TREE BASED METHODS

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INTRODUCTION TO DECISION TREES

MOTIVATION

- In many real-world applications, decisions need to be made based on complex, multi-dimensional data.
- One goal of statistical analysis is to provide insights and guidance to support these decisions.
- Decision trees provide a way to organize and summarize information in a way that is easy to understand and use in decision-making.

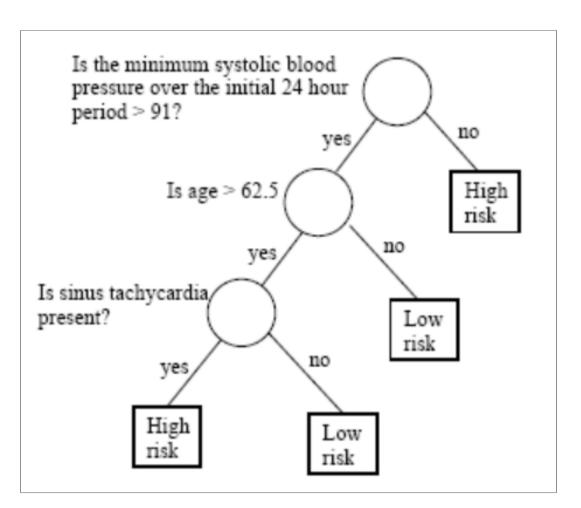
EXAMPLES (1)

- A bank need to have a way to decide if/when a customer can be granted a loan.
- A doctor may need to decide if an oncological patient has to undergo a surgery or a less aggressive treatment.
- A company may need to decide about investing in new technologies or stay with the traditional ones.

In all those cases a decision tree may provide a structured approach to decision-making that is based on data and can be easily explained and justified.

EXAMPLES (2)

 Similarly as would do a doctor, patients are classified into one of two classes: high risk versus low risk based on: systolic blood pressure, age and tachycardia.



SO, WHAT IS A DECISION TREE?

- A decision tree is a graphical representation of a series of decisions and their potential outcomes.
- It is obtained by recursively *stratifying* or *segmenting* the *feature space* into a number of simple regions.
- Each region (decision) corresponds to a *node* in the tree, and each potential outcome corresponds to a *branch*.
- The tree structure can be used to guide decision-making based on data.

WHAT DO WE NEED TO LEARN?

 We need context and also, we need to learn how to build, evaluate and optimize trees.

Context

- When is it appropriate to rely on decision trees?
- When would other approaches be preferable?
- What type of decision trees can be used?

Build the tree

- How do we construct the tree?
- How do we optimize the tree?
- How do we evaluate it?

MORE ABOUT CONTEXT

- Decision trees are non parametric, data guided predictors, well suited in many situations such as:
 - Non-linear relationships.
 - High-dimensional data.
 - Interaction effects.
 - Non-parametric data.
 - Mixed data types.
- They are not so appropriate for complex datasets, or complex problems, that require expert knowledge.

TYPES OF DECISION TREES

- Two main types: Classification and Regression Trees (CART).
 - Classification Trees are built when the response variable is categorical.
 - They aim to classify a new observation based on the values of the predictor variables.
 - Regression Trees are used when the response variable is numerical.
 - They aim to predict the value of a continuous response variable based on the values of the predictor variables.

CLASSIFICATION VS REGRESSION TREES

Aspect	Regression Trees	Classification Trees	
Outcome var. type	Continuous	Categorical	
Goal	To predict a numerical value	To predict a class label	
Splitting criteria	Mean Squared Error, Mean Abs. Error, etc.	Gini Impurity, Entropy, etc.	
Leaf node prediction	Mean or median of the target variable in that region	Mode or majority class of the target variable	
Tree visualization	Sequence of splits leading to a numerical predic	Sequence of splits leading to a categorical pr	
Examples of use cases	Predicting housing prices, predicting stock prices	Predicting customer churn, predicting the like	
Evaluation metric	Mean Squared Error, Mean Absolute Error, R-square	Accuracy, Precision, Recall, F1-score, etc.	

Aspect	Regression Trees	Classification Trees
Overfitting	Can suffer from overfitting if the tree is too de	Can suffer from overfitting if the tree is too
Pruning	Can be pruned to reduce overfitting	Can be pruned to reduce overfitting
Ensemble methods	Random Forest, Gradient Boosting, etc.	Random Forest, Gradient Boosting, etc.

BUILDING THE TREES

- Building the tree requires deciding:
 - how to partition ("split") the space,
 - Which *impurity* measures to use,
 - When to stop splitting
- Evaluation is similar to other classifiers.
- Optimization involves deciding:
 - How to *prune* the tree,
 - Which features are most important.

TREE BUILDING WITH R

Package	Algorithm	Dataset size	Missing data handling	Ensemble methods	Visual repr	User interface
rpart	RPART	Medium to large	Poor	No	Yes	Simple
caret	Various	Various	Depends on algorithm	Yes	Depends on algorithm	Complex
tree	CART	Small to medium	Poor	No	Yes	Simple

A "QUICK AND DIRTY" EXAMPLE IN R

The Pima Indian Diabetes data set contains 768 individuals (female) and 9 clinical variables.

```
Rows: 768
Columns: 9
$ pregnant <dbl> 6, 1, 8, 1, 0, 5, 3, 10, 2, 8, 4, 10, 10, 1, 5, 7, 0, 7, 1,
1...
$ glucose <dbl> 148, 85, 183, 89, 137, 116, 78, 115, 197, 125, 110, 168,
139,...
$ pressure <dbl> 72, 66, 64, 66, 40, 74, 50, NA, 70, 96, 92, 74, 80, 60, 72,
N...
$ triceps <dbl> 35, 29, NA, 23, 35, NA, 32, NA, 45, NA, NA, NA, NA, 23, 19,
N...
           <dbl> NA, NA, NA, 94, 168, NA, 88, NA, 543, NA, NA, NA, NA, 846,
$ insulin
17...
$ mass
           <dbl> 33.6, 26.6, 23.3, 28.1, 43.1, 25.6, 31.0, 35.3, 30.5, NA,
37....
$ pedigree <dbl> 0.627, 0.351, 0.672, 0.167, 2.288, 0.201, 0.248, 0.134,
0.158...
```

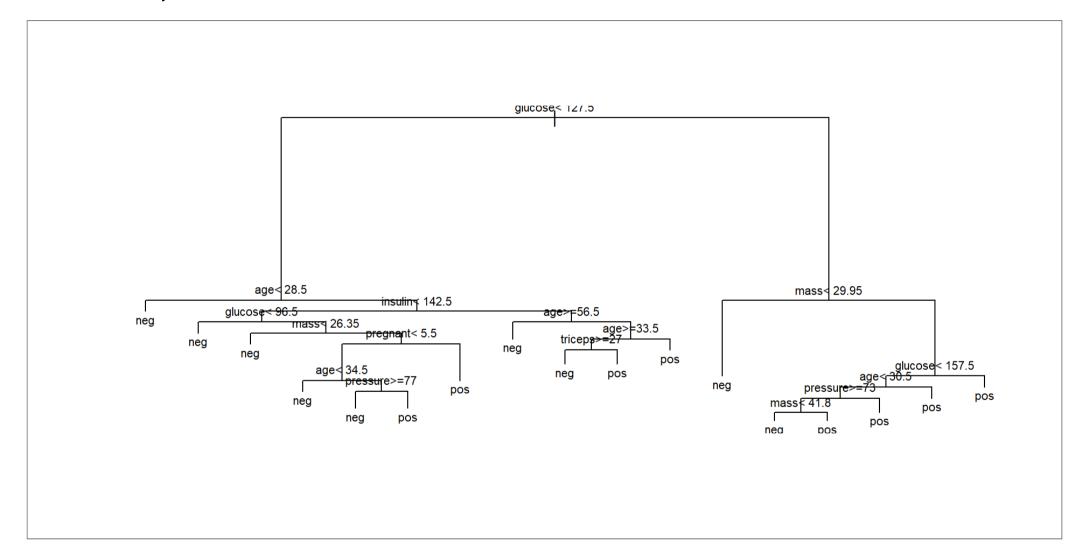
PREDICTING DIABETES ONSET

 We wish to predict the probability of individuals in being diabete-positive or negative.

```
1 library(rpart)
2 model1 <- rpart(diabetes ~., data = PimaIndiansDiabetes2)

1 plot(model1)
2 text(model1, digits = 3, cex=0.7)</pre>
```

A SIMPLE, UNPRUNNED TREE



HOW ACCURATE IS THE MODEL?

```
predicted.classes<- predict(model1, PimaIndiansDiabetes2, "class")
mean(predicted.classes == PimaIndiansDiabetes2$diabetes)</pre>
```

[1] 0.8294271

ALWAYS USE TRAIN/TEST SETS!

• A better strategy is to use train dataset to build the model and a test dataset to check how it works.

```
1 set.seed(123)
2 ssize <- nrow(PimaIndiansDiabetes2)
3 propTrain <- 0.8
4 training.indices <-sample(1:ssize, floor(ssize*propTrain))
5 train.data <- PimaIndiansDiabetes2[training.indices, ]
6 test.data <- PimaIndiansDiabetes2[-training.indices, ]</pre>
```

BUILD ON TRAIN, ESTIMATE ON TEST

• First, build the model on the train data

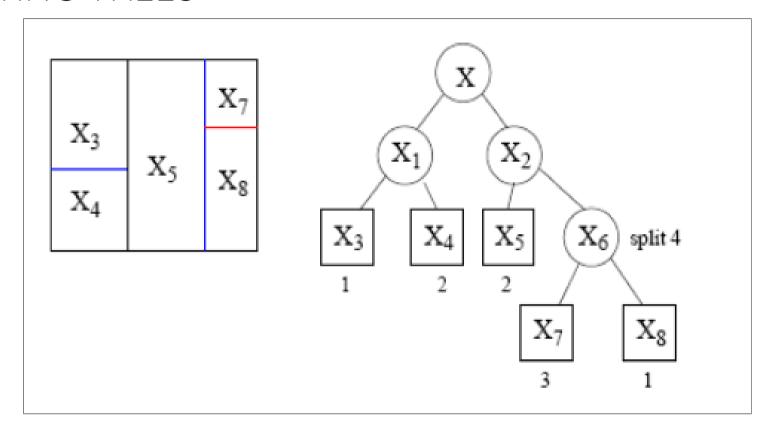
```
1 model2 <- rpart(diabetes ~., data = train.data)</pre>
```

• Then check its accuracy on the test data.

```
1 predicted.classes.test<- predict(model2, test.data, "class")
2 mean(predicted.classes.test == test.data$diabetes)</pre>
```

```
[1] 0.7272727
```

CONSTRUCTING TREES



NOTATION AND BASIC CONCEPTS

- X: Space of variables, or *feature space*
 - Usually $\mathbb{X} \subseteq \mathbb{R}^p$
 - But it can contain numerical/categorical variables.
- $X \in \mathbb{X}$: Input vector: X_1, X_2, \dots, X_p .
- Tree-structured classifiers are constructed by repeated splits of the space X into smaller and smaller subsets, beginning with X itself.
 - That is by *recursive splitting*

ADDITIONAL NOTATION

- A node is denoted by t. We will also denote the left child node by t_L and the right one by t_R .
- \bullet Denote the collection of all the nodes in the tree by T and the collection of all the leaf nodes by \tilde{T}
- A split will be denoted by s. The set of splits is denoted by S.
- Nice definition of basic terminology:

TREES PARTITION THE SPACE

- The tree represents the recursive splitting of the space.
 - Every node of interest corresponds to one region in the original space.
 - Two child nodes occupy two different regions.
 - Together, yield same region as that of the parent node.
- In the end, every leaf node is assigned with a class and a test point is assigned with the class of the leaf node it lands in.

THE TREE REPRESENTS THE SPLITTING

• Animation

CONSTRUCTION OF A TREE

It involves the following three elements:

- 1. The selection of the splits, i.e., how do we decide which node (region) to split and how to split it?
 - How to select from the pool of candidate splits?
 - What are appropriate goodness of split criteria?
- 2. If we know how to make splits ('grow' the tree), how do we decide when to declare a node terminal and *stop splitting*?
- 3. How do we assign each terminal node to a class?

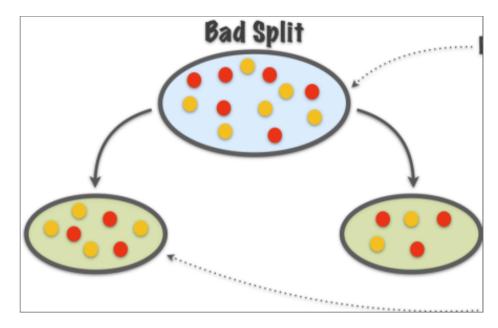
WHICH QUESTIONS TO SPLIT THE TREE

- To build a Tree, questions have to be generated that induce splits based on the value of a single variable.
- Ordered variable X_j :
 - Is $X_j \le c$? for all possible thresholds c.
 - Restricts the split line to be parallel to the coordinates.
- Categorical variables, $X_j \in \{1, 2, \dots, M\}$:
 - Is $X_j \in A$? where A is any subset of $\{1, 2, \dots, M\}$.
- ullet The pool of candidate splits for all p variables is formed by combining all the generated questions.

DETERMINING GOODNESS OF SPLIT

- The way we choose the split, is to measure every split by a 'goodness of split' measure, which depends on:
 - the split question as well as
 - the node to split.
- The 'goodness of split' in turn is measured by an impurity function.
- Intuitively, when we split the points we want the region corresponding to each leaf node to be "pure", that is, most points in this region come from the same class, that is, one class dominates.

GOOD SPLITS VS BAD SPLITS



S Good Split

Pure nodes

Purity not increased

Purity increased

MEASURING HOMOGENEITY

- In order to measure homogeneity of splits we introduce
 - Impurity functions
 - Impurity measures
- Used to measure the extent of *purity* for a region containing data points from possibly different classes.

IMPURITY FUNCTIONS

Definition: An **impurity function** is a function Φ defined on the set of all K-tuples of numbers (p_1, \dots, p_K) satisfying $p_j \geq 0$, $j = 1, \dots, K$, $\Sigma_j p_j = 1$ with the properties:

- 1. Φ achieves maximum only for the uniform distribution, that is all the p_j are equal.
- 2. Φ achieves minimum only at the points $(1,0,\ldots,0)$, $(0,1,0,\ldots,0)$, \ldots , $(0,0,\ldots,0,1)$, i.e., when the probability of being in a certain class is 1 and 0 for all the other classes.
- 3. Φ is a symmetric function of p_1, \dots, p_K , i.e., if we permute p_j , Φ remains constant.

SOME IMPURITY FUNCTIONS

Commonly used impurity functions for classification trees:

1. Entropy function: $\sum_{j=1}^K p_j \log rac{1}{p_j} = -\sum_{j=1}^K p_j \log p_j$.

If $p_j=0$, use the limit $\lim p_j \to \log p_j=0$.

- 2. Misclassification rate: $1 \max_j p_j$.
- 3. Gini index: $\sum_{j=1}^{K} p_j (1-p_j) = 1 \sum_{j=1}^{K} p_j^2$.

IMPURITY MEASURES FOR A SPLIT

• Definition: Given an impurity function Φ , define the impurity measure, denoted as i(t), of a node t as:

$$i(t) = \phi(p(1 \mid t), p(2 \mid t), \ldots, p(K \mid t))$$

- where $p(j \mid t)$ is the estimated posterior probability of class j given a point is in node t.
 - That is, the impurity measure is the impurity function when computed on probabilities associated (conditional) with a node.

GOODNESS OF A SPLIT

• Once we have i(t), we define the goodness of split s for node t, denoted by $\Phi(s,t)$:

$$\Phi(s,t) = \Delta i(s,t) = i(t) - p_R i\left(t_R
ight) - p_L i\left(t_L
ight)$$

• The best split for the single variable X_j is the one that has the largest value of $\Phi(s,t)$ over all $s \in \mathcal{S}_j$, the set of possible distinct splits for X_j .

IMPURITY SCORE FOR A NODE

- The impurity of a node i(t) doesn'y account for its size.
- This is done by the *impurity score* of node t, defined as: $I(t) = i(t) \cdot p(t),$
- i(t) is based solely on the estimated posterior probabilities of the classes in that node.
- I(t) is the weighted impurity measure of node t, taking into account not only the estimated posterior probabilities of the classes, but also the estimated proportion of data that go to node t.

APPLICATIONS OF I(t)

- I(t) can be used to:
 - Define the aggregated impurity of a tree, by adding the impurity scores of all terminal leaves.
 - Provide a weighted measure of impurity decrease for a split: $\Delta I(s,t) = p(t)\Delta i(s,t).$
 - Define a criteria for stop splitting a tree (see below).

ENTROPY AS AN IMPURITY MEASURE

• The entropy of a node, t, that is split in n child nodes t_1 , t_2 , ..., t_n , is:

$$H(t) = -\sum_{i=1}^{n} P\left(t_i
ight) \log_2 P\left(t_i
ight)$$

GOODNESS OF SPLIT BASED ON ENTROPY

- From here, an information gain (that is impurity decrease) measure can be introduced.
- Information theoretic approach that compares
 - the entropy of the parent node before the split to
 - that of a weighted sum of the child nodes after the split where the weights are proportional to the number of observations in each node.

INFORMATION GAIN

• For a split s and a set of observations (a node) t, information gain is defined as:

$$IG(t,s) =$$
(original entropy) $-$ (entropy after the split)

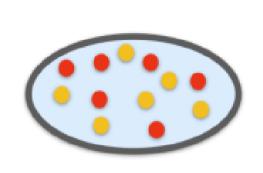
$$IG(t,s) = H(t) - \sum_{i=1}^{n} rac{|t_i|}{t} H\left(x_i
ight)$$

EXAMPLE

Consider the problem of designing an algorithm to automatically differentiate between apples and pears (class labels) given only their width and height measurements (features).

Width	Height	Fruit
7.1	7.3	Apple
7.9	7.5	Apple
7.4	7.0	Apple
8.2	7.3	Apple
7.6	6.9	Apple
7.8	8.0	Apple
7.0	7.5	Pear
7.1	7.9	Pear
6.8	8.0	Pear
6.6	7.7	Pear
7.3	8.2	Pear
7.2	7.9	Pear

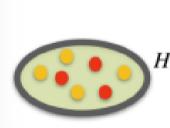
EXAMPLE. ENTROPY CALCULATION



$$H(X) = \sum_{i=1}^{n} P(x_i) log_2 P(x_i)$$

$$= -\frac{6}{12} \cdot log_2(\frac{6}{12}) - \frac{6}{12} \cdot log_2(\frac{6}{12})$$

$$= \frac{1}{2} + \frac{1}{2} = 1$$

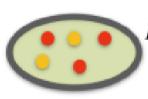


$$H(X) = -\frac{4}{7} \cdot log_2(\frac{4}{7}) - \frac{3}{7} \cdot log_2(\frac{3}{7})$$

$$= 0.4613 + 0.5239 = 0.9852$$

$$H(X) = -\frac{3}{5} \cdot log_2(\frac{3}{5}) - \frac{2}{5} \cdot log_2(\frac{2}{5})$$

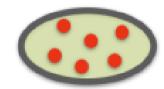
$$= 0.4422 + 0.5288 = 0.9710$$



$$H(X) = -\frac{3}{5} \cdot log_2(\frac{3}{5}) - \frac{2}{5} \cdot log_2(\frac{2}{5})$$

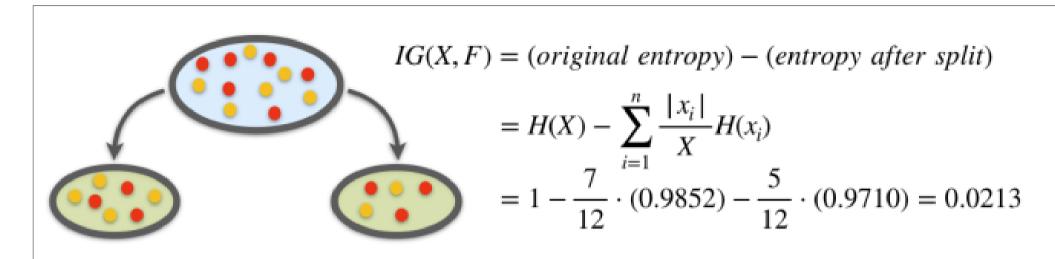


$$H(X)=-\frac{6}{6}\cdot log_2(\frac{6}{6})=0$$



$$H(X) = -\frac{6}{6} \cdot log_2(\frac{6}{6}) = 0$$

EXAMPLE. INFORMATION GAIN



$$IG(X, F) = 1 - \frac{6}{12} \cdot (0) - \frac{6}{12} \cdot (0) = 1$$

WHEN TO STOP GROWING

- Maximizing information gain is one possible criteria to choose among splits.
- In order to avoid excessive complexity it is usually decided to stop splitting when "information gain does not compensate for increase in complexity".
- In practice stop splitting if:

$$\max_{s \in S} \Delta I(s,t) < eta$$

CLASS ASSIGNMENT RULES (1)

- The decision tree classifies new data points as follows.
 - We let a data point pass down the tree and see which leaf node it lands in.
 - The class of the leaf node is assigned to the new data point. Basically, all the points that land in the same leaf node will be given the same class. This is similar to k-means or any prototype method.

CLASS ASSIGNMENT RULES (2)

- A class assignment rule assigns a class $j=1,\cdots,K$ to every terminal (leaf) node $t\in \tilde{T}.$
- The class is assigned to node $t. \, \tilde{T}$ is denoted by $\kappa(t)$,
- E.g., if $\kappa(t)=2$, all the points in node t would be assigned to class 2.

CLASS ASSIGNMENT RULES (3)

• If we use 0-1 loss, the class assignment rule is very similar to k-means (where we pick the majority class or the class with the maximum posterior probability):

$$\kappa(t) = rg \max_{j} p(j \mid t)$$

ESTIMATING THE ERROR RATE (1)

- Let's assume we have built a tree and have the classes assigned for the leaf nodes.
- Goal: estimate *the classification error rate* for this tree.
- We need to introduce the resubstitution estimate r(t) for the probability of misclassification, given that a case falls into node t. This is:

$$r(t) = 1 - \max_{j} p(j \mid t) = 1 - p(\kappa(t) \mid t)$$

ESTIMATING THE ERROR RATE (2)

- Denote R(t) = r(t)p(t), that is the miscclassification error rate weighted by the probability of the node.
- The resubstitution estimation for the overall misclassification rate ${\cal R}(T)$ of the tree classifier ${\cal T}$ is:

$$R(T) = \sum_{t \in ilde{T}} R(t)$$

OPTIMIZING THE TREE

- Trees obtained by looking for optimal splits tend to overfit: good for the data in the tree, but generalize badly and tend to fail more in predictions.
- In order to reduce complexity and overfitting while keeping the tree as good as possible tree pruning may be applied.
- Essentially pruning works by removing branches that are unlikely to improve the accuracy of the model on new data.

PRUNING METHODS

- There are different pruning methods, but the most common one is the *cost-complexity* pruning algorithm, also known as the *weakest link pruning*.
- The algorithm works by adding a penalty term to the misclassification rate of the terminal nodes:

$$R_{lpha}(T) = R(T) + lpha |T|$$

where α is the parameter that controls the trade-off between tree complexity and accuracy.

COST COMPLEXITY PRUNING

- Start by building a large tree that overfits the data.
- Then, use cross-validation to estimate the optimal value of alpha that minimizes the generalization error.
- Finally, prune the tree by removing the branches that have a smaller improvement in impurity than the penalty term multiplied by alpha.
- Iterate the process until no more branches can be pruned, or until a minimum tree size is reached.

REGRESSION TREES

REGRESSION MODELLING WITH TREES

- When the response variable is numeric, decision trees are regression trees.
- Option of choice for distinct reasons
 - The relation between response and potential explanatory variables is not linear.
 - Perform automatic variable selection.
 - Easy to interpret, visualize, explain.
 - Robust to outliers and can handle missing data

REGRESSION VS CLASSIFICATION TREES

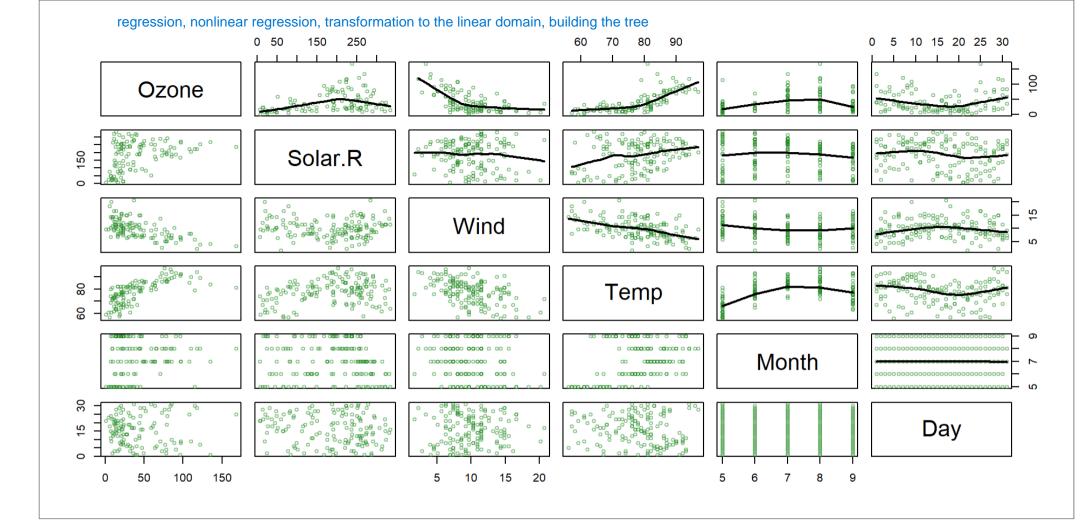
- Some differences with classification trees:
 - Splitting criteria based on mean squared error or mean absolute error.
 - Leaf node prediction based on mean/median of the target variable.
 - Evaluation metrics based on measures of the difference between the predicted and actual values.

REGRESSION TREE EXAMPLE

- The airquality dataset from the datasets package contains daily air quality measurements in New York from May through September of 1973 (153 days).
- The main variables include:
 - Ozone: the mean ozone (in parts per billion) ...
 - Solar.R: the solar radiation (in Langleys) ...
 - Wind: the average wind speed (in mph) ...
 - Temp: the maximum daily temperature (°F) ...
- Main goal: Predict ozone concentration.

NON LINEAR RELATIONSHIPS!

```
1 aq <- datasets::airquality
2 color <- adjustcolor("forestgreen", alpha.f = 0.5)
3 ps <- function(x, y, ...) { # custom panel function
4  panel.smooth(x, y, col = color, col.smooth = "black", cex = 0.7, lwd = 2)
5 }
6 pairs(aq, cex = 0.7, upper.panel = ps, col = color)</pre>
```



BUILDING THE TREE (1): SPLITTING

- Consider:
 - all predictors X_1, \ldots, X_n , and
 - ullet all values of cutpoint s for each predictor and
- ullet For each predictor find boxes R_1,\dots,R_J that minimize the RSS, given by $\sum_{j=1}^J \sum_{i\in R_i} \left(y_i \hat{y}_{R_j}
 ight)^2$

where \hat{y}_{R_j} is the mean response for the training observations within the j th box.

BUILDING THE TREE (2): SPLITTING

• To do this, define the pair of half-planes

$$R_1(j,s) = \{X \mid X_j < s\} \ ext{ and } R_2(j,s) = \{X \mid X_j \geq s\}$$

and seek the value of j and s that minimize the equation:

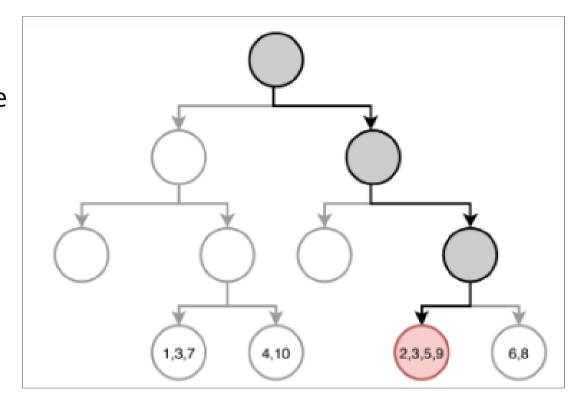
$$\sum_{i: x_i \in R_1(j,s)} ig(y_i - \hat{y}_{R_1}ig)^2 + \sum_{i: x_i \in R_2(j,s)} ig(y_i - \hat{y}_{R_2}ig)^2.$$

greedy algorithm

BUILDING THE TREE (3): PREDICTION

- Once the regions have been created we predict the response using the mean of the training observations in the region to which that observation belongs.
- In the example, for an observation belonging to the shaded region, the prediction would be:

$$\hat{(}y)=rac{1}{4}(y_2+y_3+y_5+y_9)$$



the mean of the terminal nodes

EXAMPLE: A REGRESSION TREE

```
1 set.seed(123)
2 train <- sample(1:nrow(aq), size = nrow(aq)*0.7)
3 aq_train <- aq[train,]
4 aq_test <- aq[-train,]
5 aq_regresion <- tree::tree(formula = Ozone ~ ., mean squre error data = aq_train, split = "deviance")
7 summary(aq_regresion)</pre>
```

```
Regression tree:

tree::tree(formula = Ozone ~ ., data = aq_train, split = "deviance")

Variables actually used in tree construction:

[1] "Temp" "Wind" "Solar.R" "Day"

Number of terminal nodes: 8

Residual mean deviance: 285.6 = 21420 / 75

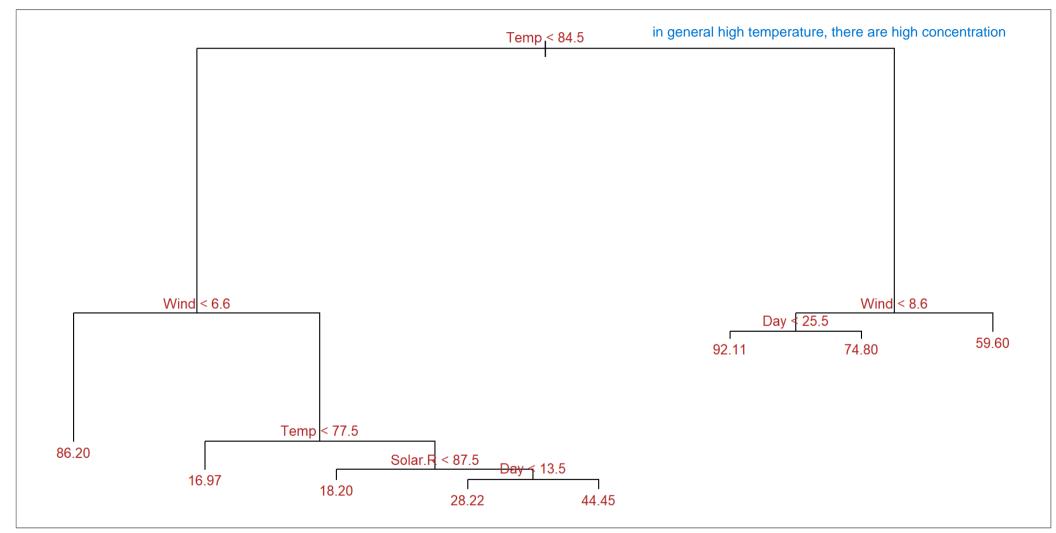
Distribution of residuals:

Min. 1st Qu. Median Mean 3rd Qu. Max.

-58.2000 -7.9710 -0.4545 0.0000 5.5290 81.8000
```

EXAMPLE: PLOT THE TREE

air quality



PRUNNING THE TREE (1)

- As before, cost-complexity prunning can be applied
- We consider a sequence of trees indexed by a nonnegative tuning parampter α .

mean squared error + regularization

• For each value of α there corresponds a subtree $T \subset T_0$ such that:

$$\sum_{m=1}^{|T|} \sum_{i:} ig(y_i \in R_m - \hat{y}_{R_m}ig)^2 + lpha |T| \quad (*)$$
 regularization

is as small as possible.

purity of the nodes

TUNING PARAMETER α

- α controls a trade-off between the subtree's complexity and its fit to the training data.
- When $\alpha = 0$, then the subtree T will simply equal T_0 .
- As α increases, there is a price to pay for having a tree with many terminal nodes, and so (*) will tend to be minimized for a smaller subtree.
- Equation (*1) is reminiscent of the lasso.
- α can be chosen by cross-validation.

OPTIMIZING THE TREE (α)

- 1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.
- 2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of α .
- 3. Use K-fold cross-validation to choose α . That is, divide the training observations into K folds. For each $k=1,\ldots,K$:
 - 1. Repeat Steps 1 and 2 on all but the k th fold of the training data.
 - 2. Evaluate the mean squared prediction error on the data in the left-out k th fold, as a function of α .

Average the results for each value of α . Pick α to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of α .

EXAMPLE: PRUNE THE TREE

```
Regression tree:

tree::tree(formula = Ozone ~ ., data = aq_train, split = "deviance")

Variables actually used in tree construction:

[1] "Temp" "Wind" "Solar.R" "Day"

Number of terminal nodes: 8

Residual mean deviance: 285.6 = 21420 / 75

Distribution of residuals:

Min. 1st Qu. Median Mean 3rd Qu. Max.

-58.2000 -7.9710 -0.4545 0.0000 5.5290 81.8000
```

In this example pruning does not improve the tree.

REFERENCES AND RESOURCES

REFERENCES

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RESOURCES

- Applied Data Mining and Statistical Learning (Penn Statte-University)
- R for statistical learning
- CART Model: Decision Tree Essentials
- An Introduction to Recursive Partitioning Using the RPART Routines