S&DS 265 / 565

Introductory Machine Learning

Trees

September 28

Yale

Classification and Regression Trees (CART)

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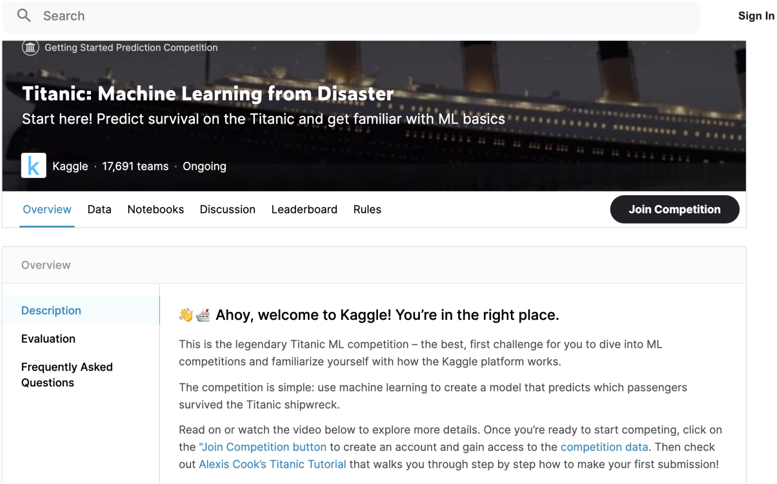
- Response variables can be categorical or quantitative
- Yields a set of interpretable decision rules
- Predictive ability is mediocre, *but* can be improved by combining multiple trees (resampling, ensemble methods)

Titanic data



Titanic data

- **Survived**: Outcome of survival (0 = No; 1 = Yes)
- **Pclass**: Socio-economic class (1 = Upper class; 2 = Middle class; 3 = Lower class)
- **Name**: Name of passenger
- **Sex**: Sex of the passenger
- **Age**: Age of the passenger (Some entries contain `NaN`)
- **SibSp**: Number of siblings and spouses of the passenger aboard
- **Parch**: Number of parents and children of the passenger aboard
- **Ticket**: Ticket number of the passenger
- **Fare**: Fare paid by the passenger
- **Cabin** Cabin number of the passenger (Some entries contain `NaN`)
- **Embarked**: Port of embarkation of the passenger (C = Cherbourg; Q = Queenstown; S = Southampton)

Trees

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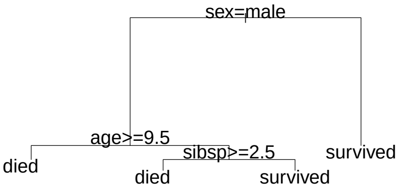
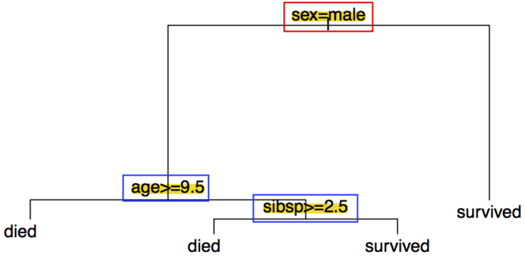
Modeling Titanic survival:



Tree terminology

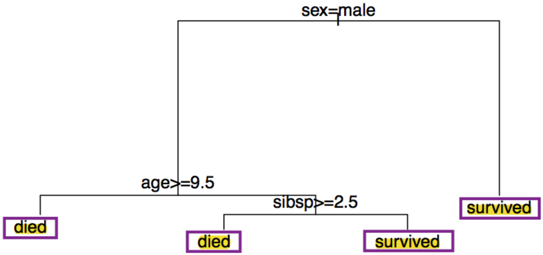
Internal nodes are points where the predictor space is split.



The internal node at the top is the **root** of the tree.

Tree terminology

Terminal nodes (or **leaves**) are the ends of the tree where no further splitting occurs.



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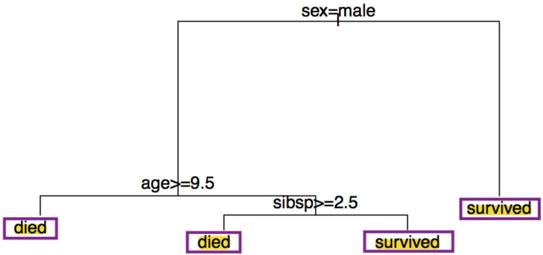
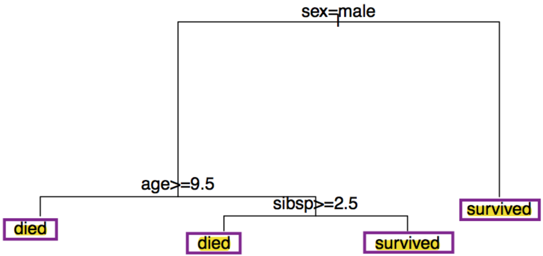


Denote these J regions as $R_1, \ldots, R_J$.

Tree terminology



- $R_1 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i \geq 9.5\}$
- $R_2 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i < 9.5 \cap \text{sibsp}_i \geq 2.5\}$
- $R_3 = \{i : \text{sex}_i = \text{male} \cap \text{age}_i < 9.5 \cap \text{sibsp}_i < 2.5\}$
- $R_4 = \{i : \text{sex}_i \neq \text{male}\}$

Let's go to the Titanic demo

Bias-variance

- As tree is grown deeper, bias decreases
- But the variance increases
- How to choose the right size of tree?

Stopping criterion

Once we stop, we relabel the terminal nodes to be $R_1, \ldots, R_J$ and compute $\bar{y}_{R_j}$ (means within each region) to serve as $\widehat{y}$ values.

But when do we stop?

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Many options – resulting in tuning parameters that are hard to deal with.

Tree pruning

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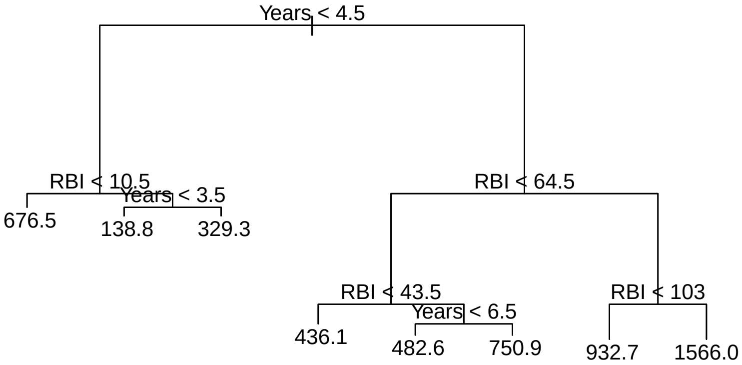

Tree pruning

How do we prune?

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- cross validation

Tree pruning

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- cross validation
- cost-complexity pruning

Cost-complexity pruning

$$C(T) = \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \widehat{y}_{R_m})^2 + \alpha|T|$$

α is a tuning parameter that controls for the complexity of the model.

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α is a tuning parameter that controls for the complexity of the model.

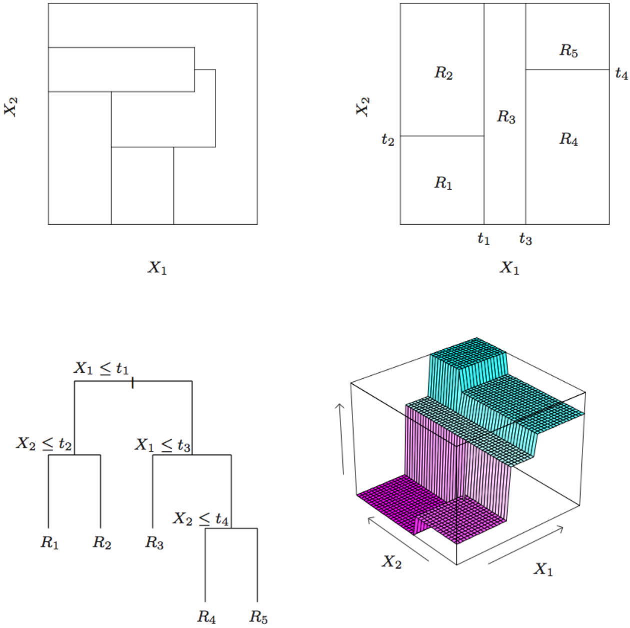
- $\alpha = 0$ implies the full tree
- Larger α implies higher penalty for complexity of model

Tree pruning

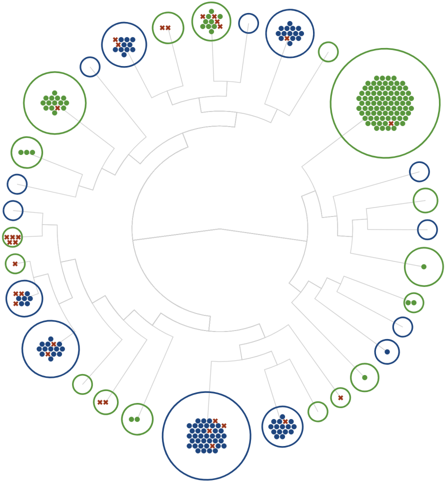
1. Grow a big tree on a *training set*.
2. Obtain a nested set of subtrees $T_L \subset \cdots \subset T_2 \subset T_1 \subset T_0$ corresponding to a sequence of α values.
3. Use K-fold cross-validation to identify the subtree/α that does best.

So far

- Give interpretable decision rules
- Deep trees have low bias, high variance
- Trees can be grown greedily to be full, then pruned back
- Predictive power is ... meh


X_2
X_1
R_2
R_5
t_4
R_3
R_4
t_2
R_1
t_1
t_3
X_2
X_1
$X_1 \leq t_1$
$X_2 \leq t_2$
$X_1 \leq t_3$
$X_2 \leq t_4$
R_1
R_2
R_3
R_4
R_5
X_2
X_1

Beautiful demo `http://www.r2d3.us/`



Summary from today

- Trees give interpretable, nonlinear prediction rules
- Deep trees have low bias, high variance
- Shallow trees have high bias, low variance
- Deep trees are pruned back using cross-validation to find best bias/variance tradeoff.