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

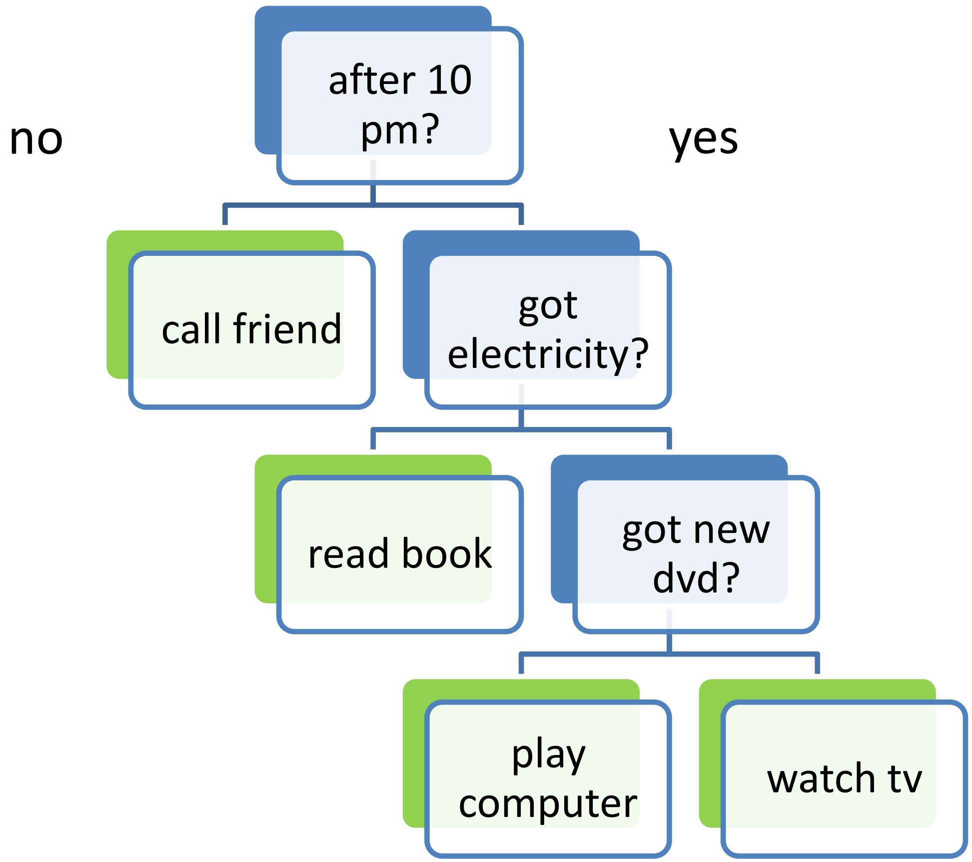
- “Elements of Statistical Learning”
- http://statweb.stanford.edu/~tibs/ElemStatLearn/

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

Next Topics

- Tree classifier
- Bagging
- Random Forest

Decision Tree



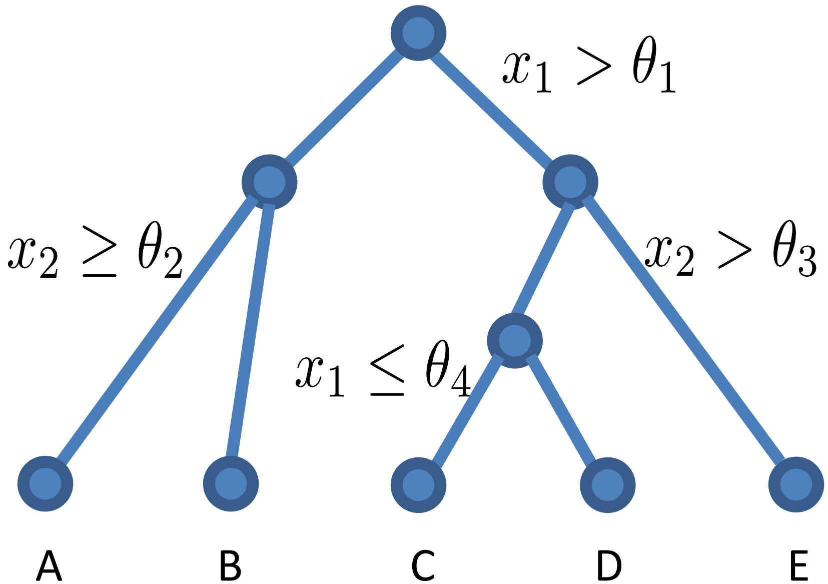
Decision Trees

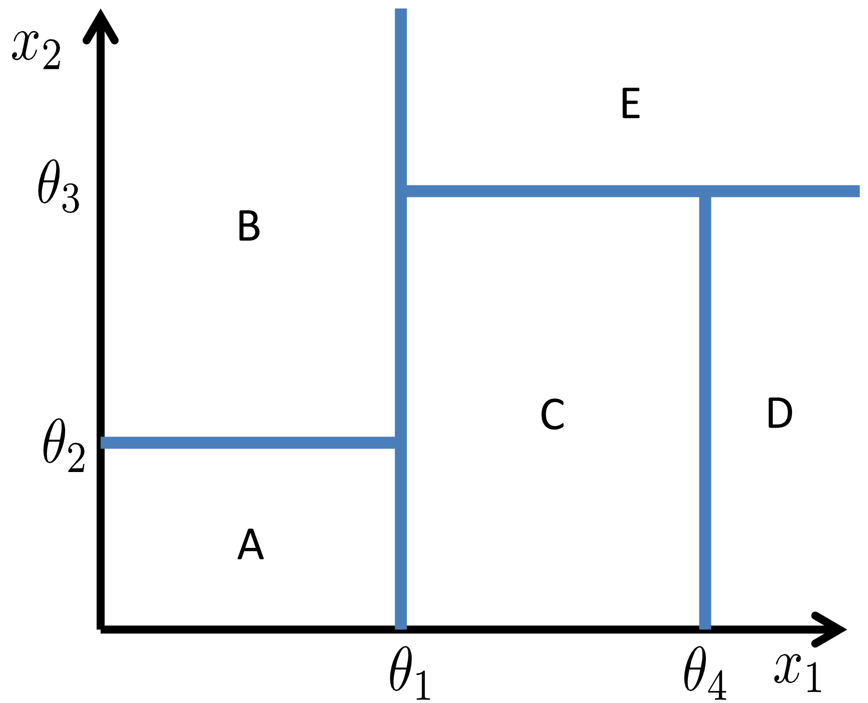
- Fast training
- Fast prediciton
- Easy to understand
- Easy to interpret

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





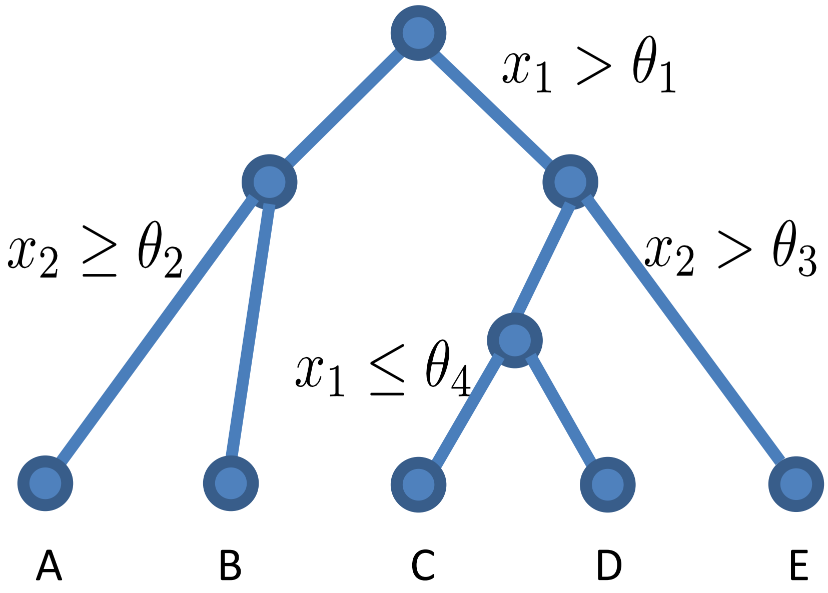
Bishop, "Pattern Recognition and Machine Learning", Springer, 2006

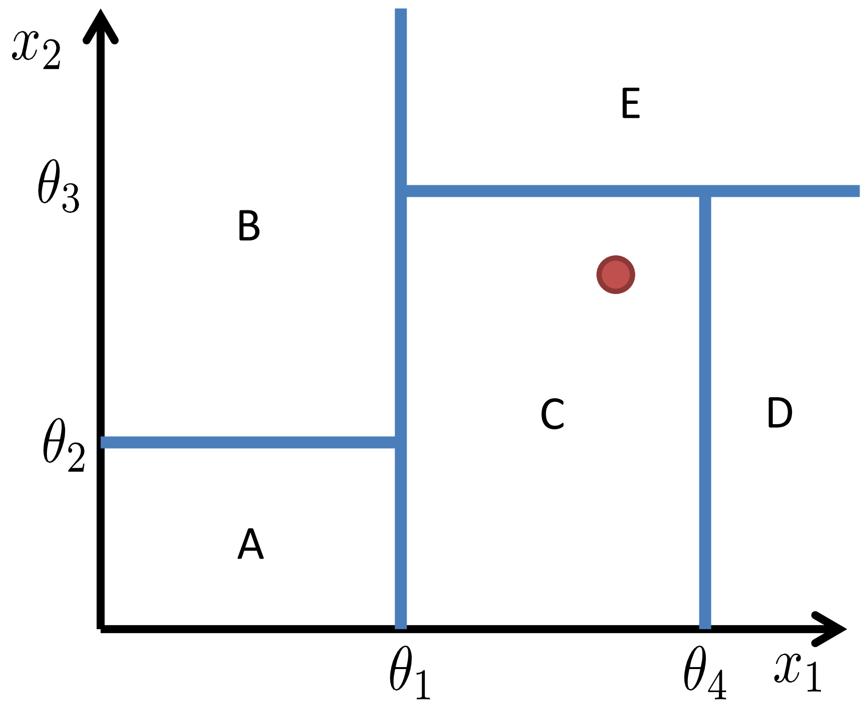
Decision Tree - Idea

- What is a the benefit of using only one feature at a time?

- What is the drawback?

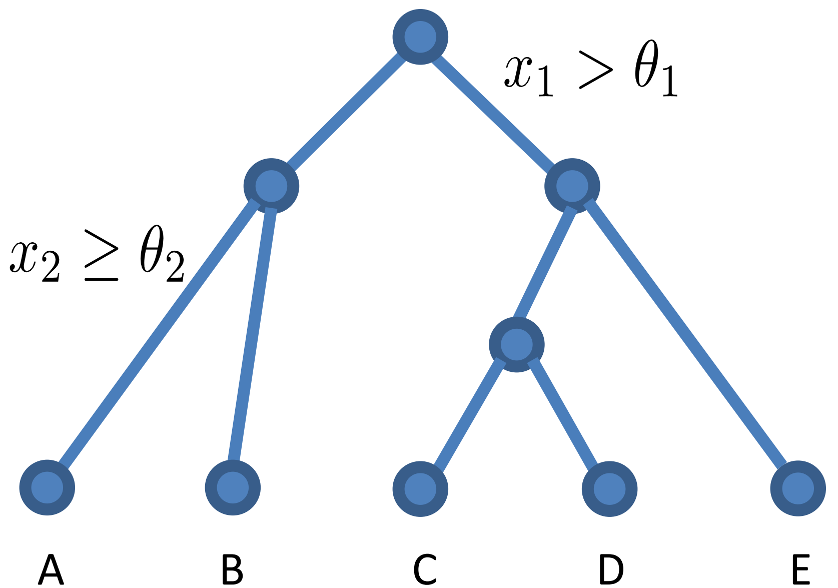
Decision Tree - Prediction



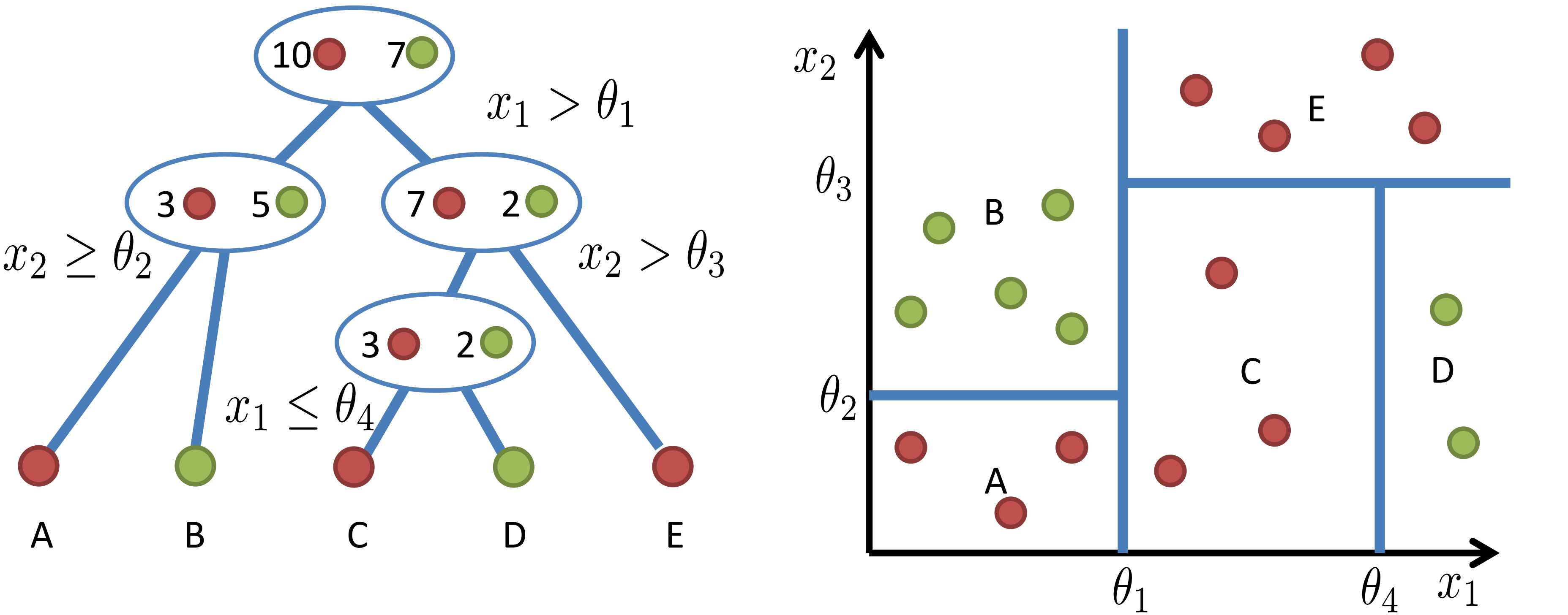


Decision Tree -Training

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



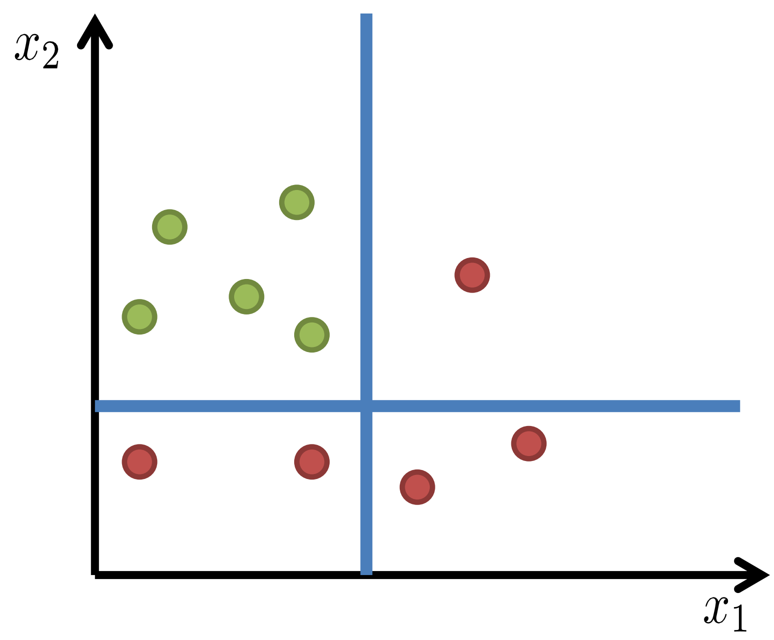
Node Purity



10 7
$x_1 > \theta_1$
3 5
7 2
$x_2 \geq \theta_2$
$x_2 > \theta_3$
3 2
$x_1 \leq \theta_4$
A
B
C
D
E
x_2
θ_3
E
B
C
D
θ_2
A
θ_1
θ_4
x_1

Gini Impurity

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



Gini Impurity

Example:

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)

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

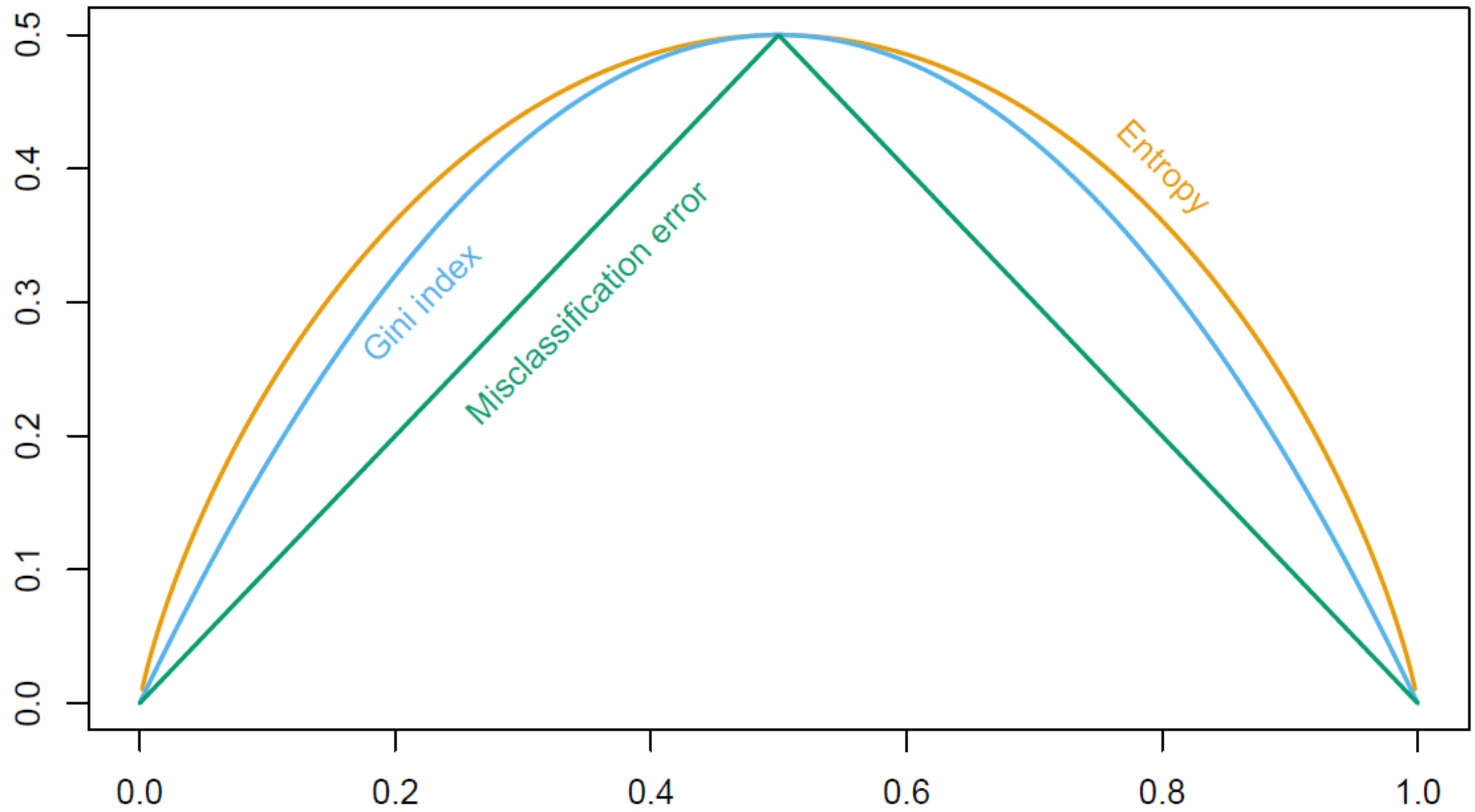
- gini impurity: **0.24** + **0.21** + **0.21** = 0.66

Gini Impurity

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

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

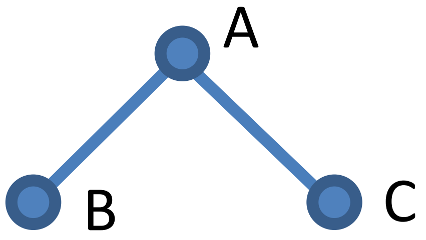
Gini Impurity



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

Node Purity Gain

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



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

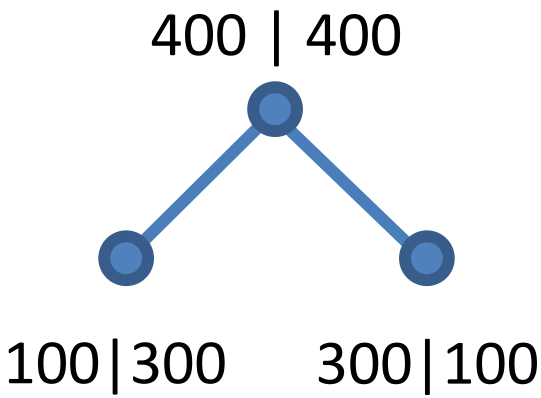
Misclassification

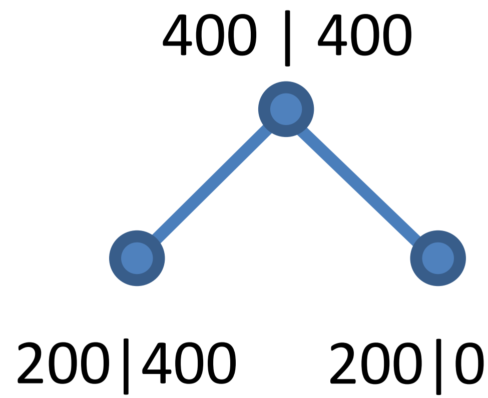
- $\frac{1}{N}\sum_{i}^{N}\mathbf{1}(\hat{\mathrm{y}}_i \neq y_i)$

- 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

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

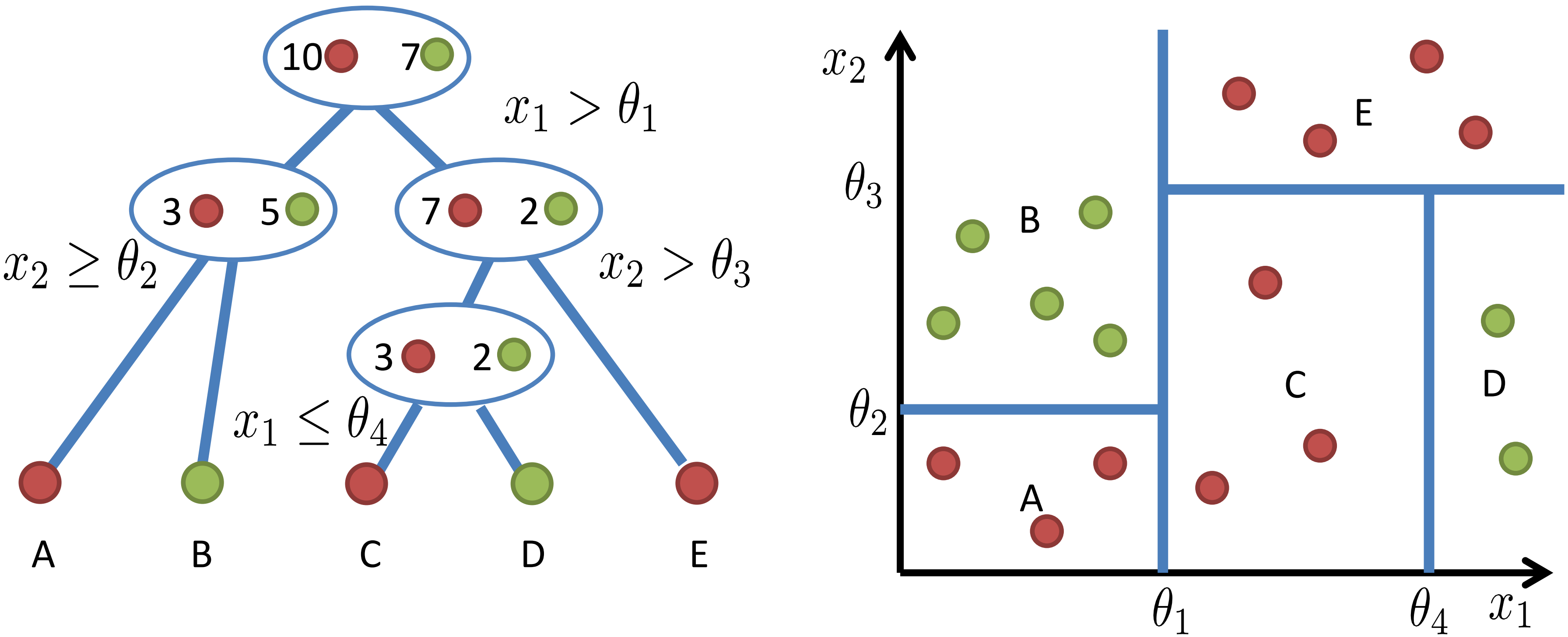
- Does this produce an optimal tree?
- What does optimal tree mean?

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

When to Stop

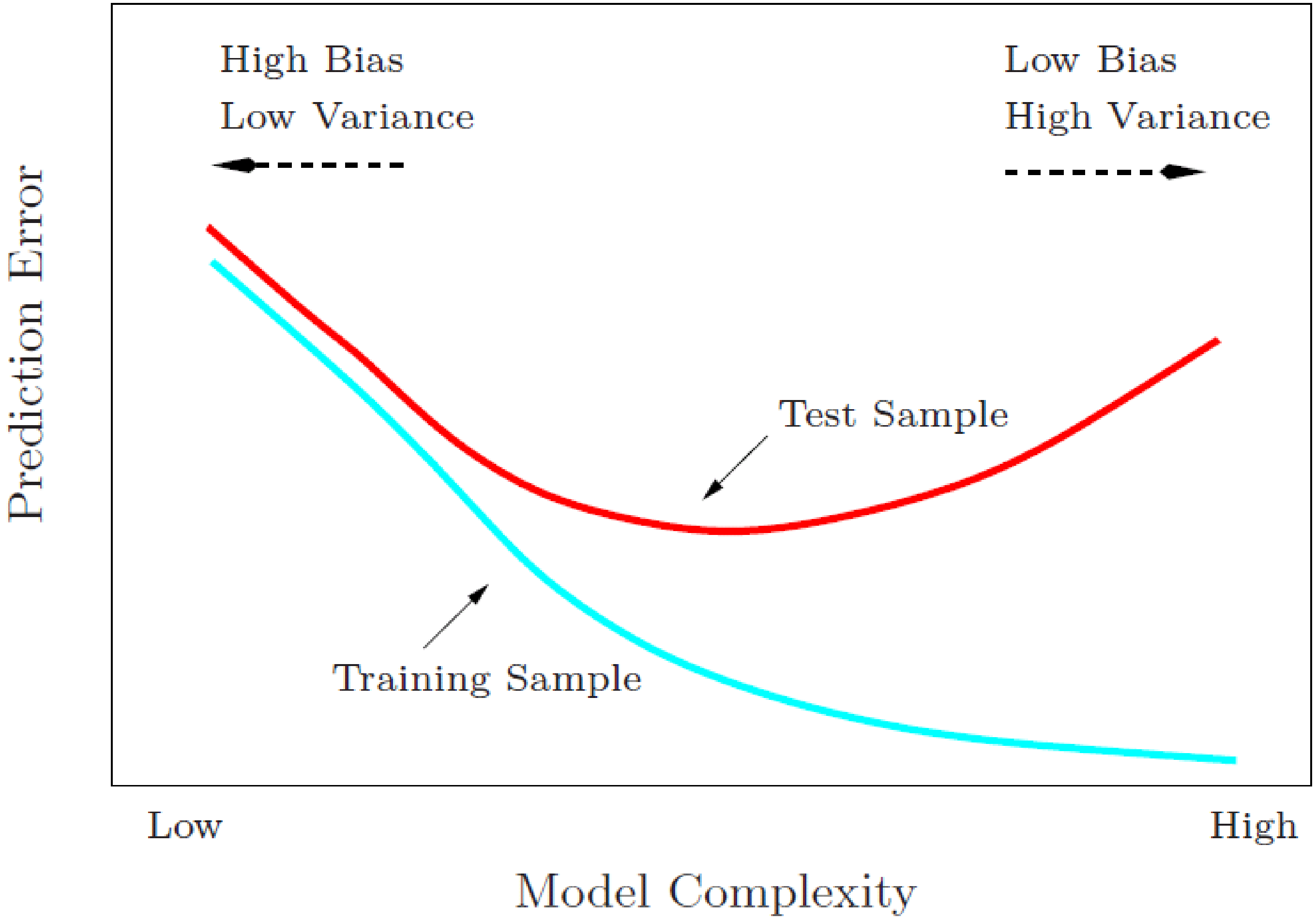
- node contains only one class
- node contains less than x data points
- max depth is reached
- node purity is sufficient
- you start to overfit => cross-validation

Tree Pruning



How do you make a prediction for the merged cell?

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

Characteristic	SVM	Trees
Natural handling of data of "mixed" type	▼	▲
Handling of missing values	▼	▲
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	▲	▼

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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:

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

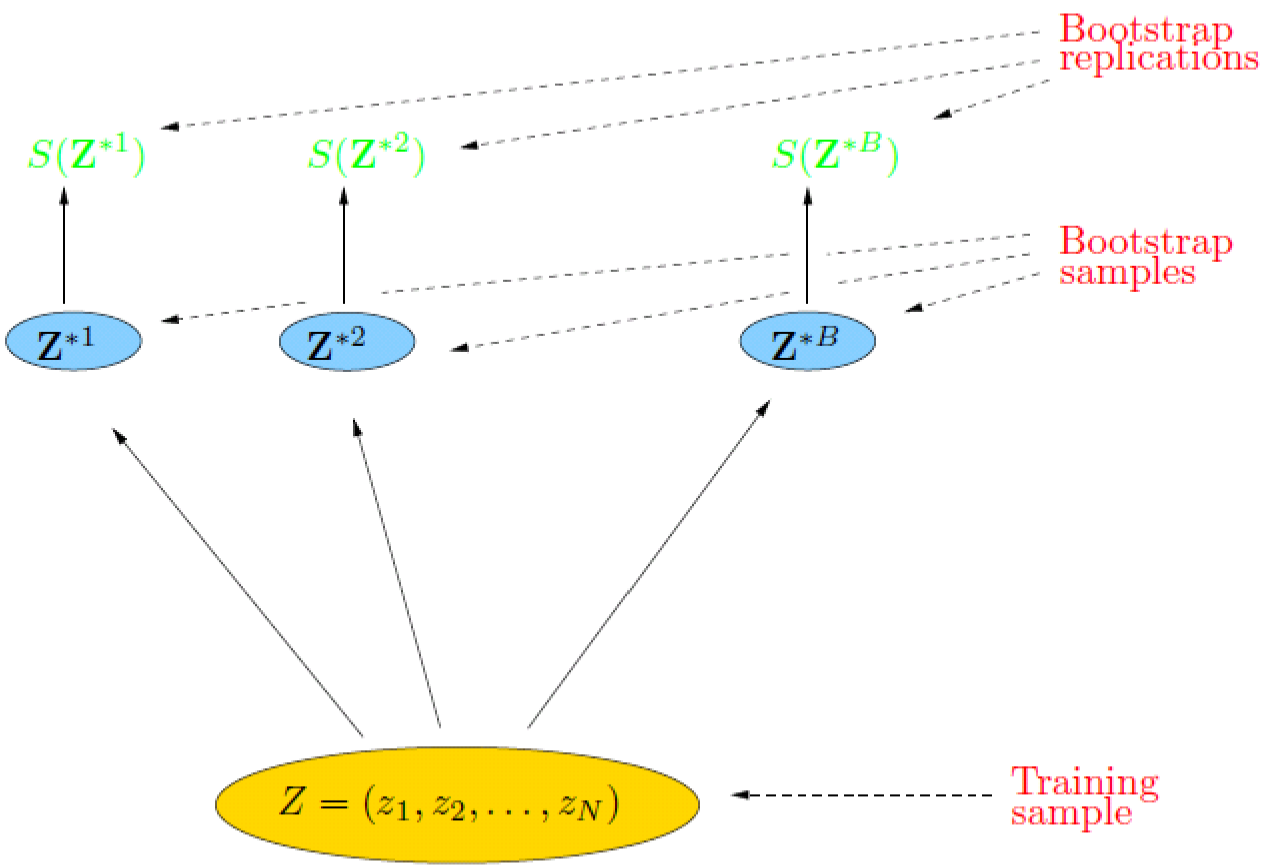
Bootstrap

- 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



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

Bootstrap

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

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.

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

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.

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

$$\approx 0.632$$

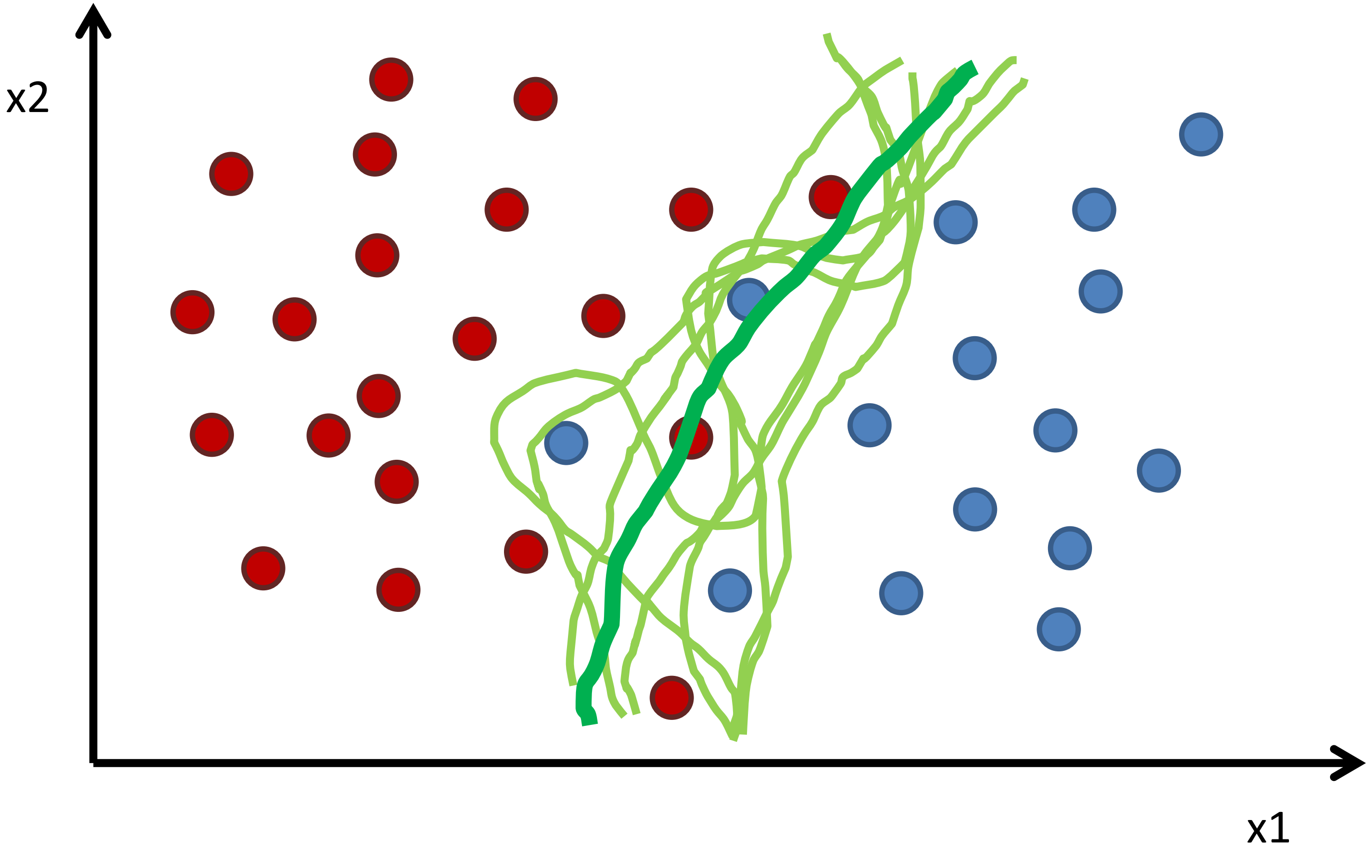
This number is important later

Bagging

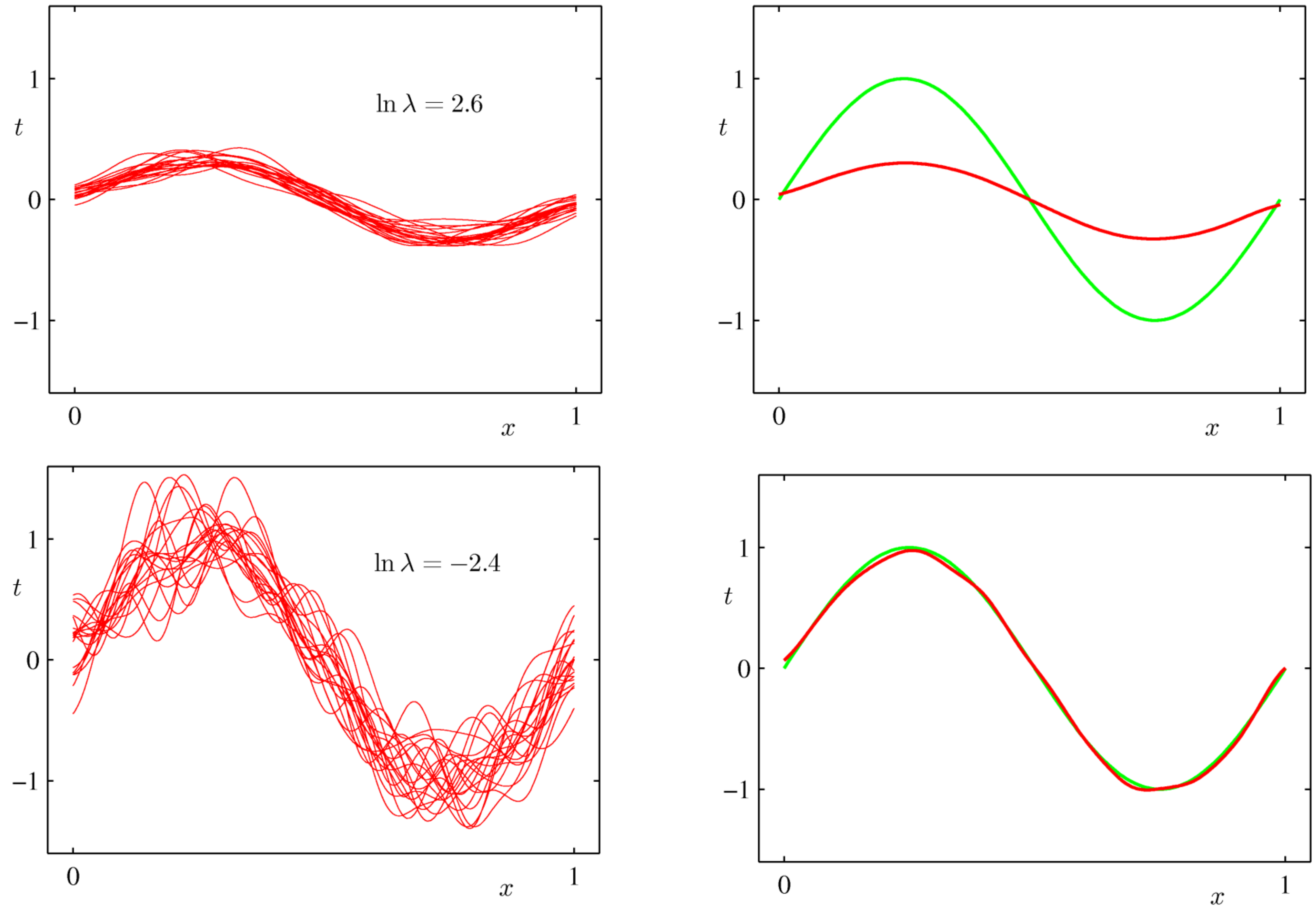
- Bootstrap aggregating

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

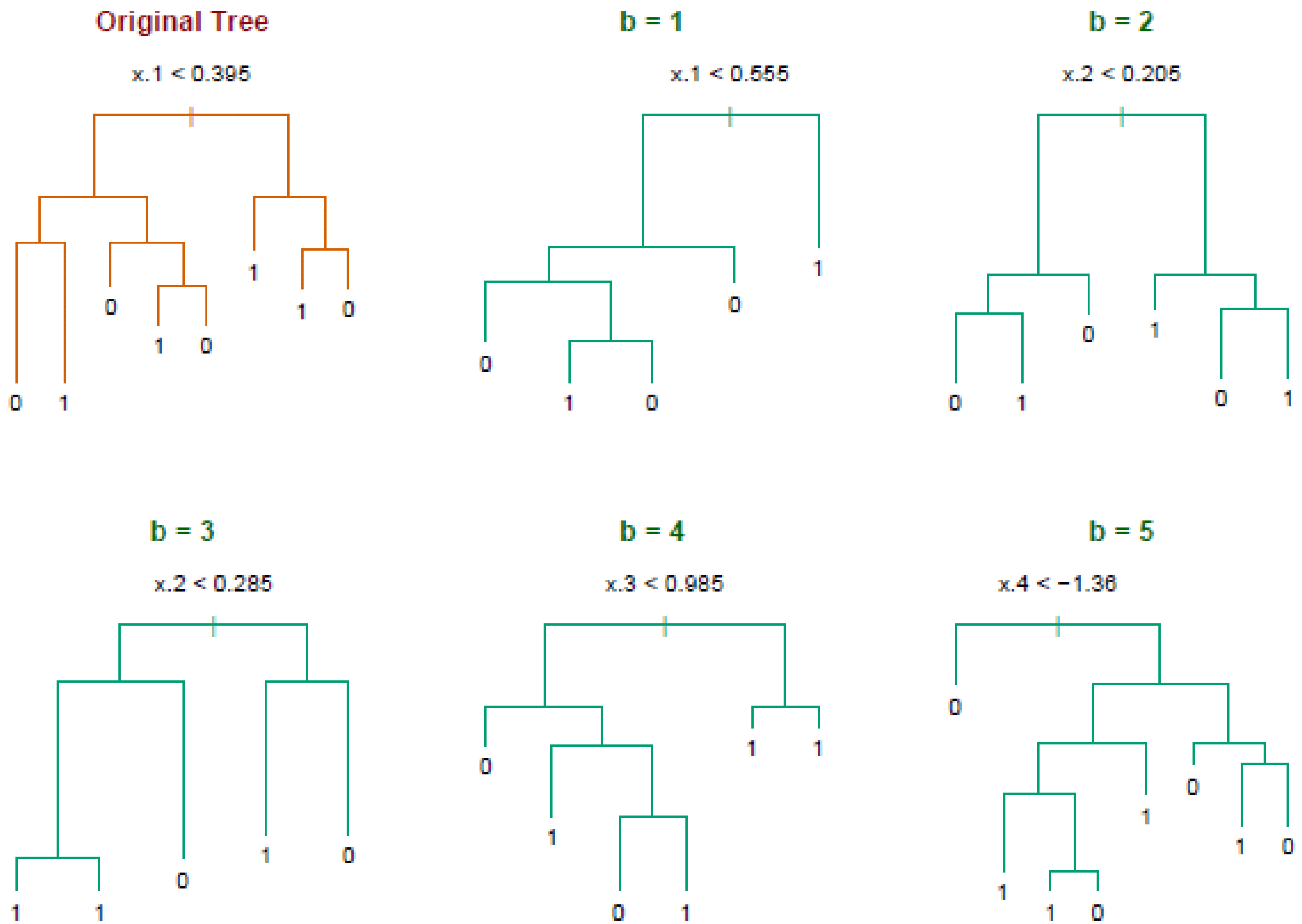
Bagging Example



Bias-Variance Trade-off



Bagging Decision Trees



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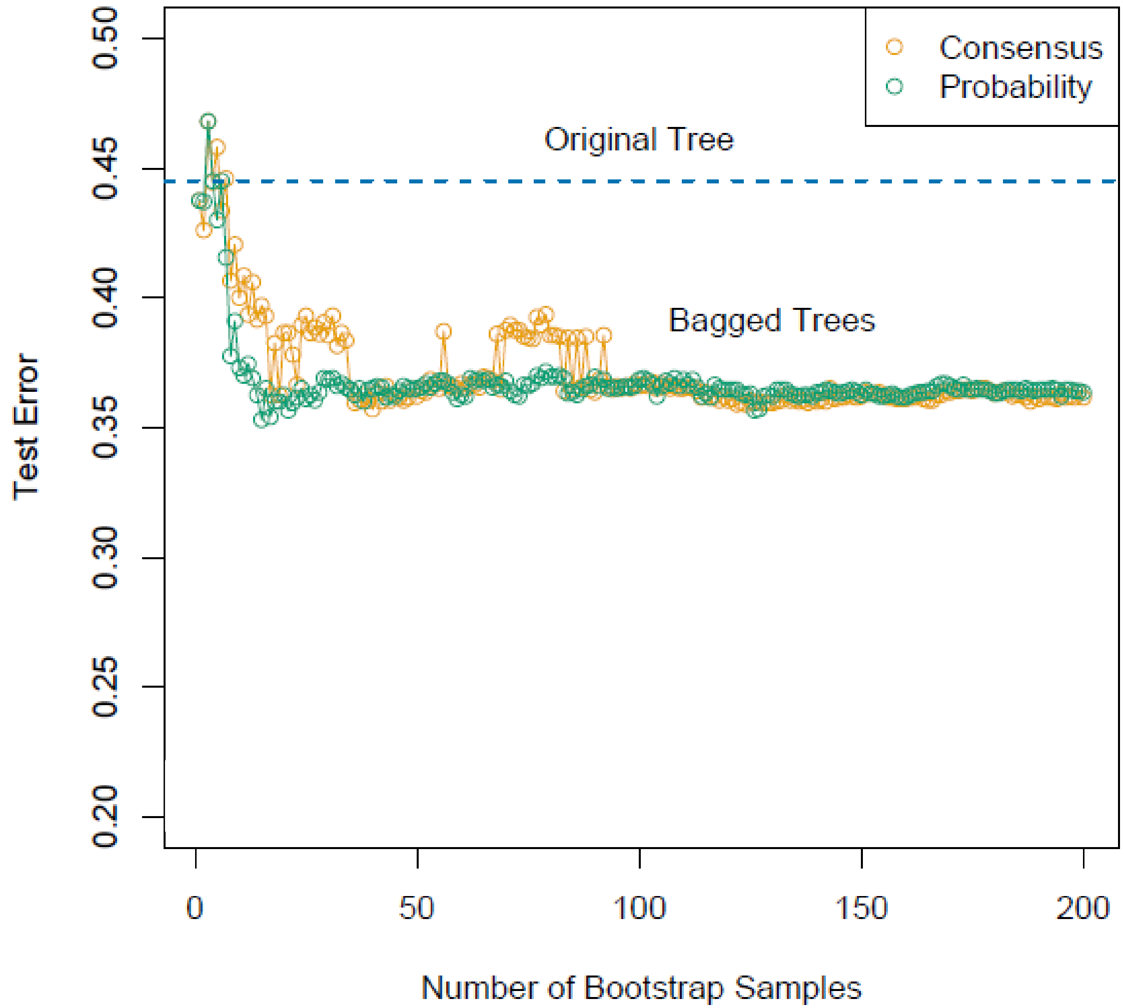
Bagging Decision Trees



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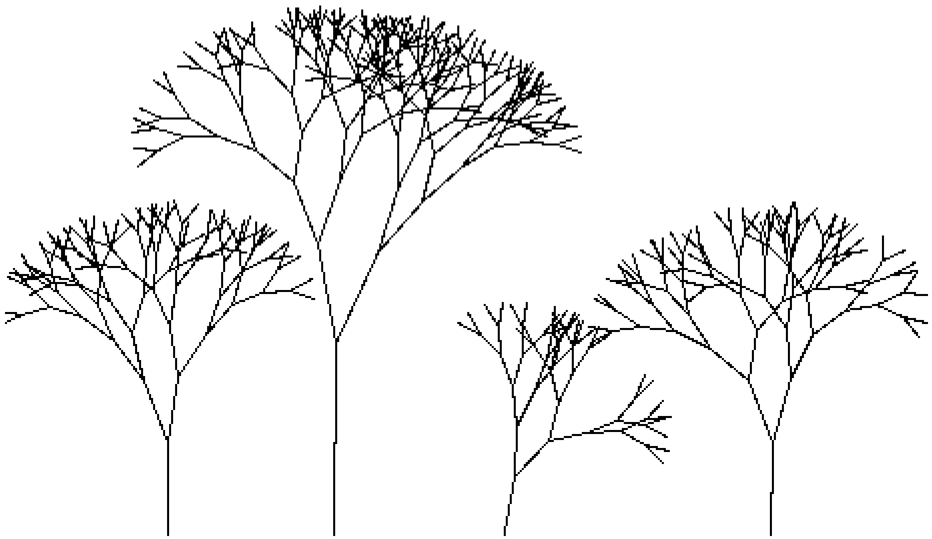
Bagging

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

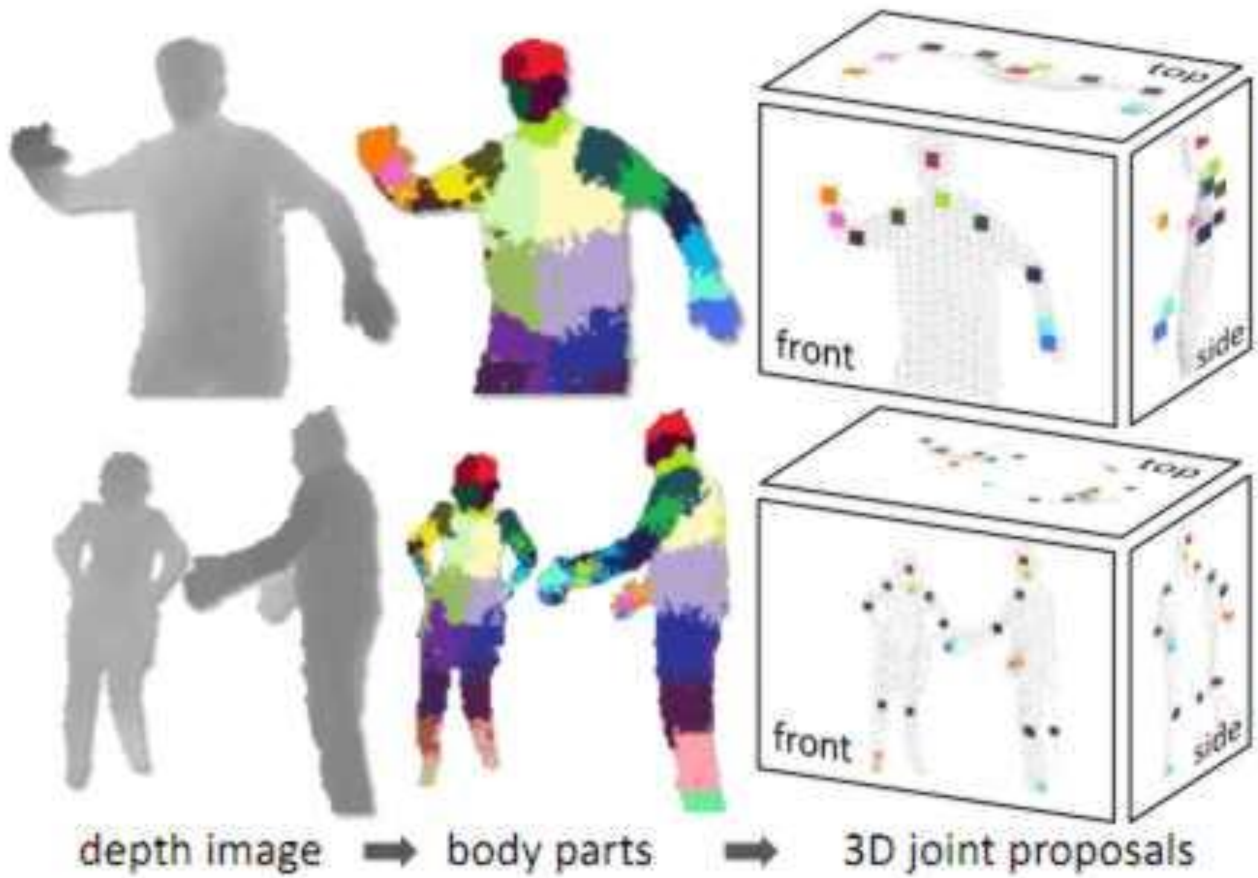
Random Forest

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



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)

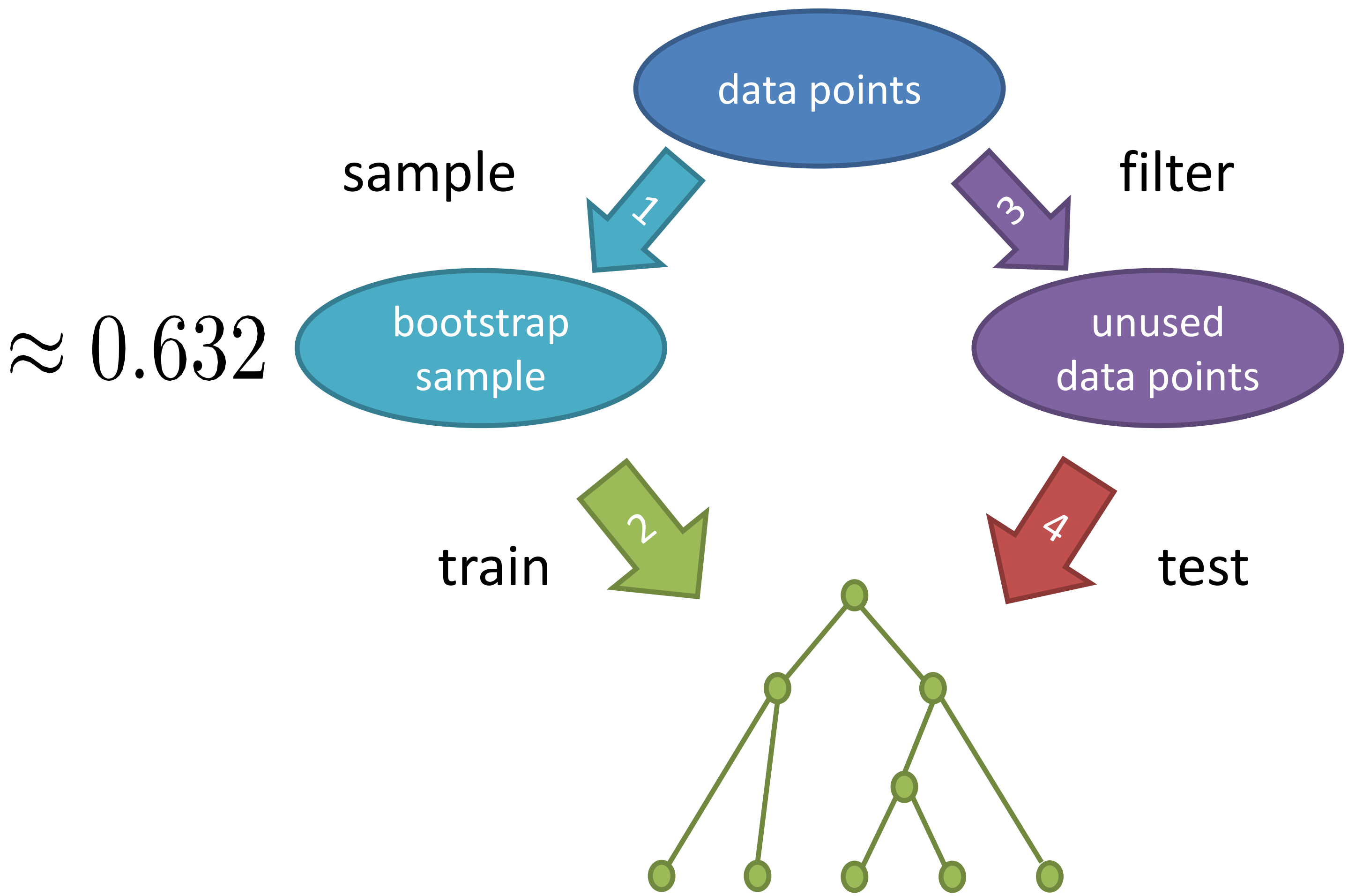
- Increasing number of features for each split:
  - Increases correlation
  - Increases strength of single trees

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



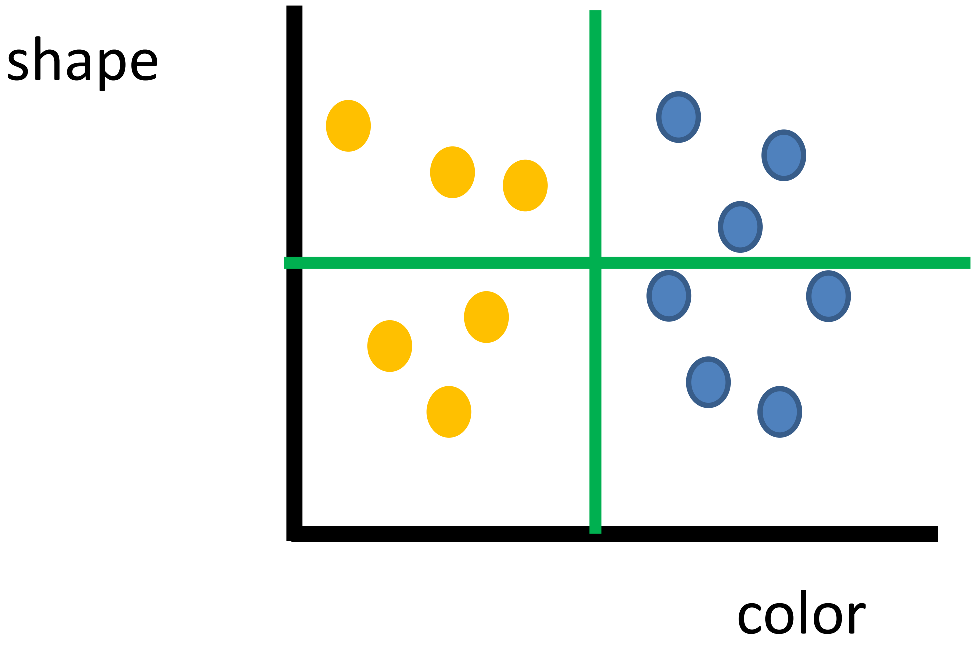
Out of Bag Error

- 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

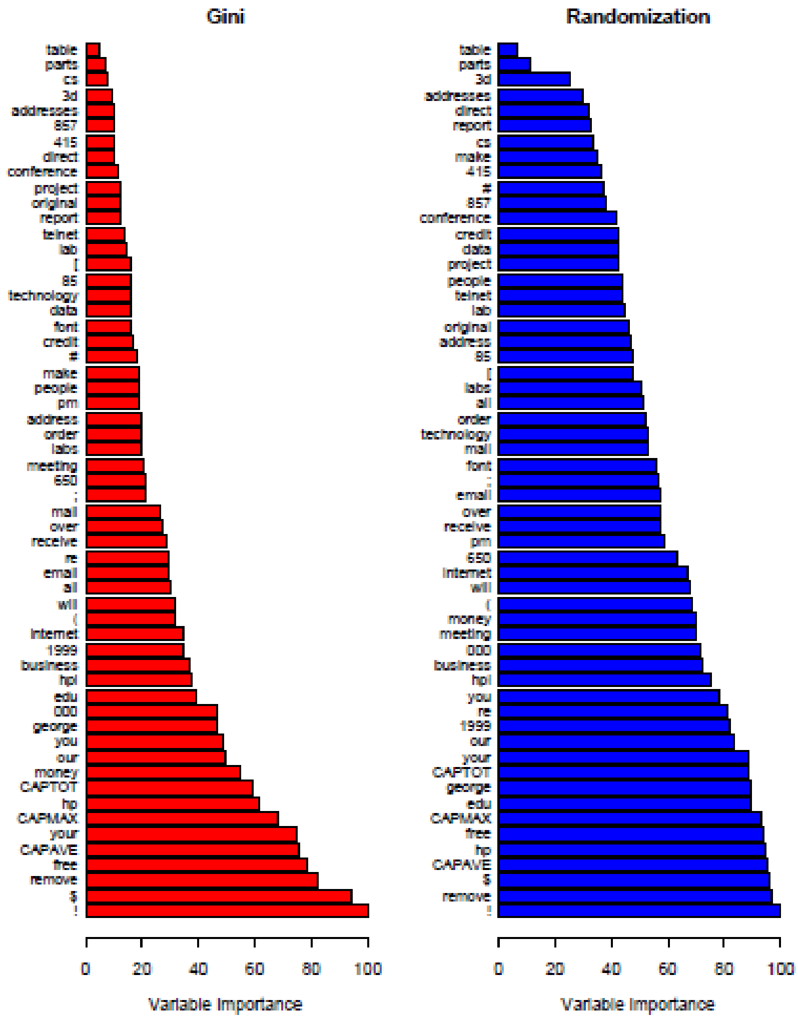
Variable Importance - 1



Variable Importance - 2

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

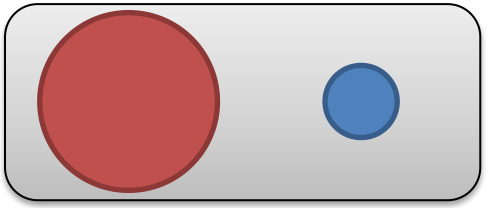
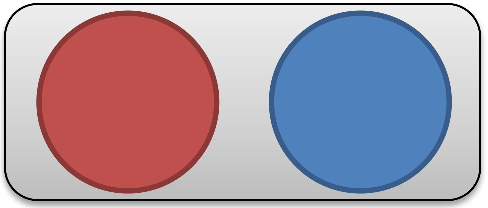
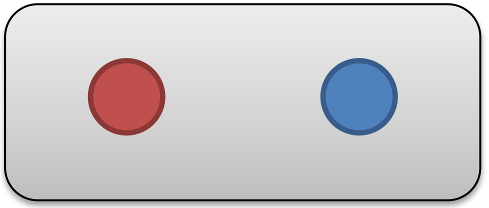
Example: Spam classification



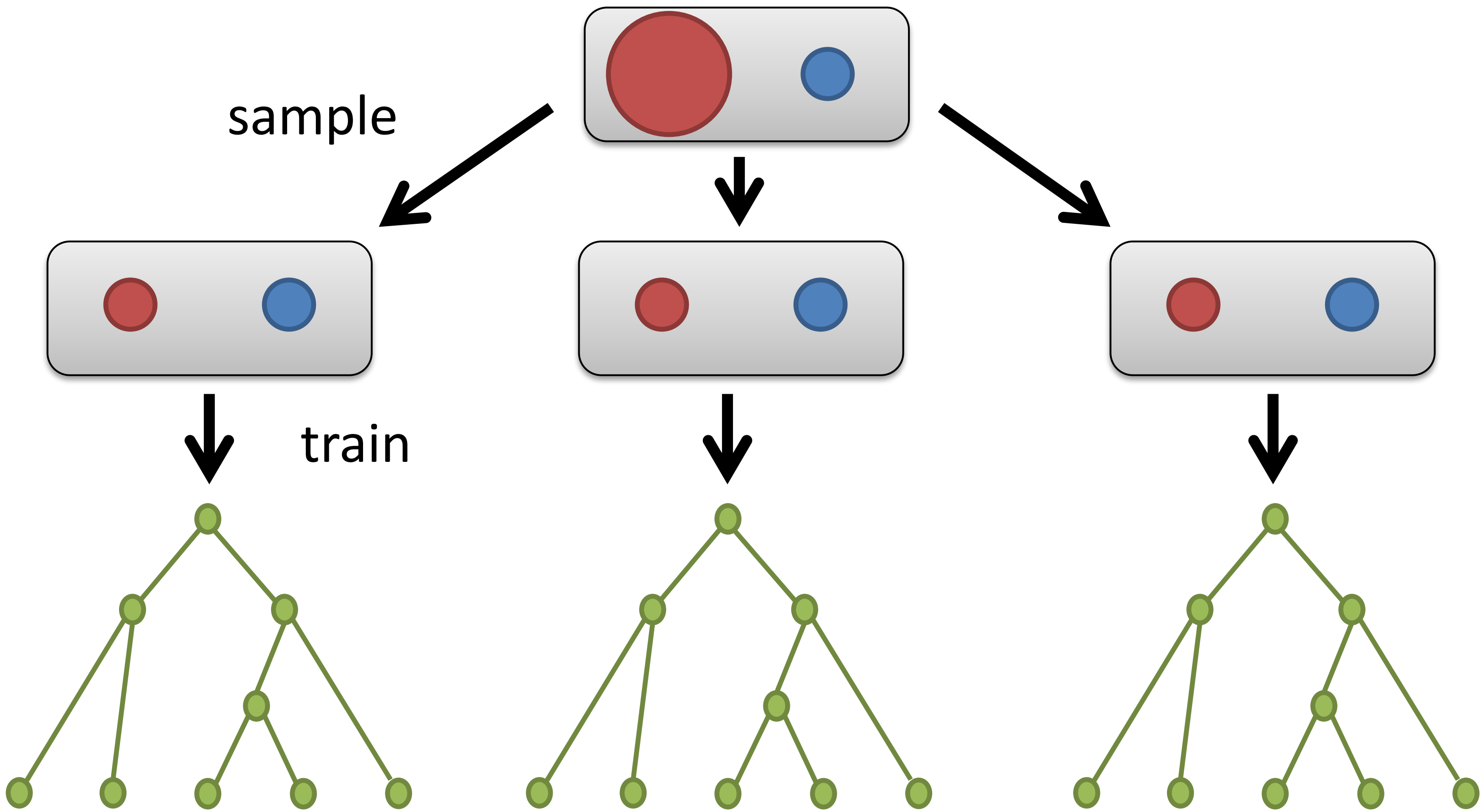
Randomization tends to spread out the variable importance more uniformly.

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