Machine Learning: Chenhao Tan

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LECTURE 19

Slides adapted from Jordan Boyd-Graber, Chris Ketelsen

Logistics

- Homework 4 is due on Sunday!
- Project proposal feedback.

Learning objectives

- Understand the general idea behind ensembling
- Understand bagging
- Learn about Adaboost

Overview

Ensemble methods

Bagging and random forest

General idea of boosting

Outline

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Outline of CSCI 4622

We've already covered stuff in blue!

- Problem formulations: classification, regression
- Supervised techniques: decision trees, nearest neighbors, perceptron, linear models, neural networks, support vector machine, kernel methods
- Unsupervised techniques: clustering, linear dimensionality reduction
- "Meta-techniques": ensembles, expectation-maximization
- Understanding ML: limits of learning, practical issues, bias & fairness
- Recurring themes: (stochastic) gradient descent

Ensemble methods

We have learned

- Decision trees
- Perceptron
- KNN
- Naïve Bayes
- Logistic regression
- Neural networks
- Support vector machines

A meta question: why do we only use a single model?

Ensemble methods

We have learned

- Decision trees
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A meta question: why do we only use a single model?
In practice, especially to win competitions, many models are used together.

Ensemble methods

There are many techniques to use multiple models.

- Bagging
  - Train classifiers on subsets of data
  - Predict based on majority vote
- Boosting
  - Build a sequence of dumb models
  - Modify training data along the way to focus on difficult examples
  - Predict based on weighted majority vote of all the models
- Stacking
  - Take multiple classifiers' outputs as inputs and train another classifier to make final prediction

Outline

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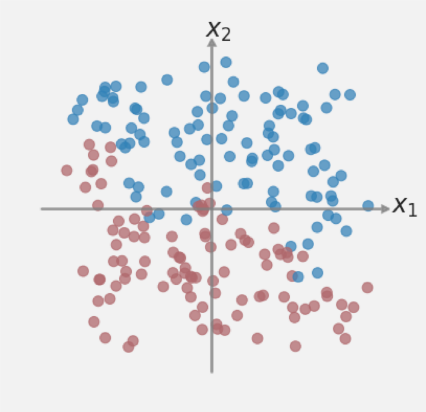
Recap of decision tree

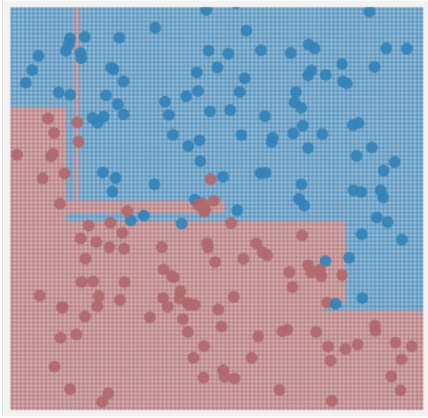
Algorithm: DTREETRAIN

Data: data D, feature set Φ
Result: decision tree
if *all examples in* D *have the same label* y*, or* Φ *is empty and* y *is the best guess*
then
  return LEAF(y);
else
  for *each feature* ϕ *in* Φ **do**
    partition D into D_0 and D_1 based on ϕ-values;
    let mistakes(ϕ) = (non-majority answers in D_0) + (non-majority answers in D_1);
  end
  let ϕ^* be the feature with the smallest number of mistakes;
  return NODE(ϕ^*, {0 $\rightarrow$ DTREETRAIN($D_0, \Phi \setminus \{\phi^*\}$), 1 $\rightarrow$ DTREETRAIN($D_1, \Phi \setminus \{\phi^*\}$)});
end

Recap of decision tree

Full decision tree classifiers tend to overfit



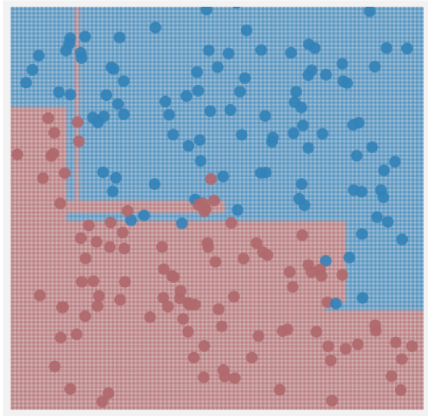


Recap of decision tree

Full decision tree classifiers tend to overfit

We could alleviate this a bit with pruning.

- Prepruning
  - Don’t let the tree have too many levels
  - Stopping conditions
- Postpruning
  - Build the complete tree
  - Go back and remove vertices that don’t affect performance too much



Bagging

We will see how we can use many decision trees.
General idea:

- Train numerous slightly different classifiers
- Use each classifier to make a prediction on a test instance
- Predict by taking majority vote from individual classifiers

Bagging

Today we will look at two different types of ensembled decision tree classifiers. The simplest is called *bootstrapped aggregation* (or bagging).

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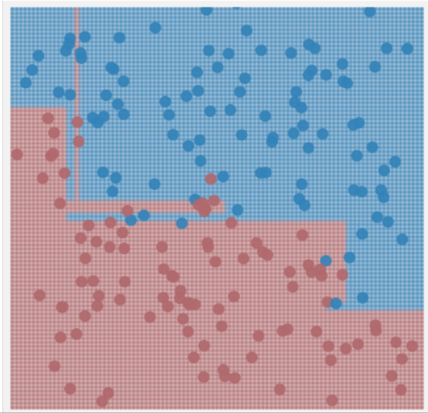
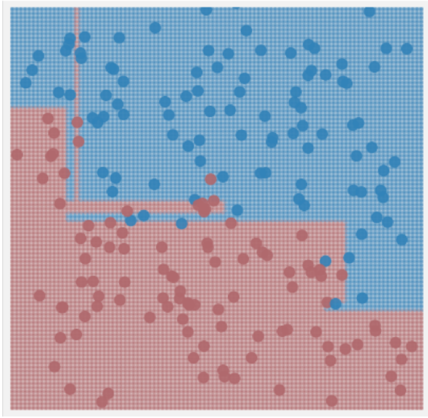
Idea: What would have happened if those training examples that we clearly overfit to weren't there?



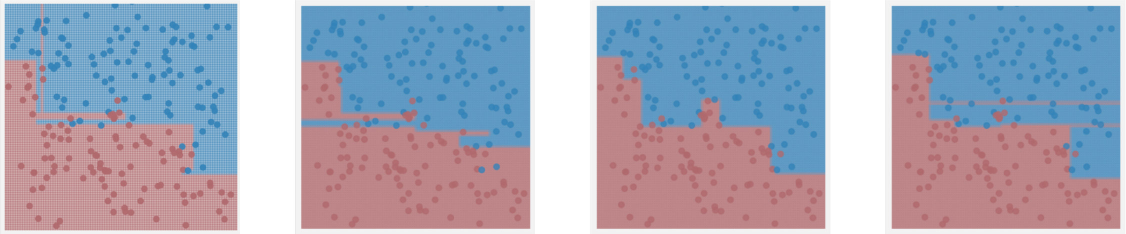
Bagging

The simplest is called *bootstrapped aggregation* (or bagging).

- Sample n training examples with replacement
- Fit decision tree classifier to each sample
- Repeat many times
- Aggregate results by majority vote



Bagging



Bagging

How many unique instances show up in n samples with replacement?

Bagging

How many unique instances show up in n samples with replacement?
The likelihood that an instance is never chosen in n draws is
$\lim_{n\to\infty}(1-\frac{1}{n})^n = \frac{1}{e}$

Bagging

In general, assume that $y \in \{-1, 1\}$ and each individual DCT has h_k
Then we can define the bagged classifier as

$$H(x) = \text{sign} \sum_{k=1}^{K} h_k(x)$$

Bagging Pros and Cons

Pros:

- Results in a much lower variance classifier than a single decision tree

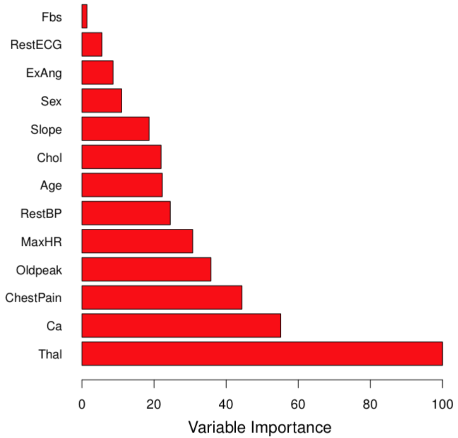
Cons:

- Results in a much less interpretable model

We essentially give up some interpretability in favor of better prediction accuracy. But we can still get insight into what our model is doing using bagging.

Bagging and feature importance

Although we cannot follow the tree structure any more, we can estimate average feature importance of single features.
Feature importance in a single tree can be defined as information gain achieved by splitting on this feature.



An even better approach: random forests

It turns out, we can take the bagging idea and make it even better.
Suppose you have a particular feature that is a very strong predictor for the response.
So strong that in almost all Bagged Decision Trees, it's the first feature that gets split on.

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Maybe always splitting on the same feature isn't the best idea.

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So strong that in almost all Bagged Decision Trees, it's the first feature that gets split on.
When this happens, the trees can all look very similar. They're too correlated.
Maybe always splitting on the same feature isn't the best idea.
Maybe, like with bootstrapping training examples, we split on a random subset of features too.

Random forests

- Still doing bagging, in the sense that we fit bootstrapped resamples of training data
- But every time we have to choose a feature to split on, don't consider all p features
- Instead, consider only $\sqrt{p}$ features to split on

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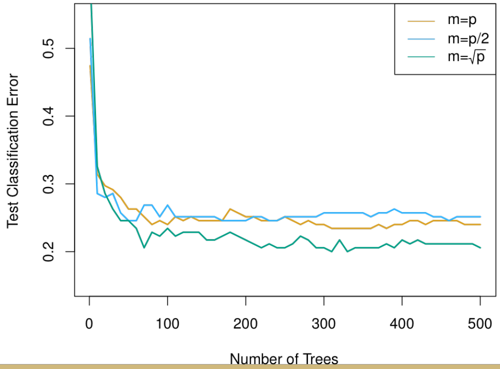
- But every time we have to choose a feature to split on, don't consider all p features
- Instead, consider only $\sqrt{p}$ features to split on

Advantages:

- Since at each split, considering less than half of features, this gives very different trees
- Very different trees in your ensemble decreases correlation, and gives more robust results
- Also, slightly cheaper because you don't have to evaluate each feature to choose best split

Random forests

Look at expression of 500 different genes in tissue samples. Predict 15 cancer states



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General idea of boosting

Boosting intuition

Boosting is an ensemble method, but with a different twist.
Idea:

- Build a sequence of dumb models
- Modify training data along the way to focus on difficult to classify examples
- Predict based on weighted majority vote of all the models

Challenges:

- What do we mean by dumb?
- How do we promote difficult examples?
- Which models get more say in vote?

Boosting intuition

What do we mean by dumb?
Each model in our sequence will be a weak learner

$$\text{err} = \frac{1}{m}\sum_{i=1}^{m} I(y_i \neq h(\mathbf{x}_i)) = \frac{1}{2} - \gamma, \gamma > 0$$

Most common weak learner in Boosting is a decision stump - a decision tree with a single split

Boosting intuition

How do we promote difficult examples?

After each iteration, we'll increase the importance of training examples that we got wrong on the previous iteration and decrease the importance of examples that we got right on the previous iteration

Each example will carry around a weight w_i that will play into the decision stump and the error estimation

Weights are normalized so they act like a probability distribution

$$\sum_{i=1}^{m} w_i = 1$$

Boosting intuition

Which models get more say in vote?
The models that performed better on training data get more say in the vote
For our sequence of weak learners: $h_1(\mathbf{x}), h_2(\mathbf{x}), \ldots, h_K(\mathbf{x})$
Boosted classifier defined by

$$H(\mathbf{x}) = \text{sign}\left[\sum_{k=1}^{K} \alpha_k h_k(\mathbf{x})\right]$$

Weight α_k is measure of accuracy of h_k on training data