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

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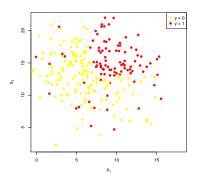
Course Overview

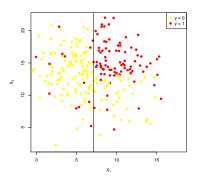
- ▶ Day 1: Single trees
 - ▶ Introduction to recursive partitioning methods (CART)
 - Unbiased recursive partitioning
 - Model-based recursive partitioning
 - Trees for clustered / multilevel data
- ▶ Day 2: Ensemble methods
 - Bagging, Boosting and Random Forests
 - Interpretation: Variable importance
 - Tuning parameters
 - Requests?

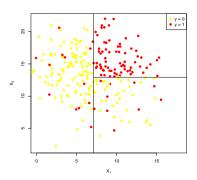
Recursive partitioning

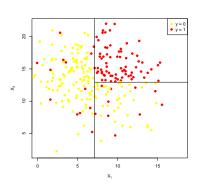
aim: predict Y from X_1, \ldots, X_p

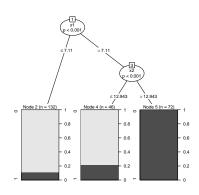
how: find subgroups, characterized by values of X_1, \ldots, X_p , that are most similar in terms of outcome Y (within each subgroup)











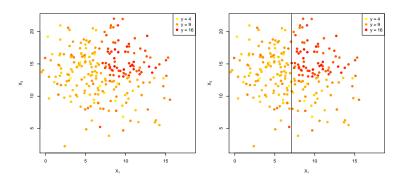
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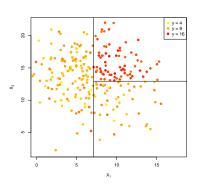
note: a partition can theoretically take any shape. To turn the partitioning into a feasible task, (most) RPMs:

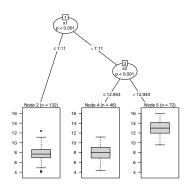
- split the data (variable space) recursively
- using one variable per split (rectangular areas)
- create binary splits only

Continuous Y



Continuous Y





1. How is the tree built?

2. How can we make predictions from the tree?

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- 2. How can we make predictions from the tree?
 - drop new observation down the tree
 - terminal node yields prediction:
 - majority class (classification)
 - mean (regression)

Tree building - multiway or binary

traditional recursive partitioning algorithms:

- multiway splitting (of categorical variables only): C4.5 (Quinlan, 1993)
 implemented in Weka, available through RWeka
- binary splitting: CART (Breiman et al., 1984)
 implemented in packages and functions rpart and tree

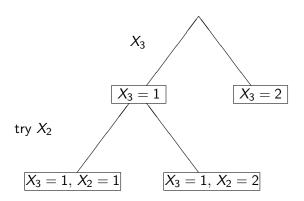
Multiway splitting (C4.5)

from the starting node

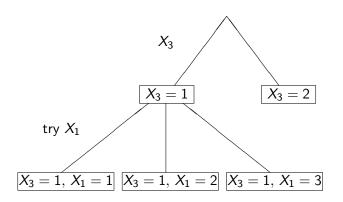
- produce as many nodes as categories
- select variable for splitting if most informative with respect to impurity reduction

. . .

Multiway splitting (C4.5)



Multiway splitting (C4.5)



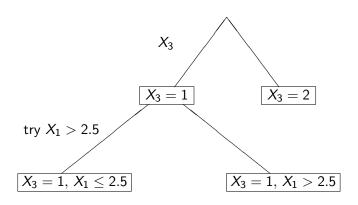
Binary splitting

from the current node

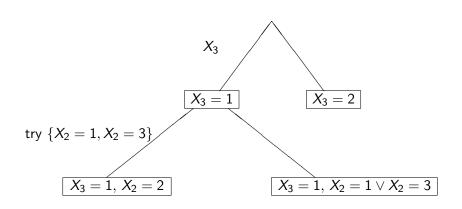
- try all possible cutpoints for all variables
- split using the best cutpoint = produce two nodes

. . .

Binary splitting - continuous predictor variables



Binary splitting - categorical predictor variables



Tree building - multiway or binary?

Any multi-way split can be represented as a series of binary splits.

Binary splitting

continuous, ordinal

$$y = 1$$

$$y = 0$$

$$X_{j}$$

categorical

$$AB|CD$$
 or $A|BCD$ or $AD|BC$ or $C|ABD$...

note: to reduce number of possible splits, CART 'orders' the levels of categorical variables by the mean of the outcome (regression) or the proportion of class 1 observations (classification)



Cutpoint selection in CART

for current node C and daughter nodes C_{L,c_j} and C_{R,c_j}

select the best cutpoint c_j* within the range of each predictor variable X_j with respect to impurity reduction

$$c_{j}^{*} = rg \max_{c_{j}} \Delta \Im \left(C, C_{L,c_{j}}, C_{R,c_{j}} \right)$$

(in regression: improvement in SSE instead of impurity reduction)

Impurity reduction

impurity reduction = impurity before splitting - impurity after splitting (weighted mean over nodes)

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$$\Delta \Im \left(C, C_{L,c_j}, C_{R,c_j}\right) = \Im(C) - \left(\frac{n_{L,c_j}}{n} \Im(C_{L,c_j}) + \frac{n_{R,c_j}}{n} \Im(C_{R,c_j})\right)$$

where n_{L,c_j} is the number of observations in C that are assigned to the left node

(e.g., for a continuous predictor,
$$n_{L,c_j} = \sum_i \mathsf{I}(x_{ij} \leq c_j)$$
)

Impurity measures

Gini index (used in CART)

$$\mathfrak{I}(C) = \sum_{k=0}^K \hat{p}_k (1 - \hat{p}_k)$$

Shannon entropy (used in C4.5)

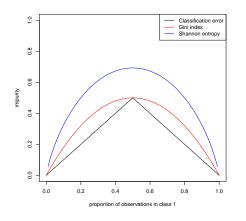
$$\Im(C) = -\sum_{k=0}^{K} \hat{p}_k \log \hat{p}_k$$

Classification error (never or rarely used)

$$\Im(C) = 1 - \max_{k} \hat{p}_{k}$$

Impurity measures

Impurity measures for K = 2 response classes:



Impurity in a node is:

0, if all observations are of the same class.

max, if each class is held by the same number of observations.

► tree building:

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 - recursively select splitting variable and cutpoint

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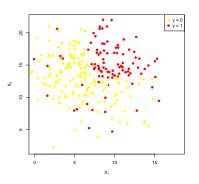
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 - the impurity reduction does not exceed a (user) pre-specified threshold

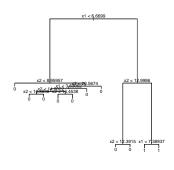
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 - ▶ prune (Hastie et al., 2001) if necessary

Pruning

Full tree likely to overfit:





Pruning

- ▶ Find the optimal number of nodes |T| for tree T
- Create a range of subtrees T_M through T_1 ,
 - ▶ T_M is the full tree, T_1 is a tree with 1 node
 - ▶ In every subtree T_m , the node that least improved impurity is removed from tree T_{m+1}
- Full tree T was build by minimizing $\sum_{m=1}^{M} \sum_{x_i \in C_m} L(y_i \hat{y}_i)$ in the training data
- Find optimal number of nodes |T| by minimizing $\sum_{m=1}^{|T|} \sum_{x_i \in C_m} L(y_i \hat{y}_i) + \alpha |T| \text{ in the training data}$
- ▶ Optimal value of α is determined through k-fold CV

Short detour: Model validation

aim: evaluate model performance and compare models usually based on prediction error estimates

$$\frac{1}{n}\sum_{i=1}^n\mathsf{I}(\hat{y}_i\neq y_i)$$

in classification

$$\frac{1}{n}\sum_{i=1}^n(\hat{y}_i-y_i)^2$$

in regression

Naive approach

- fit model on training sample
- estimate error on same training sample

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- estimate error on same training sample

bad idea!

Naive approach

- error estimation would be overoptimistic
- especially for models that overfit, i.e. that
 - fit too closely to random variation in the training sample
 - are not generalizable to other samples from the same data generating process
 - ⇒ rewards overfitting

test sample should not be identical to the training sample!

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- set aside part of the original sample as a test sample
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 - better: more than one test sample
- k-fold cross validation

Cross validation (CV)

k-fold CV: randomly separate original training sample into k subsets



- ▶ in *k* steps:
- ▶ fit model on training sample minus *k*th subset
- ▶ assess prediction error on kth subset (test sample)⇒ gives k error estimates
- average over k error estimates

Cross validation (CV)

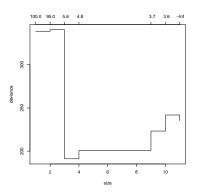
How many folds to use?

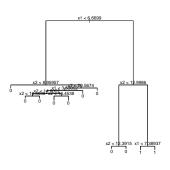
Extreme case: *N*-fold-CV (leave-one-out-CV, can be overly optimistic)

Rule of thumb: k = 10 gives realistic estimates of prediction error Kohavi (1995)

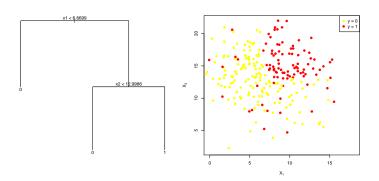
Note: Whenever you perform cross-validation, or random sampling, make sure you can exactly reproduce your results by setting the random seed (e.g, set.seed(42)).

Back to pruning





Prune tree



Classification and regression trees

- missing values
 by means of surrogate variables (Hastie et al., 2001)
- observation weights useful if classes are unbalanced, or if different costs are associated with different types of misclassifications

Growing CARTs with package tree

tree options and other functions controlling tree growing and size:

na.action =	function to filter missing data. The default is na.pass as	
	tree handles missing values by dropping them down the	
	tree as far as possible.	
mincut =	minimum number of observations to include in either child	
	node. The default is 5.	
minsize =	smallest allowed node size. The default is 10.	
mindev =	The within-node deviance must be at least this times that of	
	the root node for the node to be split. Default is .01.	
cv.tree()	Performs k -fold CV cost-complexity (pruning) parameter.	
prune.tree()	Prunes tree to size found with cv.tree.	

Interpretation

variables that appear in the tree are (supposed to be) more relevant than those that do not appear in the tree

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Note: only descriptive (beware of causal attributions)!

	regression tree	linear model
model	$f(\mathbf{x}) = \sum_{m} \hat{y}_{m} I(\mathbf{x} \in C_{m})$	$f(\mathbf{x}) = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_1 + \dots$

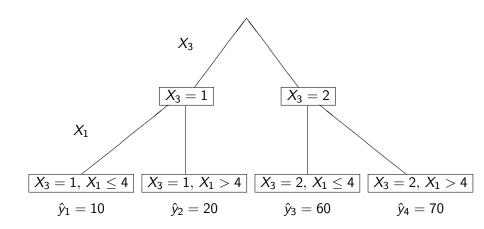
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N < p	can deal	cannot, need penalized regression

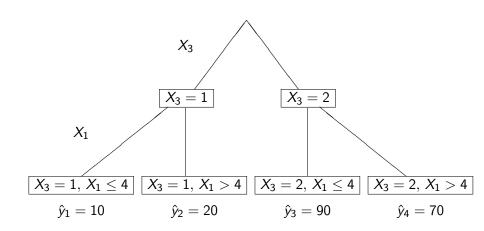
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main effect	?	$\hat{\beta}_1 \cdot x_1$
interaction	?	$\hat{eta}_1 \cdot extit{x}_1 \ \hat{eta}_{1,2} \cdot extit{x}_1 \cdot extit{x}_2$

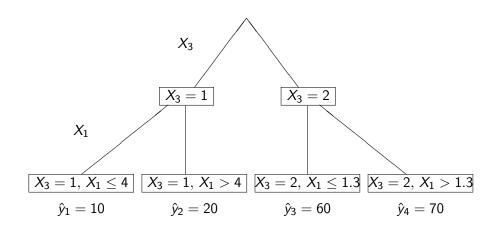
Interpretation: Two main effects



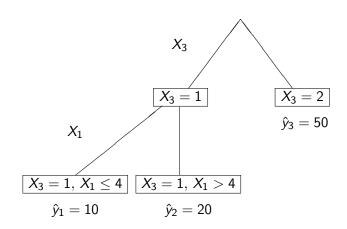
Interpretation: Interaction



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continuous variables and variables with many categories, as well es variables with missing values, are preferred in original CART and C4.5 (cf., e.g., White and Liu, 1994, Loh and Shih, 1997, Jensen and Cohen, 2000, Kim and Loh, 2001, Dobra and Gehrke, 2001)

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 - \Rightarrow p-value of optimally selected (χ^2 , rank or Gini) statistic (Shih, 2004, Lausen et al., 2004, Strobl et al., 2007) correct for optimal choice of cutpoint
 - ⇒ separate variable and cutpoint selection (Loh and Shih, 1997, Kim and Loh, 2001, Hothorn et al., 2006)

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- ▶ package party or partykit for unbiased recursive partitioning (Hothorn et al., 2006, 2017, Hothorn and Zeileis, 2015)
 - ▶ function ctree for classification, regression and survival trees

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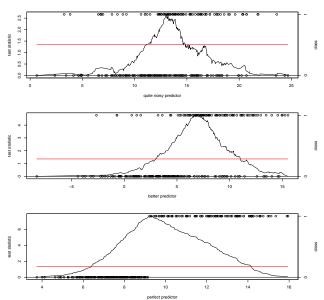
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- package party or partykit for unbiased recursive partitioning (Hothorn et al., 2006, 2017, Hothorn and Zeileis, 2015)
 - ▶ function ctree for classification, regression and survival trees
- splitting based on p-values of conditional inference tests, that also serve as a stopping criterion
 - ⇒ separates variable and split selection
 - ⇒ no overfitting
 - ⇒ pruning not necessary

Conditional inference trees (Hothorn et al., 2006)

- 1. Test the global null hypothesis of independence between any of the m covariates and the response. If null hypothesis can be rejected, select the covariate X_j^* with strongest association to Y. Otherwise, stop.
- 2. Select the splitting value for X_j^* that optimally separates the observations in terms of outcome Y.
- 3. Split the observations and repeat the procedure in each of the resulting daughternodes.

Test statistics for selecting splitting value



ctree function

ctree options controlling tree growing process:

mincriterion =	value of the test statistic or (1-p)-value that must
	be exceeded in order to implement a split.
maxdepth =	maximum depth of the tree. The default
	maxdepth = Inf means that no restrictions
	are applied to tree sizes.
minsplit =	the minimum sum of weights in a node in order
	to be considered for splitting.
minbucket =	the minimum sum of weights in a terminal node
minprob =	proportion of observations needed to establish
	a terminal node
splittry =	number of variables that are inspected for
	admissible splits if the best split doesn't
	meet the sample size constraint

ctree function

ctree options controlling tree growing process:

multiway =	a logical indicating if multiway splits for all factor
	levels are implemented for unordered factors.
maxsurrogate =	number of surrogate splits to evaluate. Note that
	currently only surrogate splits in ordered
	covariables are implemented.
majority =	if TRUE, observations which can't be classified to
	a daughter node because of missing information
	are randomly assigned (following the node
	distribution). If FALSE, they go with the
	majority (the default in ctree).

Model-based recursive partitioning

Rationale:

Global parametric model (e.g., $Y = X\beta + \epsilon$) may not fit the data well. When additional covariates are available, it may be possible to partition the data with respect to these covariates and find better-fitting models in each cell of the partition.

Zeileis et al. (2008)

Model-based recursive partitioning

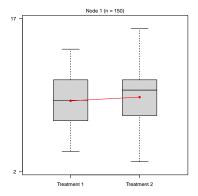
- 1. Fit a parametric model (e.g., estimate $\hat{\beta}$ for a (G)LM) to all observations in the current node.
- 2. Test whether the parameter estimates are stable with respect to every ordering of U_1, \ldots, U_q . If null hypothesis of parameter stability can be rejected, select covariate U_j^* associated with the highest instability. Otherwise, stop.
- 3. Select the splitting value for U_j^* that locally optimizes the loss function in each of the resulting daughter nodes.
- 4. Split the observations and repeat the procedure in each of the resulting daughternodes.

Example: Linear-model based recursive partitioning

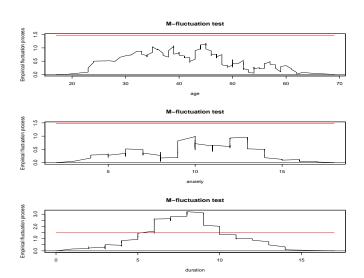
Dataset of N=150 patients receiving one of two treatments for depression.

- X: treatment indicator
- ▶ *Y*: post-treatment depressive symptom score
- $ightharpoonup Z_1, \ldots, Z_p$: age, anxiety, duration

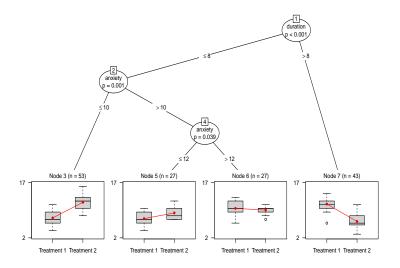
Global linear model



Parameter stability tests for linear model



Linear model tree



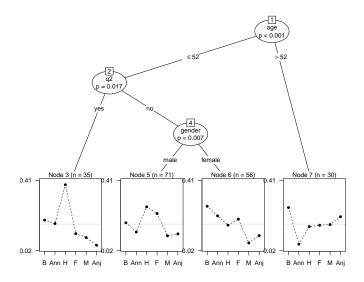
Example: Bradley-Terry model based recursive partitioning

Dataset of N = 192 respondents, who judged the attractiveness of the top six contestants on Germany's Next Topmodel 2007.

- preference: Preferences for all 15 paired comparisons from 6 contestants: Barbara, Anni, Hana, Fiona, Mandy, and Anja.
- $ightharpoonup Z_1, \ldots, Z_p$: gender, age, q1, q2, q3
 - q1: Do you recognize the women on the pictures?
 - q2: Did you watch Germany's Next Topmodel regularly?
 - q3: Do you know who won Germany's Next Topmodel?

Further reference: Strobl et al. (2011) and R-package psychotree.

Bradley-Terry tree



Clustered / multilevel / longitudinal data

Lower-level observations nested within higher-level units \Rightarrow Linear mixed-effects model: $y = X\beta + Ub + \epsilon$

Recursive partitioning of mixed-effects models:

- ▶ replace fixed-effects part $X\beta$ by f(X), found through recursive partitioning
- estimate random-effects parameters as usual

Example: mixed-effects model based recursive partitioning

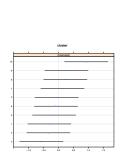
Dataset of ${\it N}=150$ patients receiving one of two treatments for depression.

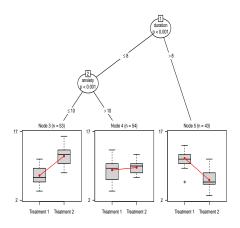
- ▶ X: treatment indicator
- Y: post-treatment depressive symptom score
- \triangleright Z_1, \ldots, Z_p : age, anxiety, duration
- ▶ U: dummy indicators for treatment center (n = 10)

Further reference: Fokkema et al. (2015) and R-package glmertree.

Linear mixed-effects model tree

$$Y = X\beta_j + Ub + \epsilon$$





References I

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