S&DS 265 / 565

Introductory Machine Learning

Trees and Forests

October 3

Yale

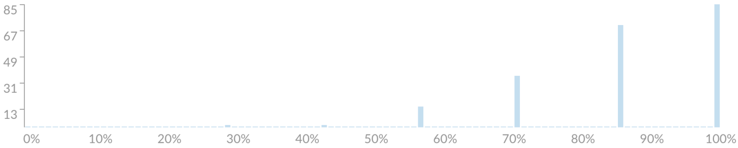
Reminders

- Assn 2 out; due Thursday at midnight
- Quiz 2 last week
- Midterm in class on Tuesday, October 17
- Questions?

Quiz Summary

Section Filter ▾ | Student Analysis | Item Analysis

Average Score	High Score	Low Score	Standard Deviation	Average Time
87%	100%	29%	0.99	13:54



Communication

Important: For any communication regarding assignments, late work, etc. that requires email:

- Email the instructor John Lafferty (john.lafferty@yale.edu) **and** course manager Joanne Chen (haoting.chen@yale.edu)
- State that this is for Introductory Machine Learning (S&DS 265)
- Any email to me alone may go unanswered

Classification and Regression Trees (CART)

Trees provide ways of modeling nonlinear relationships by carving out *rectangular regions* in the feature space.

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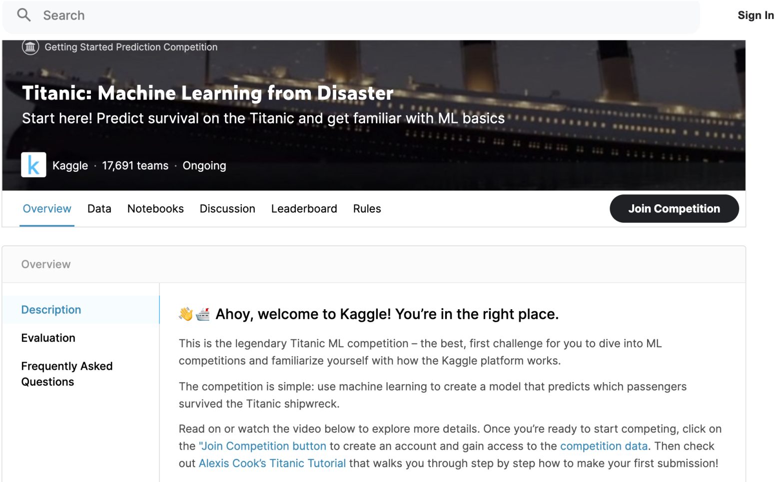
- Response variables can be categorical or quantitative
- Yields a set of interpretable decision rules
- Predictive ability is mediocre, *but* can be improved by combining multiple trees (resampling, ensemble methods)

Titanic data



Titanic data

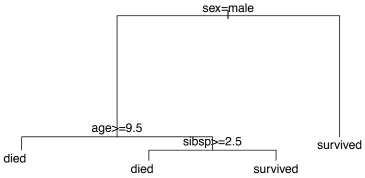
- **Survived**: Outcome of survival (0 = No; 1 = Yes)
- **Pclass**: Socio-economic class (1 = Upper class; 2 = Middle class; 3 = Lower class)
- **Name**: Name of passenger
- **Sex**: Sex of the passenger
- **Age**: Age of the passenger (Some entries contain `NaN`)
- **SibSp**: Number of siblings and 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

Trees

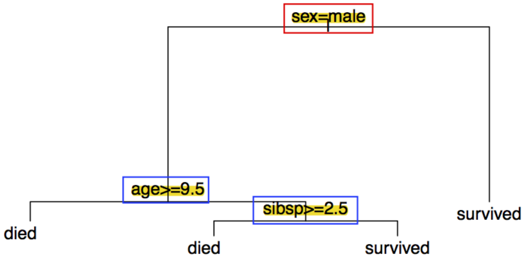
Trees

Modeling Titanic survival:



Tree terminology

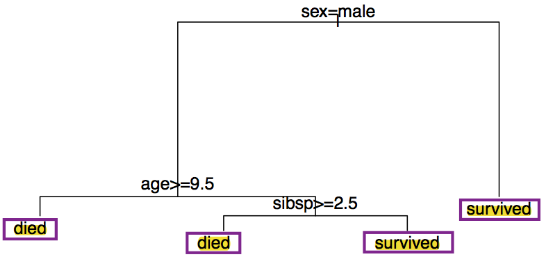
Internal nodes are points where the predictor space is split.



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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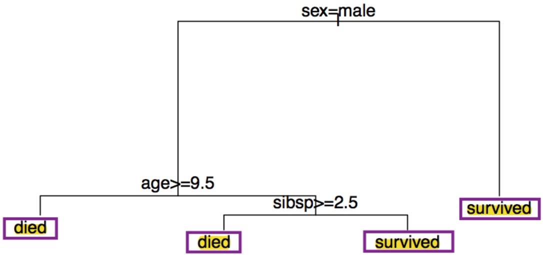
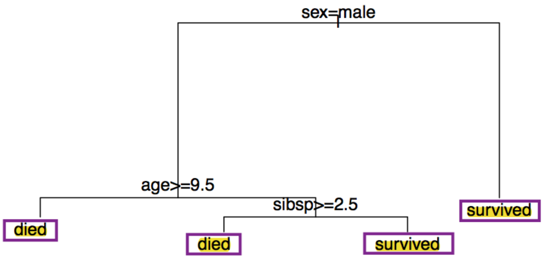


Denote these J regions as $R_1, \ldots, R_J$.

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

- Nodes are split by greedily choosing the best question (greatest reduction in error)
- 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.

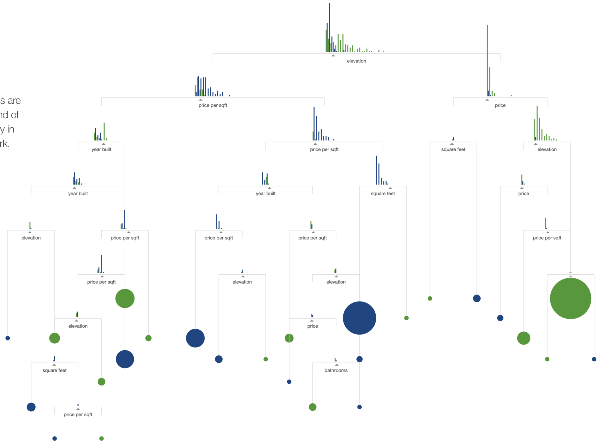
Tree pruning

Another way to get around the overfitting problem is to grow a large tree and then **prune** it back.

Typically, pruning involves looking at subtrees of the fully-grown tree, and comparing how well the subtrees perform.

Tree pruning

You could even continue to add branches until the tree's predictions are **100% accurate**, so that at the end of every branch, the homes are purely in San Francisco or purely in New York.



Tree pruning

How do we prune?

- cross validation
- cost-complexity pruning

Cost-complexity pruning

$$\text{Minimize:} \qquad \text{Loss}(T) + \lambda \{\text{\# of nodes in T}\}$$
$$= \sum_{m=1}^{|T|} \sum_{i \in R_m} (y_i - \widehat{y}_{R_m})^2 + \lambda |T|$$

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

Cost-complexity pruning

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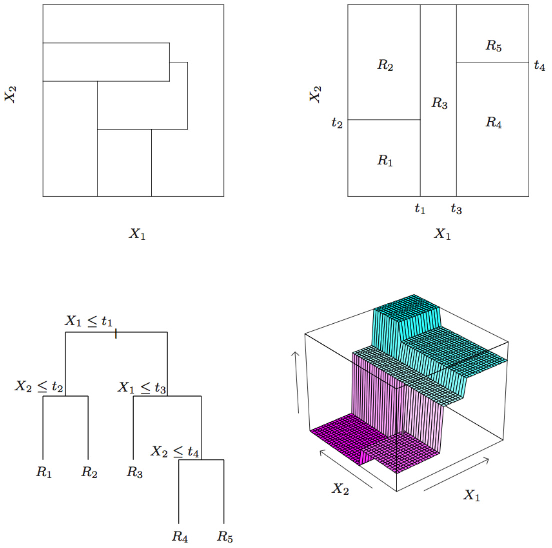
λ is a tuning parameter that controls for the complexity of the model.

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

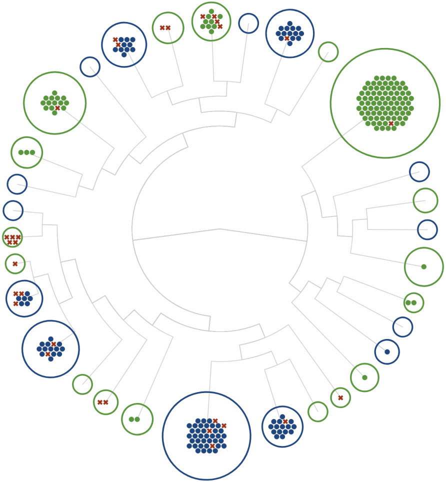
Tree pruning

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 λ values.
3. Use (leave-one-out or k-fold) cross-validation to identify the subtree/λ that does best.



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

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



This demo gives a nice description of bias-variance tradeoff for trees. It's well worth a look!

Trees vs. other methods

Decision trees are similar in spirit to k-nearest neighbors.

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- Both produce simple predictions (averages/maximally occurring) based on “neighborhoods” in the predictor space.
- Neighborhoods chosen very differently

Trees vs. other methods

Recall that linear regression fits models of the form

$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$

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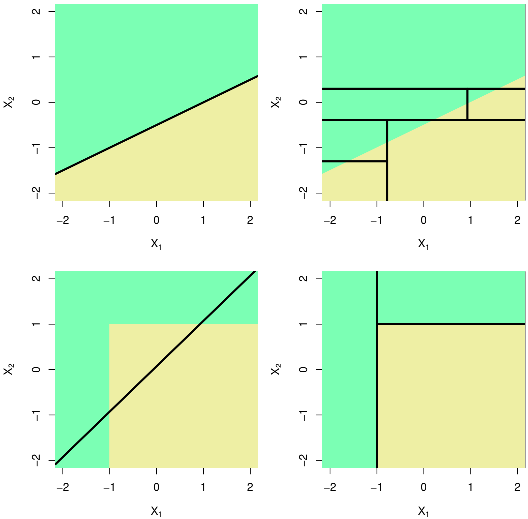
$$f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$$

Regression trees are like fitting linear regression models with a bunch of indicators

$$f(X) = \sum_{j=1}^{J} \beta_j \mathbb{1}\left\{X \in R_j\right\}$$

Trees vs. other methods

Are trees always better than linear methods?



Summary so far

- 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.

Random Forests

- Grow many trees and average their predictions
- Trees are grown deep, to have low bias, but high variance
- To “decorrelate” the trees and reduce variance, each tree is
  - grown on a bootstrap sample of the data
  - grown with random subsets of the predictors at each split
- Tree growing can be done in parallel

Leo Breiman—“Keep it simple”

Random Forests Algorithm

1. For $b = 1$ to B:
   (a) Draw a bootstrap sample Z^* of size n from the training data
   (b) Grow a random-forest tree T_b to the bootstrapped data, recursively repeating following steps, until minimum node size reached:
      i. Select m variables at random from the p variables
      ii. Pick the best variable/split-point among the m
      iii. Split the node into two children nodes
2. Output the ensemble of trees $\{T_b\}_{b=1}^{B}$.

Random Forests Algorithm

To make a prediction at a new point x:

Regression: Average $\widehat{f}^B_{rf}(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$

Classification: Majority vote of the individual trees

Out of bag (OOB) prediction

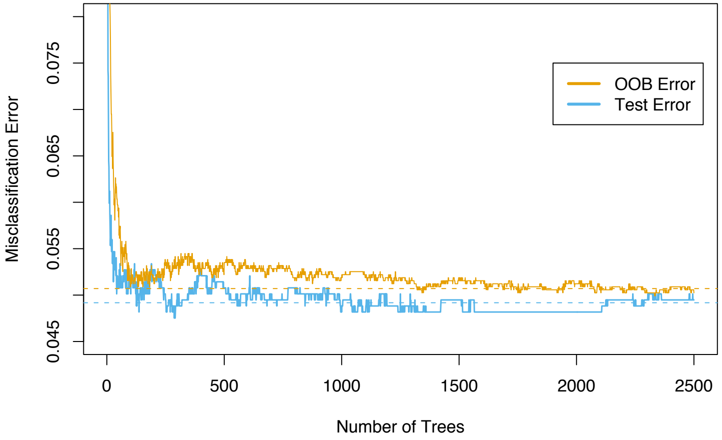
A bootstrap sample, or "bag" of data, is a n data points sampled with replacement from the original set of n data points. Will contain repetitions.

Each tree is grown on such a sample, which contains about $\frac{2}{3}$ of the original data (with repetitions). The remaining $\frac{1}{3}$ can be used as validation data

- For each observation $z_i = (x_i, y_i)$, construct its random forest predictor by averaging only those trees corresponding to bootstrap samples in which z_i did not appear
- Thus, cross-validation can be performed "along the way"

Chance a sample x_i does not appear in a bootstrap sample is $\left(1 - \frac{1}{n}\right)^n \longrightarrow \frac{1}{e} \approx 0.37$

Out of bag (OOB) prediction



Performance on email spam task

Single tree: 8.7%

Random forest: 5.1%

(standard error of the estimates is $\approx 0.6\%$)

Variable importance

Random forests improve upon the predictive ability of trees, but sacrifices the interpretability of the single tree model

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A good tool for interpreting a forest is **variable importance**

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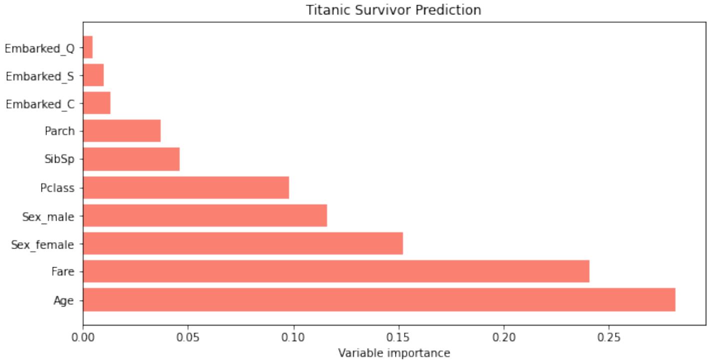
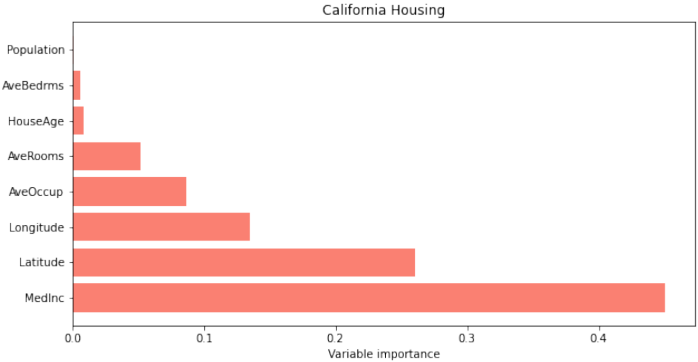
A good tool for interpreting a forest is **variable importance**

Variable importance is the amount that the RSS (or other loss) is reduced due to splits over a given predictor, averaged over all trees in the forest

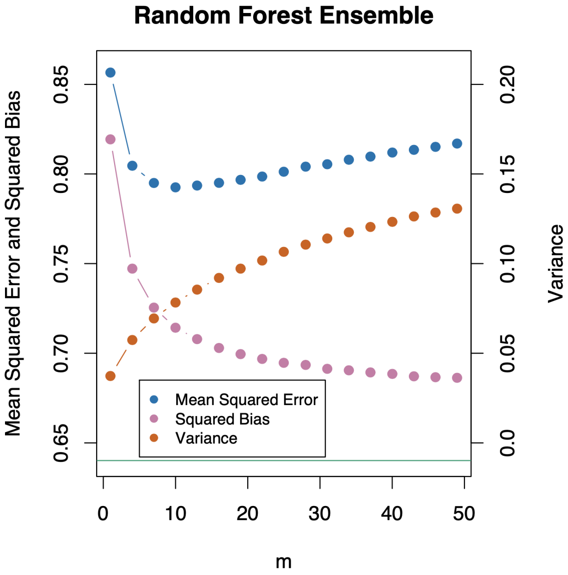
Variable importance



Variable importance



Random forest MSE



Understanding the bias-variance tradeoff for random forests

- Each tree has low (squared) bias, because it is deep
- The bootstrap sample and random subset of questions allowed at a given split result in “diversity” among of the trees
- This diversity translates to decorrelation, and tends to reduce the variance
- As we increase the number *m* in the random subset of questions allowed at each split, the complexity increases—variance goes up, squared bias goes down

Let’s go to the notebook

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
```

In [2]:
```
titanic_train = pd.read_csv('https://raw.githubusercontent.com/minsuk-heo/kaggle-titanic/master/input/train.csv')
titanic_test = pd.read_csv('https://raw.githubusercontent.com/minsuk-heo/kaggle-titanic/master/input/test.csv')
titanic_train
```

Out[2]:

	PassengerId	Survived	Pclass	Name	Sex	Age	SibSp	Parch	Ticket	Fare	Cabin	Embarked
0	1	0	3	Braund, Mr. Owen Harris	male	22.0	1	0	A/5 21171	7.2500	NaN	S
1	2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Th...	female	38.0	1	0	PC 17599	71.2833	C85	C
2	3	1	3	Heikkinen, Miss. Laina	female	26.0	0	0	STON/O2. 3101282	7.9250	NaN	S
3	4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female	35.0	1	0	113803	53.1000	C123	S
4	5	0	3	Allen, Mr. William Henry	male	35.0	0	0	373450	8.0500	NaN	S
...	...	...	...	...	...	...	...	...	...	...	...	...
886	887	0	2	Montvila, Rev. Juozas	male	27.0	0	0	211536	13.0000	NaN	S
887	888	1	1	Graham, Miss. Margaret Edith	female	19.0	0	0	112053	30.0000	B42	S
888	889	0	3	Johnston, Miss. Catherine Helen "Carrie"	female	NaN	1	2	W./C. 6607	23.4500	NaN	S
889	890	1	1	Behr, Mr. Karl Howell	male	26.0	0	0	111369	30.0000	C148	C
890	891	0	3	Dooley, Mr. Patrick	male	32.0	0	0	370376	7.7500	NaN	Q

891 rows × 12 columns

Summary

- Trees give interpretable, nonlinear prediction rules
- Deep trees have low bias, high variance
- Random forests are a way of combining trees
- Want: Different trees should capture different aspects of the data
- How: Grow each tree on a random (bootstrap) sample of the data and choosing from a random set of questions at each split