

Ordinal forests

Roman Hornung

Introduction

Method

mplementatic

Application & comparison to alternatives

Estimating conditional class probabilities and considering the ordinal scale in the

# Ordinal forests: Prediction and covariate importance ranking with ordinal response variables

#### Roman Hornung

Institute for Medical Information Processing, Biometry and Epidemiology,
University of Munich

December, 21th, 2020



#### Introduction

#### Ordinal forests

Roman Hornung

#### Introduction

ivietnoa

mplementati

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the
ranking of the

- Ordinal forests (OFs) are a method for the prediction of ordinal outcomes using covariate information.
- They are **regression forests** that use **score values**  $s_1, \ldots, s_J$  in place of the class values  $1, \ldots, J$  of the ordinal outcome.
- **score values**  $s_1, \ldots, s_J$  **optimized** in such a way that the OF features an **optimal** (out-of-bag (OOB)) estimated **performance**
- concept of OF based on latent variable assumption: ordinal outcome assumed to be coarsened version of a latent metric variable



## Algorithm

Ordinal forests

Roman Hornun

Introduction

Method

mplementat

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the

#### Optimize score set:

- s<sub>1</sub>,...,s<sub>J</sub> optimized by: 1) generating many score sets randomly, 2) constructing an OF for each and 3) averaging across the ones associated with the best performance
- performance measured via the out-of-bag observations of the trees in the forests using a **performance measure**  $g(\cdot)$
- Different choices of  $g(\cdot)$  lead to different kinds of performance.
- 2 Grow a **OF**  $f_{\text{final}}$  with  $B_{\text{final}}$  trees (e.g.  $B_{\text{final}} = 10^4$ ) using  $s_1, \ldots, s_J$  as score set.



### Performance measure $g(\cdot)$

Ordinal forests

Roman Hornung

Introductio

#### Method

. . . . .

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the
ranking of the
variables

- "Equal": Classify observations from all classes with the same accuracy.
- "Proportional": Classify correctly as many observations as possible (larger classes are given more weight).
- "Oneclass": Maximize the performance with respect to a specific class, disregarding the other classes.
- NEW: "Probability": Allow conditional class probability estimation (by using the ranked probability score).



#### R package ordinalForest

Ordinal forests

Roman Hornung

Introductio

Metho

Implementation

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the
ranking of the
variables

on CRAN, version 2.4-1

ordinalForest uses (code from) R package ranger (fast!) to construct the regression forests

- variable importance measure (VIM) two variants:
  - based on misclassification error rate importance with respect to class point prediction
  - **NEW**: based on ranked probability score importance with respect to conditional class probability estimation



### Real data analysis - study design

Ordinal forests

Roman Hornung

Introductio

Metho

Implementati

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the
ranking of the

#### ■ five real datasets

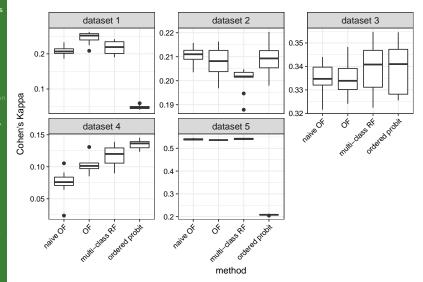
- four methods: 1) OF using 1,..., J as score values ("naive OF"), 2) OF, 3) multi-class Random Forests (RF), 4) ordered probit regression
- **goal**: Assess **prediction performance**.
- performance metrics: Cohen's Kappa, weighted Kappa
- validation scheme: 10 times repeated 10-fold cross-validation



#### Real data analysis - results: Cohen's Kappa

#### Ordinal forests

Application & comparison to alternatives





#### Real data analysis - results: linearly weighted Kappa

Ordinal forests

Roman Hornung

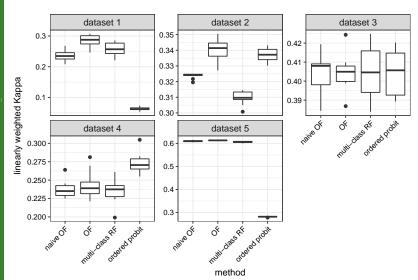
Introductio

Metho

Implementat

Application & comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
the ordinal
scale in the
ranking of the





#### Simulation results

Ordinal forests

Roman Hornung

Introductio

Method

plementati

Application & comparison to alternatives

Estimating conditional class probabilities and considering the ordinal scale in the ranking of the

■ three considered methods: 1) naive OF, 2) OF, 3) multi-class RF

- prediction performance: For all settings (with not negligibly small signal) OF better than naive OF and multi-class RF
- variable importance (based on misclassification error rate): OF better than multi-class RF, no improvement over naive OF
- OF particularly effective when the low and high classes are smaller (common in practice)



### Outlook: Estimating conditional class probabilities and considering the ordinal scale in the ranking of the variables

Ordinal forests

Outlook: Estimating conditional class probabilities considering the ordinal scale in the ranking of the variables

#### Background:

- 1 in its original form (Hornung (2020a)) OF only suitable for point class prediction, not conditional class probability estimation
- 2 Buri & Hothorn (2020): introduce Ordinal Transformation Forests (OTFs); find that available performance measures ("equal" and "proportional") do not perform well for conditional class probability estimation using OFs.
- ⇒ New performance measure: Use of (negative) ranked probability score (RPS):

$$\mathsf{RPS} = \frac{1}{n} \sum_{i=1}^{n} \frac{1}{J-1} \sum_{i=1}^{J} \left[ \widehat{\mathbb{P}}(Y_i \leq j | \boldsymbol{X}_i = x_i) - I(Y_i \leq j) \right]^2$$



## Outlook: Estimating conditional class probabilities and considering the ordinal scale in the ranking of the variables

Ordinal forests

Roman Hornung

Introductio

Metho

mplementa

Application & comparison to alternatives

Outlook: Estimating conditional class probabilities and considering the ordinal scale in the ranking of the

- Evaluated OFs for probability estimation with the negative RPS using the same simulation design as Buri & Hothorn (2020).
  - ⇒ Much better performance than for performance measures "equal" and "proportional"; performance comparable to OTFs (depending on setting: similar, better or worse).
- New VIM based on RPS:

$$VIM_{j} = \frac{1}{ntree} \sum_{i=1}^{ntree} RPS_{tree,i}^{(OOB-permuted j)} - RPS_{tree,i}$$

- To Do: Performance evaluation of new VIM...



Ordinal forests

Roman Hornung

Introduction

Method

Implementatio

Application & comparison to

Outlook: Estimating conditional class probabilities and considering the ordinal scale in the ranking of th

## Thank you for your attention!



#### References

Ordinal forests

Roman Hornung

Introductio

Application &

comparison to alternatives

Outlook:
Estimating
conditional
class
probabilities
and
considering
she ordinal
scale in the
variables

Ben-David, A. (2008).

Comparison of classification accuracy using Cohen's Weighted Kappa.

Expert Systems with Applications **34**, 825–832.

Buri, M. and Hothorn, T. (2020).

Model-based random forests for ordinal regression.

International Journal of Biostatistics 16(2), 20190063.

Hornung, R. (2020a).
Ordinal Forests

Ordinal Forests.

Journal of Classification 37, 4–17.

Hornung, R. (2020b).

ordinalForest: Ordinal Forests: Prediction and Variable Ranking with Ordinal Target Variables.

R package version 2.4-1.

http://cran.R-project.org/package=ordinalForest

Janitza, S., Tutz, G., and Boulesteix, A.-L. (2016).

Random forest for ordinal responses: prediction and variable selection.

Computational Statistics and Data Analysis **96**, 57–73.

Wright, M. and Ziegler, A. (2017).

ranger: A Fast Implementation of Random Forests for High Dimensional Data in C++ and R.

Journal of Statistical Software 77, 1–17.



### Performance measures $g(\cdot)$ for different purposes

Ordinal forests

Roman Hornun Be Yind $(y, \hat{y}, j)$  Youden's index for predicting class j, where  $y / \hat{y}$  is the vector of true / predicted classes, then:

 $\blacksquare$  equal classification performance for **all classes**  $\Rightarrow$ 

$$g(\mathbf{y}, \widehat{\mathbf{y}}) = \frac{1}{J} \sum_{j=1}^{J} \text{Yind}(\mathbf{y}, \widehat{\mathbf{y}}, j)$$

■ equal classification performance for **all observations** ⇒

$$g(\boldsymbol{y}, \widehat{\boldsymbol{y}}) = \sum_{i=1}^{J} \frac{\#\{y_i = j : i \in \{1, \dots, n\}\}}{n} \; \mathsf{Yind}(\boldsymbol{y}, \widehat{\boldsymbol{y}}, j)$$

 $\blacksquare$  optimal prediction performance for class  $I \Rightarrow$ 

$$g(y, \widehat{y}) = \text{Yind}(y, \widehat{y}, l)$$



### Real data analysis - datasets

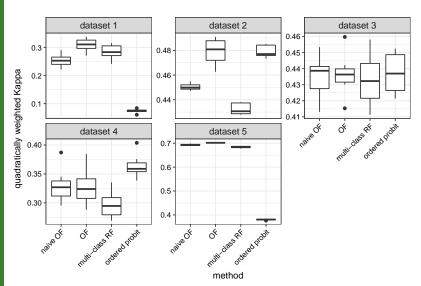
Ordinal forests

Dataset	# observ.	# classes	class frequenc.	# covariates
mammography	412	3	234, 104, 74	5
nhanes	1914	5	198, 565, 722, 346, 83	26
supportstudy	798	5	310, 104, 57, 7, 320	15
vlbw	218	9	33, 16, 19, 15, 25, 27, 35, 36, 12	10
winequality	4893	6	20, 163, 1457, 2198, 880, 175	11



## Real data analysis - results: quadratically weighted Kappa

Ordinal forests





### Simulation - study design

Ordinal forests

Romar Hornun

- three methods: 1) naive OF, 2) OF, 3) multi-class RF
- **30 settings**, 100 datasets per setting
- setting parameters:
  - correlations among covariates
  - sample size
  - number of covariates
  - numbers of classes of ordinal outcome
  - known true intervals considered for latent variable underlying ordinal outcome



#### Simulation - results II

Ordinal forests

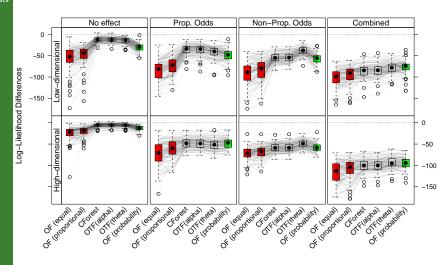
Roman Hornung

■ partition  $[0, b_1], [b_1, b_2], \dots ]b_{J-1}, 1]$  of [0, 1] corresponding to the optimized scores  $s_1, \dots, s_J$  NO meaningful indicator of actual "class widths"



## Performance regarding class probability estimation: Predicted out-of-sample log-likelihood minus true log-likelihood

Ordinal forests

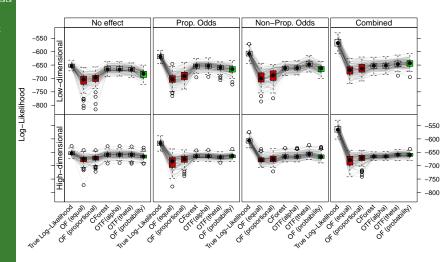




## Performance regarding class probability estimation: Predicted out-of-sample log-likelihood

Ordinal forests

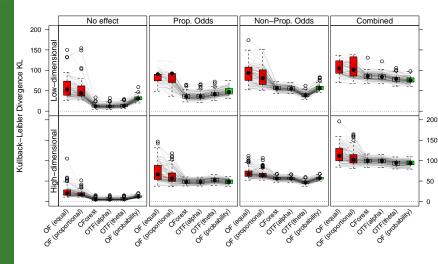
Romar Hornun





Performance regarding class probability estimation: Kullback-Leibler divergence -  $\mathbb{P}(Y=y|\boldsymbol{X}=x)$  vs.  $\widehat{\mathbb{P}}(Y=y|\boldsymbol{X}=x)$ 

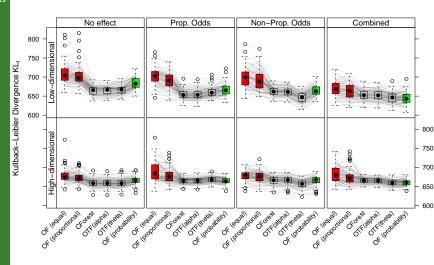
Ordinal forests





Performance regarding class probability estimation: Kullback-Leibler divergence - Y vs.  $\widehat{\mathbb{P}}(Y=y|\boldsymbol{X}=x)$ 

Ordinal forests





## Performance regarding point prediction: Kullback-Leibler divergence - $\widehat{Y}$ vs. $\mathbb{P}(Y = y | X = x)$

Ordinal forests

