# INTRO TO DATA SCIENCE LECTURE 15: ENSEMBLE METHODS

Paul Burkard 08/13/2015

RECAP 2

## **LAST TIME:**

- RECOMMENDER SYSTEMS
- CONTENT-BASED RECOMMENDERS
- COLLABORATIVE FILTERING

## **QUESTIONS?**

#### **AGENDA**

I. ENSEMBLE TECHNIQUES
II. PROBLEMS IN CLASSIFICATION
III. BAGGING
IV. BOOSTING
HANDS-ON: ENSEMBLE METHODS

#### **LEARNING GOALS**

- ▶ What are Ensemble Methods?
  - ▶ Why do we need them?
  - What are some common types?
- What are bagging and boosting?

# I. ENSEMBLE METHODS

## **ENSEMBLE TECHNIQUES**

Q: What are ensemble techniques?

A: Methods of improving classification accuracy by aggregating predictions over several base classifiers.

Ensembles are often much more accurate than the base classifiers that compose them.

Of course we can extend these ideas to things like regression, clustering, or other ML techniques.

#### **ENSEMBLE TECHNIQUES**

In order for an ensemble classifier to outperform a single base classifier, the following conditions must be met:

1) the bc's must be accurate: they must outperform random guessing

2) the bc's must be diverse: their misclassifications must occur on different training examples

## Q: How do you create an ensemble classifier?

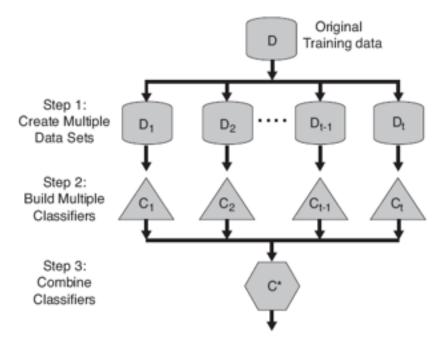


Figure 5.31. A logical view of the ensemble learning method.

#### **CREATING AN ENSEMBLE PREDICTION**

- Q: How do you generate several base classifiers?
- A: There are several ways to do this:

- manipulating the training set
- manipulating the output labels
- manipulating the learning algorithm itself

We will talk about a few examples of each of these.

# II. PROBLEMS IN CLASSIFICATION

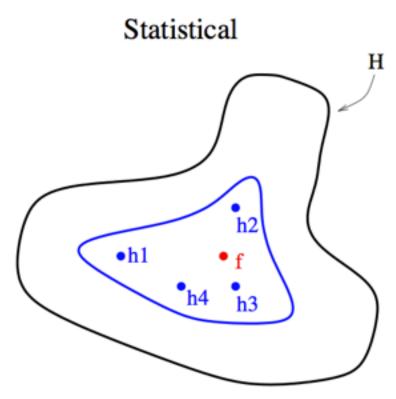
In any supervised learning task, our goal is to make predictions of the true feature-output mapping function f by finding a learner h.

There are three main problems that can prevent this:

- statistical problem
- computational problem
- representational problem

If the amount of training data available is small, the base classifier will have difficulty converging to f.

An ensemble classifier can mitigate this problem by "averaging out" base classifier predictions to improve convergence.



#### NOTE

The true function f is best approximated as an average of the base classifiers.

## THE COMPUTATIONAL PROBLEM

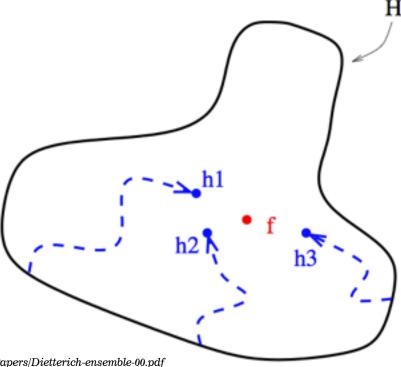
Even with sufficient training data, it may still be computationally difficult to find the best learner h.

For example, if our base classifier is a decision tree, an exhaustive search of the hypothesis space of all possible classifiers is extremely complex.

An ensemble composed of several BC's with different starting points can provide a better approximation to f than any individual BC.

#### THE COMPUTATIONAL PROBLEM

## Computational



#### NOTE

The true function f is often best approximated by using several starting points to explore the hypothesis space.

 $source: http://www.cs.iastate.edu/\sim jtian/cs573/Papers/Dietterich-ensemble-00.pdf$ 

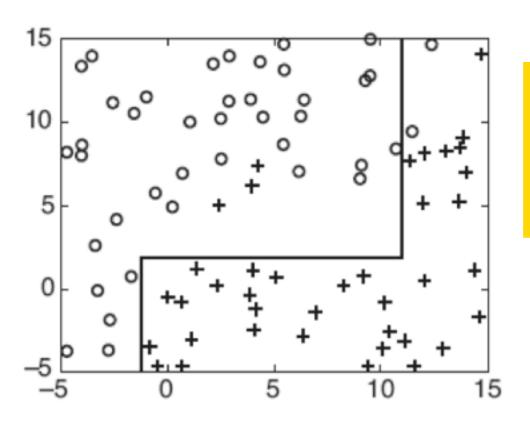
#### THE REPRESENTATIONAL PROBLEM

Sometimes f cannot be expressed in terms of our hypothesis at all.

To illustrate this, suppose we use a decision tree as our base classifier.

A decision tree works by forming a rectilinear partition of the feature space.

#### THE REPRESENTATIONAL PROBLEM — 2D DECISION TREE



#### NOTE

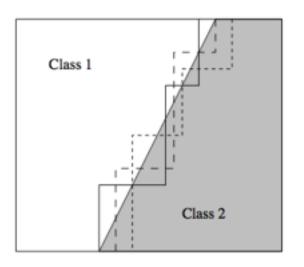
What is a *rectilinear* decision boundary?

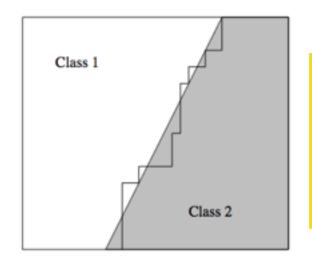
One whose segments are *orthogonal* to the x & y axes.

But what if f is a diagonal line?

Then it cannot be represented by finitely many rectilinear segments, and therefore the true decision boundary cannot be obtained by a decision tree classifier.

However, it may be still be possible to approximate f or even to expand the space of representable functions using ensemble methods.



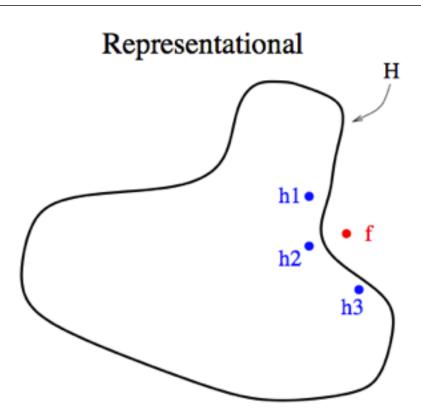


#### NOTE

An ensemble of decision trees can approximate a diagonal decision boundary.

Fig. 4. The left figure shows the true diagonal decision boundary and three staircase approximations to it (of the kind that are created by decision tree algorithms). The right figure shows the voted decision boundary, which is a much better approximation to the diagonal boundary.

#### THE REPRESENTATIONAL PROBLEM — EXPANDING THE HYPOTHESIS SPACE



#### NOTE

Ensemble classifiers can be effective even if the true decision boundary lies outside the hypothesis space.

# III. BAGGING

**Bagging** (bootstrap aggregating) is a method that involves manipulating the training set by resampling.

#### NOTE

Resampling means that some training records may appear in a sample more than once, or even not at all.

We learn k base classifiers on k different samples of training data.

These samples are independently created by resampling the training data using uniform weights (eg, a uniform sampling distribution).

**Bagging** (bootstrap aggregating) is a method that involves manipulating the training set by resampling.

#### NOTE

Each training sample is the same size as the original training set.

We learn k base classifiers on k different samples of training data.

These samples are independently created by resampling the training data using uniform weights (eg, a uniform sampling distribution).

Bagging reduces the variance in our generalization error by aggregating multiple base classifiers together (provided they satisfy our earlier requirements).

If the base classifier is stable, then the ensemble error is primarily due to bc bias, and bagging may not be effective.

Since each sample of training data is equally likely, bagging is not very susceptible to overfitting with noisy data.

# RANDOM FORESTS

## RANDOM FORESTS

A random forest is a common ensemble of decision trees where each base classifier is grown using a random effect.

- 1) Select a sample of the original training set and build a tree as follows:
  - 1) Randomly select m features out of the M available
  - 2) Pick the best split based on just those m variables
- 2) Repeat (1) for N iterations
- 3) Predict based on majority vote of N trees

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# IV. BOOSTING

Boosting is an iterative procedure that adaptively changes the sampling distribution of training records at each iteration.

The first iteration uses uniform weights (like bagging). In subsequent iterations, the weights are adjusted to emphasize records that were misclassified in previous iterations.

The final prediction is constructed by a weighted vote (where the weights for a bc depends on its training error).

- 1) Start with a training set where each item has equal weight
- 2) Build a classifier G
- 3) Compute the error e(G) of the classifier (% incorrect)
- 4) Build a new training set where the incorrect instances are weighted (repeated) by the error e(G) of the classifier
- 5) Repeat
- 6) Predict based on majority vote (or vote based on accuracy inverse error)

Like in bagging, sampling is done with replacement, and as a result some records may not appear in a given training sample.

These omitted records will likely be misclassified, and given greater weight in subsequent iterations once the sampling distribution is updated.

So even if a record is left out at one stage, it will be emphasized later.

Updating the sampling distribution and forming an ensemble prediction leads to a nonlinear combination of the base classifiers.

# HANDS-ON: RECOMMENDERS