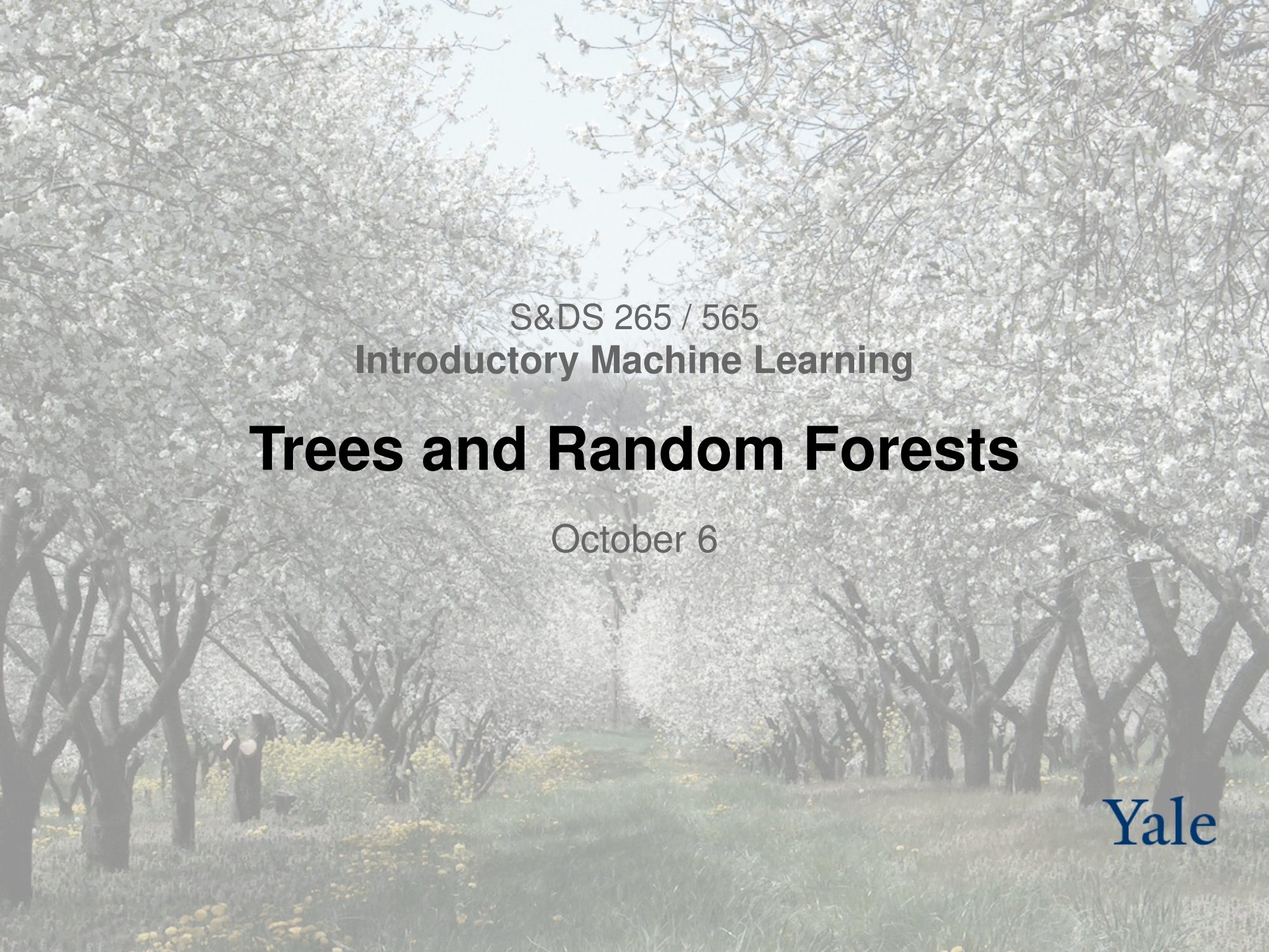


S&DS 265 / 565

Introductory Machine Learning

Trees and Random Forests

October 6

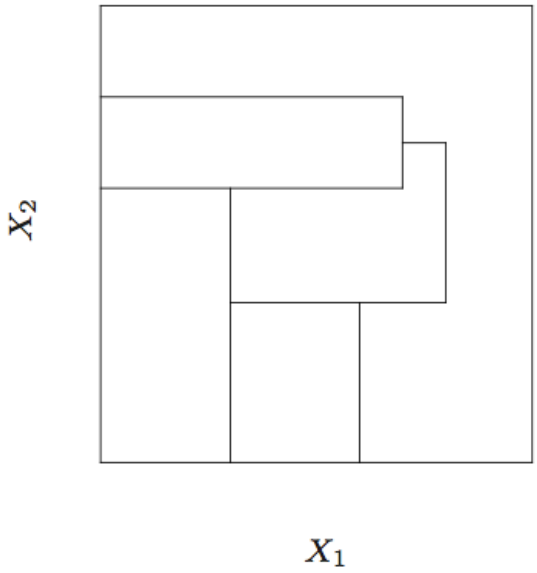
Yale

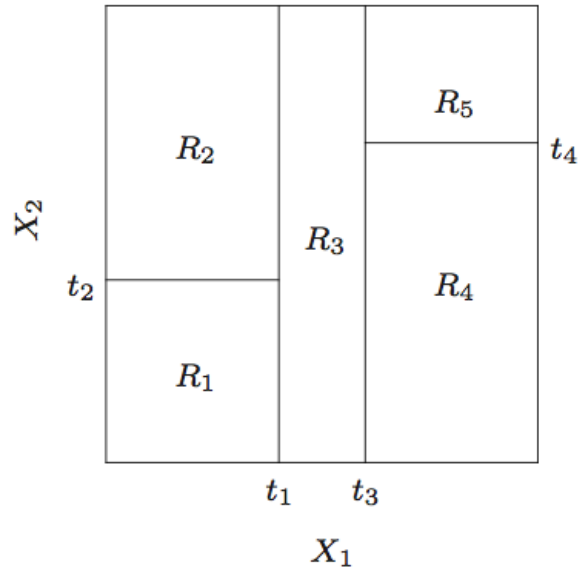
Reminders

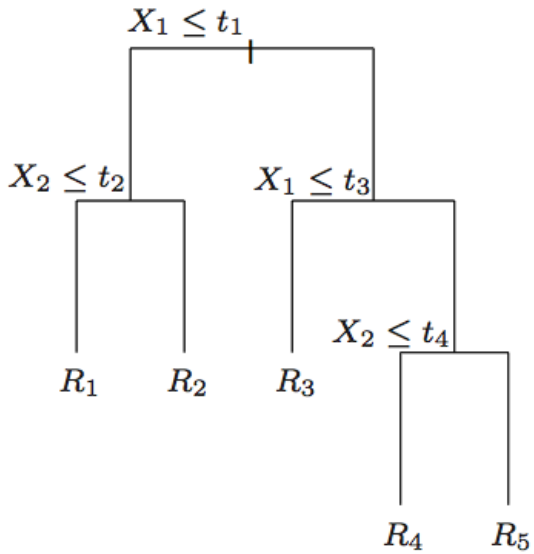
- Assn 2 out; due week from today
- Quiz 3 available 10:30am today (48 hours, 20 minutes)
- Midterm in class on October 18
- Practice midterms have been posted
- Review sessions TBA
- Questions?

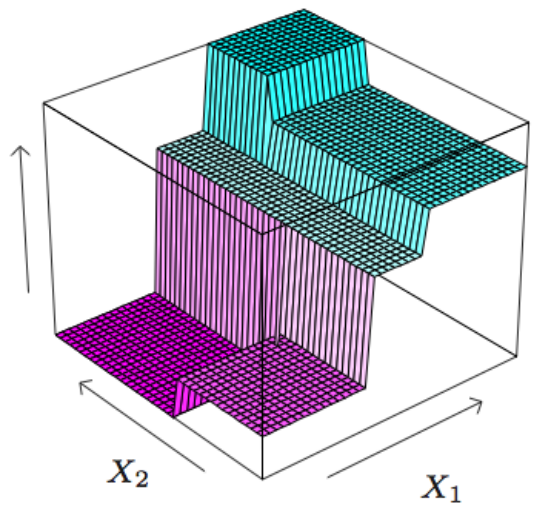
Last time: trees

- 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

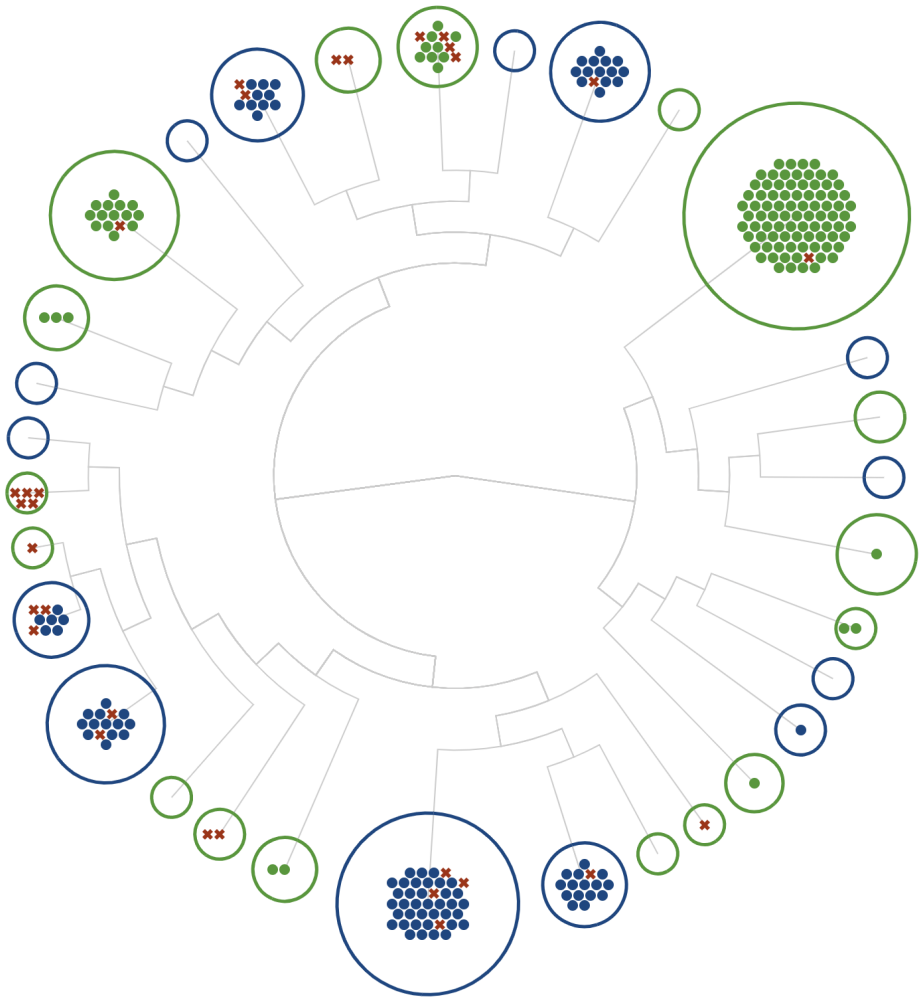

X_2
X_1


R_1
R_2
R_3
R_4
R_5
t_1
t_2
t_3
t_4
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/visual-intro-to-machine-learning-part-2



Classification Trees

- $\widehat{y}_i$ for all $i \in R_j$ is *most commonly occurring class* of training observations in R_j.

$$\widehat{y}_{R_j} = \arg\max_k \widehat{p}_{jk},$$

  where $\widehat{p}_{jk}$ is the proportion of training observations with label k in rectangle (leaf) R_j.
- No longer want to minimize RSS, but instead minimize...
  - classification error rate

$$E = \sum_{j=1}^{J} |R_j|(1 - \max_k(\widehat{p}_{jk}))$$

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$$E = \sum_{j=1}^{J} |R_j|(1 - \max_k(\widehat{p}_{jk}))$$

  - Gini index

$$G = \sum_{j=1}^{J} |R_j| \sum_{k=1}^{K} \widehat{p}_{jk}(1 - \widehat{p}_{jk})$$

    Encourages higher **node purity**.

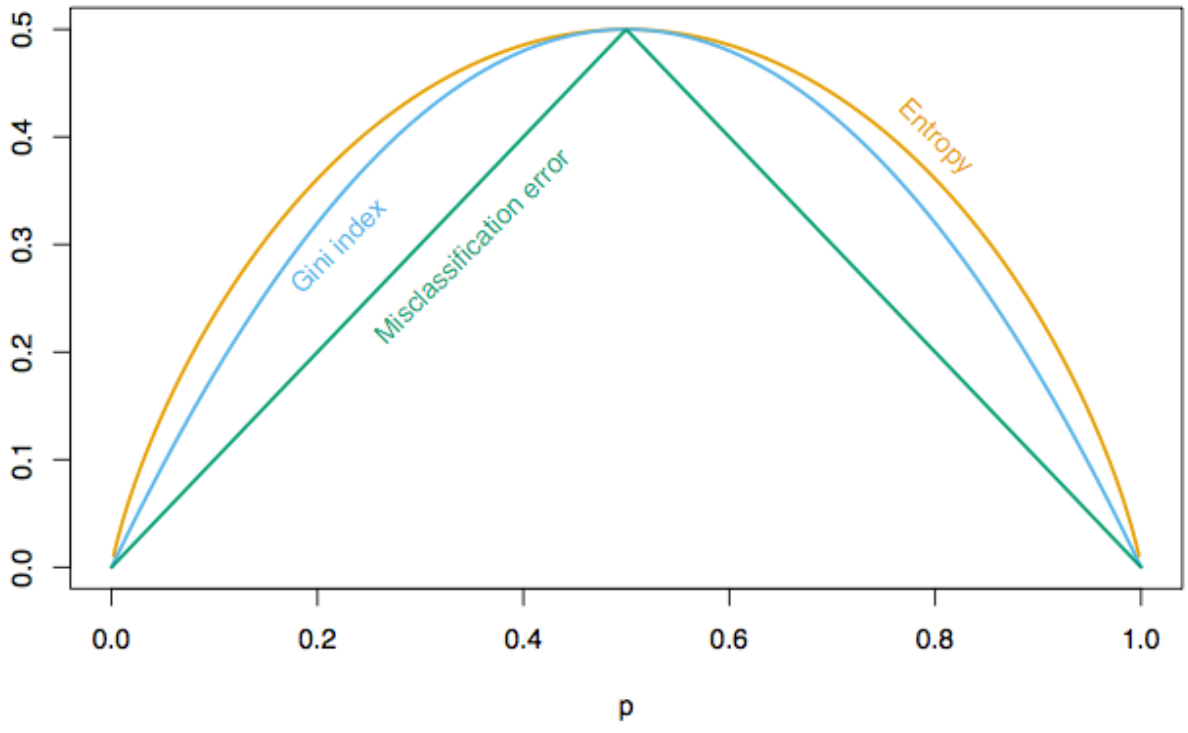
Impurity measures

Define node proportion of class k

$$\begin{aligned} \widehat{p}_{mk} &= \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k) \\ k(m) &= \arg\max_k \widehat{p}_{mk} \end{aligned}$$

- Misclassification error: $1 - \widehat{p}_{mk(m)}$
- Gini index: $\sum_{k=1}^{K} \widehat{p}_{mk}(1 - \widehat{p}_{mk})$
- Entropy: $-\sum_{k=1}^{K} \widehat{p}_{mk} \log \widehat{p}_{mk}$

Impurity measures



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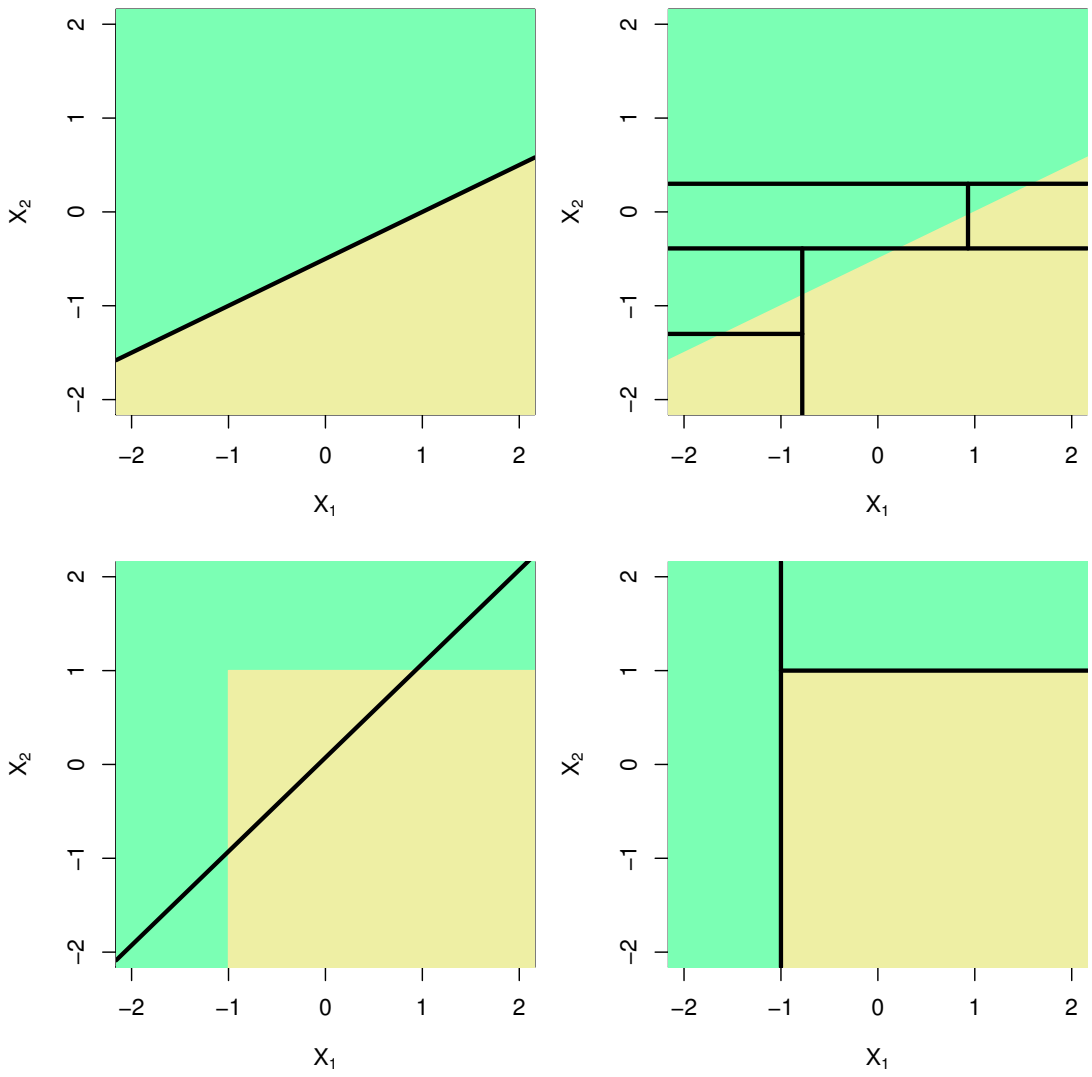
Regression trees are like fitting linear regression models with a bunch of indicators

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

Trees vs. other methods

Are trees always better than linear methods?



Summary

- trees are intuitive
- prediction rules easy to explain, interpret
- trees are sensitive to underlying data
- trees produce non-smooth prediction surfaces
- prediction accuracy can be so-so

Ensemble methods

Ensemble methods pool together multiple models to arrive at more reliable predictions.

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Ensemble methods pool together multiple models to arrive at more reliable predictions.

- bagging
- random forests
- boosting

Bootstrap samples

- We have n data points
- Randomly sample exactly n of them *with replacement*
- Contains about $\frac{2}{3}$ of the data, with duplicates

Chance a particular example does not appear in sample:

$$\left(1 - \frac{1}{n}\right)^n \longrightarrow \frac{1}{e} \approx 0.37$$

https://inferentialthinking.com/chapters/13/2/Bootstrap.html

Bagging

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Create B bootstrap samples, grow tree (without pruning) using each $\widehat{f}^{*1}, \widehat{f}^{*2}, \ldots \widehat{f}^{*B}$. For prediction at x, we take an average:

$$\widehat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \widehat{f}^{*b}(x)$$

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Classification trees: For prediction at x, $\widehat{f}_{bag}(x)$ is decided by *majority vote*.

Leo Brieman – “Keep it Simple”

Out-of-Bag error estimation

Each bagged tree uses about 2/3 of all observations (with repeats).

The remaining data—*out-of-bag* (OOB) observations—can be put to good use.

Out-of-Bag error estimation

	Bagging iteration					OOB Est.
Obs	1	2	3	...	B	
1	OOB	train	train	...	train	$\widehat{y}_1$
2	train	OOB	train	...	train	$\widehat{y}_2$
3	train	train	OOB	...	train	$\widehat{y}_3$
4	OOB	train	train	...	OOB	$\widehat{y}_4$
...	...	...	...	...	...	...
n	train	train	OOB	...	train	$\widehat{y}_n$

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...	...	...	...	...	...	...
n	train	train	OOB	...	train	$\widehat{y}_n$

- For each bagged tree, we can make predictions for the OOB observations.
- At the end, we can aggregate over all predictions for the i-th observation to arrive at a OOB prediction $\widehat{y}_i$.
- We can compute prediction error based on these OOB predictions $\widehat{y}_1, \ldots, \widehat{y}_n$.

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While bagging improves upon the predictive ability of trees, it kills off the interpretability of the model.

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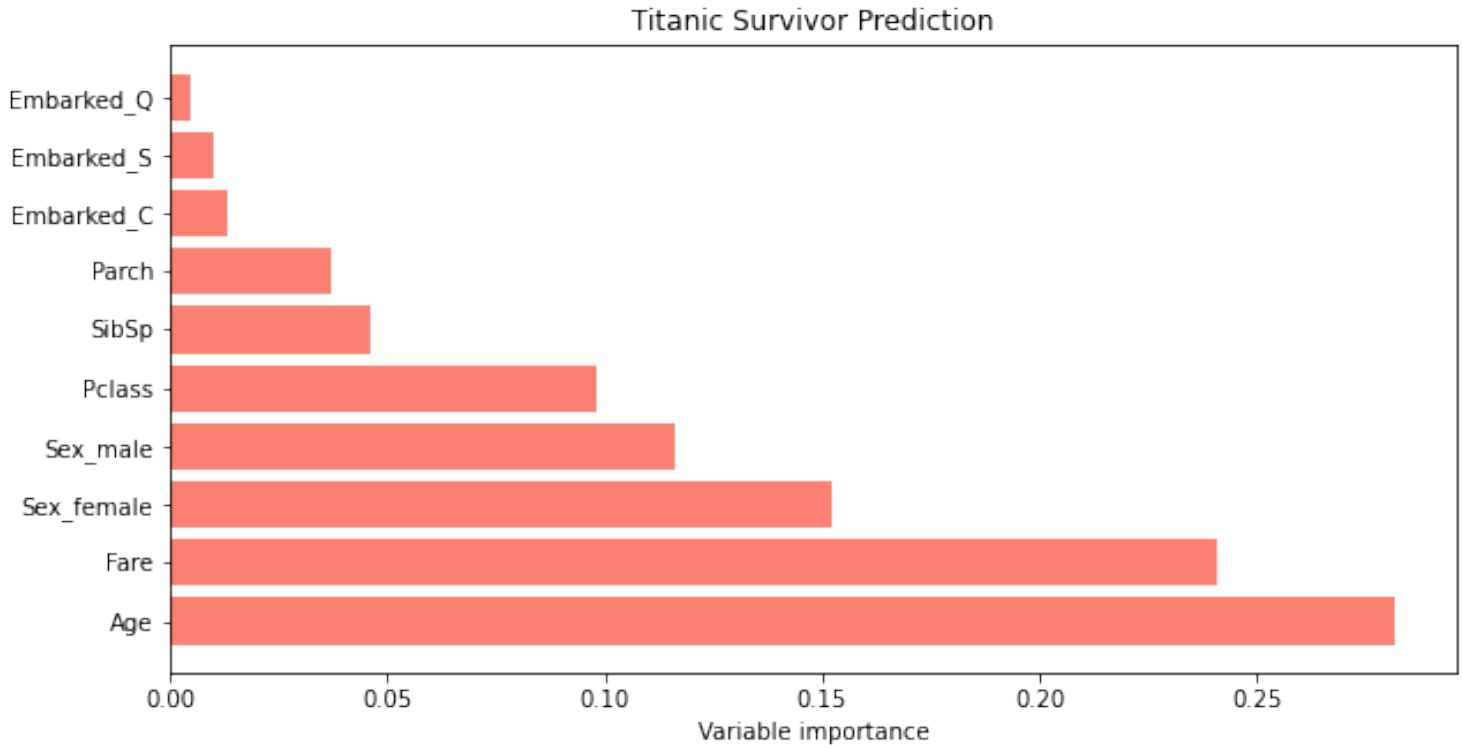
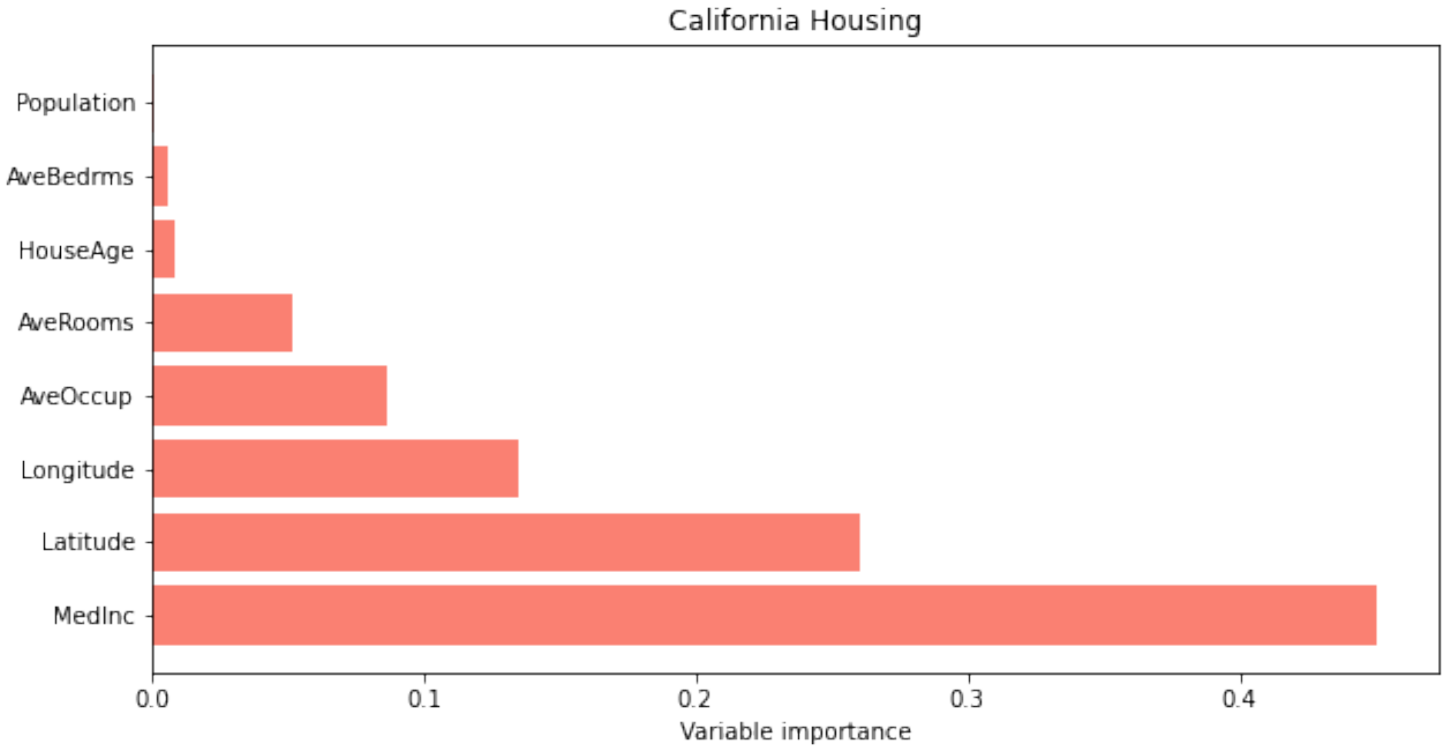
A good tool for interpreting a bagged tree model (and other tree-based ensemble methods like forests) is the **variable importance measure**.

Variable importance can be measured by the amount that the RSS (or Gini index) is reduced due to splits over a given predictor, averaged over all B trees.

Variable importance



Variable importance



Random Forests

Similar to bagging, but takes the averaging idea even further – averaging uncorrelated things decreases the error!

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Similar to bagging, but takes the averaging idea even further – averaging uncorrelated things decreases the error!

Still use bootstrap samples, but only use m out of p predictors at each split, *chosen randomly*

Bagging and Random Forests

- Grow many trees and average their predictions
- Trees are grown deep, to have low bias, but high variance
- To “decorrelate” the predictors, 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

Guess who?

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 fo trees $\{T_b\}_{b=1}^{B}$.

To make a prediction at a new point x:

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

Classification: Majority vote of the individual trees

Random forests–recommended parameters

- For classification, default value of m is $\lfloor \sqrt{p} \rfloor$ and the minimum node size is one.
- For regression, the default values of m is $\lfloor p/3 \rfloor$ and the minimum node size is five.

(you don't need to remember this)

MSRP: Manufacturer's Suggested Randomization Parameters

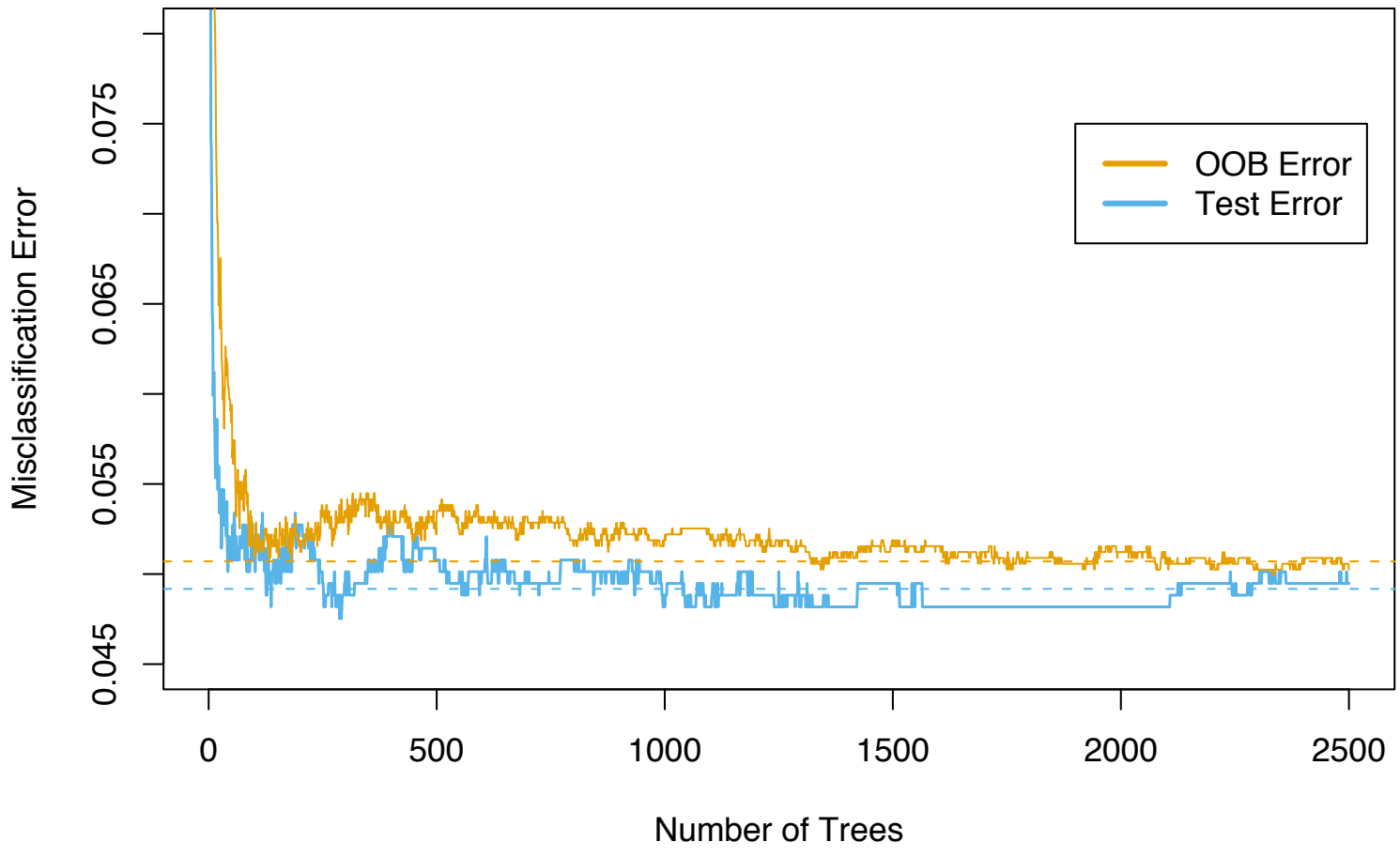
Out of bag (OOB) prediction

As before, can use out-of-bag (OOB) samples:

- 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



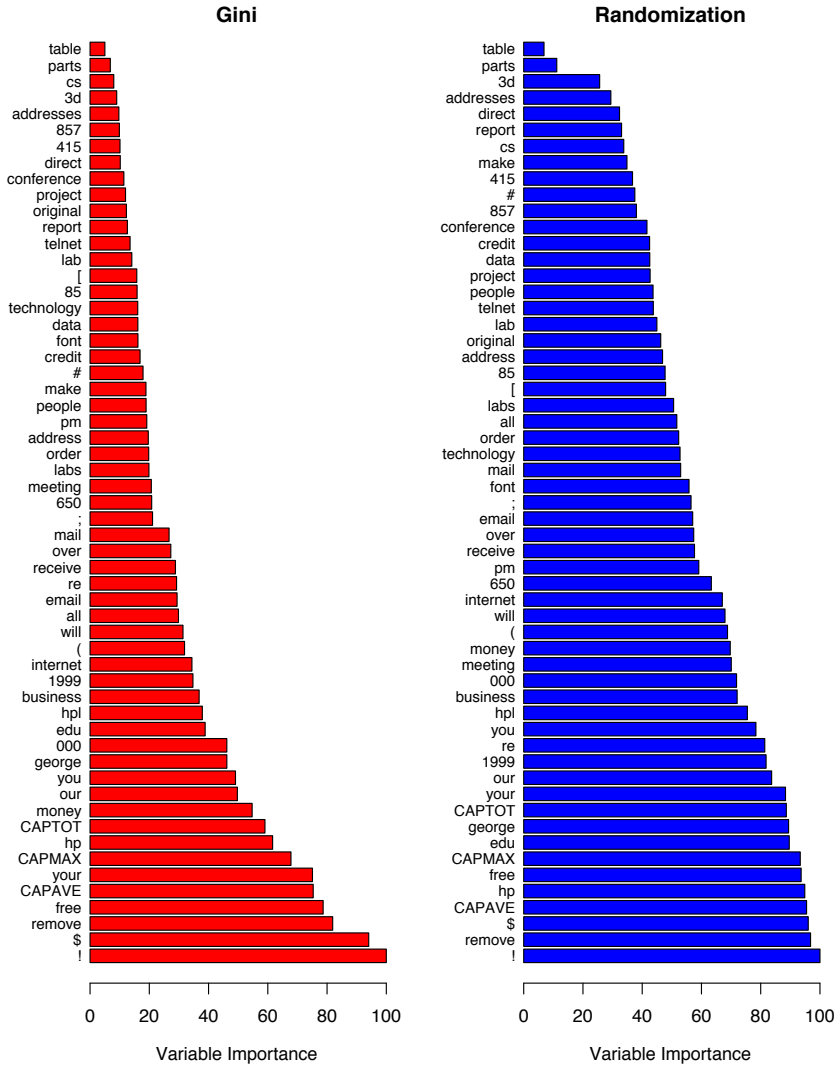
Performance on email spam task

Single tree: 8.7%

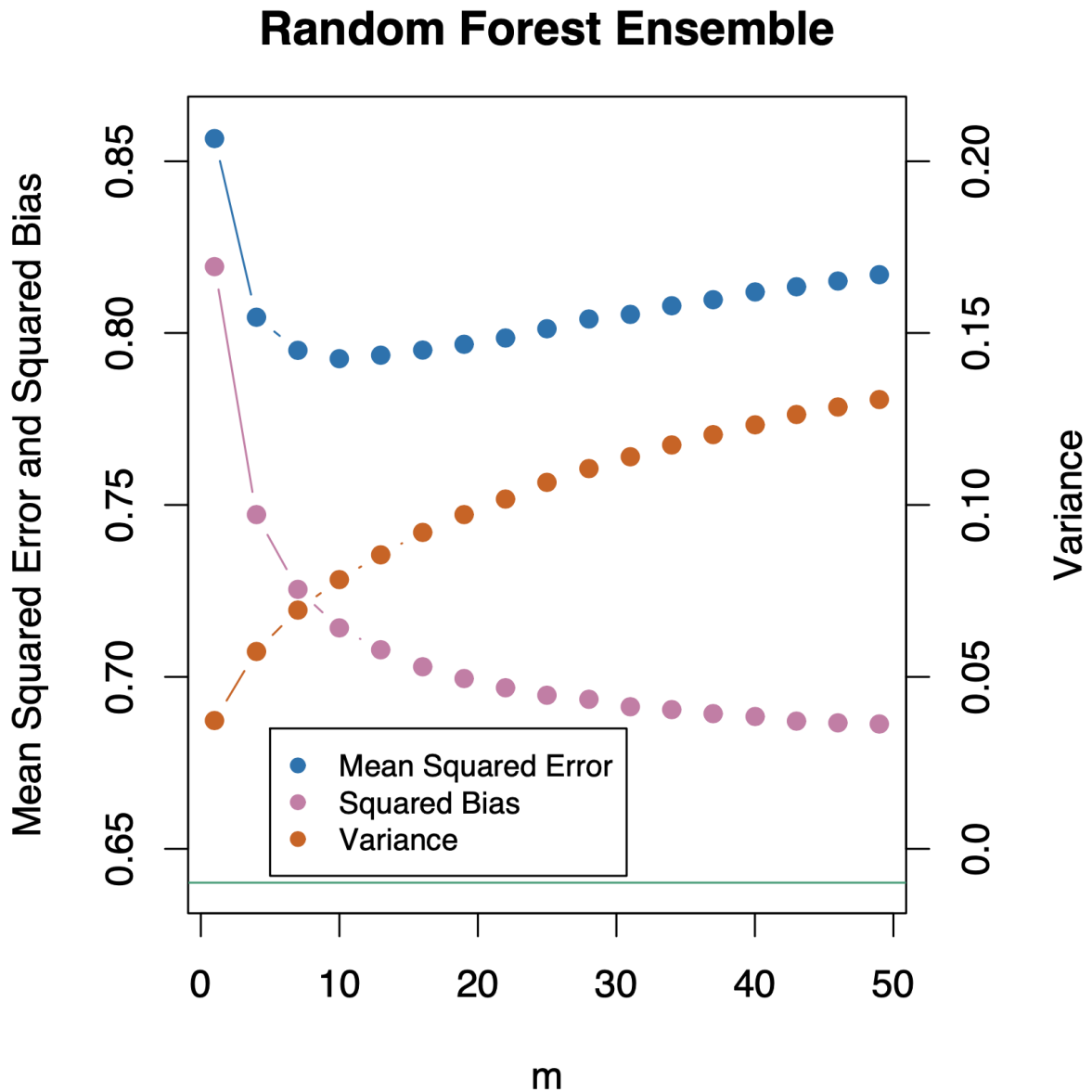
Random forests: 5.1%

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

Important features: Spam



Random forest MSE



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

What did we learn today?

- Bagging tries to reduce variance by averaging many trees
- Random forests decorrelate by random sampling of predictors
- Manage bias-variance tradeoff with randomization