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Lecture 6

Prediction/classification using logistic regression models
Classification And Regression Trees (CART)

Lecture 5 Review: Prediction/classification

- Data: $(\bigcirc{Y_1}, X_1), ..., (\bigcirc{Y_n}, X_n)$ where X_i is a $(\underbrace{p+1})\times 1$ vector of exposures/predictors.
- Model: $logit[Pr(Y_i = 1|X_i)] = \boxed{X_i'\beta}$
- Fit the Model: $\boxed{\hat{\beta}} \rightarrow \underbrace{\hat{\mu}_i = \frac{exp(X_i'\hat{\beta})}{1+exp(X_i'\hat{\beta})}} = \underbrace{\hat{Pr}(Y_i=1|X_i)}$

▶ Define a classification rule:

$$d_i(\hat{\mu}_i, c) = \begin{cases} 1 & \hat{\mu}_i > c \\ 0 & \hat{\mu}_i \le c \end{cases}$$

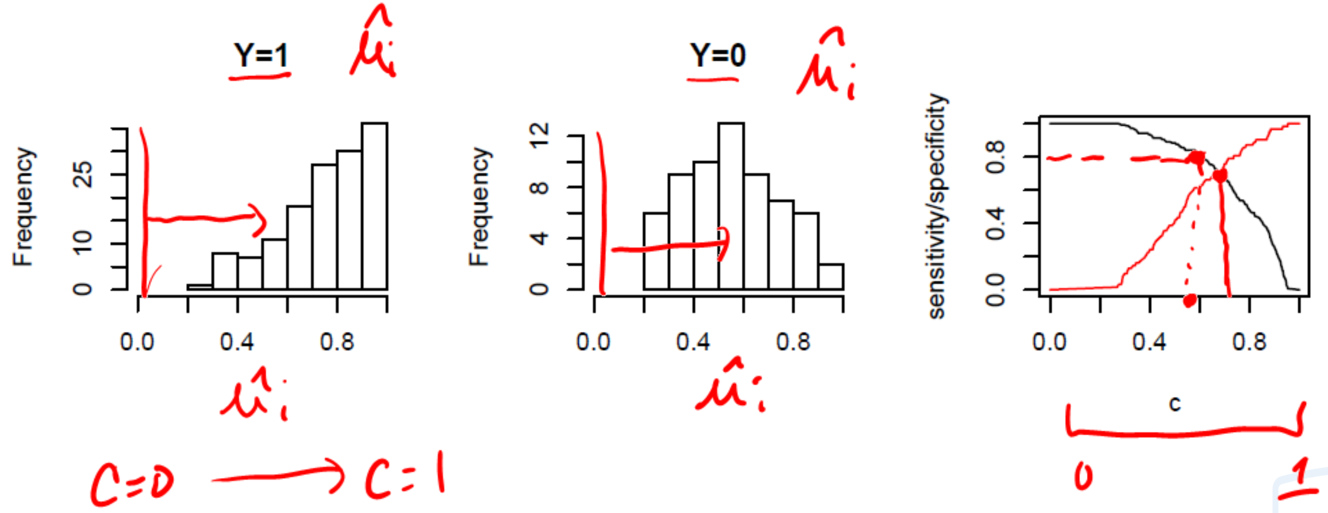
▶ Define sensitivity and specificity based on the classification rule:

$$Sens = Pr(d_i(\hat{\mu}_i, c) = 1 \mid Y_i = 1) = Pr(\hat{\mu}_i > c \mid Y_i = 1)$$

$$Spec = Pr(d_i(\hat{\mu}_i, c) = 0 \mid Y_i = 0) = Pr(\hat{\mu}_i \le c \mid Y_i = 0)$$

Defining and evaluating the classifier

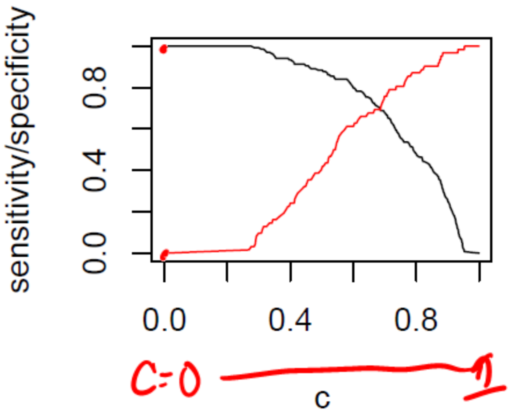
- Set c so we can maximize both sensitivity and specificity
  - Plot sens and spec as a function of c

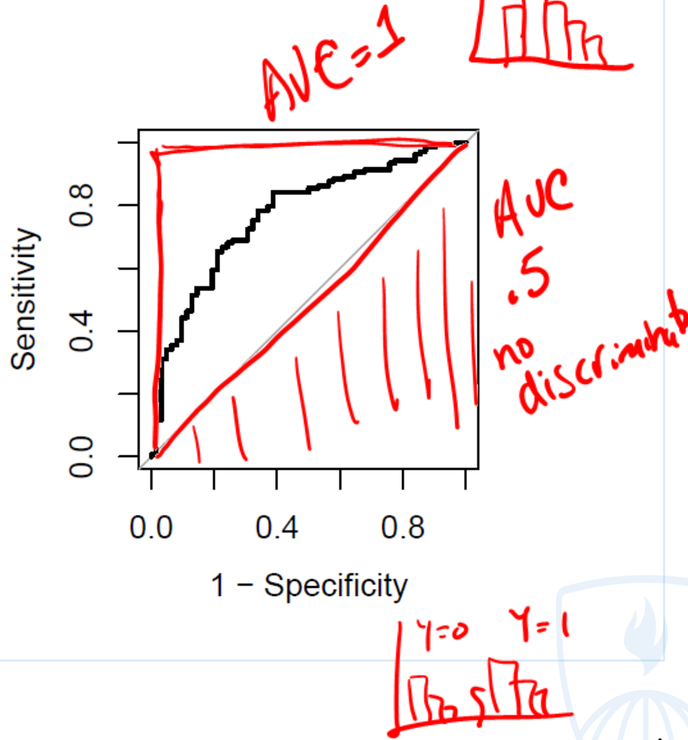


$C=0 \longrightarrow C=1$

Defining and evaluating the classifier

- Evaluate the entire model upon which the classifier is based
  - Receiver Operating Characteristic (ROC) curve
  - Plot sens vs. 1-spec for each c





Classification and Regression Trees (CART)

- So far, we have considered using a logistic regression model to define a classifier.
  - This approach requires that we build the regression model, i.e. we know the key predictors, including functional form for continuous variables and important interactions, etc.

- Instead of building a logistic regression model for developing a classifier, we will consider a classification and regression tree.
  - Removes the need for us to specify the model.

- We will give a very brief introduction to statistical learning methods
  - Classification and regression trees (CART) (today) ✓
  - Random forests (Thursday)
  - 3rd term Machine Learning course by Vadim
  - Chapter 9 in HTF text

- Classification and regression trees (CART)
  - Leo Breiman, Professor of Statistics at UC Berkeley, Richard Olshen, Jerry Friedman and others in 1984
  - Breiman spent the rest of his career developing important statistical learning (SL) (aka "machine learning - ML") tools including "bagging", "boosting" and "random forests".

CART

- Data will be partitioned into a
  - Training set: used to construct the model
  - Test/validation set: used to evaluate the quality/fit of the model (compared to competing models)

- Goal is to generate predictions for linear/continuous or categorical (binary or many than 2 categories) responses

- Algorithm goal: minimize a measure of prediction error

- Break the predictor space into M non-overlapping rectangular predictor sub-spaces
  - assign a predicted value within each subspace
  - Linear outcome: predicted value in each subspace is the sample mean
  - Binary outcome: predicted value in each subspace is most frequently occurring outcome (0 vs. 1) in that subspace

Regression Trees

- Approximates E(Y|X) via a step function!

$$\underbrace{f(X)}^{E(Y|X)} = \sum_{m=1}^{M} \underline{c_m} I(X \in \underline{R_m}).$$

- R_m are selected to minimize

$$\underbrace{\sum_{i=1}^{n}\{y - \sum_{m=1}^{M} c_m I(X \in R_m)\}^2}$$

sums of squared residuals

sums of squared errors in predictn

- c_m are estimated via the mean Y in R_m

$$\hat{c}_m = ave(y_i | x_i \in R_m)$$

Regression Trees

- CART uses a greedy algorithm

- To find the first split:
  - Search over all predictors X_j and split points *s*

$$\underbrace{R_1(j,s) = \{X|X_j \leq s\}}_{} \text{ and } \underbrace{R_2(j,s) = \{X|X_j > s\}}_{}$$

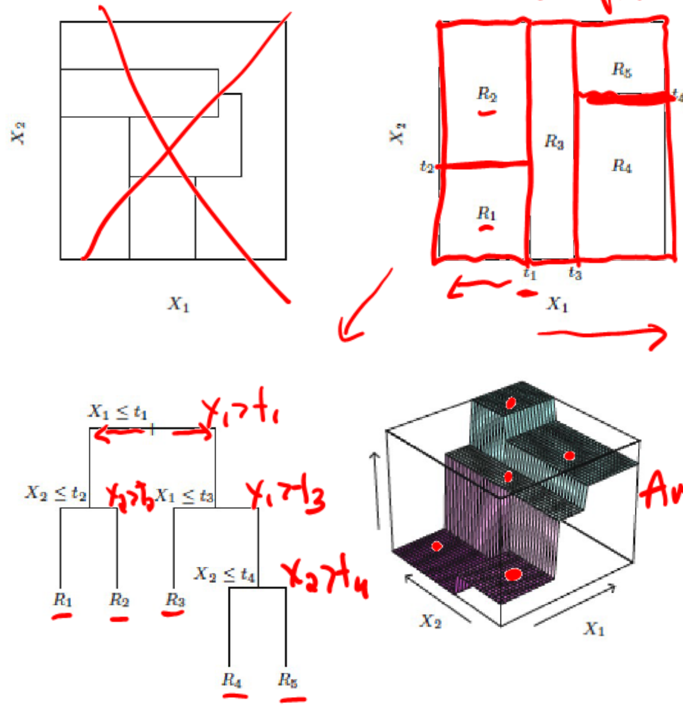
  - Find j and s that satisfy:

$$\min_{j,s}\left[\min_{c1} \sum_{x_i \in R_1(j,s)} (y_i - c1)^2 + \min_{c2} \sum_{x_i \in R_2(j,s)} (y_i - c2)^2\right]$$

  - Repeat

HTF Figure 9.2

$\bar{Y}$ = prediction with 0 splits



$E(Y|X_1,X_2) =$

$c_1 I(X_1 \le t_1) \times I(X_2 \le t_2)$

$+ c_2 I(X_1 \le t_1) \times I(X_2 > t_2)$

$+ c_3 I(X_1 > t_1) \times I(X_1 \le t_3)$

$+ c_4 I(X_1 > t_3) \times I(X_2 \le t_4)$

$+ c_5 I(X_1 > t_3) \times I(X_2 > t_4)$

$\text{Ave}(Y|X \in R_m)$

Regression Trees: When do we stop?

- Tree size, i.e. number of groups M, is determined by user-specified parameters

- Recommendation is to start by growing a large tree, call this T_0, to determine M by setting a minimum node size (e.g. each node must include at least 5 observations).
  - Then "prune" the true using a "cost complexity parameter"

$\hookrightarrow$ AIC

Regression Trees: Cost complexity parameter

- Called "cp" in the output

- Define a subtree T which is contained in T_0
  - Obtained by collapsing internal nodes
  - |T| denotes the number of terminal nodes in subtree T

$$N_m = \#\{x_i \in R_m\}$$

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i$$

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

loss function

$$\underline{C_\alpha(T)} = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$$

Regression Trees: Cost complexity parameter

- CART finds the unique tree T_α that minimizes $C_\alpha(T)$ for each α.
- α defines the trade-off between tree size and goodness of fit.
- α values are estimated via a cross-validation procedure; see details in Chapter 9 of HTF
- Final tree can be selected among the T_α that yields the smallest cross-validated sums of squared error (MSE).

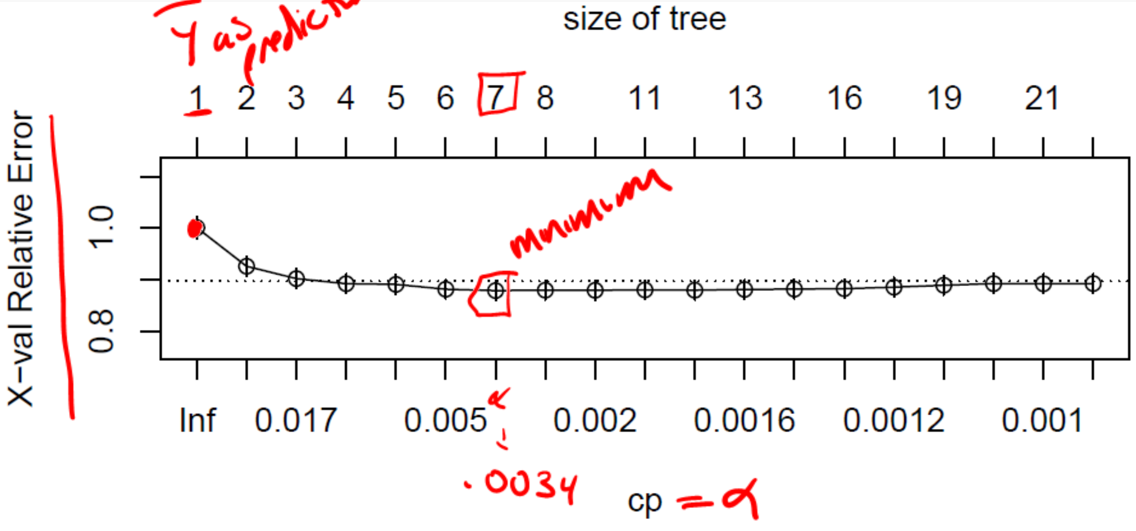
Example: Predict log(expenditures + 1) within NMES

e

```
set.seed(123454321)
dat.train=dat[train<-sample(1:nrow(dat),floor(nrow(dat)/2)),]
dat.test=dat[-train,]
```

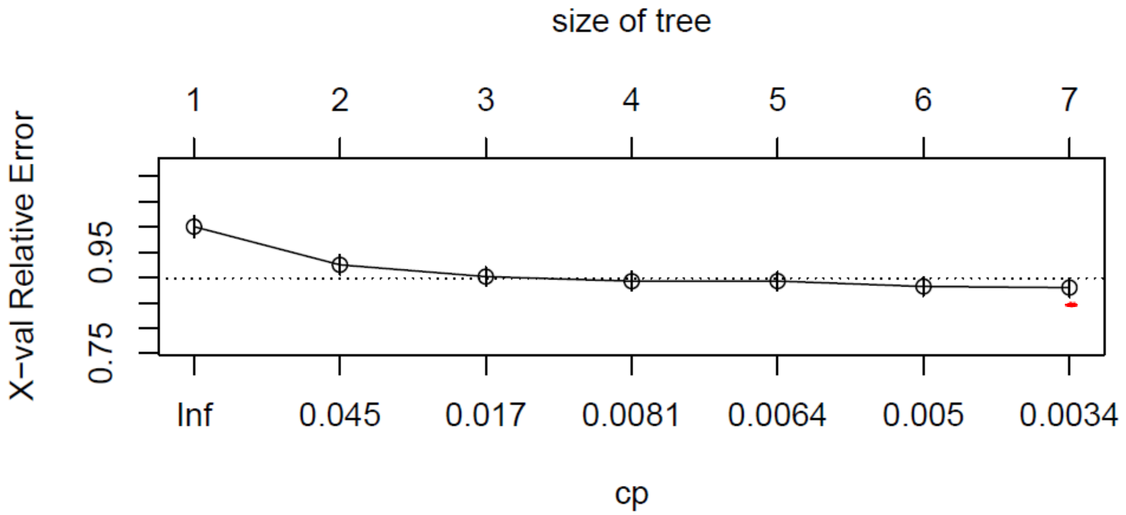
```
## Fit a first tree settting the "cp" parameter to 0.001
tree0=rpart(e~.,data=dat.train,method="anova",control=rpart.control(minsize=20,cp=.001))
par(mfrow=c(2,1),mar=c(5,5,5,1))
plotcp(tree0)
```

Y as predictor



Example: Predict log(expenditures + 1) within NMES

```
tree=rpart(e~.,data=dat.train,method="anova",control=rpart.control(minsize=20,cp=.0030))
plotcp(tree)
```



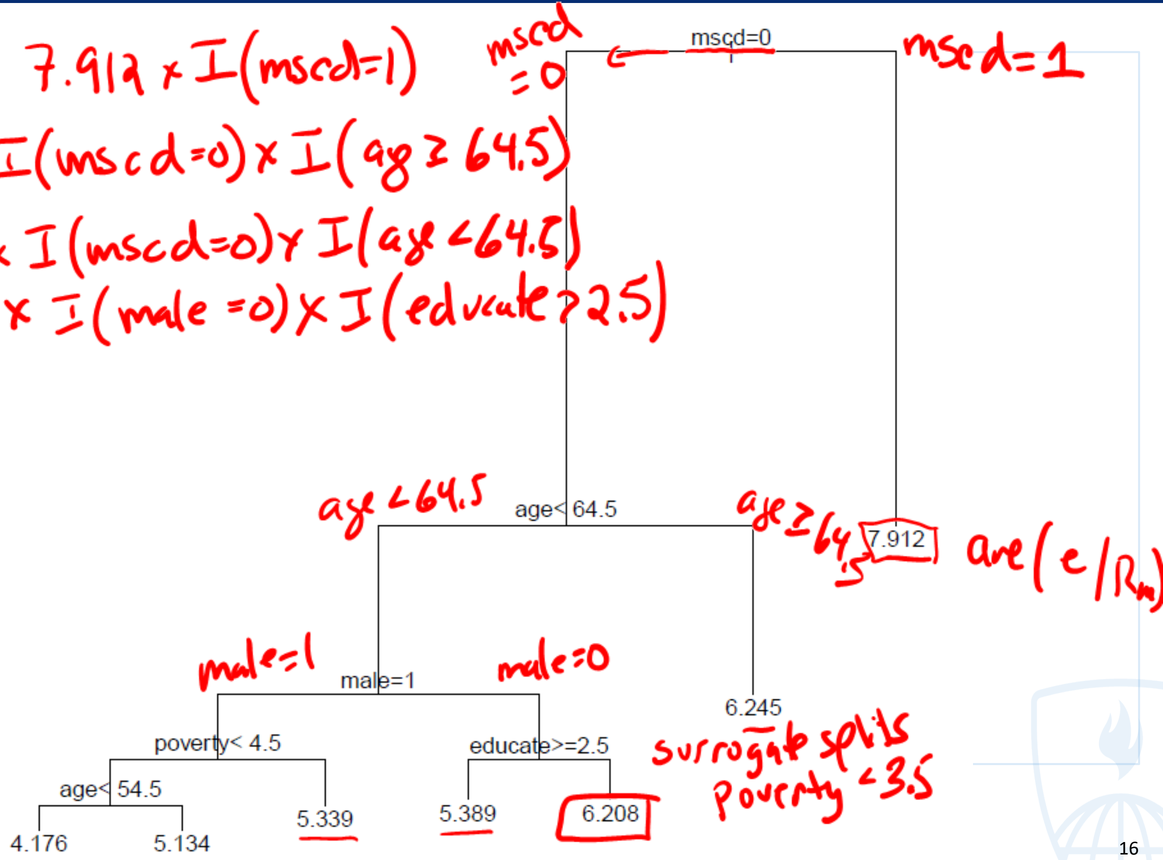
Example: Predict log(expenditures + 1) within NMES

```
##           α CP nsplit rel error    y-axis xerror       xstd
## 1 0.075345979      0 1.0000000 1.0004711 0.02089362
## 2 0.026861159      1 0.9246540 0.9251182 0.01917377
## 3 0.010320801      2 0.8977929 0.9018284 0.01866638
## 4 0.006407304      3 0.8874721 0.8927497 0.01854963
## 5 0.006319377      4 0.8810648 0.8929794 0.01855866
## 6 0.003940150      5 0.8747454 0.8822941 0.01838046
## 7 0.003000000      6 0.8708052 0.8801729 0.01836491
##
## Variable importance
##     mscd      age educate     male married poverty
##       53       22       8        7       5       4
```

- Measure of importance: sum of the goodness of split measures for each split where the variable is the primary variable (plus additional piece related to whether this variable is a surrogate), scaled to total 100 across all variables

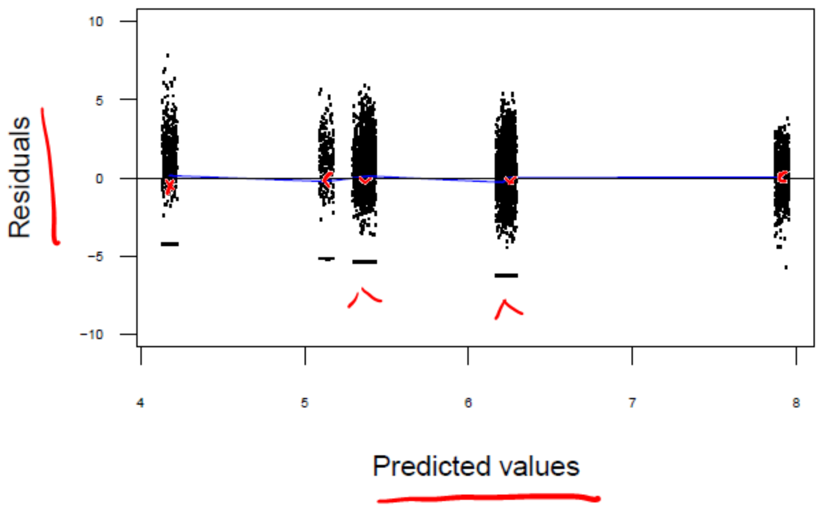
Example: Predict log(expenditure + 1) within NMES

$$\hat{E}(e \mid X) = 7.912 \times I(mscd=1)$$
$$+ 6.245 \times I(mscd=0) \times I(age \geq 64.5)$$
$$+ 6.208 \times I(mscd=0) \times I(age < 64.5) \times I(male=0) \times I(educate \geq 2.5)$$
$$+$$



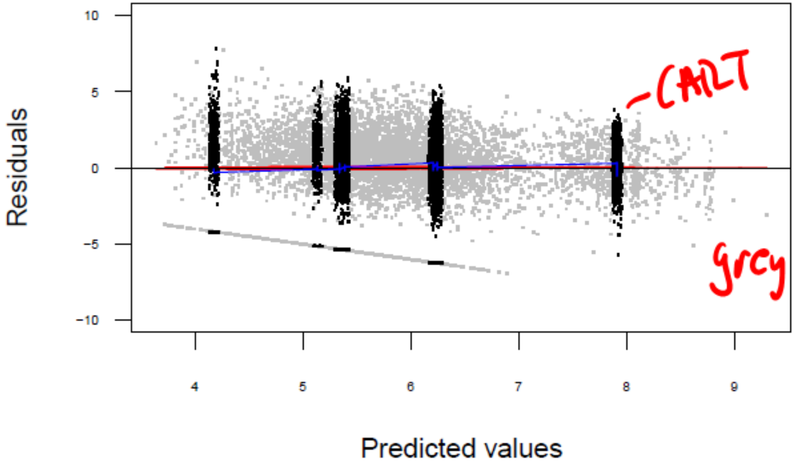
Regression trees: evaluating the fit of the model

```
# Generate predicted values
tree.yhat=predict(tree,newdata=dat.test,na.action=na.pass)
# Compute the residuals
res.tree.test=dat.test$e-tree.yhat
# Compute the MSE = sums of squared residuals / n for the
# test/validation dataset
mse.tree.test=sum(res.tree.test^2)/length(res.tree.test)
```



Regression trees: comparing to a parametric model

```
# Fit a parametric model, using the training data
model=lm(data=dat.train,e~ns(age,2)*male*mscd + as.factor(poverty)*as.factor(educate))
# Get predictions, residuals based on test/validation sample
model.yhat=predict(model,newdata=dat.test)
res.model.test=dat.test$e-model.yhat
# Compute the MSE for the parametric model
mse.model.test=sum(res.model.test^2)/length(res.model.test)
```



MSE comparison:

CART: 5.806; Linear Model: 5.68

CART: General comments

Some comments about CART to read further about in THF Chapter 9.2.4:

- interactions at the core
- must produce rectangles in X space
- specific tree, but not necessarily predictions, are unstable to perturbations in X - makes interpretation of tree unreliable
- poorly represents smooth functional relationships
- has natural extensions to the GLM family
- handles missing data reasonably well through surrogate variables
- tends to favor variable selection for factors with lots of levels

↓ random forests

Classification trees

- Same procedure
  - Different goodness of fit criteria

For classification trees, define

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

Observations in node m are classified in category k based on the category k with highest $\hat{p}_{mk}$.

Different measures of node impurity $Q_m(T)$ include the misclassification error, Gini index and cross-entropy or deviance. When we are constructing a classification tree for a binary response where $p = Pr(Y = 1)$, these measures are:

$$\text{Misclassification error: } 1 - max(p, 1 - p)$$

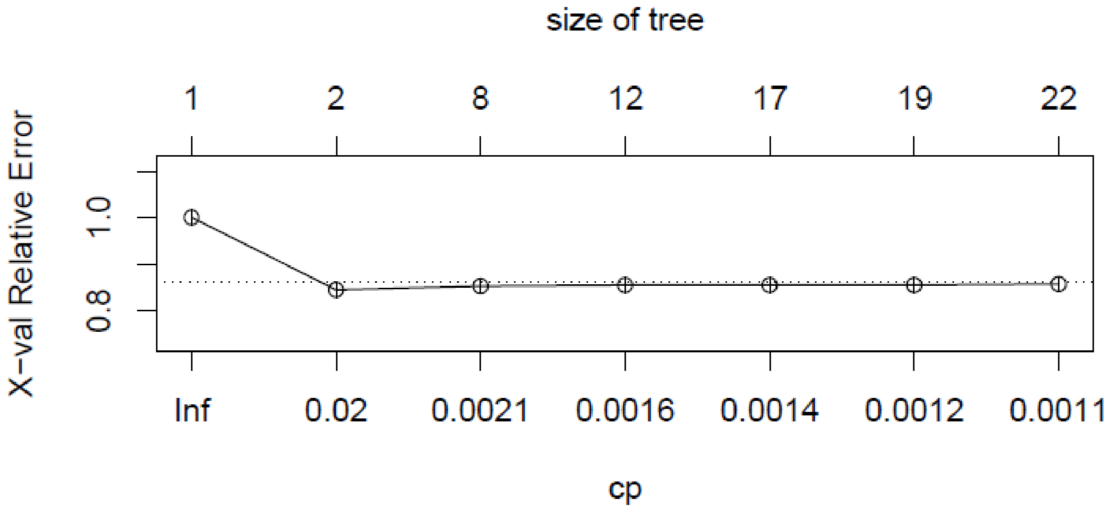
$$\text{Gini index: } 2p(1 - p)$$

$$\text{Cross entropy or deviance: } -plog(p) - (1 - p)log(1 - p)$$

The Gini index or cross-entropy impurity measures are often used to construct the tree where the misclassification error is used for tree pruning.

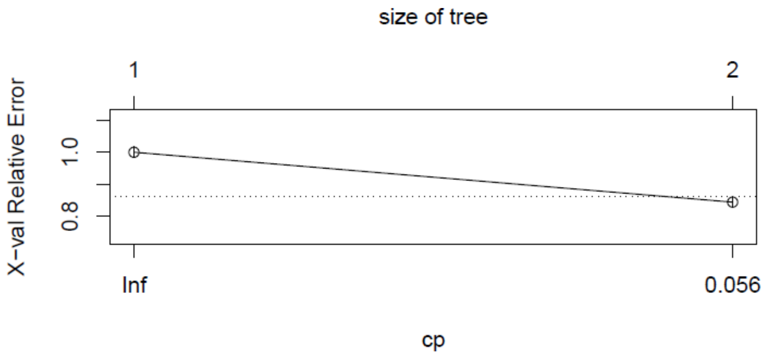
Example: Predict a big expenditure

```
set.seed(123454321)
dat1.train=dat1[train<-sample(1:nrow(dat),floor(nrow(dat)/2)),]
dat1.test=dat1[-train,]
tree0=rpart(big~.,data=dat1.train,method="class",control=rpart.control(minsize=20,cp=.001))
par(mfrow=c(2,1),mar=c(5,5,5,1))
plotcp(tree0)
```

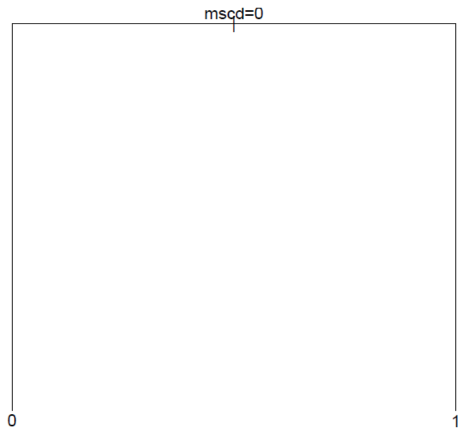


Example: Predict a big expenditure

```
tree=rpart(big~.,data=dat1.train,method="class",control=rpart.control(minsize=20,cp=.02))
plotcp(tree)
```



```
##           CP nsplit rel error    xerror       xstd
## 1 0.1555751      0 1.0000000 1.0000000 0.01667776
## 2 0.0200000      1 0.8444249 0.8444249 0.01600726
##
## Variable importance
## mscd
##  100
```

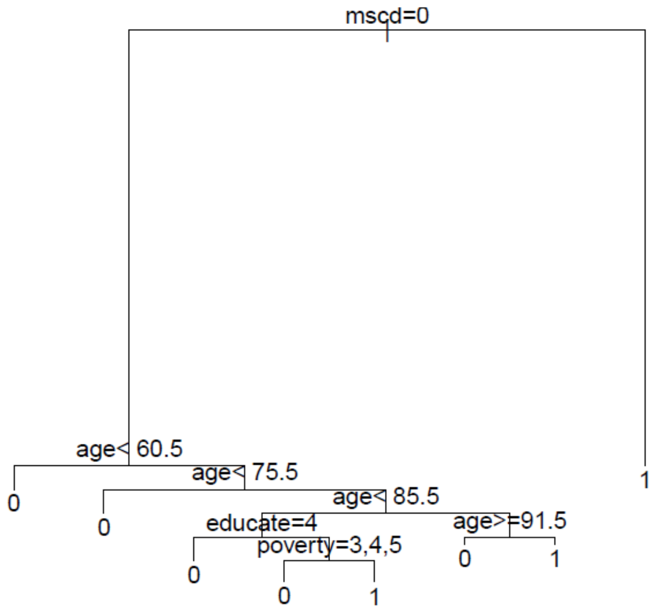


Example: Predict a big expenditure

- Change the CART criteria

```
treetest0=rpart(big~.,data=dat1.train,method="class",control=rpart.control(minsize=5,cp=.001))
```

```
bestcp <- treetest0$cptable[which.min(treetest0$cptable[,"xerror"]),"CP"]
tree.pruned <- prune(treetest0, cp = bestcp)
plot(tree.pruned);text(tree.pruned,pretty=3)
```



Example: Predict a big expenditure

- Compare to a parametric model

```
# comparison to logistic model
model=glm(data=dat1.train,big~ns(age,2)*male*mscd
          + as.factor(poverty)*as.factor(educate),
          family=binomial())

# Get the predicted values from the logistic regression model
model.yhat=predict.glm(model,newdata=dat1.test,type="response")
# The ROCR package requires that you first create a "prediction"
# object using the prediction function,
# this function takes the predicted probabilities + true values
pred.model.test=prediction(model.yhat,dat1.test$big)
# The performance function will compute several measures of
# performance for the classification scheme
# here we are selecting true positive rate, false positive rate
perf.model.test=performance(pred.model.test,"tpr","fpr")
# Use the performance object and ask for AUC
auc.model.test=performance(pred.model.test,"auc")
```

Example: Predict a big expenditure

```r
# Compare the performance of the parametric model
# to the classification tree
tree.yhat=as.vector(predict(tree,newdata=dat1.test,na.action=na.pass)[,2])
# Same as before, create the prediction object and
# compute auc
pred.tree.test=prediction(tree.yhat,dat1.test$big)
auc.tree.test=performance(pred.tree.test,"auc")
```

```r
# Compare the performance of the parametric model
# to the classification tree
tree.yhat2=as.vector(predict(tree.pruned,newdata=dat1.test,na.action=na.pass)[,2])
# Same as before, create the prediction object and
# compute auc
pred.tree.test2=prediction(tree.yhat2,dat1.test$big)
auc.tree.test2=performance(pred.tree.test2,"auc")
```

Example: Predict a big expenditure

- Compare the AUC values

```
auc.model.test@y.values[[1]]
```

```
## [1] 0.6762746
```

```
auc.tree.test@y.values[[1]]
```

```
## [1] 0.588122
```

```
auc.tree.test2@y.values[[1]]
```

```
## [1] 0.6463928
```

Where to next?

- Based on some of the earlier limitations we pointed out, we will consider random forests!