# INTRO TO DATA SCIENCE LECTURE 10: ENSEMBLE TECHNIQUES

RECAP 2

# **LAST TIME:**

- DECISION TREES
- OPTIMIZATION FUNCTIONS & OVERFITTING
- DECISION TREES IN SCIKIT-LEARN

## **QUESTIONS?**

#### **AGENDA**

- I. ENSEMBLE TECHNIQUES
  II. PROBLEMS IN CLASSIFICATION
- III. BAGGING
- IV. BOOSTING
- V. RANDOM FORESTS

# **EXERCISE:**

**VI. ADABOOST** 

Q: What are ensemble techniques?

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

Base classifiers and ensemble classifiers are sometimes called weak learners and strong learners.

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

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

1) the bc's must be accurate: low bias

2) the bc's must be diverse: uncorrelated

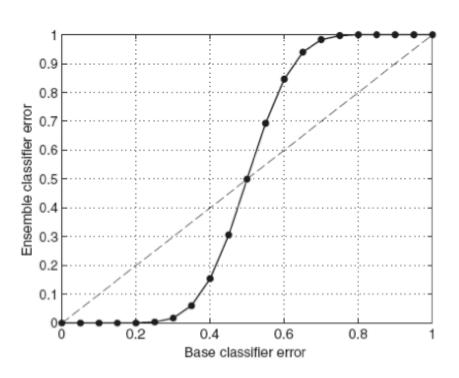
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#### NOTE

Ideally, we would also like the base classifiers to be *unstable* to variations in the training set.

In other words, *high* variance.



#### NOTE

dashed line = perfectly correlated bc's (no improvement using ensemble)

solid line = perfectly uncorrelated bc's (some improvement for unbiased bc's)

Figure 5.30. Comparison between errors of base classifiers and errors of the ensemble classifier.

# II. PROBLEMS IN CLASSIFICATION

#### **PROBLEMS IN CLASSIFICATION**

In any supervised learning task, our goal is to make predictions of the true classification function f by learning the classifier h.

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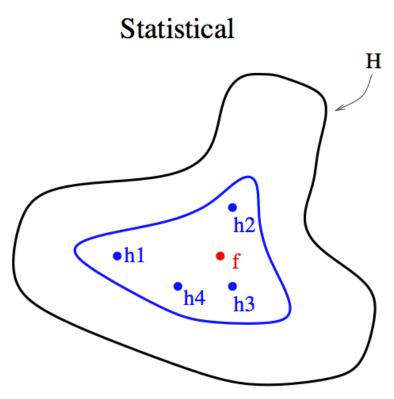
There are three main problems that can prevent this:

- statistical problem
- computational problem
- representational problem

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

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

#### THE STATISTICAL PROBLEM



#### 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 classifier 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 (NP-complete).

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Recall that this is why we used a *heuristic* algorithm (greedy search).

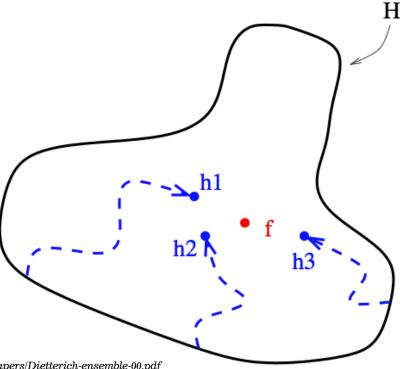
# THE COMPUTATIONAL PROBLEM

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

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

# Computational



#### NOTE

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

#### THE REPRESENTATIONAL PROBLEM

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

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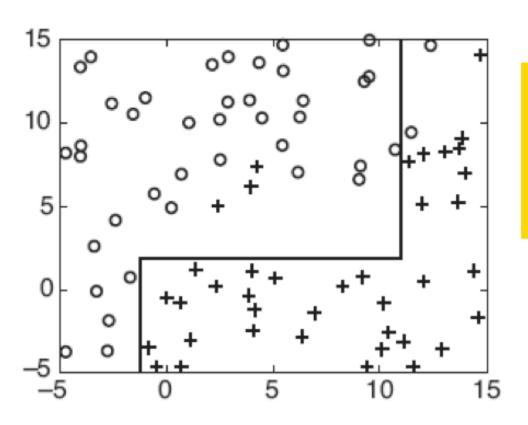
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A decision tree works by forming a rectilinear partition of the feature space.

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



#### NOTE

What is a *rectilinear* decision boundary?

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

#### THE REPRESENTATIONAL PROBLEM

But what if f is a diagonal line?

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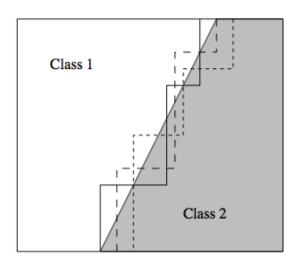
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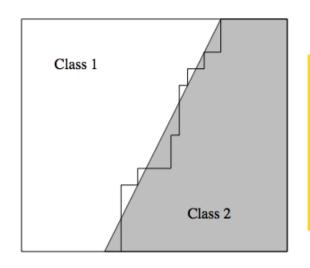
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But what if f is a diagonal line?

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.



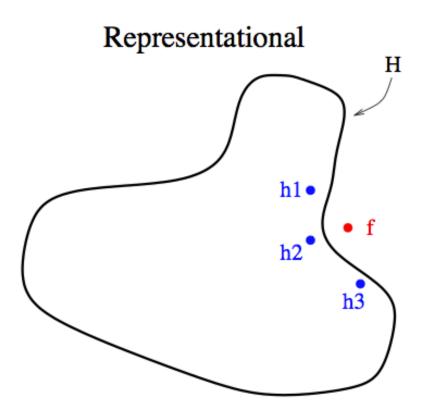


#### NOTE

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.

# **CREATING AN ENSEMBLE PREDICTION**

Q: How do you create an ensemble classifier?

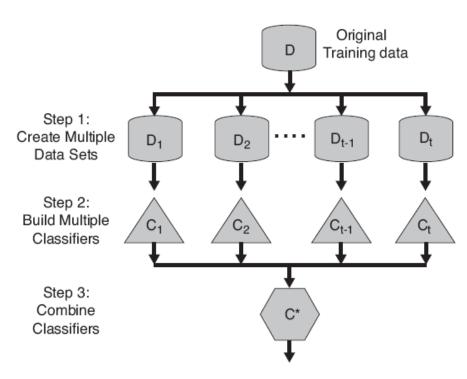


Figure 5.31. A logical view of the ensemble learning method.

### **CREATING AN ENSEMBLE PREDICTION**

Q: How do you generate several base classifiers?

- 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.

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# III. BAGGING

# **BAGGING**

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

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).

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

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The final prediction is made by taking a majority vote across be's.

# **BAGGING**

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

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

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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.

# INTRO TO DATA SCIENCE

# IV. BOOSTING

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

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#### NOTE

The bc's focus more and more closely on records that are difficult to classify as the sequence of iterations progresses.

Thus the bc's are faced with progressively more difficult learning problems.

# **BOOSTING**

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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.

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# V. RANDOM FORESTS

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For a small number of features, we can also create linear combinations of features and select splits from the enhanced feature set (Forest-RC).

Or, we can select splitting features completely at random (Forest-RI).

## RANDOM FORESTS

Random forests are about as accurate as AdaBoost, more robust to noise, and can also have better runtime than other ensemble methods (since the feature space is reduced in some cases).

# EX: ENSEMBLE METHODS IN SCIKIT-LEARN