CS109 – Data Science

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Announcements

- HW2 is due today!
- Please execute your notebooks, but without test output.

- Help with lecture material

Books

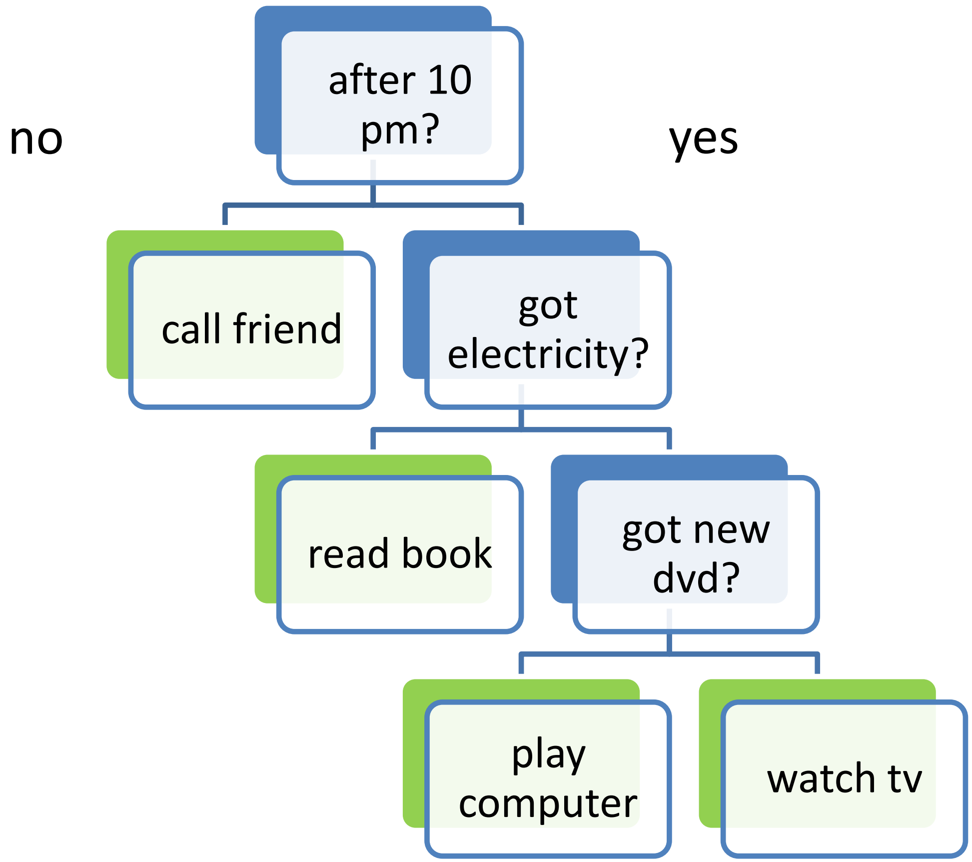
- "Elements of Statistical Learning"
- http://statweb.stanford.edu/~tibs/ElemStatLearn/

- "Pattern Recognition and Machine Learning"
- http://research.microsoft.com/en-us/um/people/cmbishop/PRML/

Next Topics

- Tree classifier
- Bagging
- Random Forest

Decision Tree



Decision Trees

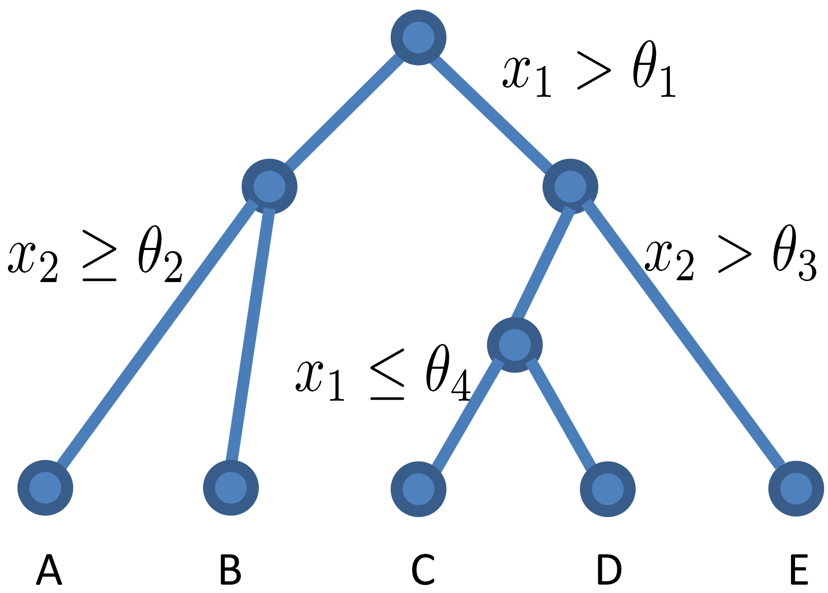
- Fast training
- Fast prediciton
- Easy to understand
- Easy to interpret

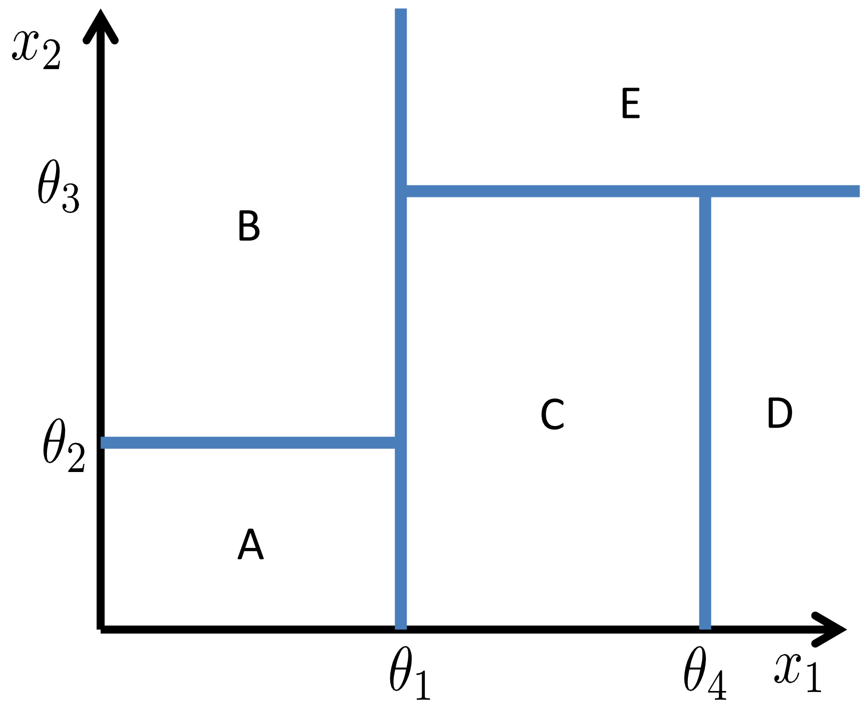
http://en.akinator.com/personnages/jeu

The link goes to a guessing game that can use 20 questions to guess an imagined character

Decision Tree - Idea

We are after a decision boundary, it's what machine learning is all about





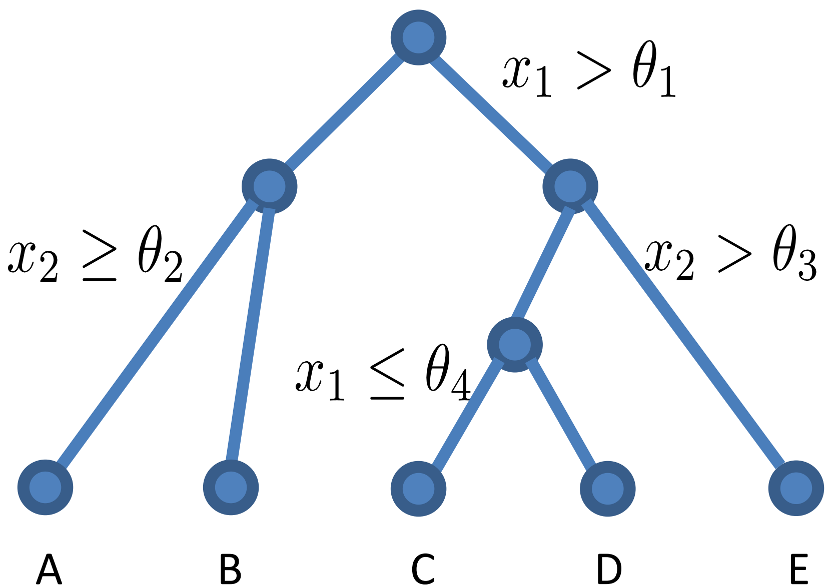
Bishop, "Pattern Recognition and Machine Learning", Springer, 2006

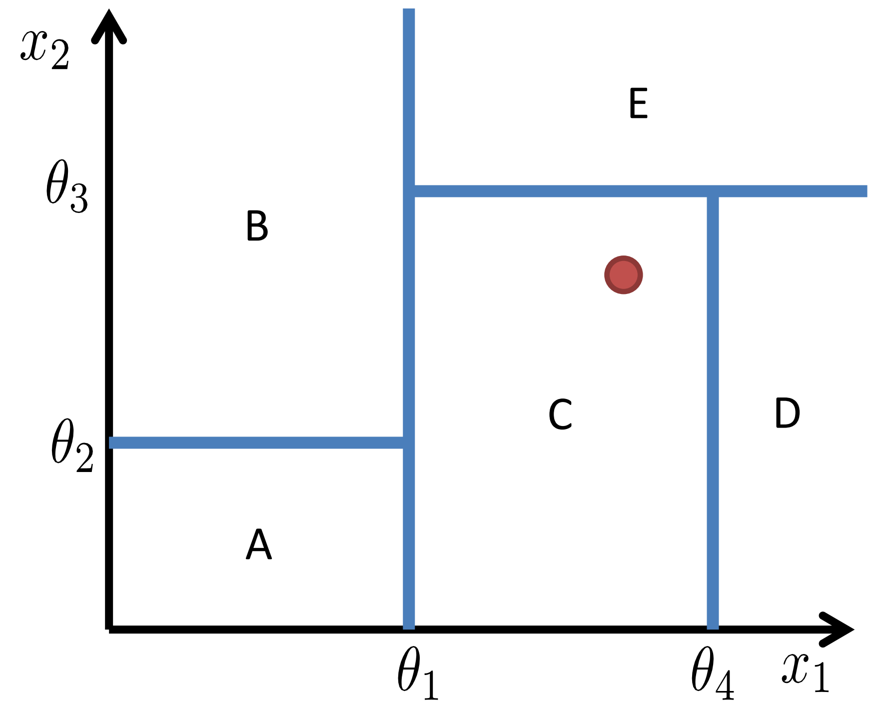
Decision Tree - Idea

- What is a the benefit of using only one feature at a time?
  - Performance. You don’t even need to look at the rest of the data once the first decision is made.
  - It is also very intuitive. It’s interpretability.
  - Sequential process as you go down the decision tree.
  - It’s also categories as the features.
  - No need to scale data given you’re only looking at one feature at a time.
- What is the drawback?

  It’s all straight lines, an axis-aligned split. You need to have high resolution should you plot this.

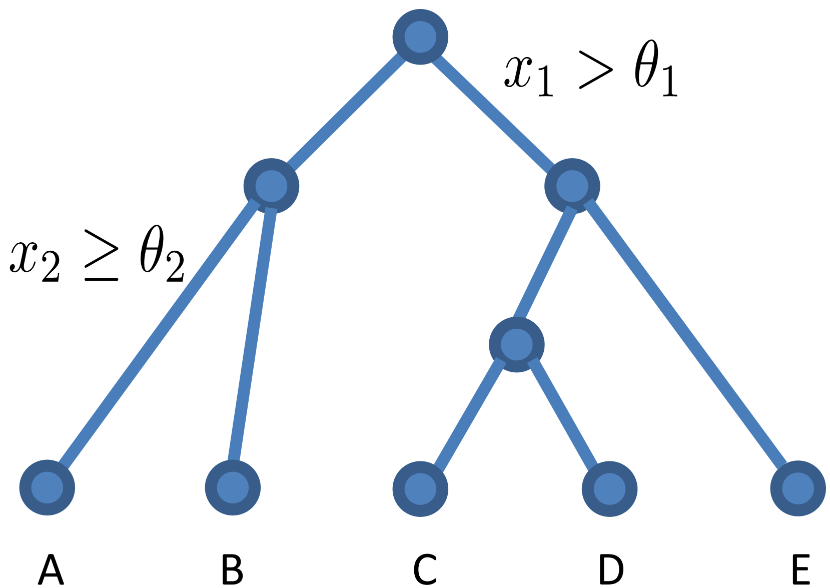
Decision Tree - Prediction





Decision Tree -Training

- Learn the tree structure:
  - which feature to query
  - which threshold to choose

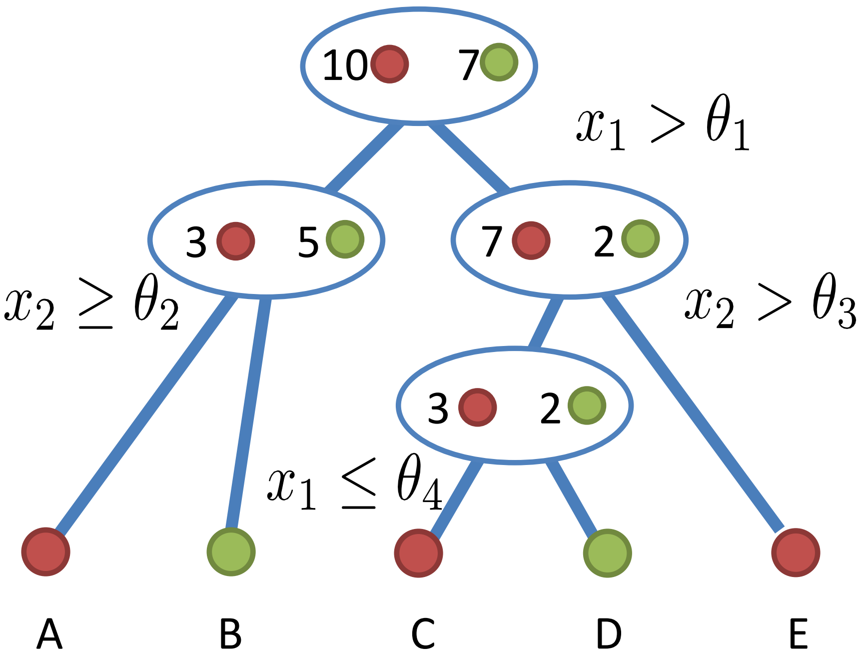


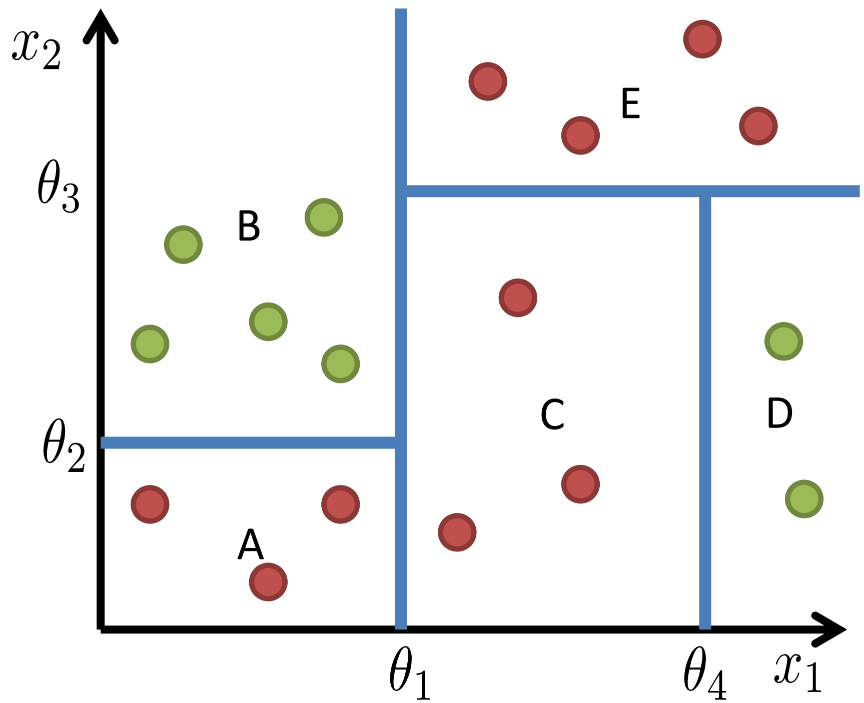
This is how to build or grow your decision tree.

This is how to determine that this feature is the right one to use for building the tree.

Node Purity

We want to come up with splits that create these cells that're 'pure' that is, only one color (class) or the other, in this case.



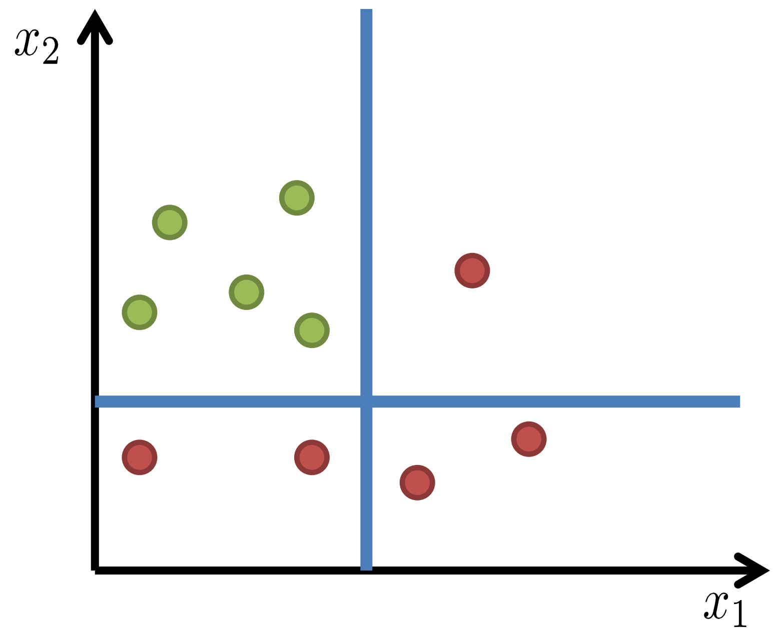


We need to express this notion of purity somehow:

Gini Impurity

Widely used in scikit learn package.

- Expected error
- if you randomly choose a sample
- and predict the class of the entire node based on it.



Gini Impurity

Example:

Multiclass:

4 **red**, 3 **green**, 3 **blue** data points

- Class probabilities:
  - red: 4/10 green: 3/10 blue: 3/10

- misclassification:
  - red: 4/10 * (3/10 + 3/10)

This is the probability of making an error.
Red prob * (Green prob + Blue prob)

Picking red

Making an error

Gini Impurity

- misclassification:
  - **red**:

  4/10 * (3/10 + 3/10) = 0.24

  - **green** and **blue**:

  3/10 * (4/10 + 3/10) = 0.21

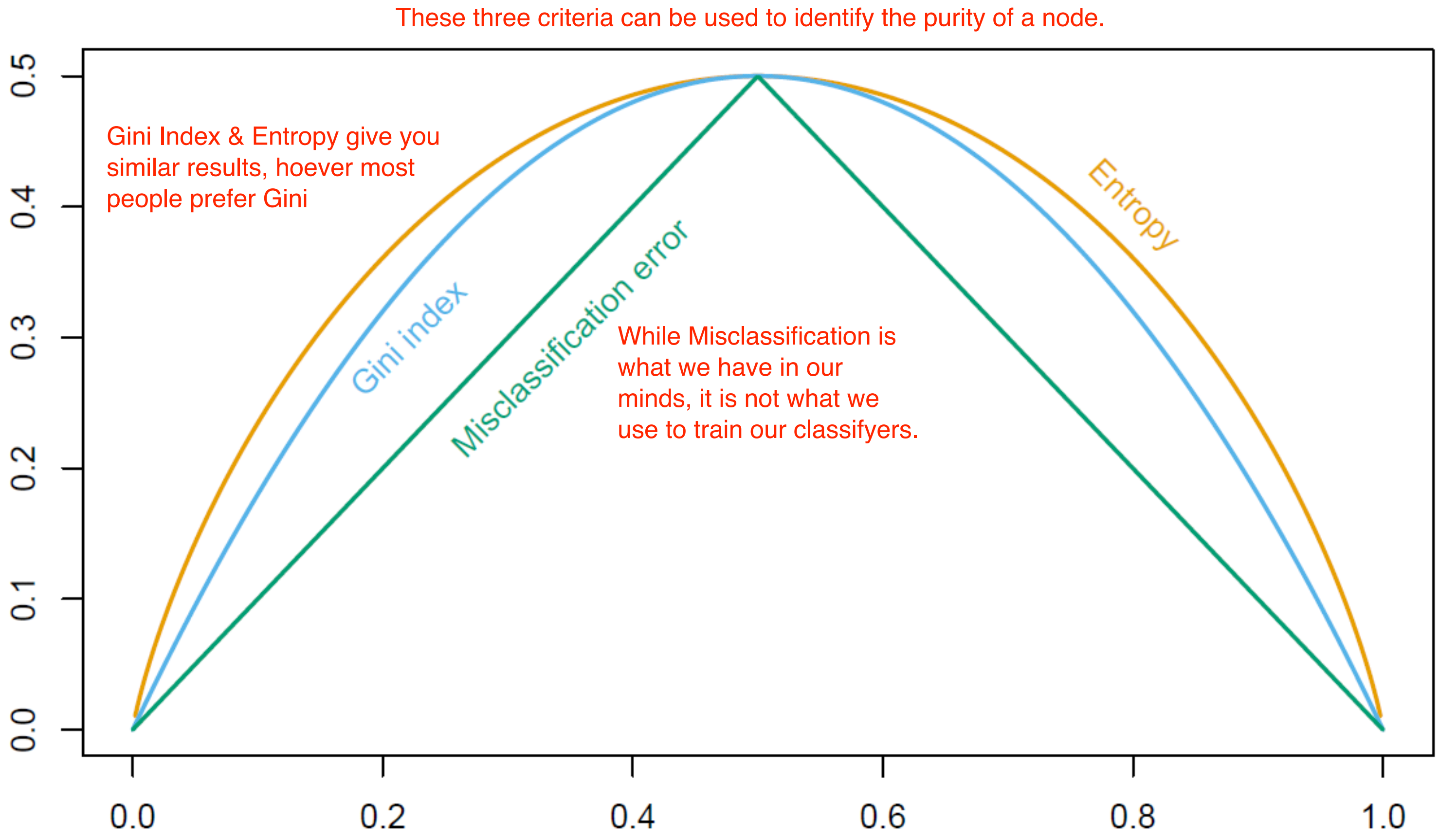
- gini impurity: **0.24** + **0.21** + **0.21** = 0.66

Gini Impurity

- Number of classes: C
- Number of data points: N
- Number of data points of class i: N_i

$$I_G = \sum_{i=1}^{C} \underbrace{\frac{N_i}{N}}_{\text{true class}} \Big(\underbrace{1 - \frac{N_i}{N}}_{\text{wrong prediction}}\Big)$$

Gini Impurity

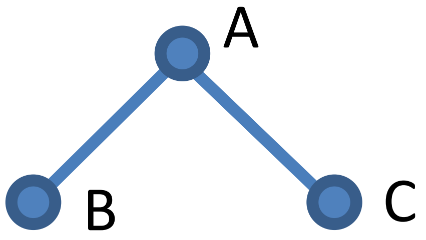


Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction", Springer (2009)

It's not enough to calculate the purity of the Parent node, you want to maximize the purity of the nodes afterwards, or the child nodes.

Node Purity Gain

- Compare:
  - Gini impurity of parent node
  - Gini impurity of child nodes



Here you look at the Gini Index you had before, and you subtract the ones after the split.

$$\boxed{\Delta I_G = I_G(A) - \frac{N(B)}{N(A)} I_G(B) - \frac{N(C)}{N(A)} I_G(C)}$$

You then weight them based on the number of points that fell into each class… or the 'gain' of purity.

Misclassification

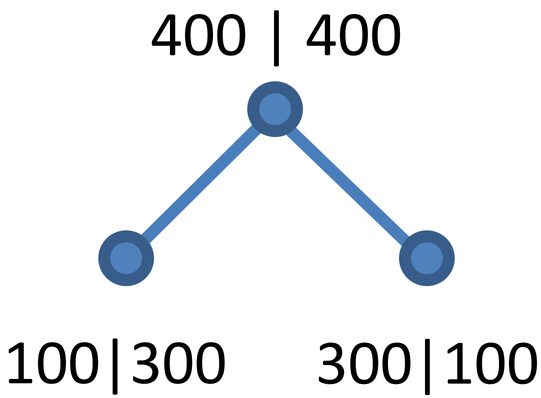
Is the predicted label the same or not the same as the one label training set.

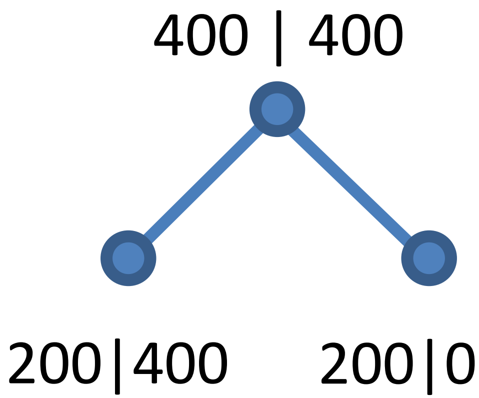
- $\frac{1}{N}\sum_{i}^{N}\mathbf{1}(\hat{y}_i \neq y_i)$

- not differentiable

Comparison Gini vs Misclassification

- Binary problem: 400 samples per class





Misclassification: 0.25
Gini gain: 0.125

Misclassification: 0.25
Gini gain: 0.166

The reason the Gini index is better here is because we got a pure cell with a lot of data points in it.

That's what the Gini Index does: It's going to chop up large chunks (data points) of pure training samples.

Pseudocode

- Check if already finished
- For each feature x_i
  - Calculate the gain from splitting on x_i
  - Let x_{best} be the feature with highest gain
- Create a decision *node* that splits on x_{best}
- Repeat on the sub-nodes

- Does this produce an optimal tree?
- What does optimal tree mean?

This is considered a greedy tree: it's always choosing the best split. If a slightly less optimal split creates a better split further down the tree, this method wouldn't be able to do so. It's not looking ahead like that.

The number of nodes is small, but others may define it in other ways.

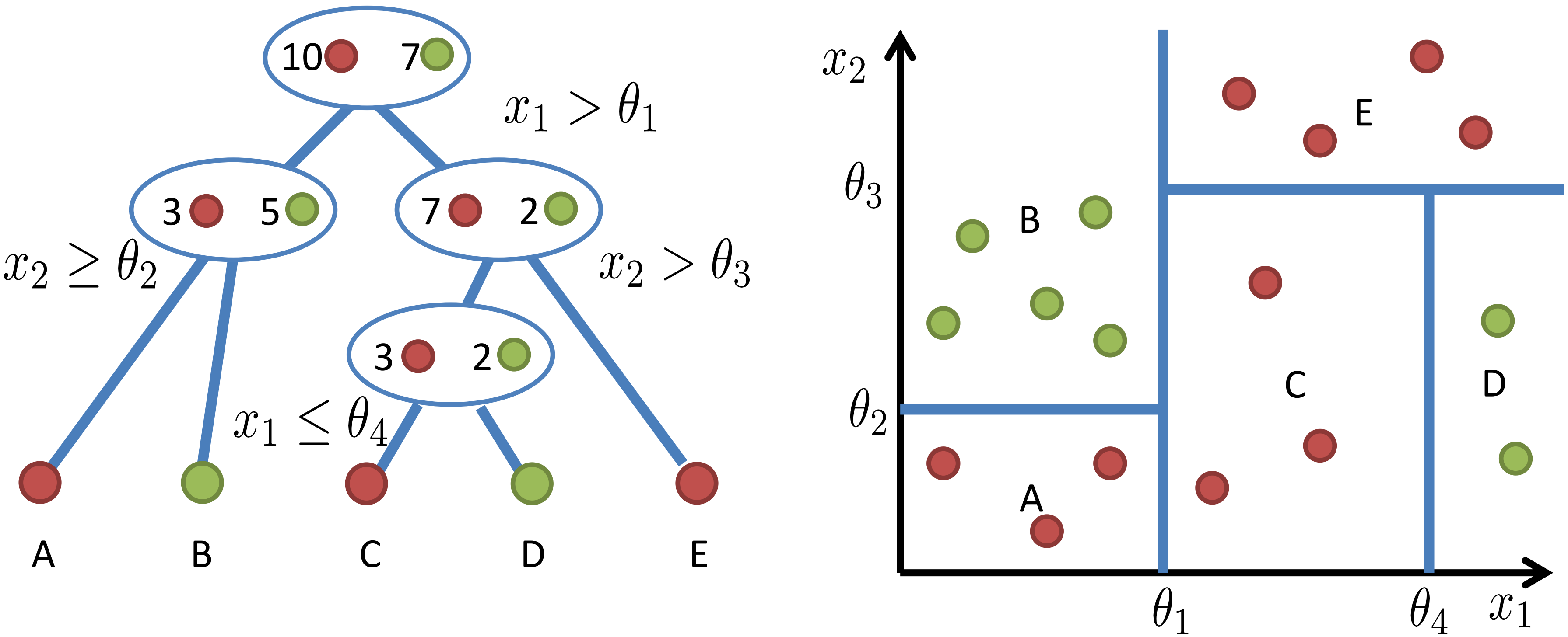
http://en.wikipedia.org/wiki/C4.5_algorithm

When to Stop

- node contains only one class
- node contains less than x data points
- max depth is reached
- node purity is sufficient
- you start to overfit => cross-validation

Grow. a tree, look at a cell and then decide
to remove that decision or cell from the tree

Tree Pruning

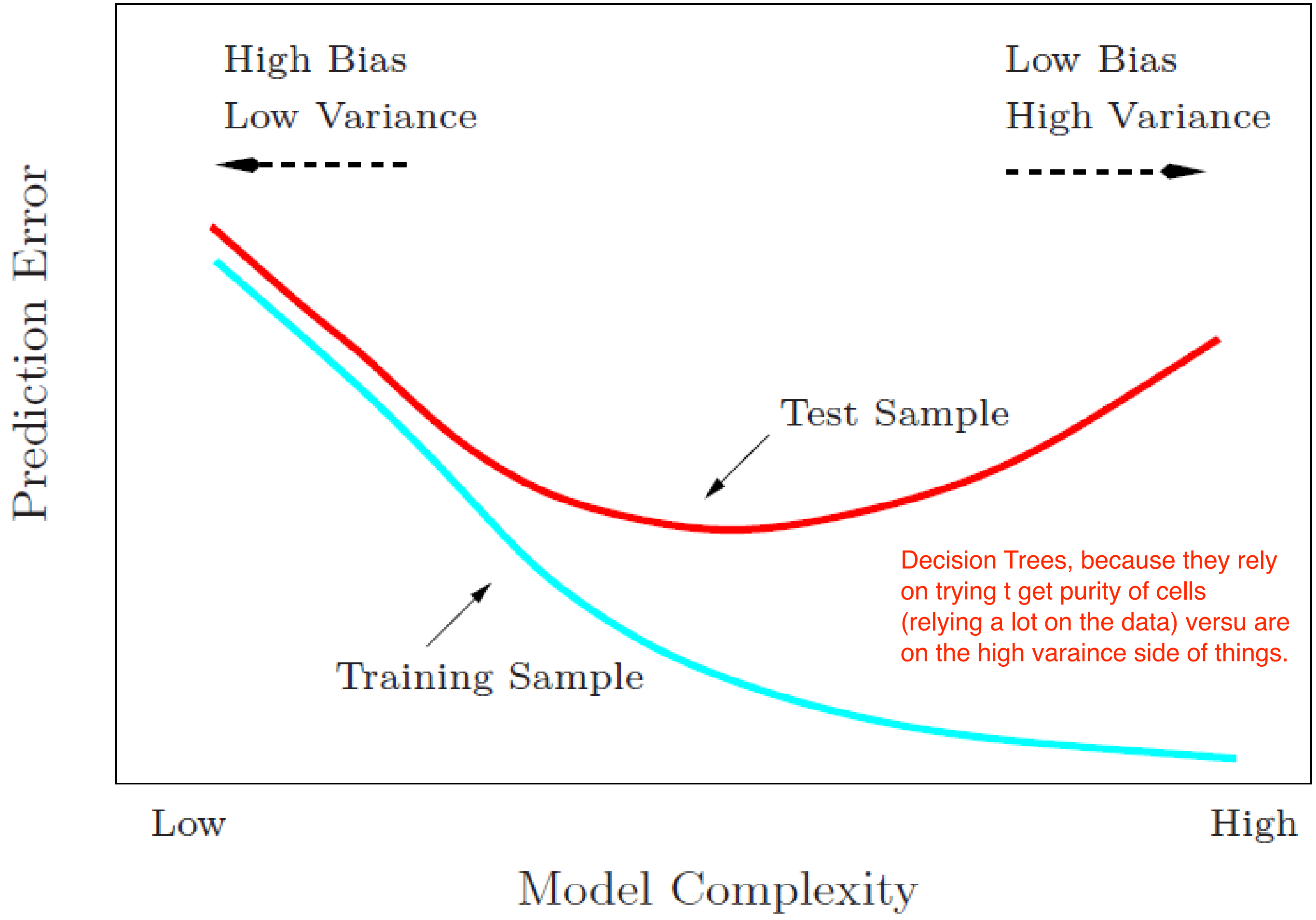


After removing the cell, you'd need to make a
prediction for the cell that's no longer as pure

How do you make a prediction for the merged cell?

Easy answer: Just give the majority vote.

Pruning and Complexity



Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction", Springer (2009)

Decision Trees - Disadvantages

- Sensitive to small changes in the data
- Overfitting
- Only axis aligned splits

Decision Trees vs SVM

(Support Vector Machine)

Characteristic	SVM	Trees	
Natural handling of data of "mixed" type	▼	▲	
Handling of missing values	▼	▲	This is in respects to training data.
Robustness to outliers in input space	▼	▲	
Insensitive to monotone transformations of inputs	▼	▲	
Computational scalability (large N)	▼	▲	
Ability to deal with irrelevant inputs	▼	▲	
Ability to extract linear combinations of features	▲	▼	
Interpretability	▼	◆	
Predictive power	▲	▼	A real bummer… it doesn't generalize well.

Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction", Springer (2009)

Wisdom of Crowds

The collective knowledge of a diverse and independent body of people typically exceeds the knowledge of any single individual, and can be harnessed by voting.

James Surowiecki

http://socialmedia4srm.wordpress.com/


Netflix Prize

Netflix Prize

- Take home messages:
  - The early gains are pretty easy then you realize all the nitty gritty little things you need to improve.It's really hard to get the 80/20 rule.
  - You plateau and then get gains with an ensemble approach.
  - 800 models needed to get the final gains. It's a big shout out to ensemble methods but ultimately a big let-down.
  - One error was making it hard to actually get the gains you want… it brings to mind how much weight to put on those kinds of data points.

Ensemble Methods

- A single decision tree does not perform well
- But, it is super fast
- What if we learn multiple trees?

We need to make sure they do not all just learn the same.

Bootstrap

A way of training decision trees all slightly differently from each other.

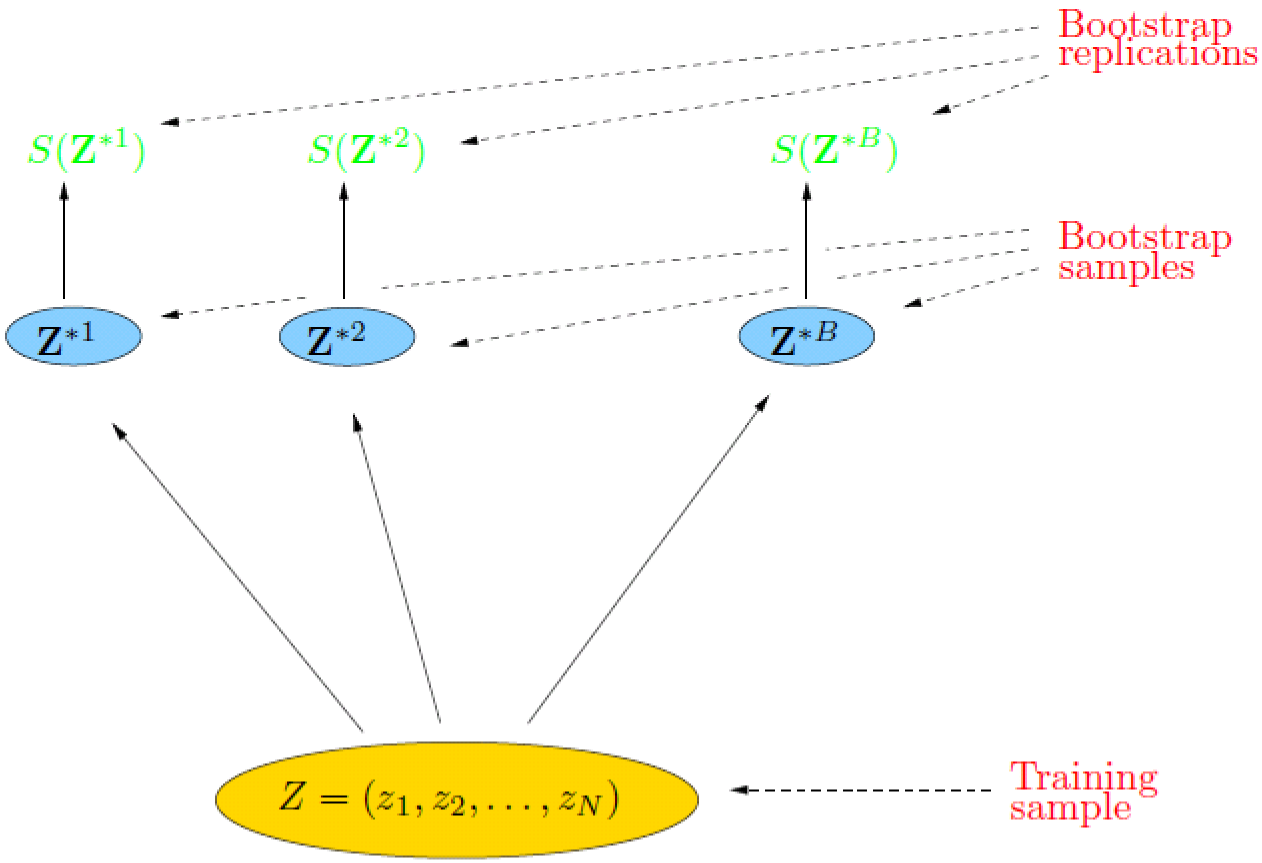
Bootstrap

- Resampling method from statistics
- Useful to get error bars on estimates

- Take N data points
- Draw N times with replacement

- Get estimate from each bootstrapped sample

Bootstrap



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Bootstrap

- I can generate more data!
- Can I do cross validation on this?

No, because it's similar data points and you'll have overlap.

Your training data would be too similar to your test data and the overlap wouldn't allow for you to get proper test performance validation.

Bootstrap vs Cross-validation

- Bootstrap has overlap in data sets

Do not use simple bootstrap to generate train and test data from same data set.

$$p(n \in Z^{*i}) = \qquad \frac{1}{N}$$

Probability of choosing n

Bootstrap vs Cross-validation

- Bootstrap has overlap in data sets

Do not use simple bootstrap to generate train and test data from same data set.

$$p(n \in Z^{*i}) = \qquad 1 - \frac{1}{N}$$

Probability of not choosing n

Bootstrap vs Cross-validation

- Bootstrap has overlap in data sets

Do not use simple bootstrap to generate train and test data from same data set.

$$p(n \in Z^{*i}) = \qquad (1 - \frac{1}{N})^N$$

Probability of not choosing n in N draws

Bootstrap vs Cross-validation

- Bootstrap has overlap in data sets

Do not use simple bootstrap to generate train and test data from same data set.

$$p(n \in Z^{*i}) = 1 - (1 - \frac{1}{N})^N$$

Probability of (not not) choosing n in N draws

Bootstrap vs Cross-validation

- Bootstrap has overlap in data sets

Do not use simple bootstrap to generate train and test data from same data set.

$$p(n \in Z^{*i}) = 1 - e^{-1}$$

$$\approx 0.632$$

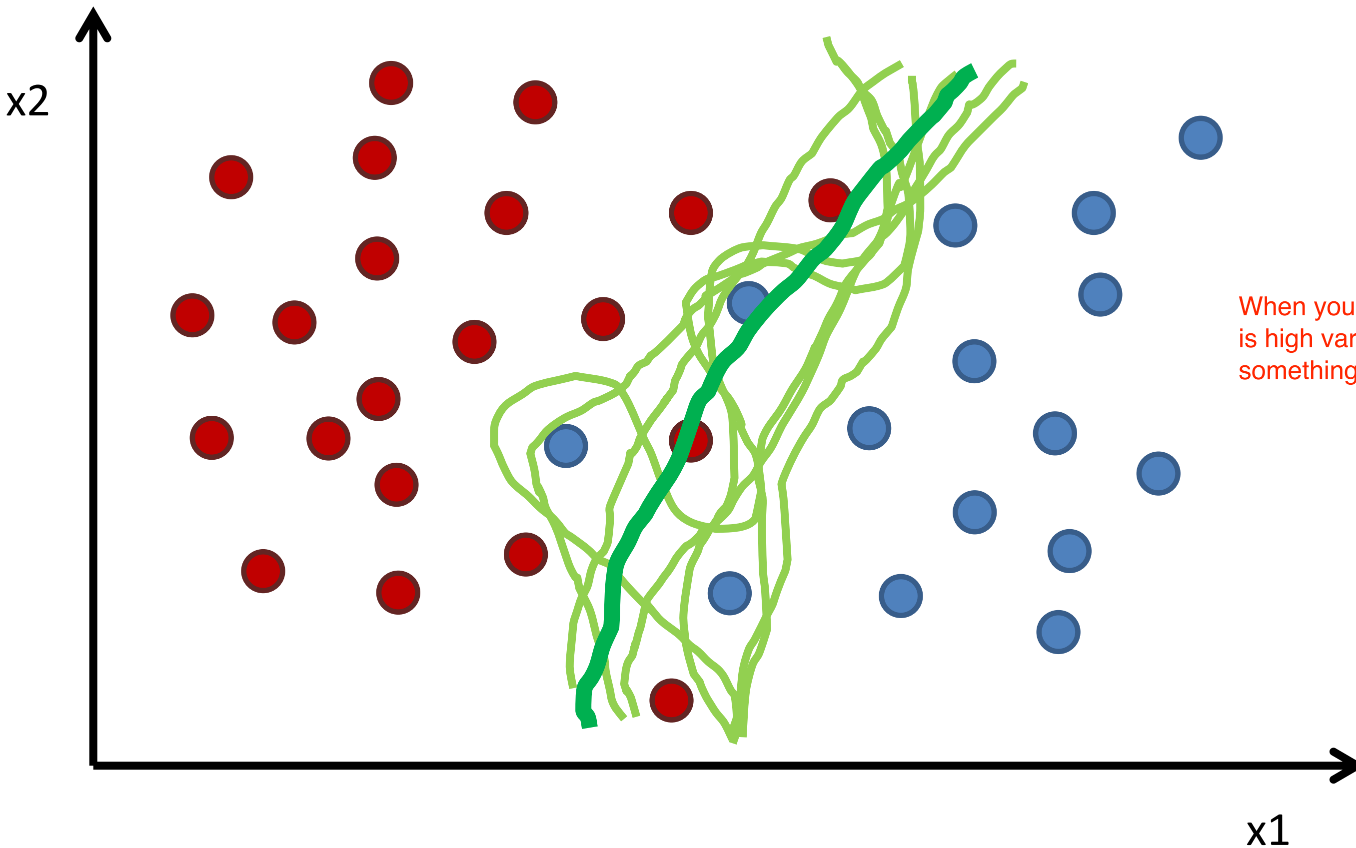
This number is important later

Bagging

- Bootstrap aggregating

- Sample with replacement from your data set
- Learn a classifier for each bootstrap sample
- Average the results

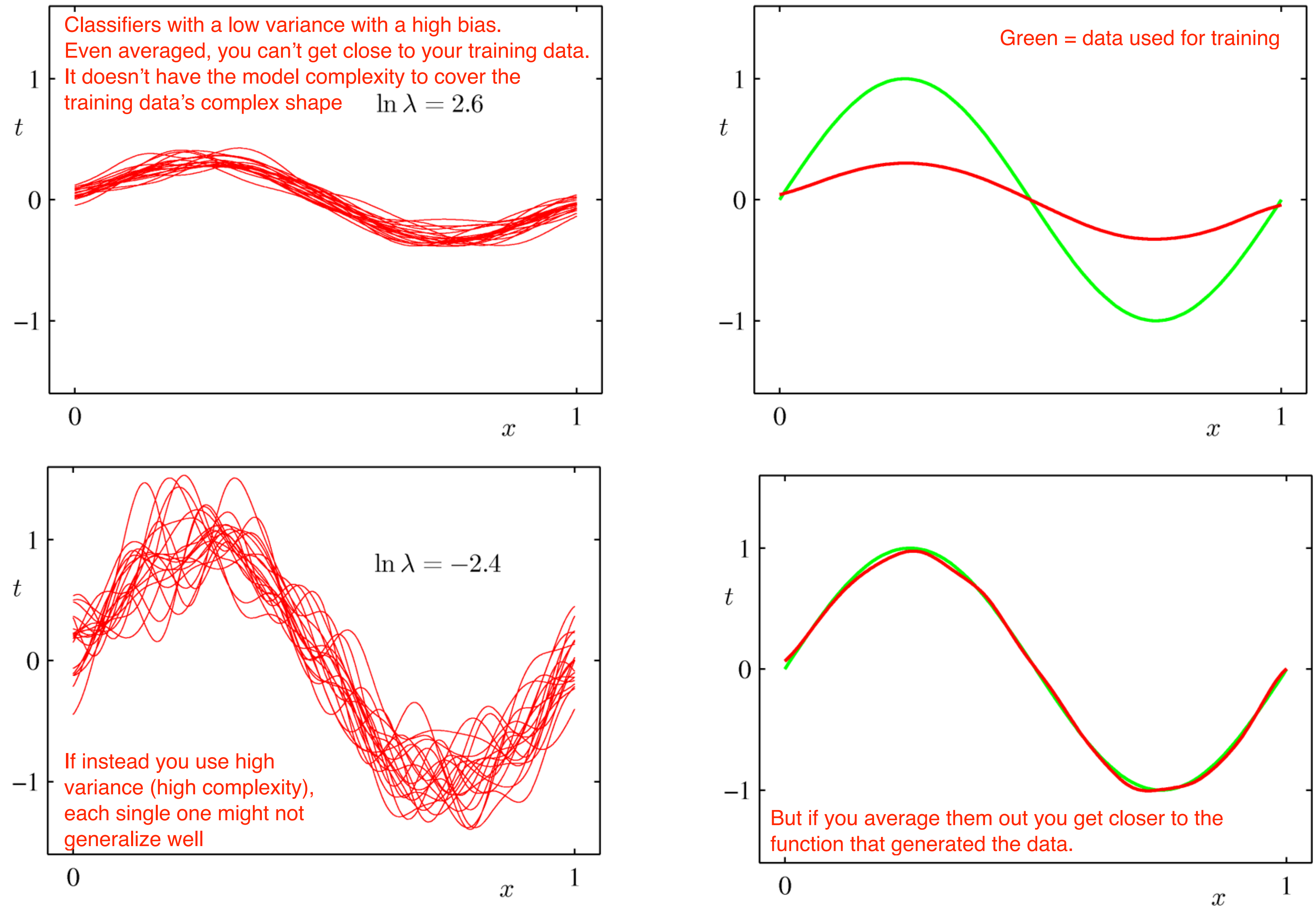
Bagging Example



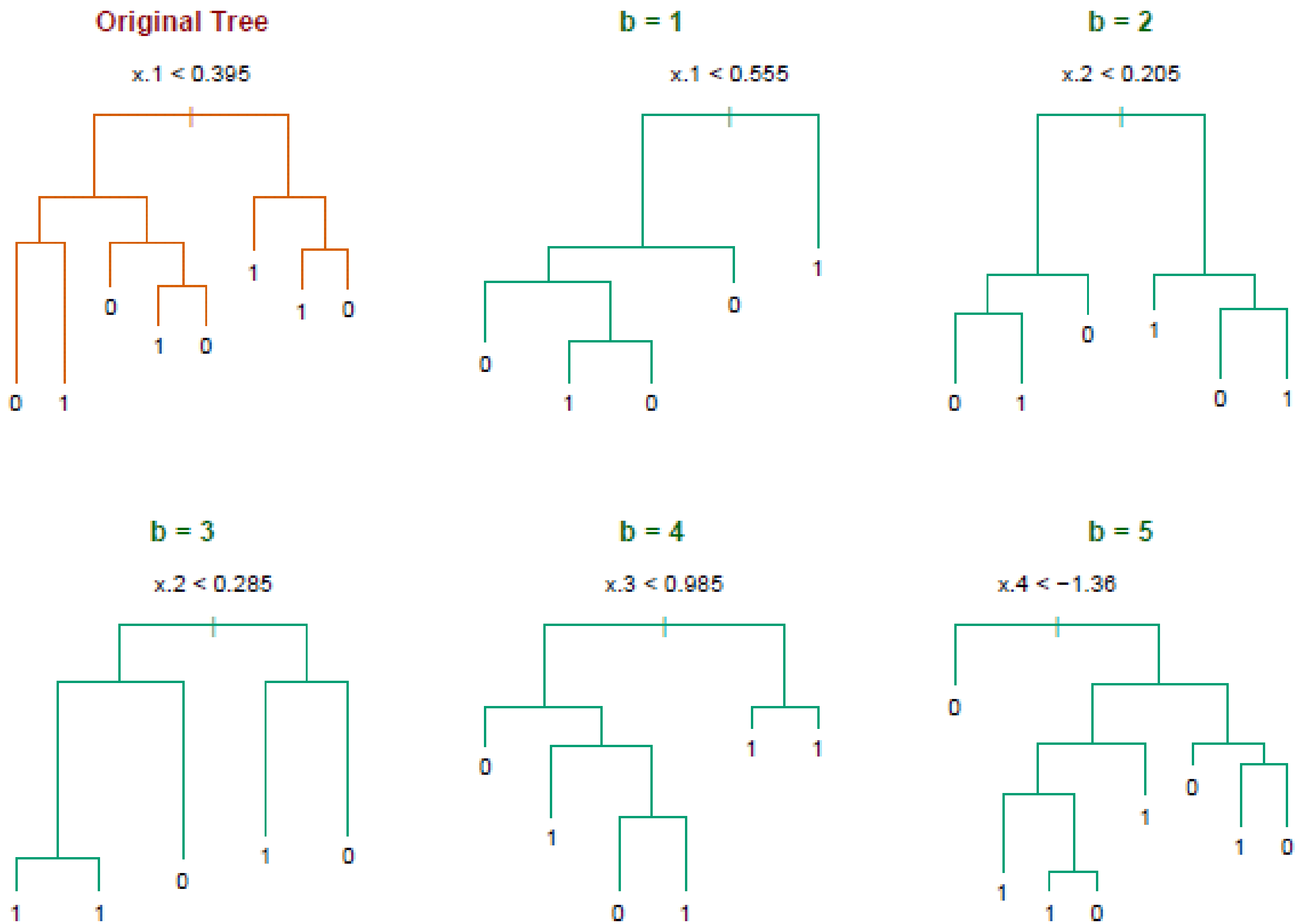
When you average something that is high variance you actually get something that is pretty smooth.

What Bagging does is trying to reduce the variance without introducing too much bias.

Bias-Variance Trade-off



Bagging Decision Trees



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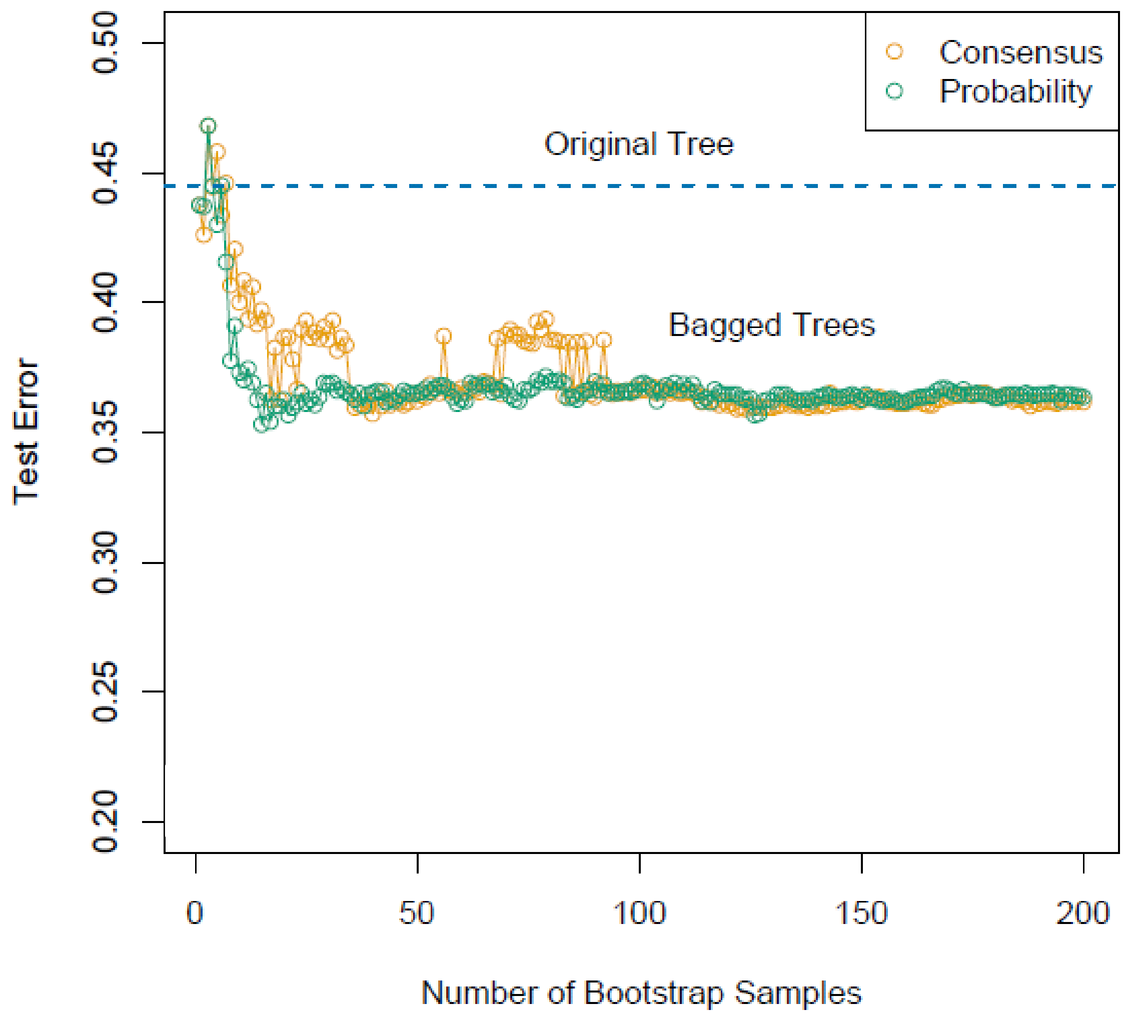
Bagging Decision Trees



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Bagging

- Reduces overfitting (variance)
- Normally uses one type of classifier
- Decision trees are popular
- Not helping with linear models
- Easy to parallelize

You can train classifiers in parallel because there is no communication going on between models/classifyers.

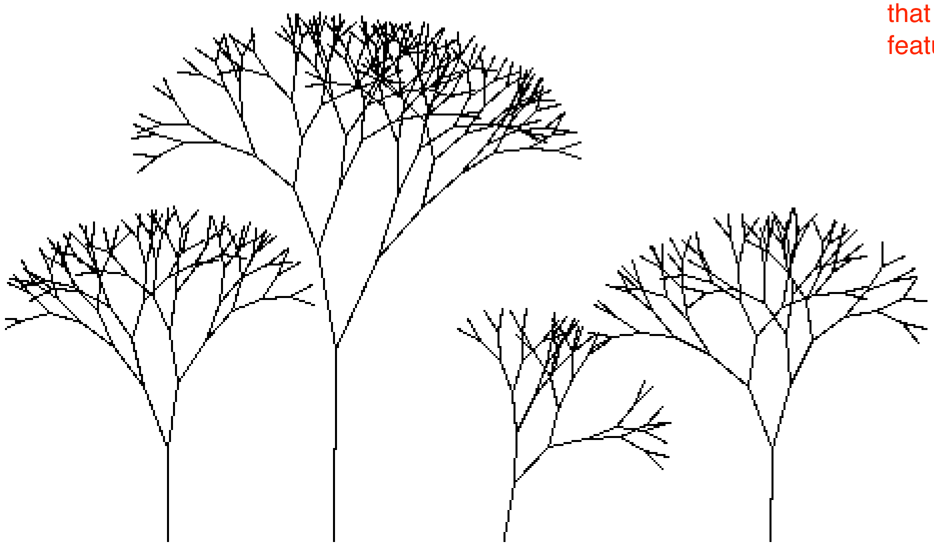
Linear models don't have high variance, vs. bagging is trying to reduce high variance.

When you're bagging you want a classifier that is capable of overfitting.

Random Forest

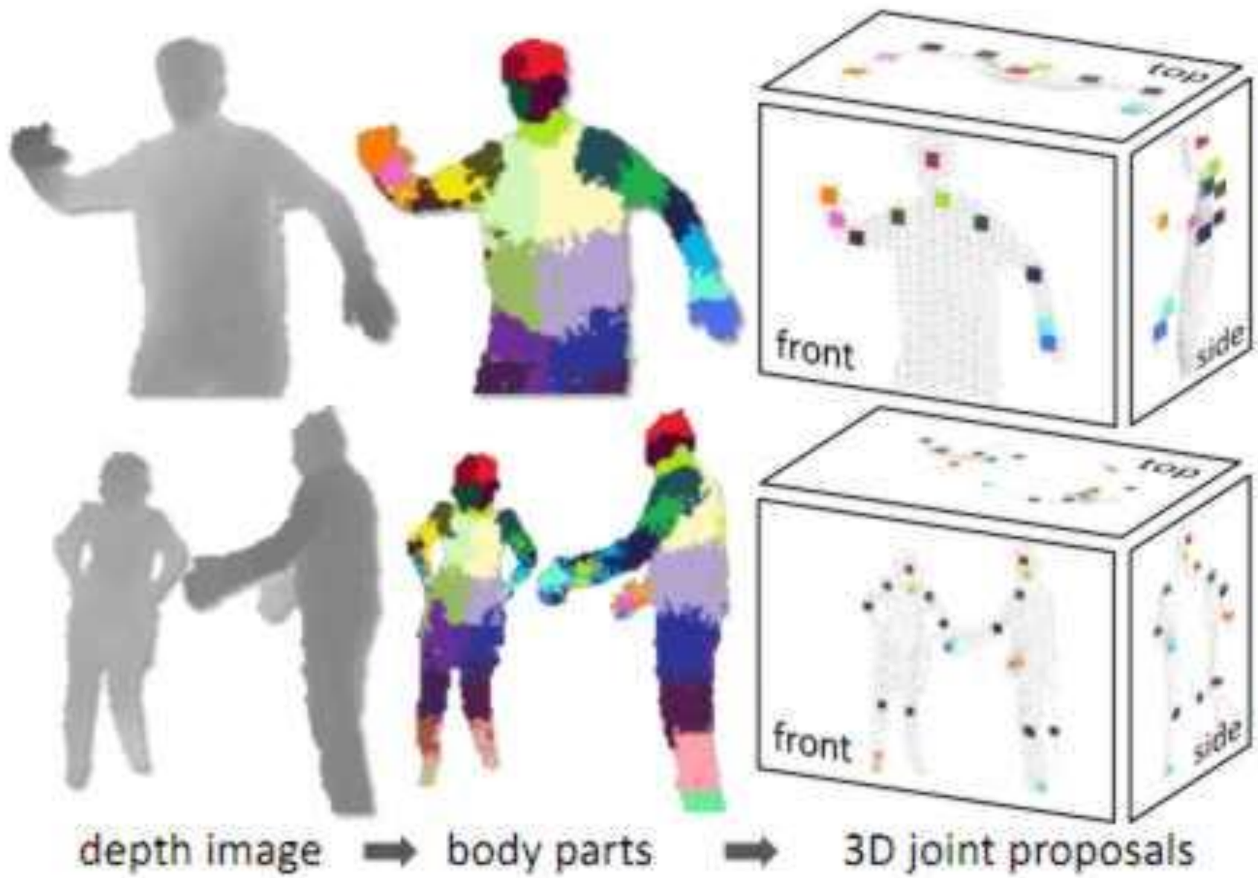
- Builds upon the idea of bagging
- Each tree build from bootstrap sample
- Node splits calculated from random feature subsets

So, instead of choosing the best feature(s) that will split the data best, a random feature(s) is chosen to split the data.



http://www.andrewbuntine.com/articles/about/fun

Random Forest – Fun Fact



hand_tracking_kinect.mp4

http://research.microsoft.com/en-us/projects/handpose/

Random Forest

- All trees are fully grown
- No pruning

- Two parameters
  - Number of trees
  - Number of features

Random Forest Error Rate

- Error depends on:
  - Correlation between trees (higher is worse)
  - Strength of single trees (higher is better)

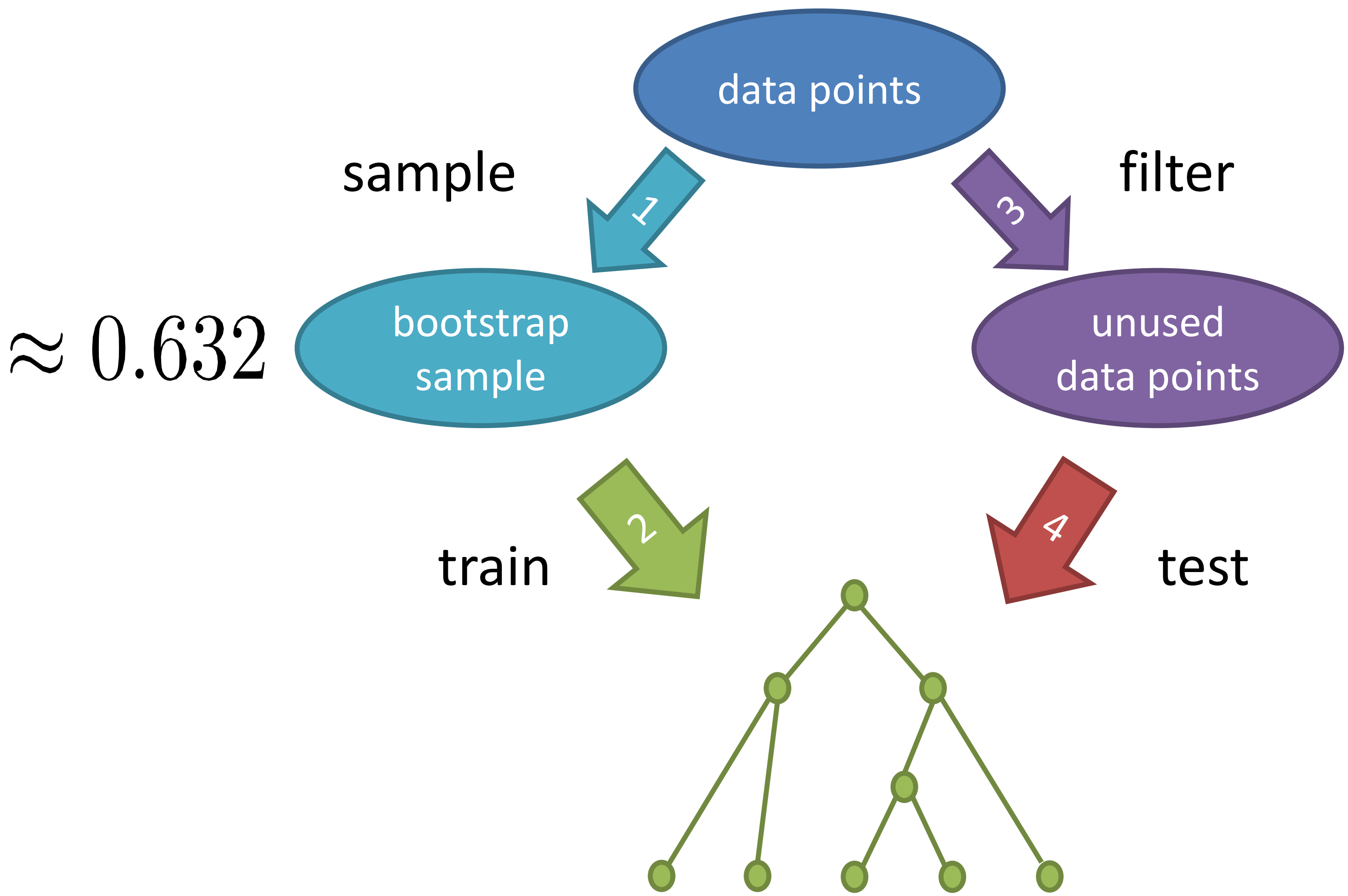
- Increasing number of features for each split:
  - Increases correlation
  - Increases strength of single trees

Out of Bag Error

- Each tree is trained on a bootstrapped sample
- About 1/3 of data points not used for training

- Predict unseen points with each tree
- Measure error

Out of Bag Error



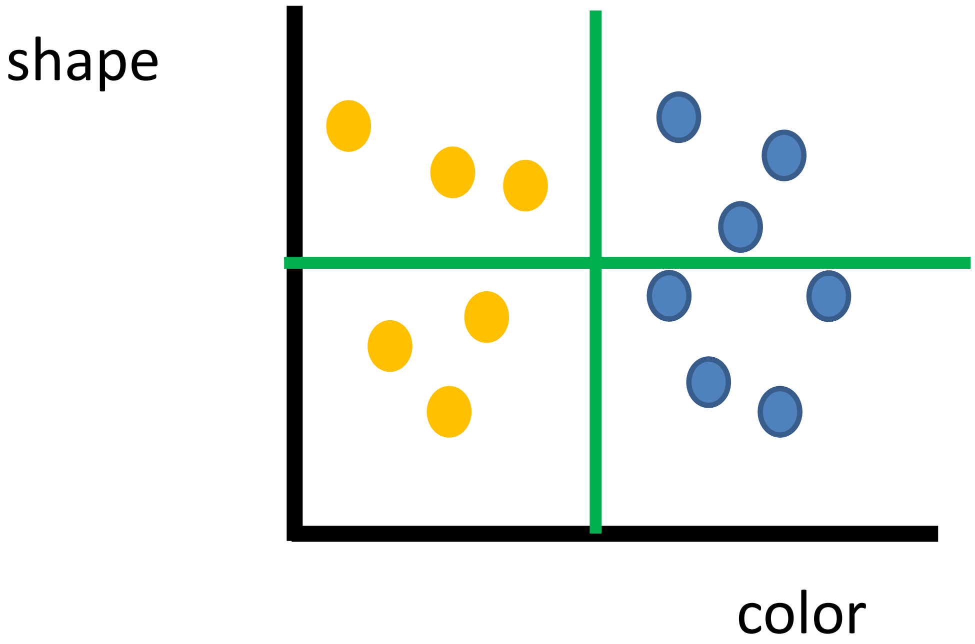
Out of Bag Error

- Very similar to cross-validation
- Measured during training
- Can be too optimistic

Variable Importance - 1

- Again use out of bag samples
- Predict class for these samples
- Randomly permute values of one feature
- Predict classes again
- Measure decrease in accuracy

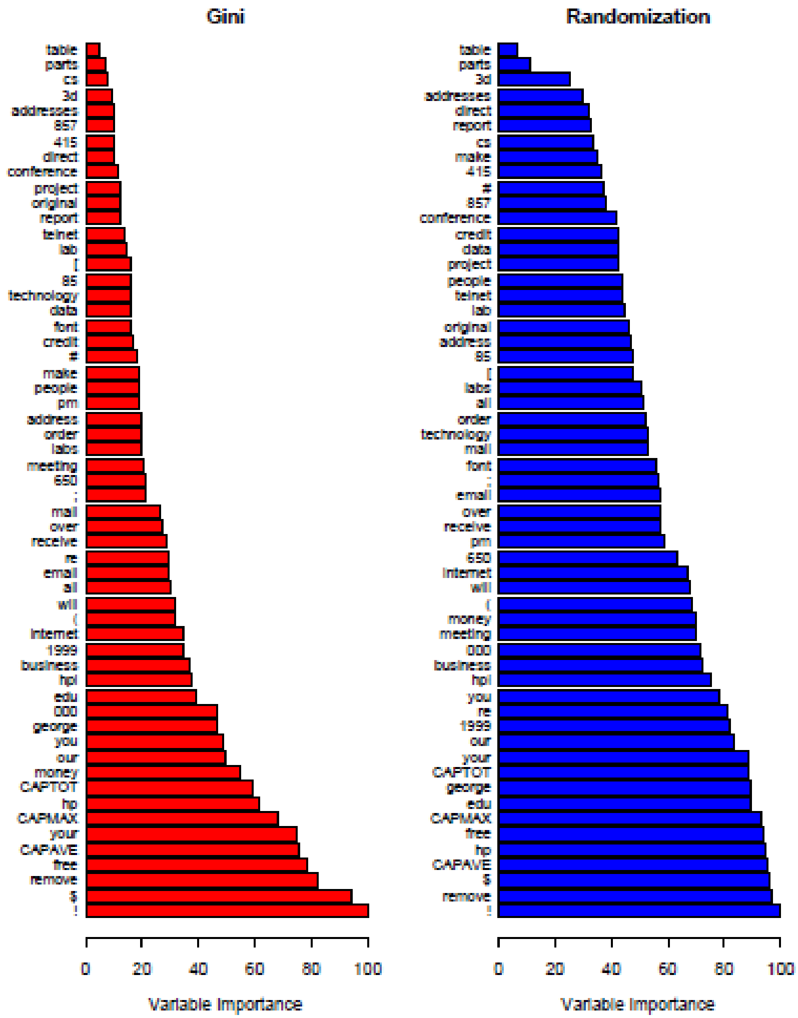
Variable Importance - 1



Variable Importance - 2

- Measure split criterion improvement
- Record improvements for each feature
- Accumulate over whole ensemble

Example: Spam classification

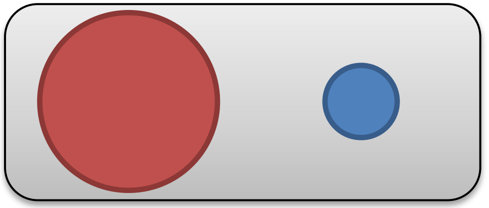


Randomization tends to spread out the variable importance more uniformly.

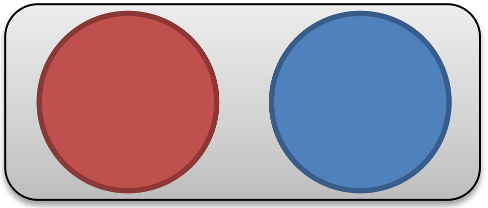
Hastie et al.,"The Elements of Statistical Learning: Data Mining, Inference, and Prediction", Springer (2009)

Unbalanced Classes

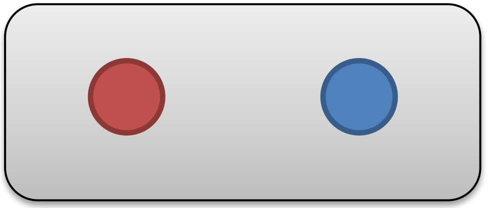
- The Problem:



- Oversample:

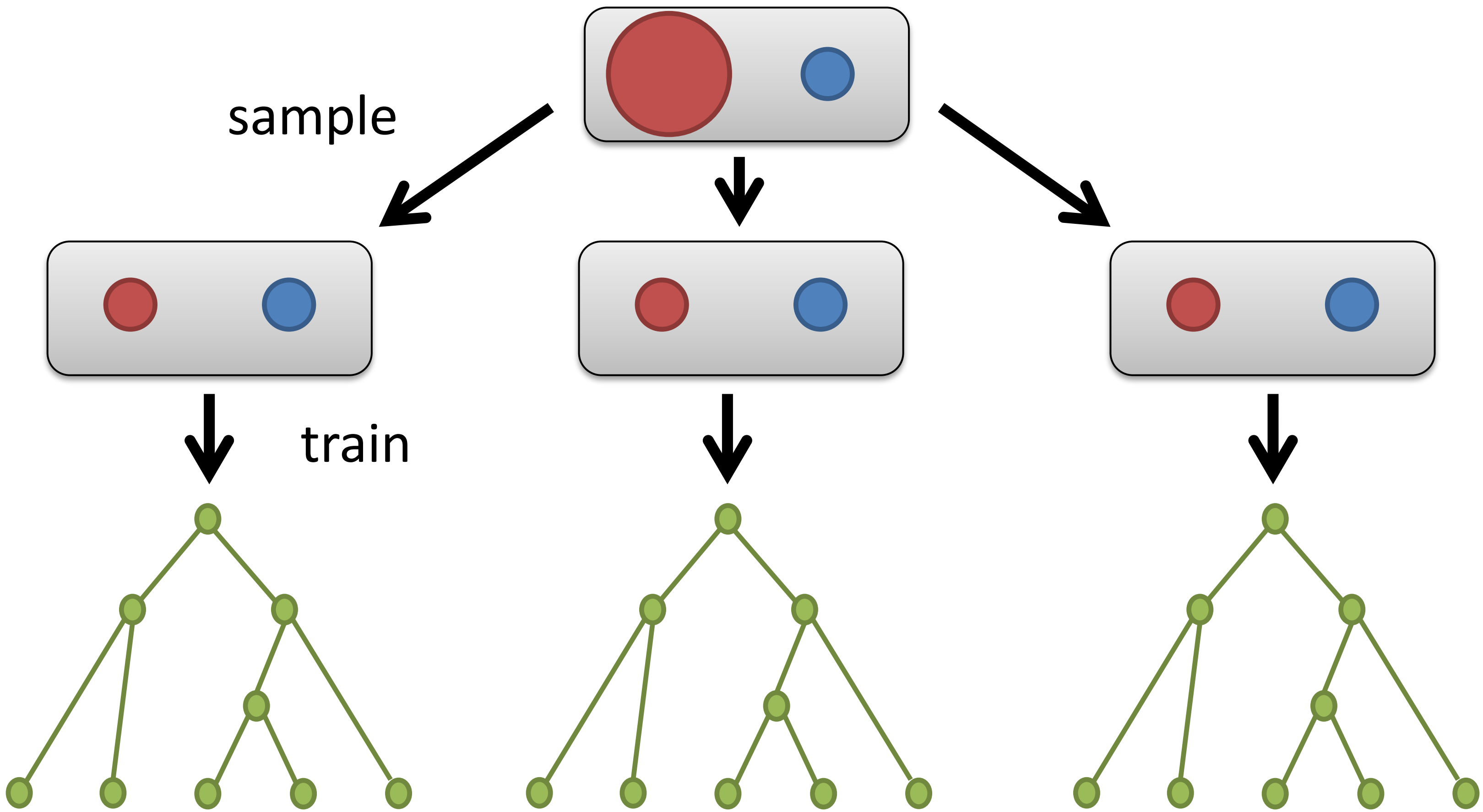


- Subsample:



- Subsample for each tree!

Random Forest Subsampling



Random Forest

- Similar to Bagging
- Easy to parallelize
- Packaged with some neat functions:
  - Out of bag error
  - Feature importance measure
  - Proximity estimation