INTRO TO DATA SCIENCE
ENSEMBLE TECHNIQUES

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

I. ENSEMBLE TECHNIQUES

Q: What are ensemble techniques?

Q: What are ensemble techniques?

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

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.

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.

NOTE

These base classifiers are sometimes called *weak learners*.

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

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

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

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**: *low bias*

2) the bc's must be **diverse**: *uncorrelated*

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**: *low bias*

2) the bc's must be **diverse**: *uncorrelated*

NOTE

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

In other words, *high variance*.

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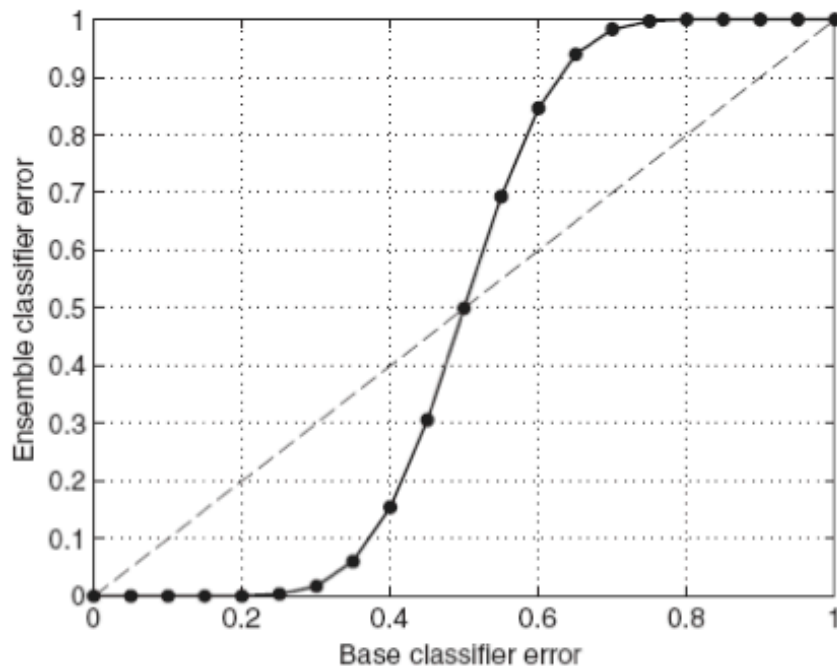
NOTE

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

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

II. 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.

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

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

Statistical

H

h2

h1   f

h4   h3
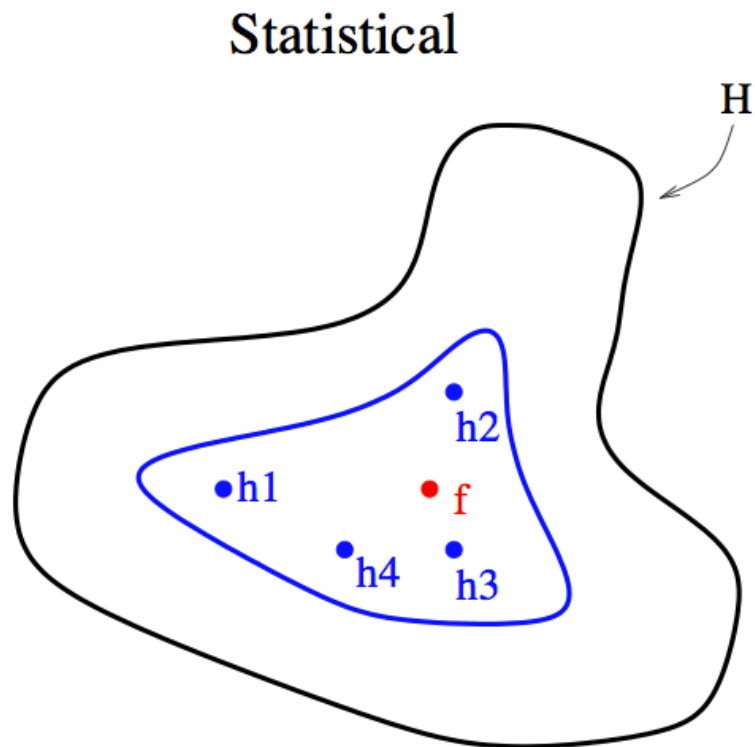
NOTE

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

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

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).

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).
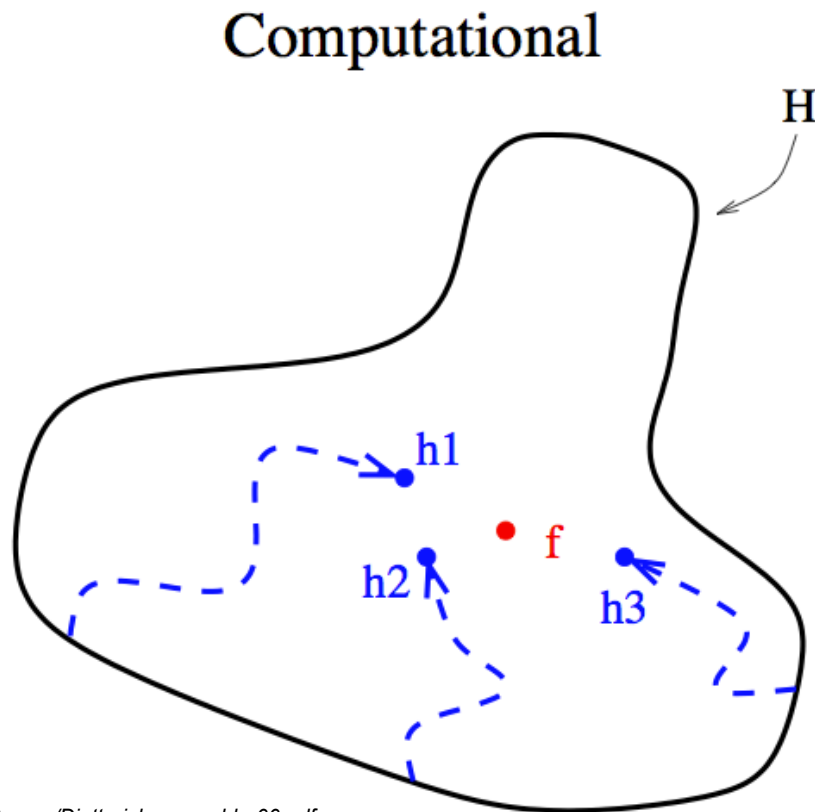
NOTE

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

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).

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

Computational

H

h1

h2   f   h3

NOTE

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

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

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.

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.
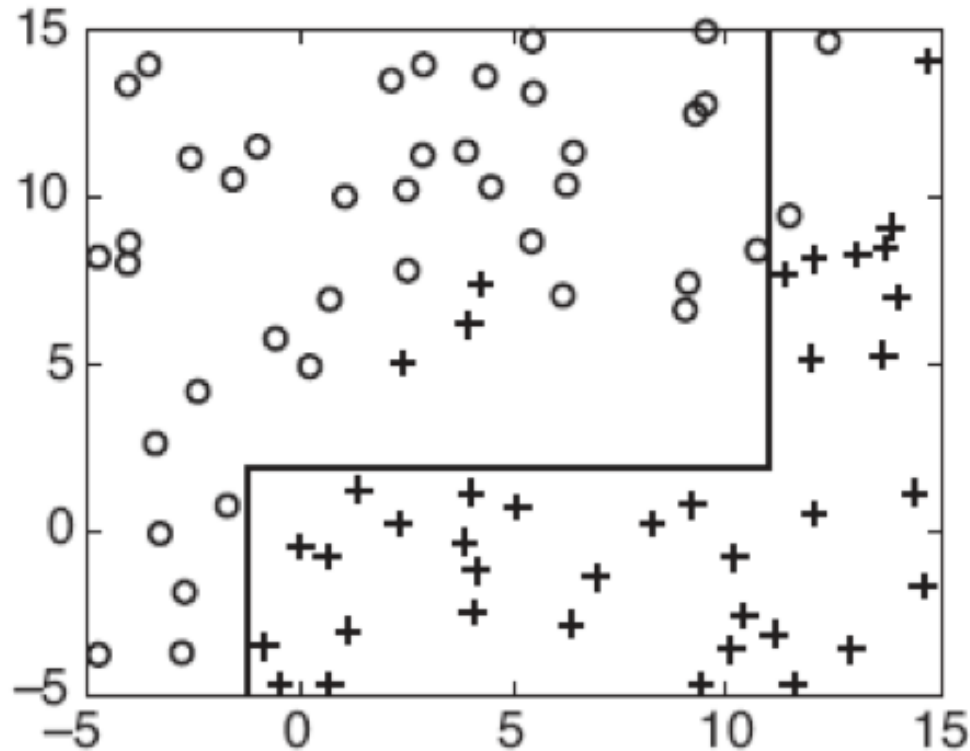
NOTE

What is a *rectilinear* decision boundary?

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

But what if *f* is a diagonal line?

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.
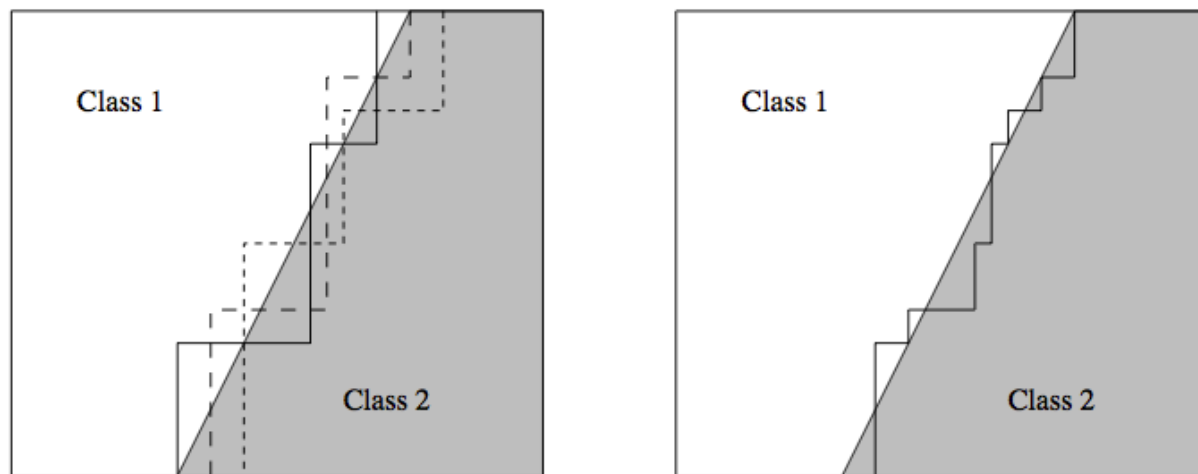
But what if f is a diagonal line?

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.

Representational

H

h1

f

h2

h3
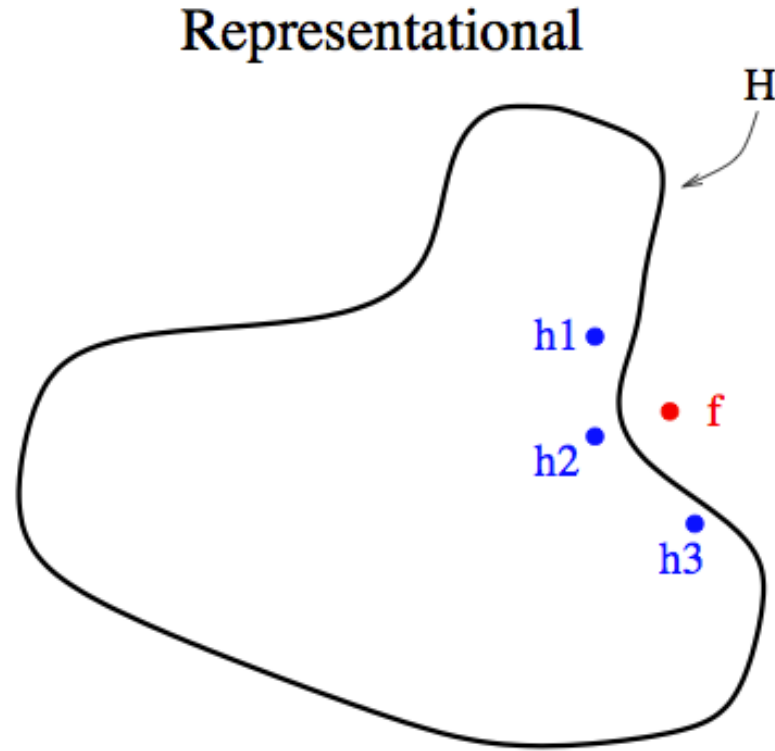
NOTE

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

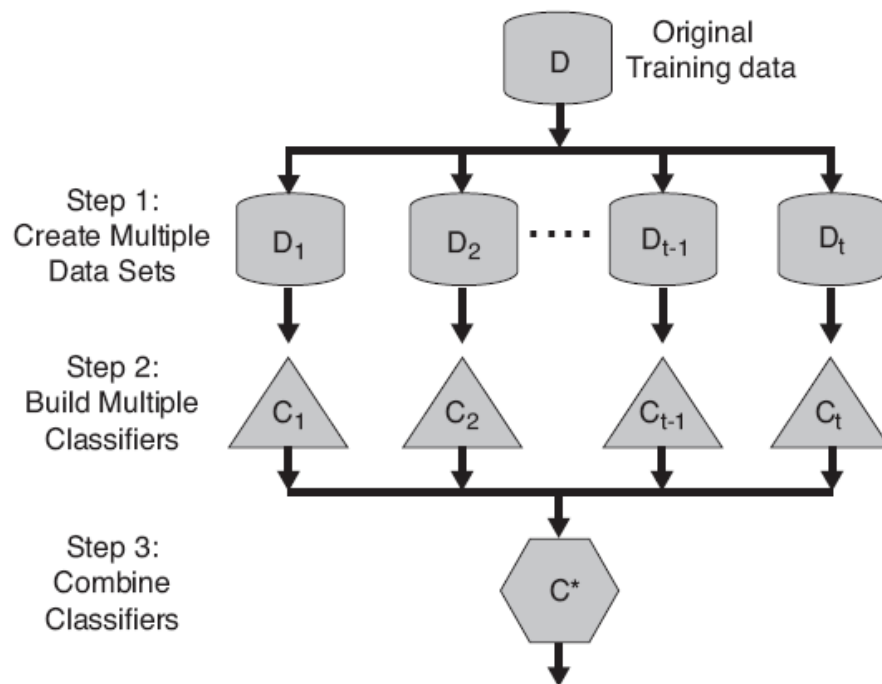Q: How do you create an ensemble classifier?

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

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.

III. BAGGING

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

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**).

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 th data using uniform weights (eg, a uniform **sampling distri**

NOTE

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

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 th[e] data using uniform weights (eg, a uniform **sampling distri**

NOTE

NOTE

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

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**).

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

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

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.

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.

IV. BOOSTING

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

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.

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).

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 su[...]
iterations, the weights are *adjusted* to emphasize records t[...]
misclassified in previous iterations.

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

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.

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

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.

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.

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 emphas

NOTE

AdaBoost is a popular boosting algorithm.

V. RANDOM FORESTS

A random forest is an ensemble of decision trees that vote to determine the final classification.

A random forest is an ensemble of decision trees that vote to determine the final classification.

There are many ways to get random trees. The most common is to take bootstrap training sets and also restrict tree growth to a random subset of features for each split.

A random forest is an ensemble of decision trees that vote to determine the final classification.

There are many ways to get random trees. The most common is to take bootstrap training sets and also restrict tree growth to a random subset of features for each split.

Other methods: Randomly generate quadratic features, randomly choose the exact feature to split on, sklearn's "extremely random forest" technique, etc.

EXERCISE