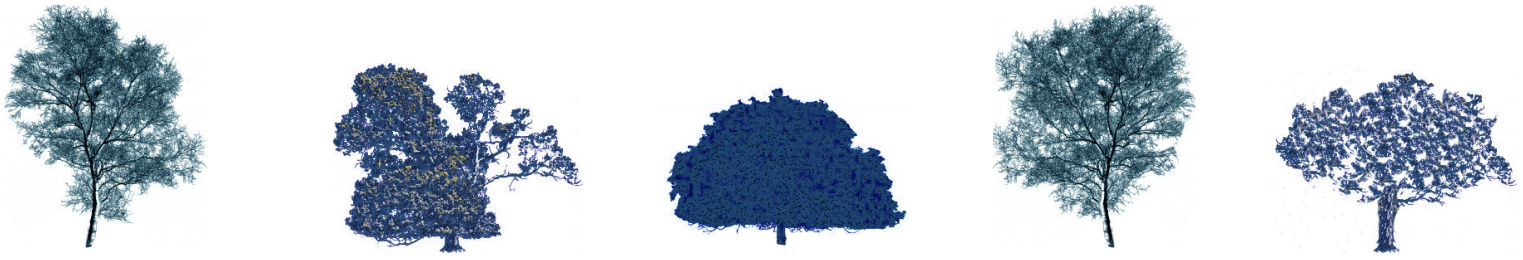
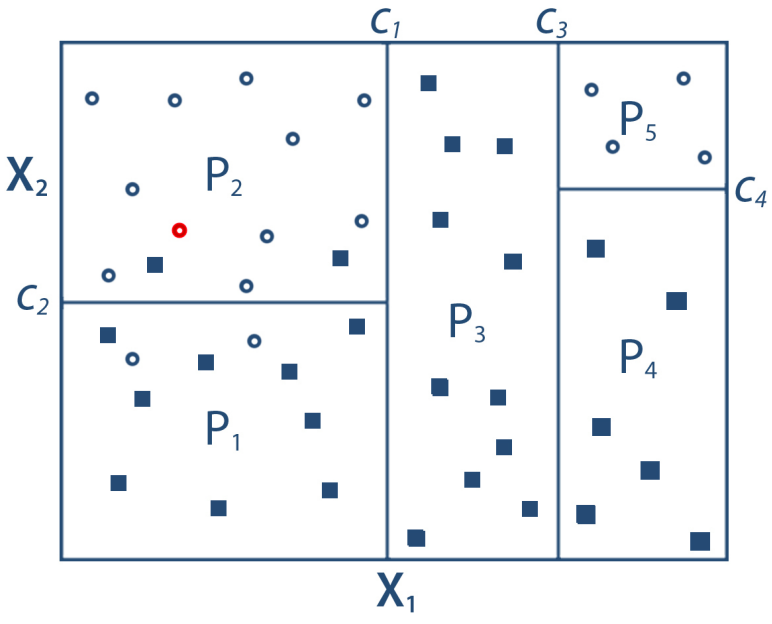


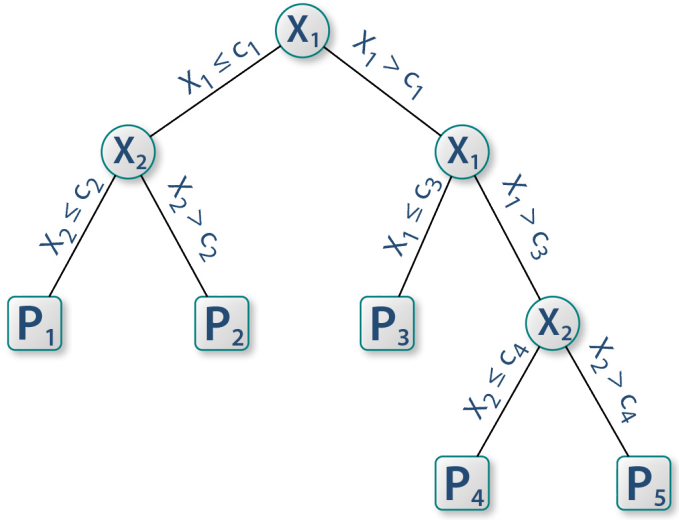


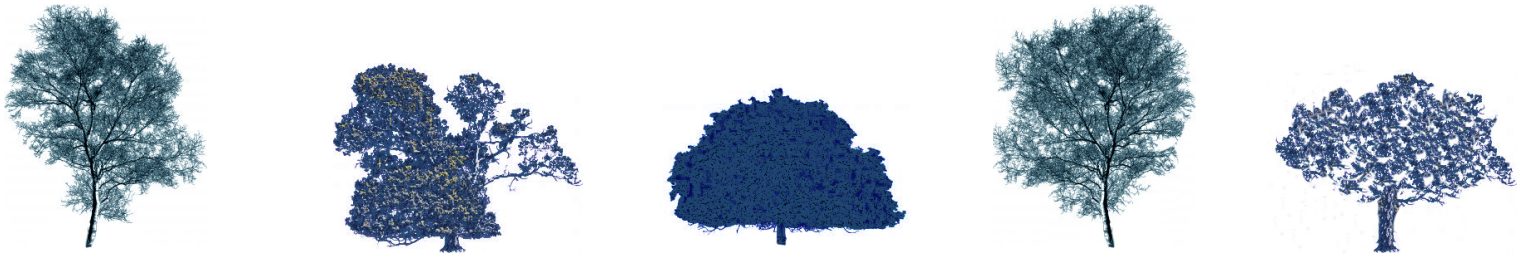


1 1 0 1 0

Random forests







1 1 0 1 0

1 according to majority vote

Random forests
Algorithm

Step 1

Draw bootstrap sample or subsample

Step 2

Grow tree

Step 3

At each node, randomly select features (`mtry` value)

Step 4

Repeat steps 1-3, average over all trees

Random forests
Algorithm

Step 1

Draw bootstrap sample or subsample

Step 2

Grow tree

Step 3

At each node, randomly select features (`mtry` value)

Step 4

Repeat steps 1-3, average over all trees

Random forests
Tuning parameters

Number of trees

- Usual default: 500
- Use more trees for high dimensional datasets

`mtry` value

Number of features selected as splitting candidates in nodes

- Usual default: $\sqrt{p}$, where $p = $ #features
- For large p use at least $p/10$

Terminal node size

Required number of observations in terminal nodes

- Determines tree size
- Typically small for classification, large for regression

Outline

1. Introduction
2. Common Claims
3. Implementations in R
4. Discussion & Conclusion

Common Claims

Claim 1: “works well without tuning”

Common Claims

Claim 1: “works well without tuning”

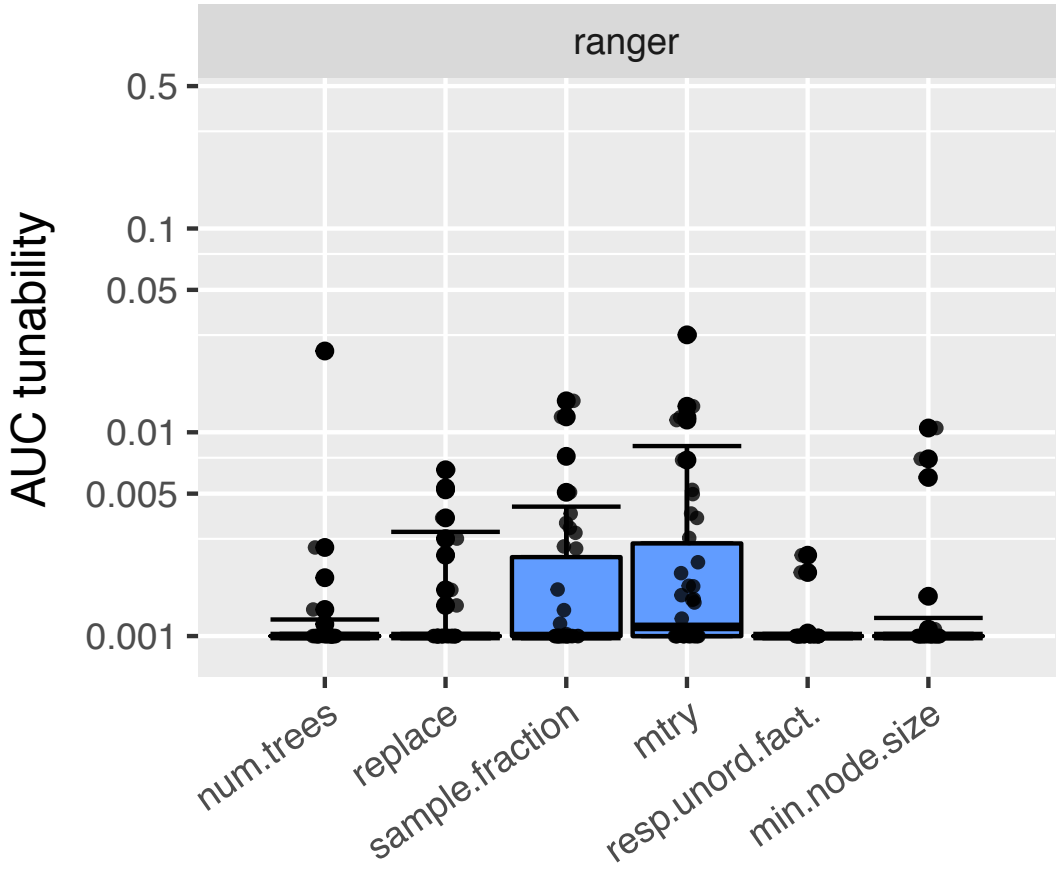
“RF is the algorithm with the smallest tunability.”

— Probst et al. 2019a

They compared `ranger`, `glmnet`, `rpart`, `kknn`, `e1071::svm`, `xgboost`.

Common Claims

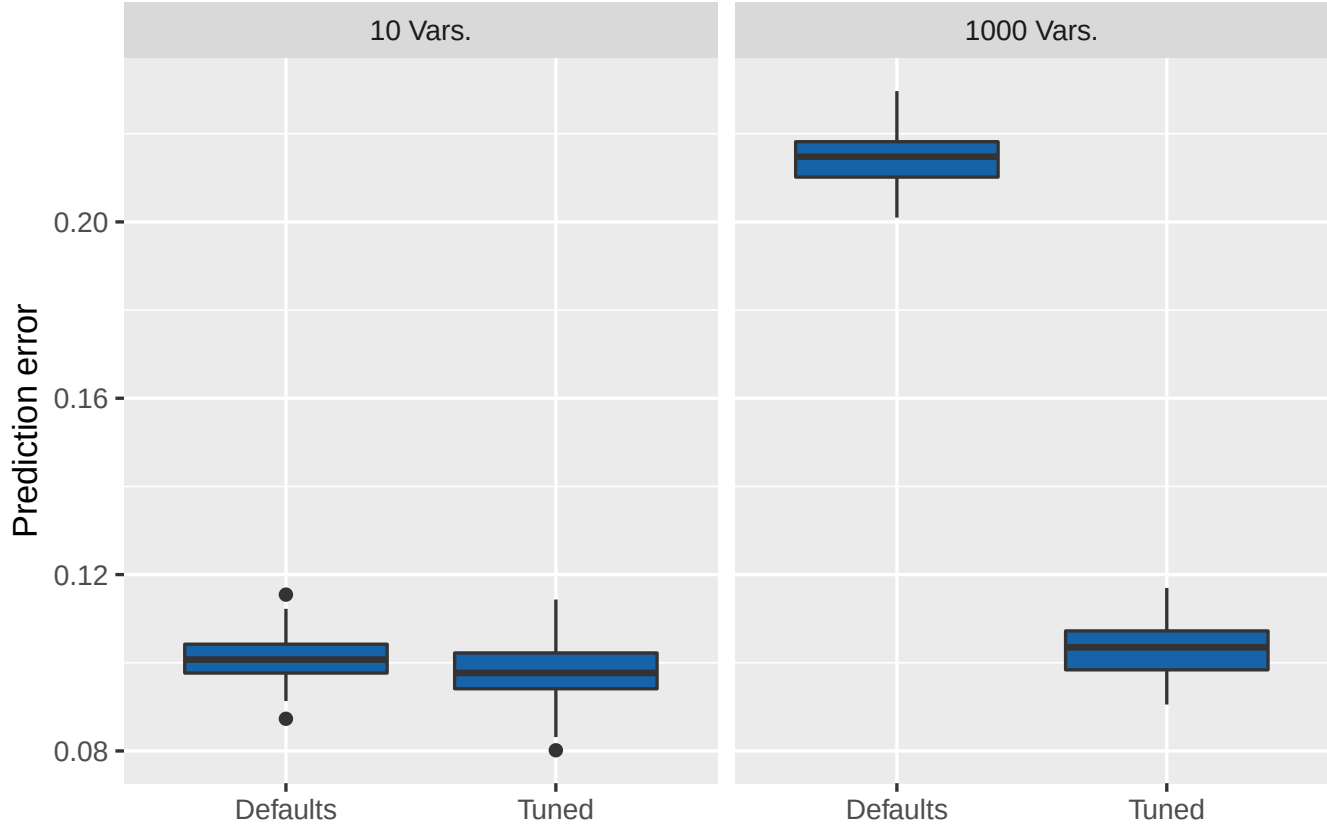
Claim 1: “works well without tuning”



Probst et al. 2019a J Mach Learn Res 20:1

Common Claims

Claim 1: “works well without tuning”



Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio

Common Claims

Claim 2: “no need to scale or recode predictors”

Common Claims

Claim 2: “no need to scale or recode predictors”

Scaling

RF invariant to monotonic transformations
$\Rightarrow$ scale-invariant

Example

Original	4.6	4.7	4.9	5.0	5.1	5.4
Scaled	-1.2	-0.9	-0.2	0.2	0.5	1.6
Logarithm	1.53	1.55	1.59	1.61	1.63	1.69

Breiman et al. 1984 ISBN 9780412048418 • Hastie et al. 2009 ISBN 9780387848570, p. 352

Common Claims

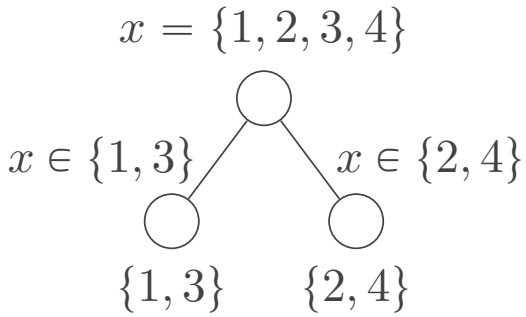
Claim 2: “no need to scale or recode predictors”

Categorical predictors

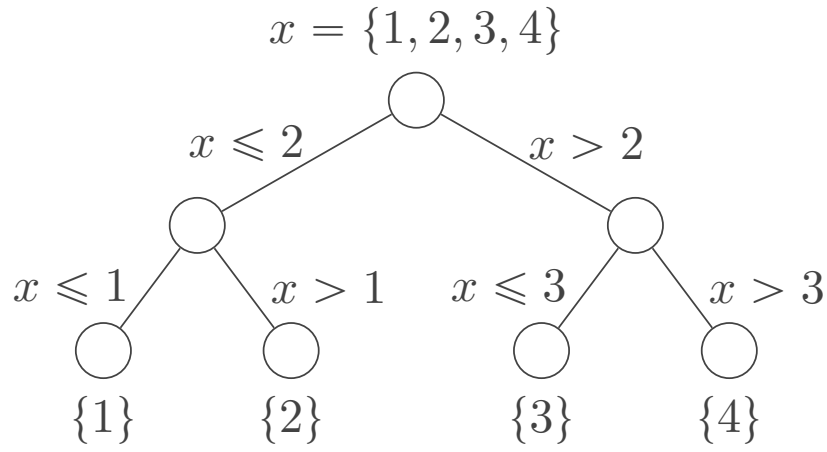
$x = \{1, 2, 3, 4\}$

Aim: Separate odd and even digits

Standard approach



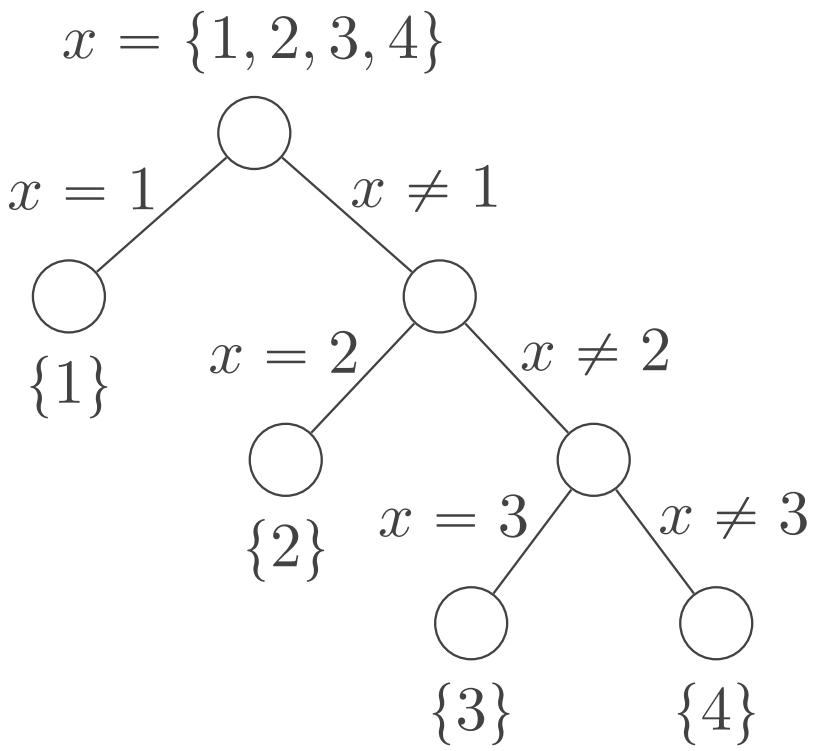
Naïve approach



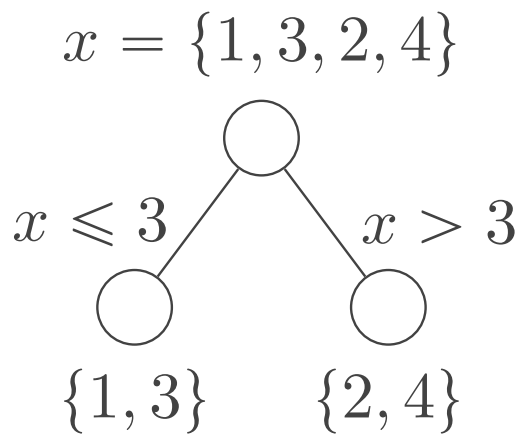
Common Claims

Claim 2: “no need to scale or recode predictors”

Dummy coding



A priori ordering



Order by average outcome

Common Claims

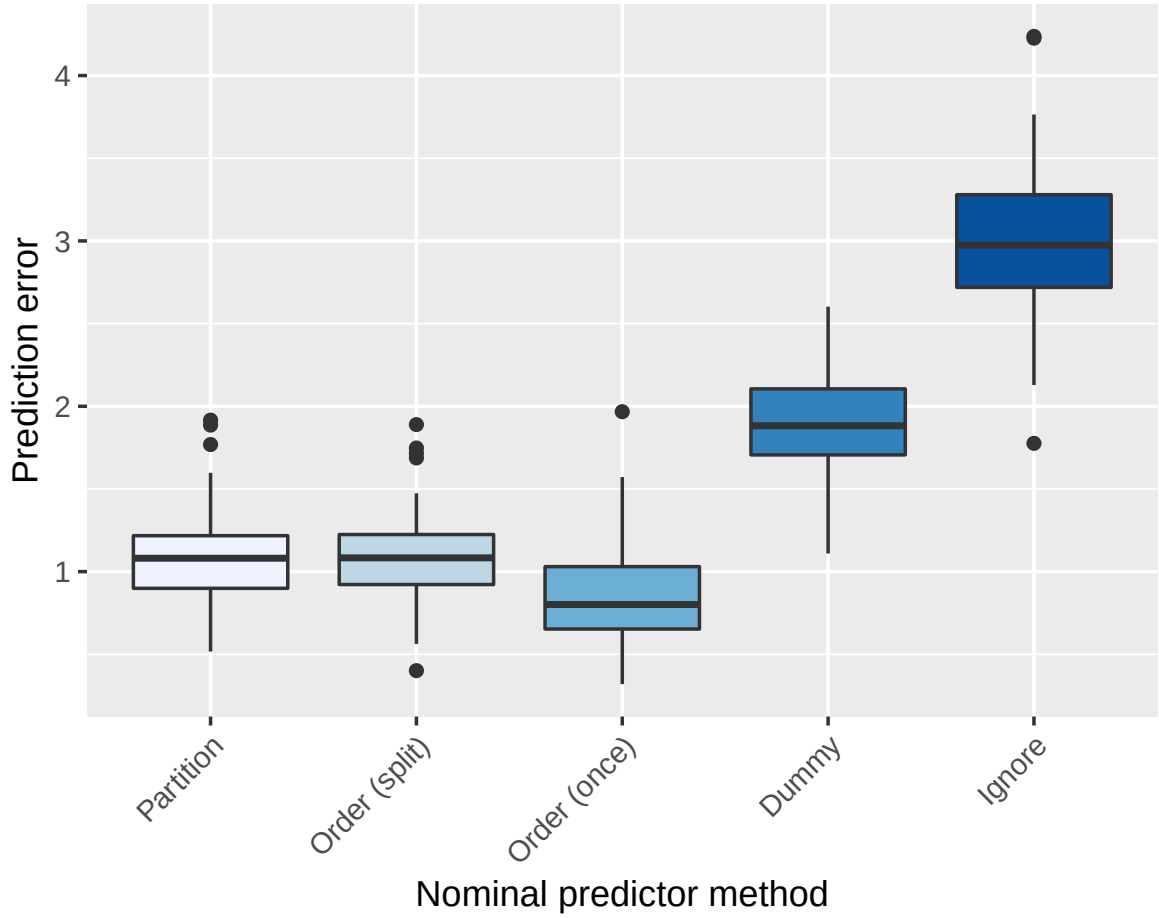
Claim 2: “no need to scale or recode predictors”

Standard approach works well only for few categories

- 4 numbers $\Rightarrow 2^{4-1} - 1 = 7$ partitions
- 28 EU countries $\Rightarrow 2^{28-1} - 1 = 1.34 \times 10^8$ partitions

Common Claims

Claim 2: “no need to scale or recode predictors”



Wright & König 2019 PeerJ 7:e6339

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors

Common Claims

Claim 3: “works well on high dimensional data”

Common Claims

Claim 3: “works well on high dimensional data”

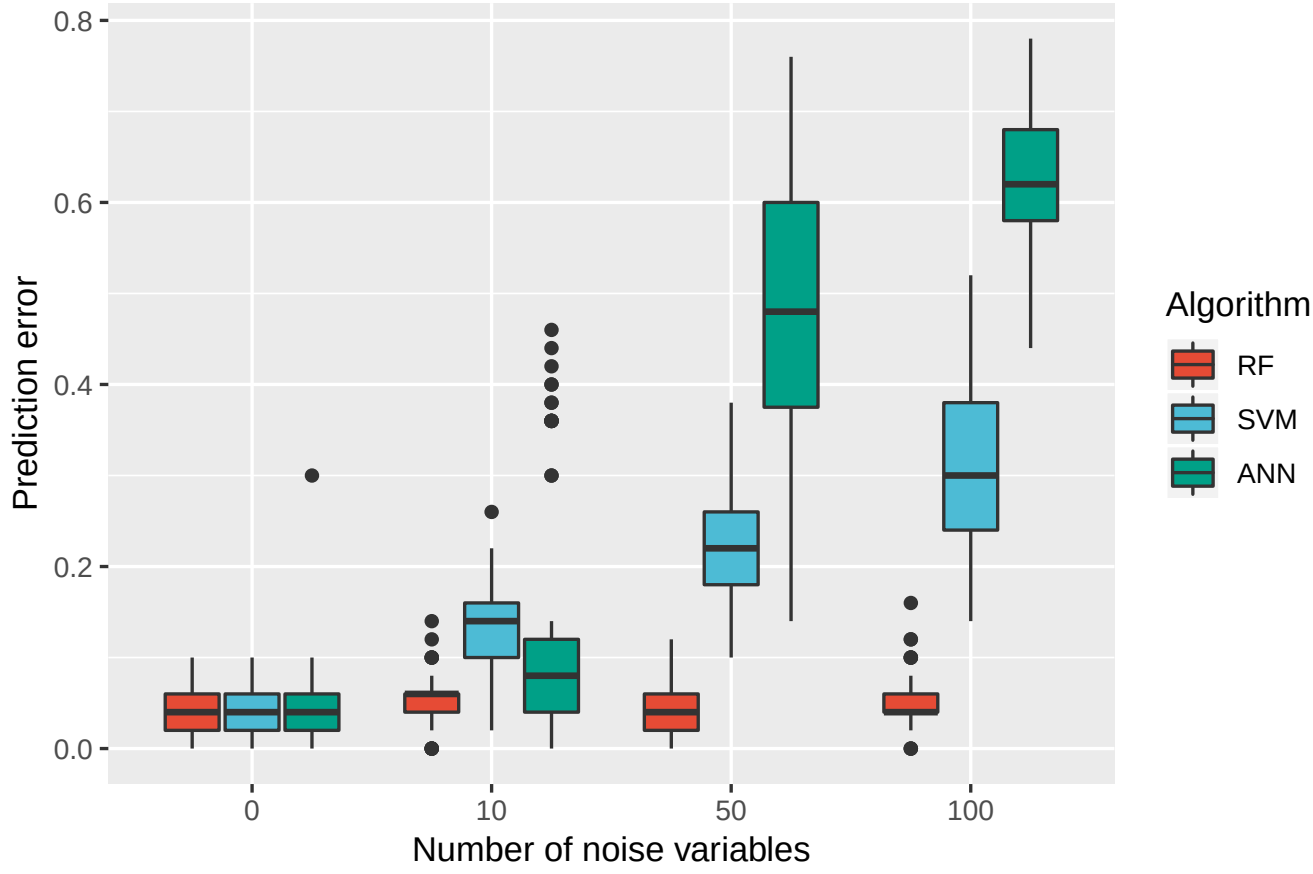
“[...] ability to deal with small sample sizes and high-dimensional feature spaces.”

“the rate of **convergence depends only on** the number $|S|$ of **strong variables**, not on the dimension p.”

— Biau & Scornet 2016

Common Claims

Claim 3: “works well on high dimensional data”



Common Claims

Claim 3: “works well on high dimensional data”

Intrinsic variable selection

- Greedy splitting algorithm selects best splitting variable
- No fitting of parameters or weights for other variables

Fast computation

See second part

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data

Common Claims

Claim 4: “cannot overfit”

Common Claims

Claim 4: “cannot overfit”

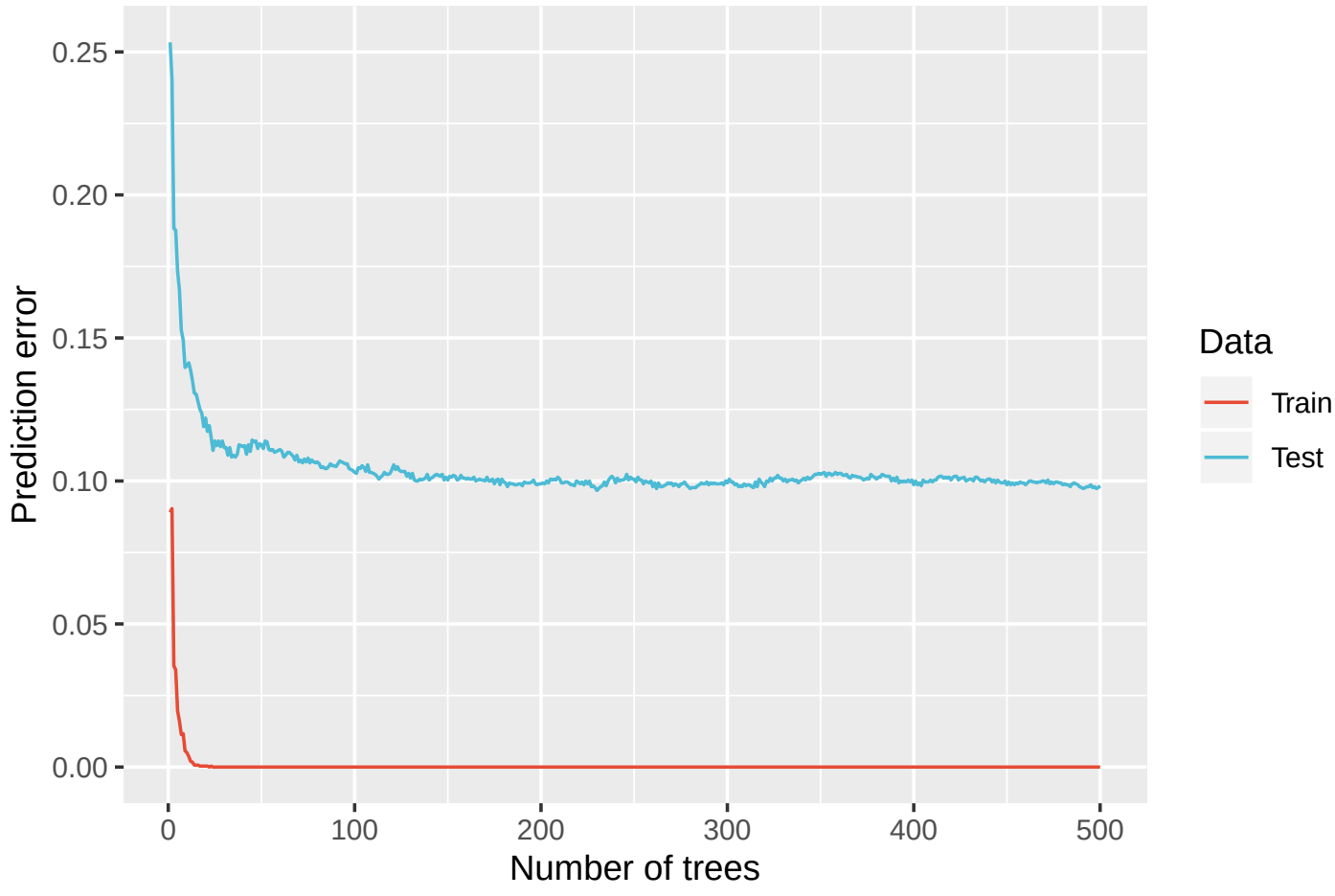
“[…] overfitting is not a problem.”

“Random forests do not overfit as more trees are added.”

— Breiman 2001

Common Claims

Claim 4: “cannot overfit”



Common Claims

Claim 4: “cannot overfit”

Definition 1

Adding trees does not hurt generalization error ✓

Definition 2

Training error is not smaller than generalization error ✗

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data
- ✓✗ Cannot overfit

Common Claims

Claim 5: “works for any kind of data”

Common Claims

Claim 5: “works for any kind of data”

Extensions

- Random survival forests: Time-to-event outcomes
- Conditional inference forests: Avoid split variable selection bias
- Quantile regression forests: Quantile regression
- Transformation forests: Predict distributions
- Block forests: Multi-omics data
- Random forests for bounded outcomes
- Generalized random forests

And many more ...

Ishwaran et al. 2008 Ann Appl Stat 2:841 • Hothorn et al. 2006 J Comp Graph Stat 15:651 • Meinshausen 2006 J Mach Learn Res 7:983 • Hothorn & Zeileis 2018 arXiv:1701.02110 • Hornung & Wright 2019 BMC Bioinformatics 20:358 • Weinhold et al. 2019 arXiv:1901.06211 • Athey et al. 2019 Ann Stat 47:1148

Common Claims

Claim 5: “works for any kind of data”

Missing extensions

- Longitudinal data, e.g. repeated measurements
- Time series, e.g. register data
- Image, speech and natural language processing (next slide)

More?

Sela & Simonoff 2012 Mach Learn 86:169 • Hajjem et al. 2014 J Stat Comput Simul 84:1313 • Capitaine et al. 2019 arXiv:1901.11279

Common Claims

Claim 5: “works for any kind of data”

“Methods like random forests regularly outperform neural networks in arbitrary domains, especially when the underlying data sizes are small and **no domain-specific insight has been used to arrange the architecture** of the underlying neural network.”

— Wang et al. 2018

Image, speech and natural language processing data

Top benchmark results are all deep learning, mostly CNN’s and RNN’s

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data
- ✓✗ Cannot overfit
- ✓ Works for almost any kind of data
  - ✗ Exception: Image, speech and natural language processing

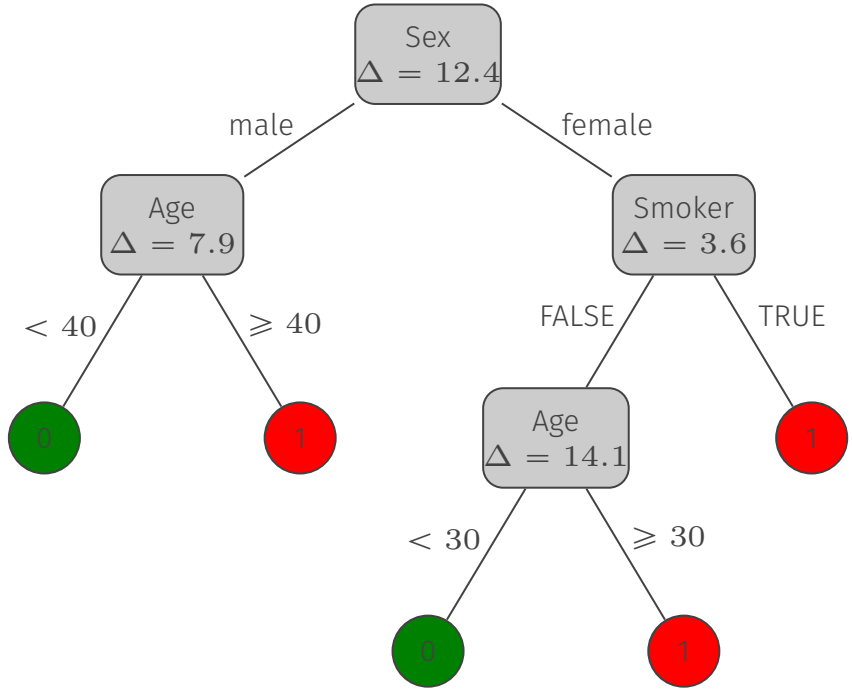
Common Claims

Claim 6: “is an interpretable model”

Common Claims

Claim 6: “is an interpretable model”

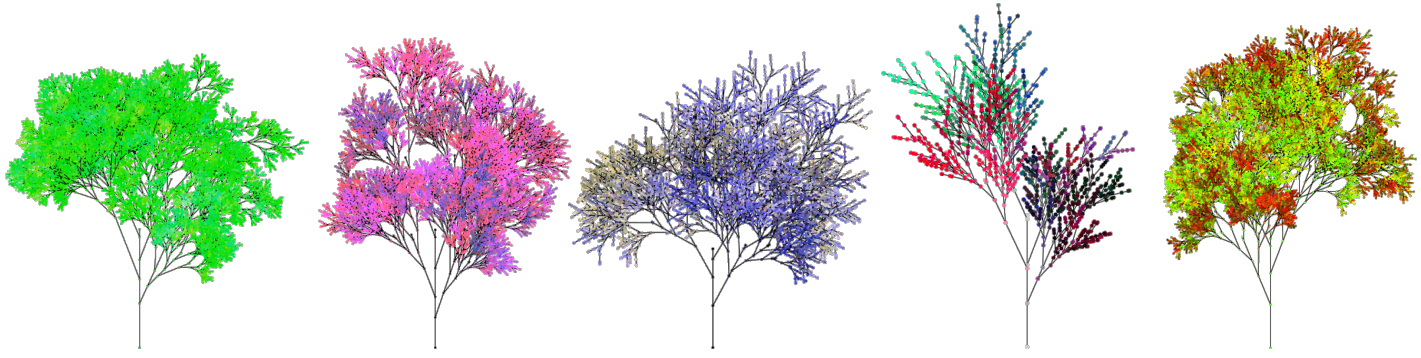
A single tree is interpretable



Common Claims

Claim 6: “is an interpretable model”

A random forest is **not** interpretable



Common Claims

Claim 6: "is an interpretable model"

Several variable importance measures available

- Gini/impurity importance: Sum of impurity measures
- Permutation importance: Permute variable, difference of prediction error
- Bias-corrected impurity importance: Difference of impurity importance to permuted version of variable
- Conditional variable importance: Conditional on other predictor variables
- Maximal subtree: Depth of first split on variable

Breiman et al. 1984 ISBN 9780412048418 • Breiman 2001 Mach Learn 45:5 • Nembrini et al. 2018 Bioinformatics 34:3711 • Strobl et al. 2008 BMC Bioinformatics 9:307 • Ishwaran et al. 2010 J Am Stat Assoc 105:205

Common Claims

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- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data
- ✓✗ Cannot overfit
- ✓ Works for almost any kind of data
  - ✗ Exception: Image, speech and natural language processing
- ✗ Is an interpretable model
  - ✓ Many variable importance measures available

Common Claims

Claim 7: “the statistical properties are well understood”

Common Claims

Claim 7: "the statistical properties are well understood"

Consistency

- Single tree not consistent
- RF consistent if $a_n/n \to 0$ and $a_n \to \infty$ (a_n/n: Subsampling rate)

Convergence rate

- Single trees slower than minimax rate
- RF achieves minimax rate. If more than 54% of variables have no effect, convergence rate faster than minimax

Asymptotic normality

- Single tree predictions asymptotically normally distributed
- RF predictions asymptotically normally distributed for subsampling

Biau et al. 2008 J Mach Learn Res 9:2015-33 • Scornet 2016 J Multiv Anal 146:72-83 • Wager et al. 2014 J Mach Learn Res 15:1625-51 • Wager & Athey 2018 J Am Stat Assoc 113:1228

Common Claims

Claim 7: “the statistical properties are well understood”

Assumptions

- Subsampling, not standard bootstrap
- Limit on subsampling rate, e.g. $a_n/n \to 0$ and $a_n \to \infty$
- Random splitting, e.g. purely random forest, selecting variable and split completely randomly

Biau et al. 2008 J Mach Learn Res 9:2015-33 • Scornet 2016 J Multiv Anal 146:72-83
Wager et al. 2014 J Mach Learn Res 15:1625-51 • Wager & Athey 2018 J Am Stat Assoc 113:1228

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- ✓✗ Cannot overfit
- ✓ Works for almost any kind of data
  - ✗ Exception: Image, speech and natural language processing
- ✗ Is an interpretable model
  - ✓ Many variable importance measures available
- ✓ The statistical properties are well understood
  - ✗ Assumptions might not hold with default settings

Common Claims

Claim 8: “the split variable selection is biased”

Common Claims

Claim 8: “the split variable selection is biased”

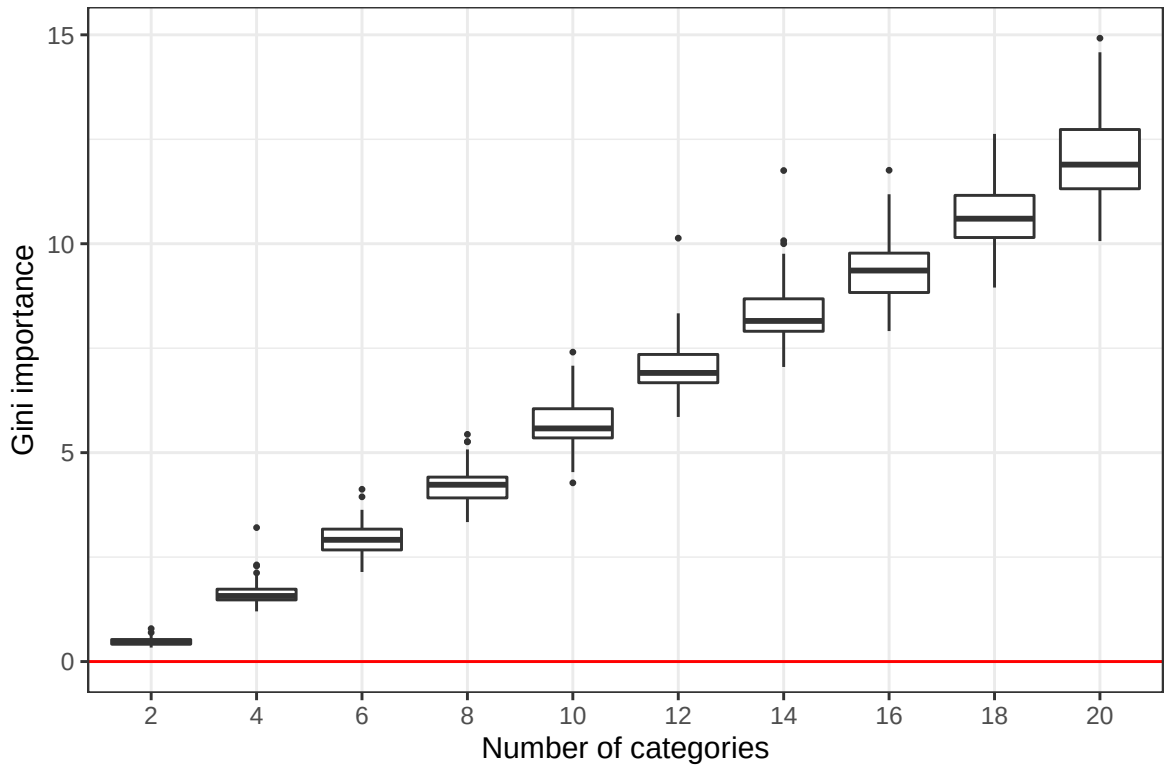
More possible split points for variables with more categories

Example

- Sex: 2 unique values
- Medication type: 5 unique values
- Age (in years): m unique values
- Biomarker: n unique values

Common Claims

Claim 8: “the split variable selection is biased”



Strobl et al. 2007 BMC Bioinformatics 8:25 • Wright et al. 2017 Stat Med 36:1272 • Nembrini et al. 2018 Bioinformatics 34:3711

Common Claims

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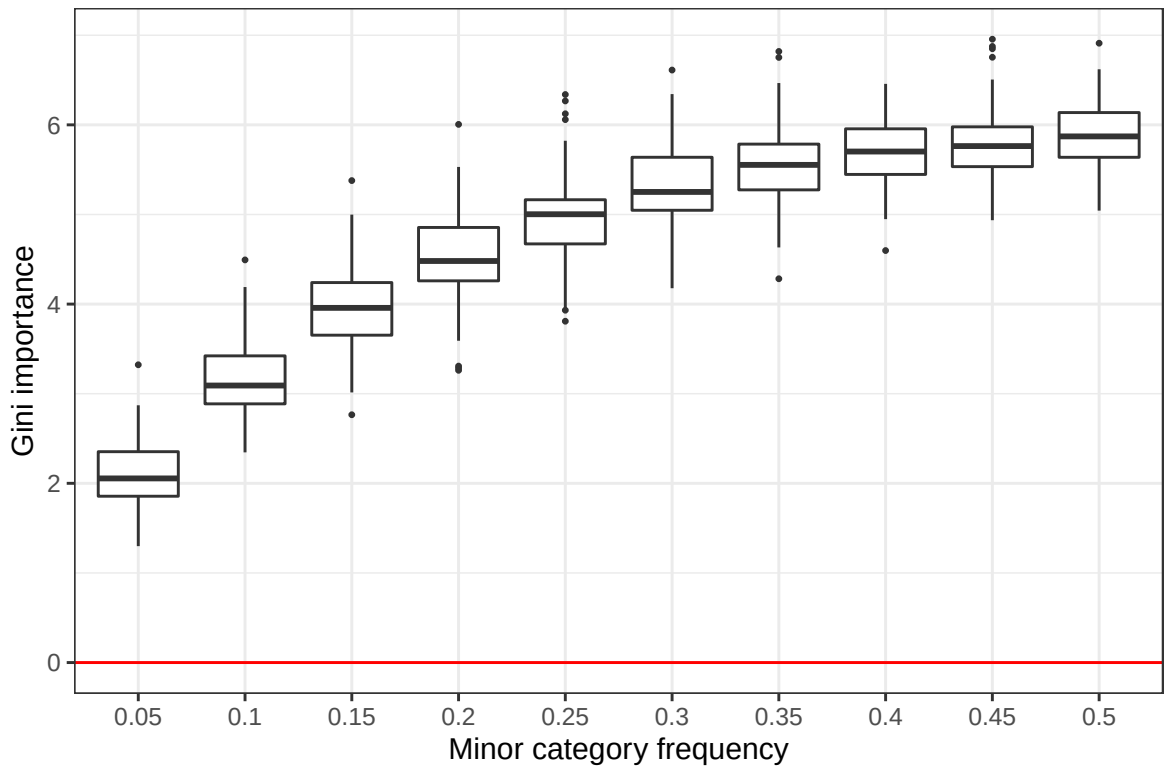


Boulesteix et al. 2012 Brief Bioinform 13:292 • Wright et al. 2017 Stat Med 36:1272 • Nembrini et al. 2018 Bioinformatics 34:3711

Common Claims

Claim 8: “the split variable selection is biased”

Solution 1
Randomized splitting rule

Solution 2
Conditional inference forests or maximally selected rank statistics

Solution 3
Bias-corrected variable importance

Geurts et al. 2006 Mach Learn 63:3 • Hothorn et al. 2006 J Comp Graph Stat 15:651 • Wright et al. 2017 Stat Med 36:1272 • Nembrini et al. 2018 Bioinformatics 34:3711

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data
- ✓✗ Cannot overfit
- ✓ Works for almost any kind of data
  - ✗ Exception: Image, speech and natural language processing
- ✗ Is an interpretable model
  - ✓ Many variable importance measures available
- ✓ The statistical properties are well understood
  - ✗ Assumptions might not hold with default settings
- ✓ The split variable selection is biased → solved

Common Claims

Claim 9: “performance is not state of the art”

Common Claims

Claim 9: “performance is not state of the art”

Gijsbers et al. 2019: Comparison of automated machine learning algorithms on 39 datasets with 4h time budget

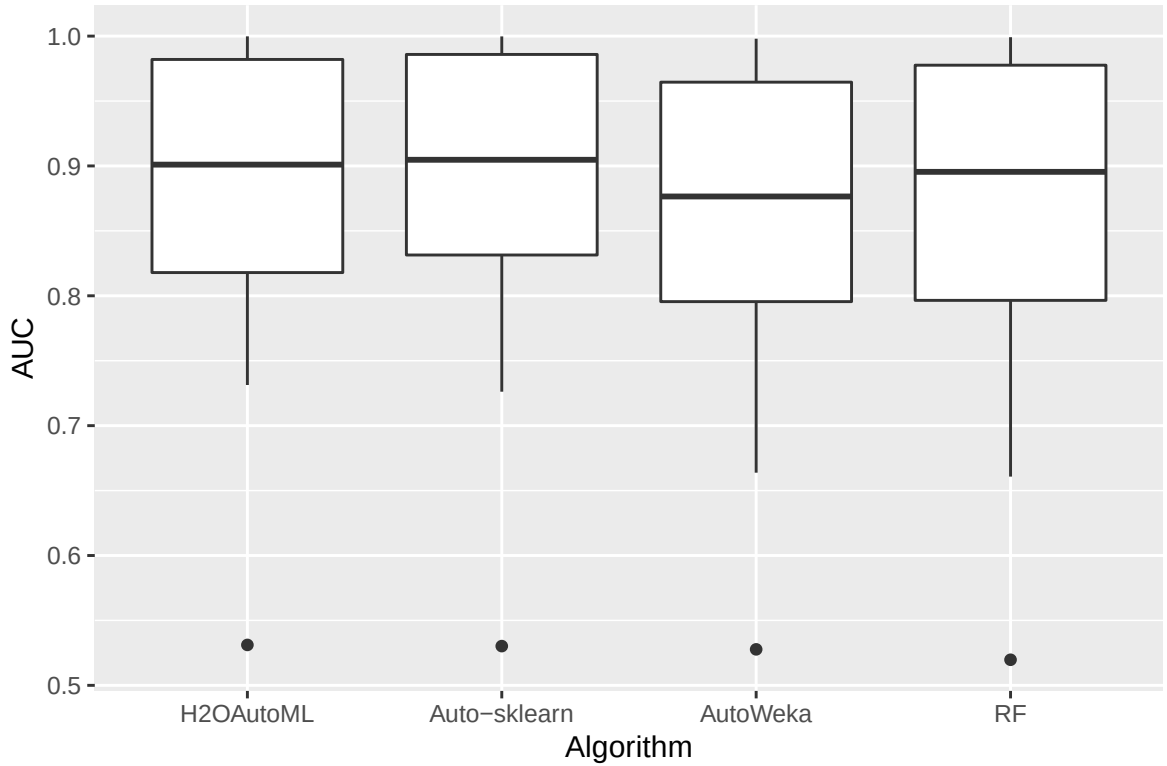
Results

Algorithms	Average rank
H2OAutoML	1.5
Auto-sklearn	2.1
AutoWeka	3.4
RF	3.0

Gijsbers et al. 2019 arXiv:1907.00909

Common Claims

Claim 9: “performance is not state of the art”



Average runtime of random forest: 16.4 seconds

Gijsbers et al. 2019 arXiv:1907.00909

Common Claims

- ✓ Works well without tuning
  - ✗ Exception: High dimensional data, low signal-to-noise ratio
- ✓ No need to scale or recode predictors
- ✓ Works well on high dimensional data
- ✓✗ Cannot overfit
- ✓ Works for almost any kind of data
  - ✗ Exception: Image, speech and natural language processing
- ✗ Is an interpretable model
  - ✓ Many variable importance measures available
- ✓ The statistical properties are well understood
  - ✗ Assumptions might not hold with default settings
- ✓ The split variable selection is biased → solved
- ✓✗ Performance is not state of the art

Common Claims

Claim 10: “detects interactions”

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“Random forests are generally **capable of capturing** gene-gene interactions, but current variable importance measures are **unable to detect** them as interactions.”

“interactions are **masked by marginal effects** and interactions cannot be differentiated from marginal effects.”

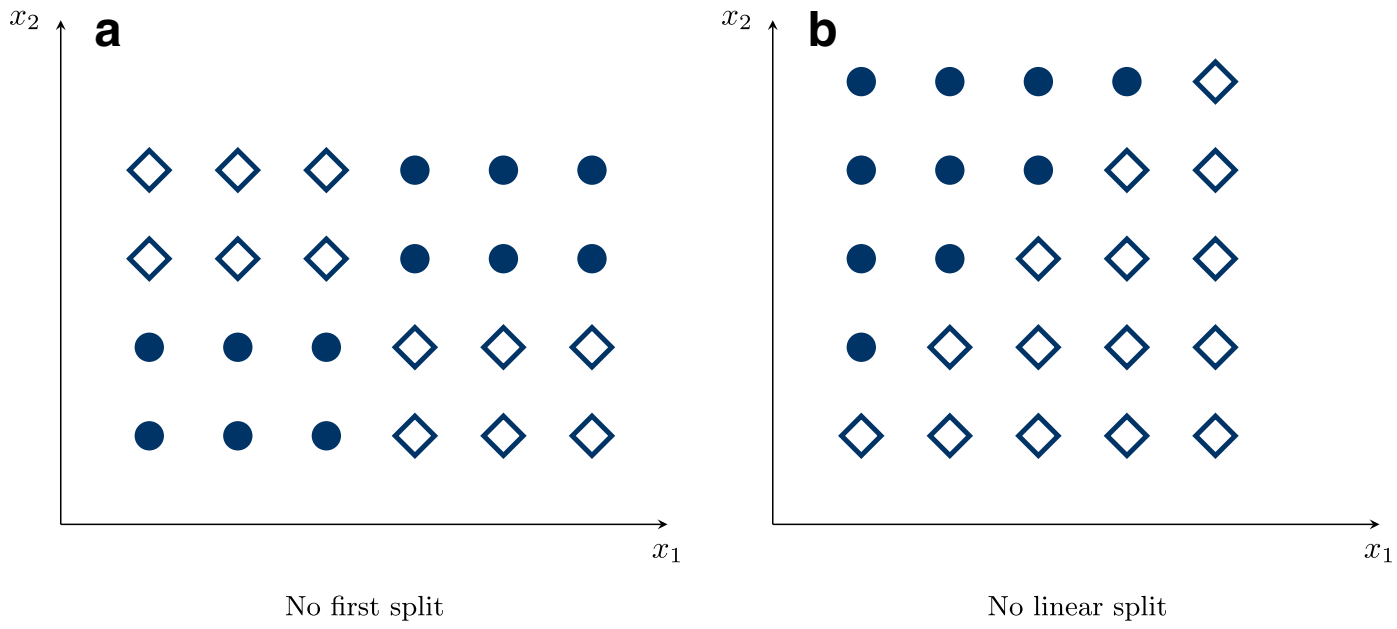
— Wright et al. 2016

“although it is able to **take interactions into account**, it **does not specifically detect them**.”

— Schmalohr et al. 2018

Common Claims

Claim 10: “detects interactions”



Wright et al. 2016 BMC Bioinformatics 17:145

Common Claims

Claim 10: “detects interactions”

Curse of dimensionality worse for interactions

Low probability to subsequently select all interacting variables in high dimensional data.

Example with $p = 100\,000$:

`mtry` $= \sqrt{p} = 316$: $p_{\text{2way}} = 0.00001$, $p_{\text{3way}} = 3 \times 10^{-8}$

`mtry` $= p/2 = 50\,000$: $p_{\text{2way}} = 0.25$, $p_{\text{3way}} = 0.125$

Need marginal effect for first split

RF splitting only detects marginal effects

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- ✓✗ Performance is not state of the art
- ✓✗ Detects interactions

Outline

1. Introduction
2. Common Claims
3. Implementations in R
4. Discussion & Conclusion

RF Implementations in R

Original RF

- `randomForest`
- `randomForestSRC`
- `Rborist`
- `ranger`

Not available anymore

- `bigrf`
- `Random Jungle`

Liaw & Wiener 2002 R News 2:18 • Ishwaran et al. 2008 Ann Appl Stat 2:841 • Seligman 2019 https://CRAN.R-project.org/package=Rborist • Wright & Ziegler 2017 J Stat Softw 77:1

RF Implementations in R

Extensions

- `party`: Conditional inference forests
- `partykit`: Conditional inference forests, model-based recursive partitioning
- `quantregForest`: Quantile regression forests
- `trtf`: Transformation forests
- `blockForest`: Block forests
- `grf`: Generalized random forests

Hothorn et al. 2006 J Comp Graph Stat 15:651 • Hothorn & Zeileis 2015 J Mach Learn Res 16:3905 • Meinshausen 2006 J Mach Learn Res 7:983 • Hothorn & Zeileis 2017 arXiv:1701.02110 • Hornung & Wright 2019 BMC Bioinformatics 20:358 • Athey et al. 2019 Ann Stat 47:1148

Runtime and memory usage

Low dimensional data

- 100,000 samples, 100 variables
- 1000 trees, `mtry`=10
- 12 CPU cores (except `randomForest`)

Package	Runtime (minutes) binary vars.	cont. vars.	Memory usage (GB)
`randomForest`	31.53	42.65	9.37
`randomForest` (MC)	5.34	7.20	13.20
`randomForestSRC`	1.72	8.35	7.26
`Rborist`	5.42	4.93	2.74
`ranger`	1.17	9.31	1.27

Slower machine than in original paper

Runtime and memory usage

Low dimensional data

- 100,000 samples, 100 variables
- 1000 trees, `mtry`=10
- 12 CPU cores (except `randomForest`)

Package	Runtime (minutes) binary vars.	cont. vars.	Memory usage (GB)
`randomForest`	31.53	42.65	9.37
`randomForest` (MC)	5.34	7.20	13.20
`randomForestSRC`	1.72	8.35	7.26
`Rborist`	5.42	4.93	2.74
`ranger`	1.17	9.31	1.27

Slower machine than in original paper

Runtime and memory usage

High dimensional data (genetic data)

- 10,000 samples, 150,000 variables (SNPs)
- 1000 trees, `mtry`=5000
- 12 CPU cores (except `randomForest`)

Package	Runtime (hours)	Memory usage (GB)
`randomForest`	93.04	52.73
`randomForest` (MC)	NA	>96
`randomForestSRC`	1.59	36.05
`Rborist`	NA	>96
`ranger`	1.19	17.71
`ranger` (GWAS mode)	0.35	0.13

Slower machine than in original paper

NA: Memory error

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Discussion

Pros

- Little or no tuning and data recoding required
- Good performance on almost any kind of data
- Overfitting not a major problem
- Variable importance measures available

Cons

- Bad performance on images, speech and natural language processing
- Not per se interpretable
- Will not win prediction challenges

Discussion

Fast implementations available

- `Rborist` fastest for continuous features and large sample sizes
- `ranger` fastest in all other cases
- Efficient analysis of genome-wide data with `ranger`

Caution

- Some packages differ in results
- Performance depends on type and size of data

Random forests: The first-choice method for every data analysis?

Conclusion

Random forests: The first-choice method for ~~every~~ most data analyses!