7

Combining Different Models for Ensemble Learning

In the previous chapter, we focused on the best practices for tuning and evaluating different models for classification. In this chapter, we will build upon those techniques and explore different methods for constructing a set of classifiers that can often have a better predictive performance than any of its individual members. We will learn how to do the following:

- Make predictions based on majority voting
- Use bagging to reduce overfitting by drawing random combinations of the training dataset with repetition
- Apply boosting to build powerful models from weak learners that learn from their mistakes

Learning with ensembles

The goal of **ensemble methods** is to combine different classifiers into a meta-classifier that has better generalization performance than each individual classifier alone. For example, assuming that we collected predictions from 10 experts, ensemble methods would allow us to strategically combine those predictions by the 10 experts to come up with a prediction that was more accurate and robust than the predictions by each individual expert. As you will see later in this chapter, there are several different approaches for creating an ensemble of classifiers. This section will introduce a basic explanation of how ensembles work and why they are typically recognized for yielding a good generalization performance.

In this chapter, we will focus on the most popular ensemble methods that use the **majority voting** principle. Majority voting simply means that we select the class label that has been predicted by the majority of classifiers, that is, received more than 50 percent of the votes. Strictly speaking, the term "majority vote" refers to binary class settings only. However, it is easy to generalize the majority voting principle to multiclass settings, which is known as **plurality voting**. (In the UK, people distinguish between majority and plurality voting via the terms "absolute" and "relative" majority, respectively.)

Here, we select the class label that received the most votes (the mode). *Figure 7.1* illustrates the concept of majority and plurality voting for an ensemble of 10 classifiers, where each unique symbol (triangle, square, and circle) represents a unique class label:

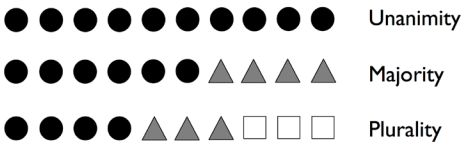


Figure 7.1: The different voting concepts

Using the training dataset, we start by training m different classifiers (C_1, ..., C_m). Depending on the technique, the ensemble can be built from different classification algorithms, for example, decision trees, support vector machines, logistic regression classifiers, and so on. Alternatively, we can also use the same base classification algorithm, fitting different subsets of the training dataset. One prominent example of this approach is the random forest algorithm combining different decision tree classifiers, which we covered in *Chapter 3*, *A Tour of Machine Learning Classifiers Using Scikit-Learn*. *Figure 7.2* illustrates the concept of a general ensemble approach using majority voting:

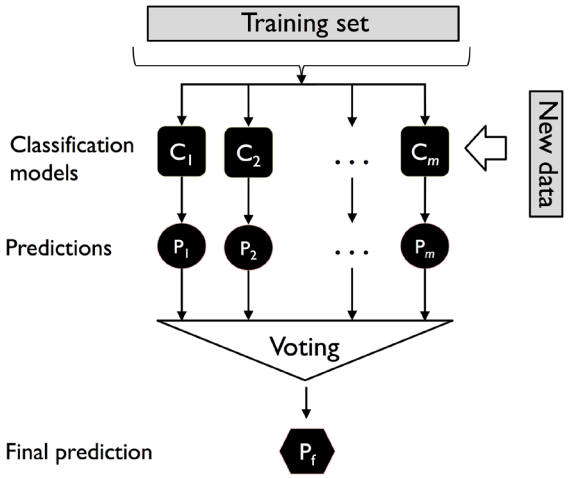


Figure 7.2: A general ensemble approach

To predict a class label via simple majority or plurality voting, we can combine the predicted class labels of each individual classifier, C_j, and select the class label, $\hat{y}$, that received the most votes:

$$\hat{y} = \text{mode}\{C_1(\boldsymbol{x}), C_2(\boldsymbol{x}), \ldots, C_m(\boldsymbol{x})\}$$

(In statistics, the mode is the most frequent event or result in a set. For example, mode{1, 2, 1, 1, 2, 4, 5, 4} = 1.)

For example, in a binary classification task where class1 = –1 and class2 = +1, we can write the majority vote prediction as follows:

$$C(\boldsymbol{x}) = \text{sign}\left[\sum_{j}^{m} C_j(\boldsymbol{x})\right] = \begin{cases} 1 & \text{if } \sum_j C_j(\boldsymbol{x}) \geq 0 \\ -1 & \text{otherwise} \end{cases}$$

To illustrate why ensemble methods can work better than individual classifiers alone, let's apply some concepts of combinatorics. For the following example, we will make the assumption that all n-base classifiers for a binary classification task have an equal error rate, ε. Furthermore, we will assume that the classifiers are independent and the error rates are not correlated. Under those assumptions, we can simply express the error probability of an ensemble of base classifiers as a probability mass function of a binomial distribution:

$$P(y \geq k) = \sum_{k}^{n} \left\langle {n \atop k} \right\rangle \varepsilon^k (1-\varepsilon)^{n-k} = \varepsilon_{\text{ensemble}}$$

Here, $\left\langle {n \atop k} \right\rangle$ is the binomial coefficient *n choose k*. In other words, we compute the probability that the prediction of the ensemble is wrong. Now, let's take a look at a more concrete example of 11 base classifiers ($n = 11$), where each classifier has an error rate of 0.25 ($\varepsilon = 0.25$):

$$P(y \geq k) = \sum_{k=6}^{11} \left\langle {11 \atop k} \right\rangle 0.25^k (1-0.25)^{11-k} = 0.034$$

The binomial coefficient

The binomial coefficient refers to the number of ways we can choose subsets of k unordered elements from a set of size n; thus, it is often called "n choose k." Since the order does not matter here, the binomial coefficient is also sometimes referred to as *combination* or *combinatorial number*, and in its unabbreviated form, it is written as follows:

$$\frac{n!}{(n-k)!\,k!}$$

Here, the symbol (!) stands for factorial—for example, 3! = 3×2×1 = 6.

As you can see, the error rate of the ensemble (0.034) is much lower than the error rate of each individual classifier (0.25) if all the assumptions are met. Note that, in this simplified illustration, a 50-50 split by an even number of classifiers, n, is treated as an error, whereas this is only true half of the time. To compare such an idealistic ensemble classifier to a base classifier over a range of different base error rates, let's implement the probability mass function in Python:

```
>>> from scipy.special import comb
>>> import math
>>> def ensemble_error(n_classifier, error):
```

```
...     k_start = int(math.ceil(n_classifier / 2.))
...     probs = [comb(n_classifier, k) *
...              error**k *
...              (1-error)**(n_classifier - k)
...              for k in range(k_start, n_classifier + 1)]
...     return sum(probs)
>>> ensemble_error(n_classifier=11, error=0.25)
0.03432750701904297
```

After we have implemented the `ensemble_error` function, we can compute the ensemble error rates for a range of different base errors from 0.0 to 1.0 to visualize the relationship between ensemble and base errors in a line graph:

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> error_range = np.arange(0.0, 1.01, 0.01)
>>> ens_errors = [ensemble_error(n_classifier=11, error=error)
...               for error in error_range]
>>> plt.plot(error_range, ens_errors,
...          label='Ensemble error',
...          linewidth=2)
>>> plt.plot(error_range, error_range,
...          linestyle='--', label='Base error',
...          linewidth=2)
>>> plt.xlabel('Base error')
>>> plt.ylabel('Base/Ensemble error')
>>> plt.legend(loc='upper left')
>>> plt.grid(alpha=0.5)
>>> plt.show()
```

As you can see in the resulting plot, the error probability of an ensemble is always better than the error of an individual base classifier, as long as the base classifiers perform better than random guessing ($\varepsilon < 0.5$).

Note that the *y* axis depicts the base error (dotted line) as well as the ensemble error (continuous line):

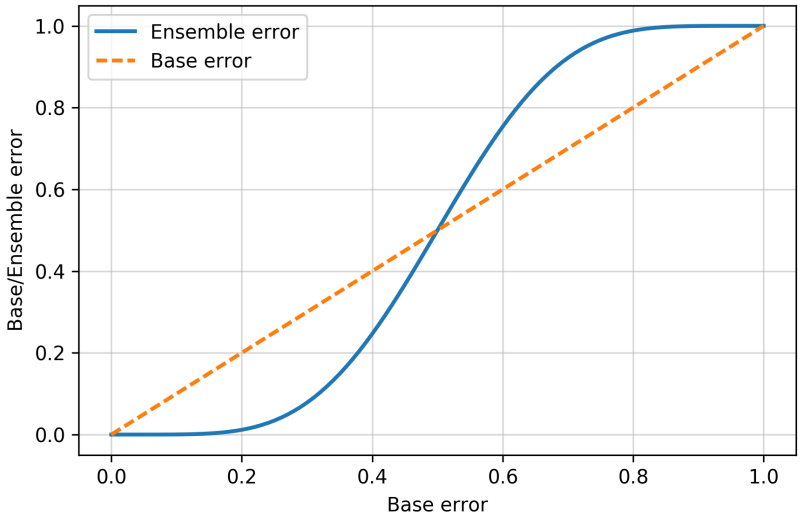


Figure 7.3: A plot of the ensemble error versus the base error

Combining classifiers via majority vote

After the short introduction to ensemble learning in the previous section, let's start with a warm-up exercise and implement a simple ensemble classifier for majority voting in Python.

Plurality voting

Although the majority voting algorithm that we will discuss in this section also generalizes to multiclass settings via plurality voting, the term "majority voting" will be used for simplicity, as is often the case in the literature.

Implementing a simple majority vote classifier

The algorithm that we are going to implement in this section will allow us to combine different classification algorithms associated with individual weights for confidence. Our goal is to build a stronger meta-classifier that balances out the individual classifiers' weaknesses on a particular dataset. In more precise mathematical terms, we can write the weighted majority vote as follows:

$$\hat{y} = \arg\max_{i} \sum_{j=1}^{m} w_j \chi_A\big(C_j(\boldsymbol{x}) = i\big)$$

Here, w_j is a weight associated with a base classifier, C_j; $\hat{y}$ is the predicted class label of the ensemble; A is the set of unique class labels; χ_A (Greek chi) is the characteristic function or indicator function, which returns 1 if the predicted class of the jth classifier matches i ($C_j(\boldsymbol{x}) = i$). For equal weights, we can simplify this equation and write it as follows:

$$\hat{y} = \text{mode}\{C_1(\boldsymbol{x}), C_2(\boldsymbol{x}), \ldots, C_m(\boldsymbol{x})\}$$

To better understand the concept of *weighting*, we will now take a look at a more concrete example. Let's assume that we have an ensemble of three base classifiers, $C_j (j \in \{1, 2, 3\})$, and we want to predict the class label, $C_j(\boldsymbol{x}) \in \{0, 1\}$, of a given example, $\boldsymbol{x}$. Two out of three base classifiers predict the class label 0, and one, C_3, predicts that the example belongs to class 1. If we weight the predictions of each base classifier equally, the majority vote predicts that the example belongs to class 0:

$$C_1(\boldsymbol{x}) \rightarrow 0, \quad C_2(\boldsymbol{x}) \rightarrow 0, \quad C_3(\boldsymbol{x}) \rightarrow 1$$

$$\hat{y} = \text{mode}\{0, 0, 1\} = 0$$

Now, let's assign a weight of 0.6 to C_3, and let's weight C_1 and C_2 by a coefficient of 0.2:

$$\hat{y} = \arg\max_i \sum_{j=1}^{m} w_j \chi_A\big(C_j(\boldsymbol{x}) = i\big)$$

$$= \arg\max_i [0.2 \times i_0 + 0.2 \times i_0, 0.6 \times i_1] = 1$$

More simply, since 3×0.2 = 0.6, we can say that the prediction made by C_3 has three times more weight than the predictions by C_1 or C_2, which we can write as follows:

$$\hat{y} = \text{mode}\{0, 0, 1, 1, 1\} = 1$$

To translate the concept of the weighted majority vote into Python code, we can use NumPy's convenient `argmax` and `bincount` functions, where `bincount` counts the number of occurrences of each class label. The `argmax` function then returns the index position of the highest count, corresponding to the majority class label (this assumes that class labels start at 0):

```
>>> import numpy as np
>>> np.argmax(np.bincount([0, 0, 1],
...           weights=[0.2, 0.2, 0.6]))
1
```

As you will remember from the discussion on logistic regression in *Chapter 3*, certain classifiers in scikit-learn can also return the probability of a predicted class label via the `predict_proba` method. Using the predicted class probabilities instead of the class labels for majority voting can be useful if the classifiers in our ensemble are well calibrated. The modified version of the majority vote for predicting class labels from probabilities can be written as follows:

$$\hat{y} = \arg\max_i \sum_{j=1}^{m} w_j p_{ij}$$

Here, p_{ij} is the predicted probability of the jth classifier for class label i.

To continue with our previous example, let's assume that we have a binary classification problem with class labels $i \in \{0, 1\}$ and an ensemble of three classifiers, $C_j (j \in \{1, 2, 3\})$. Let's assume that the classifiers C_j return the following class membership probabilities for a particular example, $\boldsymbol{x}$:

$$C_1(\boldsymbol{x}) \rightarrow [0.9, 0.1], \quad C_2(\boldsymbol{x}) \rightarrow [0.8, 0.2], \quad C_3(\boldsymbol{x}) \rightarrow [0.4, 0.6]$$

Using the same weights as previously (0.2, 0.2, and 0.6), we can then calculate the individual class probabilities as follows:

$$p(i_0|\boldsymbol{x}) = 0.2 \times 0.9 + 0.2 \times 0.8 + 0.6 \times 0.4 = 0.58$$

$$p(i_1|\boldsymbol{x}) = 0.2 \times 0.1 + 0.2 \times 0.2 + 0.6 \times 0.6 = 0.42$$

$$\hat{y} = \arg\max_i [p(i_0|\boldsymbol{x}), p(i_1|\boldsymbol{x})] = 0$$

To implement the weighted majority vote based on class probabilities, we can again make use of NumPy, using `np.average` and `np.argmax`:

```
>>> ex = np.array([[0.9, 0.1],
...                [0.8, 0.2],
...                [0.4, 0.6]])
>>> p = np.average(ex, axis=0, weights=[0.2, 0.2, 0.6])
>>> p
array([0.58, 0.42])
>>> np.argmax(p)
0
```

Putting everything together, let's now implement `MajorityVoteClassifier` in Python:

```
from sklearn.base import BaseEstimator
from sklearn.base import ClassifierMixin
from sklearn.preprocessing import LabelEncoder
from sklearn.base import clone
from sklearn.pipeline import _name_estimators
import numpy as np
import operator
class MajorityVoteClassifier(BaseEstimator, ClassifierMixin):
    def __init__(self, classifiers, vote='classlabel', weights=None):

        self.classifiers = classifiers
        self.named_classifiers = {
            key: value for key,
            value in _name_estimators(classifiers)
        }
        self.vote = vote
```

```
        self.weights = weights

    def fit(self, X, y):
        if self.vote not in ('probability', 'classlabel'):
            raise ValueError(f"vote must be 'probability' "
                             f"or 'classlabel'"
                             f"; got (vote={self.vote})")
        if self.weights and
        len(self.weights) != len(self.classifiers):
            raise ValueError(f'Number of classifiers and'
                             f' weights must be equal'
                             f'; got {len(self.weights)} weights,'
                             f' {len(self.classifiers)} classifiers')
        # Use LabelEncoder to ensure class labels start
        # with 0, which is important for np.argmax
        # call in self.predict
        self.lablenc_ = LabelEncoder()
        self.lablenc_.fit(y)
        self.classes_ = self.lablenc_.classes_
        self.classifiers_ = []
        for clf in self.classifiers:
            fitted_clf = clone(clf).fit(X,
                               self.lablenc_.transform(y))
            self.classifiers_.append(fitted_clf)
        return self
```

We've added a lot of comments to the code to explain the individual parts. However, before we implement the remaining methods, let's take a quick break and discuss some of the code that may look confusing at first. We used the `BaseEstimator` and `ClassifierMixin` parent classes to get some base functionality *for free*, including the `get_params` and `set_params` methods to set and return the classifier's parameters, as well as the `score` method to calculate the prediction accuracy.

Next, we will add the `predict` method to predict the class label via a majority vote based on the class labels if we initialize a new `MajorityVoteClassifier` object with `vote='classlabel'`. Alternatively, we will be able to initialize the ensemble classifier with `vote='probability'` to predict the class label based on the class membership probabilities. Furthermore, we will also add a `predict_proba` method to return the averaged probabilities, which is useful when computing the **receiver operating characteristic area under the curve** (**ROC AUC**):

```
    def predict(self, X):
        if self.vote == 'probability':
            maj_vote = np.argmax(self.predict_proba(X), axis=1)
        else: # 'classlabel' vote
```

```
            # Collect results from clf.predict calls
            predictions = np.asarray([
                clf.predict(X) for clf in self.classifiers_
            ]).T

            maj_vote = np.apply_along_axis(
                lambda x: np.argmax(
                    np.bincount(x, weights=self.weights)
                ),
                axis=1, arr=predictions
            )
        maj_vote = self.lablenc_.inverse_transform(maj_vote)
        return maj_vote

    def predict_proba(self, X):
        probas = np.asarray([clf.predict_proba(X)
                             for clf in self.classifiers_])
        avg_proba = np.average(probas, axis=0,
                               weights=self.weights)
        return avg_proba

    def get_params(self, deep=True):
        if not deep:
            return super().get_params(deep=False)
        else:
            out = self.named_classifiers.copy()
            for name, step in self.named_classifiers.items():
                for key, value in step.get_params(
                        deep=True).items():
                    out[f'{name}__{key}'] = value
            return out
```

Also, note that we defined our own modified version of the `get_params` method to use the `_name_estimators` function to access the parameters of individual classifiers in the ensemble; this may look a little bit complicated at first, but it will make perfect sense when we use grid search for hyperparameter tuning in later sections.

VotingClassifier in scikit-learn

Although the `MajorityVoteClassifier` implementation is very useful for demonstration purposes, we implemented a more sophisticated version of this majority vote classifier in scikit-learn based on the implementation in the first edition of this book. The ensemble classifier is available as `sklearn.ensemble.VotingClassifier` in scikit-learn version 0.17 and newer. You can find out more about `VotingClassifier` at `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.VotingClassifier.html`

Using the majority voting principle to make predictions

Now it is time to put the `MajorityVoteClassifier` that we implemented in the previous section into action. But first, let's prepare a dataset that we can test it on. Since we are already familiar with techniques to load datasets from CSV files, we will take a shortcut and load the Iris dataset from scikit-learn's `datasets` module. Furthermore, we will only select two features, *sepal width* and *petal length*, to make the classification task more challenging for illustration purposes. Although our `MajorityVoteClassifier` generalizes to multiclass problems, we will only classify flower examples from the `Iris-versicolor` and `Iris-virginica` classes, with which we will compute the ROC AUC later. The code is as follows:

```
>>> from sklearn import datasets
>>> from sklearn.model_selection import train_test_split
>>> from sklearn.preprocessing import StandardScaler
>>> from sklearn.preprocessing import LabelEncoder
>>> iris = datasets.load_iris()
>>> X, y = iris.data[50:, [1, 2]], iris.target[50:]
>>> le = LabelEncoder()
>>> y = le.fit_transform(y)
```

Class membership probabilities from decision trees

Note that scikit-learn uses the `predict_proba` method (if applicable) to compute the ROC AUC score. In *Chapter 3*, we saw how the class probabilities are computed in logistic regression models. In decision trees, the probabilities are calculated from a frequency vector that is created for each node at training time. The vector collects the frequency values of each class label computed from the class label distribution at that node. Then, the frequencies are normalized so that they sum up to 1. Similarly, the class labels of the k-nearest neighbors are aggregated to return the normalized class label frequencies in the k-nearest neighbors algorithm. Although the normalized probabilities returned by both the decision tree and k-nearest neighbors classifier may look similar to the probabilities obtained from a logistic regression model, we have to be aware that they are actually not derived from probability mass functions.

Next, we will split the Iris examples into 50 percent training and 50 percent test data:

```
>>> X_train, X_test, y_train, y_test =\
...     train_test_split(X, y,
...                      test_size=0.5,
...                      random_state=1,
...                      stratify=y)
```

Using the training dataset, we now will train three different classifiers:

- Logistic regression classifier
- Decision tree classifier
- k-nearest neighbors classifier

We will then evaluate the model performance of each classifier via 10-fold cross-validation on the training dataset before we combine them into an ensemble classifier:

```
>>> from sklearn.model_selection import cross_val_score
>>> from sklearn.linear_model import LogisticRegression
>>> from sklearn.tree import DecisionTreeClassifier
>>> from sklearn.neighbors import KNeighborsClassifier
>>> from sklearn.pipeline import Pipeline
>>> import numpy as np
>>> clf1 = LogisticRegression(penalty='l2',
...                           C=0.001,
...                           solver='lbfgs',
...                           random_state=1)
>>> clf2 = DecisionTreeClassifier(max_depth=1,
...                               criterion='entropy',
...                               random_state=0)
>>> clf3 = KNeighborsClassifier(n_neighbors=1,
...                             p=2,
...                             metric='minkowski')
>>> pipe1 = Pipeline([['sc', StandardScaler()],
...                   ['clf', clf1]])
>>> pipe3 = Pipeline([['sc', StandardScaler()],
...                   ['clf', clf3]])
>>> clf_labels = ['Logistic regression', 'Decision tree', 'KNN']
>>> print('10-fold cross validation:\n')
>>> for clf, label in zip([pipe1, clf2, pipe3], clf_labels):
...     scores = cross_val_score(estimator=clf,
...                              X=X_train,
...                              y=y_train,
```

```
...                             cv=10,
...                             scoring='roc_auc')
...     print(f'ROC AUC: {scores.mean():.2f} '
...           f'(+/- {scores.std():.2f}) [{label}]')
```

The output that we receive, as shown in the following snippet, shows that the predictive performances of the individual classifiers are almost equal:

```
10-fold cross validation:
ROC AUC: 0.92 (+/- 0.15) [Logistic regression]
ROC AUC: 0.87 (+/- 0.18) [Decision tree]
ROC AUC: 0.85 (+/- 0.13) [KNN]
```

You may be wondering why we trained the logistic regression and k-nearest neighbors classifier as part of a pipeline. The reason behind it is that, as discussed in *Chapter 3*, both the logistic regression and k-nearest neighbors algorithms (using the Euclidean distance metric) are not scale-invariant, in contrast to decision trees. Although the Iris features are all measured on the same scale (cm), it is a good habit to work with standardized features.

Now, let's move on to the more exciting part and combine the individual classifiers for majority rule voting in our `MajorityVoteClassifier`:

```
>>> mv_clf = MajorityVoteClassifier(
...     classifiers=[pipe1, clf2, pipe3]
... )
>>> clf_labels += ['Majority voting']
>>> all_clf = [pipe1, clf2, pipe3, mv_clf]
>>> for clf, label in zip(all_clf, clf_labels):
...     scores = cross_val_score(estimator=clf,
...                              X=X_train,
...                              y=y_train,
...                              cv=10,
...                              scoring='roc_auc')
...     print(f'ROC AUC: {scores.mean():.2f} '
...           f'(+/- {scores.std():.2f}) [{label}]')
ROC AUC: 0.92 (+/- 0.15) [Logistic regression]
ROC AUC: 0.87 (+/- 0.18) [Decision tree]
ROC AUC: 0.85 (+/- 0.13) [KNN]
ROC AUC: 0.98 (+/- 0.05) [Majority voting]
```

As you can see, the performance of `MajorityVotingClassifier` has improved over the individual classifiers in the 10-fold cross-validation evaluation.

Evaluating and tuning the ensemble classifier

In this section, we are going to compute the ROC curves from the test dataset to check that `MajorityVoteClassifier` generalizes well with unseen data. We must remember that the test dataset is not to be used for model selection; its purpose is merely to report an unbiased estimate of the generalization performance of a classifier system:

```
>>> from sklearn.metrics import roc_curve
>>> from sklearn.metrics import auc
>>> colors = ['black', 'orange', 'blue', 'green']
>>> linestyles = [':', '--', '-.', '-']
>>> for clf, label, clr, ls \
...     in zip(all_clf, clf_labels, colors, linestyles):
...     # assuming the label of the positive class is 1
...     y_pred = clf.fit(X_train,
...                      y_train).predict_proba(X_test)[:, 1]
...     fpr, tpr, thresholds = roc_curve(y_true=y_test,
...                                      y_score=y_pred)
...     roc_auc = auc(x=fpr, y=tpr)
...     plt.plot(fpr, tpr,
...              color=clr,
...              linestyle=ls,
...              label=f'{label} (auc = {roc_auc:.2f})')
>>> plt.legend(loc='lower right')
>>> plt.plot([0, 1], [0, 1],
...          linestyle='--',
...          color='gray',
...          linewidth=2)
>>> plt.xlim([-0.1, 1.1])
>>> plt.ylim([-0.1, 1.1])
>>> plt.grid(alpha=0.5)
>>> plt.xlabel('False positive rate (FPR)')
>>> plt.ylabel('True positive rate (TPR)')
>>> plt.show()
```

As you can see in the resulting ROC, the ensemble classifier also performs well on the test dataset (ROC AUC = 0.95). However, you can see that the logistic regression classifier performs similarly well on the same dataset, which is probably due to the high variance (in this case, the sensitivity of how we split the dataset) given the small size of the dataset:

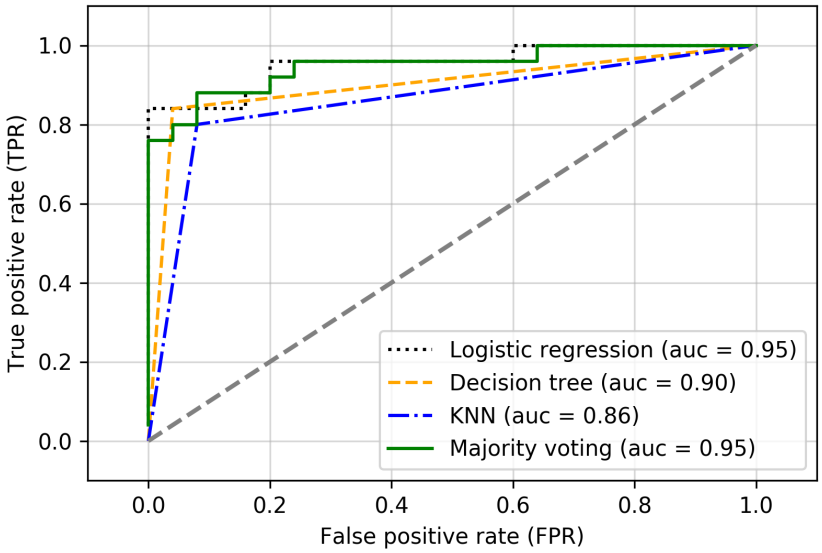


Figure 7.4: The ROC curve for the different classifiers

Since we only selected two features for the classification examples, it would be interesting to see what the decision region of the ensemble classifier actually looks like.

Although it is not necessary to standardize the training features prior to model fitting, because our logistic regression and k-nearest neighbors pipelines will automatically take care of it, we will standardize the training dataset so that the decision regions of the decision tree will be on the same scale for visual purposes. The code is as follows:

```
>>> sc = StandardScaler()
>>> X_train_std = sc.fit_transform(X_train)
>>> from itertools import product
>>> x_min = X_train_std[:, 0].min() - 1
>>> x_max = X_train_std[:, 0].max() + 1
>>> y_min = X_train_std[:, 1].min() - 1
>>>
>>> y_max = X_train_std[:, 1].max() + 1
```

```
>>> xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.1),
...                      np.arange(y_min, y_max, 0.1))
>>> f, axarr = plt.subplots(nrows=2, ncols=2,
...                         sharex='col',
...                         sharey='row',
...                         figsize=(7, 5))
>>> for idx, clf, tt in zip(product([0, 1], [0, 1]),
...                         all_clf, clf_labels):
...     clf.fit(X_train_std, y_train)
...     Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
...     Z = Z.reshape(xx.shape)
...     axarr[idx[0], idx[1]].contourf(xx, yy, Z, alpha=0.3)
...     axarr[idx[0], idx[1]].scatter(X_train_std[y_train==0, 0],
...                                   X_train_std[y_train==0, 1],
...                                   c='blue',
...                                   marker='^',
...                                   s=50)
...     axarr[idx[0], idx[1]].scatter(X_train_std[y_train==1, 0],
...                                   X_train_std[y_train==1, 1],
...                                   c='green',
...                                   marker='o',
...                                   s=50)
...     axarr[idx[0], idx[1]].set_title(tt)
>>> plt.text(-3.5, -5.,
...          s='Sepal width [standardized]',
...          ha='center', va='center', fontsize=12)
>>> plt.text(-12.5, 4.5,
...          s='Petal length [standardized]',
...          ha='center', va='center',
...          fontsize=12, rotation=90)
>>> plt.show()
```

Interestingly, but also as expected, the decision regions of the ensemble classifier seem to be a hybrid of the decision regions from the individual classifiers. At first glance, the majority vote decision boundary looks a lot like the decision of the decision tree stump, which is orthogonal to the *y* axis for *sepal width* ≥ 1.

However, you can also notice the nonlinearity from the k-nearest neighbor classifier mixed in:

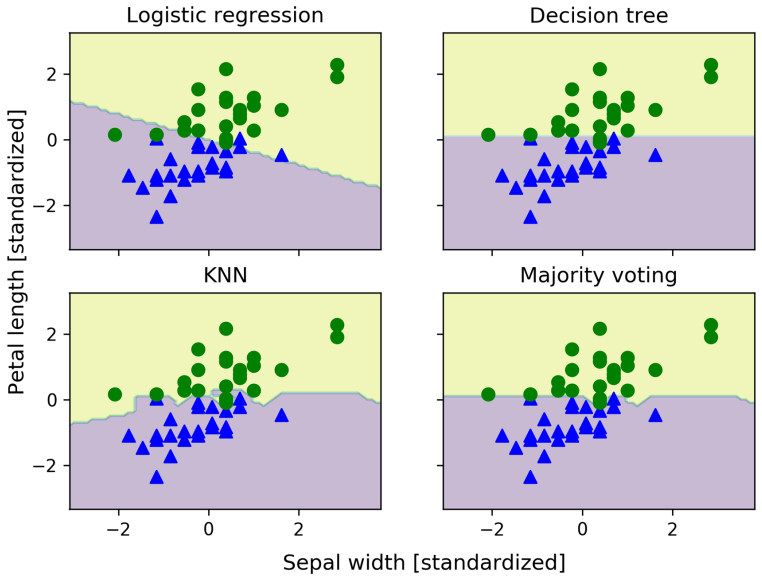


Figure 7.5: The decision boundaries for the different classifiers

Before we tune the individual classifier's parameters for ensemble classification, let's call the `get_params` method to get a basic idea of how we can access the individual parameters inside a `GridSearchCV` object:

```
>>> mv_clf.get_params()
{'decisiontreeclassifier':
 DecisionTreeClassifier(class_weight=None, criterion='entropy',
                        max_depth=1, max_features=None,
                        max_leaf_nodes=None, min_samples_leaf=1,
                        min_samples_split=2,
                        min_weight_fraction_leaf=0.0,
                        random_state=0, splitter='best'),
 'decisiontreeclassifier__class_weight': None,
 'decisiontreeclassifier__criterion': 'entropy',
 [...]
 'decisiontreeclassifier__random_state': 0,
 'decisiontreeclassifier__splitter': 'best',
 'pipeline-1':
 Pipeline(steps=[('sc', StandardScaler(copy=True, with_mean=True,
                                       with_std=True)),
                 ('clf', LogisticRegression(C=0.001,
```

```
                                          class_weight=None,
                                          dual=False,
                                          fit_intercept=True,
                                          intercept_scaling=1,
                                          max_iter=100,
                                          multi_class='ovr',
                                          penalty='l2',
                                          random_state=0,
                                          solver='liblinear',
                                          tol=0.0001,
                                          verbose=0))]),
'pipeline-1__clf':
LogisticRegression(C=0.001, class_weight=None, dual=False,
                   fit_intercept=True, intercept_scaling=1,
                   max_iter=100, multi_class='ovr',
                   penalty='l2', random_state=0,
                   solver='liblinear', tol=0.0001, verbose=0),
'pipeline-1__clf__C': 0.001,
'pipeline-1__clf__class_weight': None,
'pipeline-1__clf__dual': False,
[...]
'pipeline-1__sc__with_std': True,
'pipeline-2':
Pipeline(steps=[('sc', StandardScaler(copy=True, with_mean=True,
                                      with_std=True)),
                ('clf', KNeighborsClassifier(algorithm='auto',
                                             leaf_size=30,
                                             metric='minkowski',
                                             metric_params=None,
                                             n_neighbors=1,
                                             p=2,
                                             weights='uniform'))]),
'pipeline-2__clf':
KNeighborsClassifier(algorithm='auto', leaf_size=30,
                     metric='minkowski', metric_params=None,
                     n_neighbors=1, p=2, weights='uniform'),
'pipeline-2__clf__algorithm': 'auto',
[...]
'pipeline-2__sc__with_std': True}
```

Based on the values returned by the `get_params` method, we now know how to access the individual classifier's attributes. Let's now tune the inverse regularization parameter, `C`, of the logistic regression classifier and the decision tree depth via a grid search for demonstration purposes:

```
>>> from sklearn.model_selection import GridSearchCV
>>> params = {'decisiontreeclassifier__max_depth': [1, 2],
...           'pipeline-1__clf__C': [0.001, 0.1, 100.0]}
>>> grid = GridSearchCV(estimator=mv_clf,
...                     param_grid=params,
...                     cv=10,
...                     scoring='roc_auc')
>>> grid.fit(X_train, y_train)
```

After the grid search has completed, we can print the different hyperparameter value combinations and the average ROC AUC scores computed via 10-fold cross-validation as follows:

```
>>> for r, _ in enumerate(grid.cv_results_['mean_test_score']):
...     mean_score = grid.cv_results_['mean_test_score'][r]
...     std_dev = grid.cv_results_['std_test_score'][r]
...     params = grid.cv_results_['params'][r]
...     print(f'{mean_score:.3f} +/- {std_dev:.2f} {params}')
0.983 +/- 0.05 {'decisiontreeclassifier__max_depth': 1,
                'pipeline-1__clf__C': 0.001}
0.983 +/- 0.05 {'decisiontreeclassifier__max_depth': 1,
                'pipeline-1__clf__C': 0.1}
0.967 +/- 0.10 {'decisiontreeclassifier__max_depth': 1,
                'pipeline-1__clf__C': 100.0}
0.983 +/- 0.05 {'decisiontreeclassifier__max_depth': 2,
                'pipeline-1__clf__C': 0.001}
0.983 +/- 0.05 {'decisiontreeclassifier__max_depth': 2,
                'pipeline-1__clf__C': 0.1}
0.967 +/- 0.10 {'decisiontreeclassifier__max_depth': 2,
                'pipeline-1__clf__C': 100.0}
>>> print(f'Best parameters: {grid.best_params_}')
Best parameters: {'decisiontreeclassifier__max_depth': 1,
                  'pipeline-1__clf__C': 0.001}
>>> print(f'ROC AUC : {grid.best_score_:.2f}')
ROC AUC: 0.98
```

As you can see, we get the best cross-validation results when we choose a lower regularization strength (`C=0.001`), whereas the tree depth does not seem to affect the performance at all, suggesting that a decision stump is sufficient to separate the data. To remind ourselves that it is a bad practice to use the test dataset more than once for model evaluation, we are not going to estimate the generalization performance of the tuned hyperparameters in this section. We will move on swiftly to an alternative approach for ensemble learning: **bagging**.

Building ensembles using stacking

The majority vote approach we implemented in this section is not to be confused with stacking. The stacking algorithm can be understood as a two-level ensemble, where the first level consists of individual classifiers that feed their predictions to the second level, where another classifier (typically logistic regression) is fit to the level-one classifier predictions to make the final predictions. For more information on stacking, see the following resources:

- The stacking algorithm has been described in more detail by David H. Wolpert in *Stacked generalization*, *Neural Networks*, 5(2):241–259, 1992 (`https://www.sciencedirect.com/science/article/pii/S0893608005800231`).
- Interested readers can find our video tutorial about stacking on YouTube at `https://www.youtube.com/watch?v=8T2emza6g80`.
- A scikit-learn compatible version of a stacking classifier is available from mlxtend: `http://rasbt.github.io/mlxtend/user_guide/classifier/StackingCVClassifier/`.
- Also, a `StackingClassifier` has recently been added to scikit-learn (available in version 0.22 and newer); for more information, please see the documentation at `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.StackingClassifier.html`.

Bagging – building an ensemble of classifiers from bootstrap samples

Bagging is an ensemble learning technique that is closely related to the `MajorityVoteClassifier` that we implemented in the previous section. However, instead of using the same training dataset to fit the individual classifiers in the ensemble, we draw bootstrap samples (random samples with replacement) from the initial training dataset, which is why bagging is also known as *bootstrap aggregating*.

The concept of bagging is summarized in *Figure 7.6*:

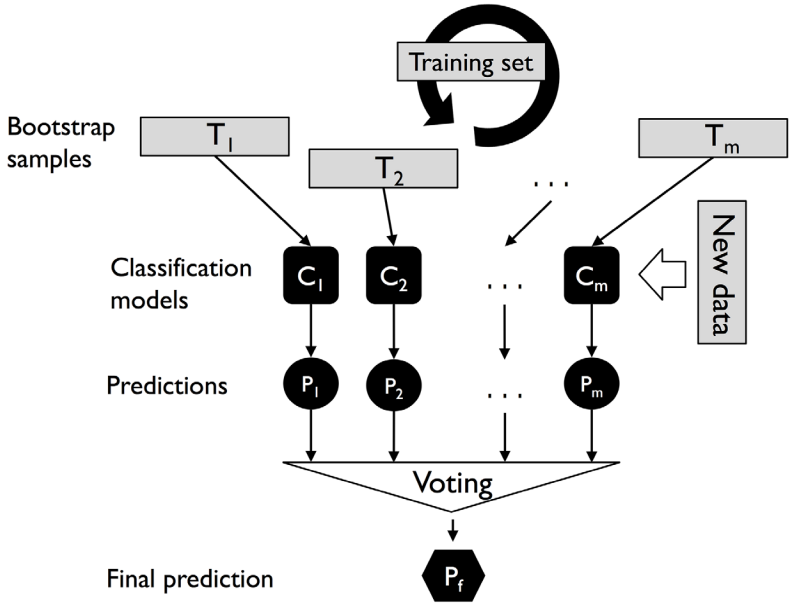


Figure 7.6: The concept of bagging

In the following subsections, we will work through a simple example of bagging by hand and use scikit-learn for classifying wine examples.

Bagging in a nutshell

To provide a more concrete example of how the bootstrap aggregating of a bagging classifier works, let's consider the example shown in *Figure 7.7*. Here, we have seven different training instances (denoted as indices 1-7) that are sampled randomly with replacement in each round of bagging. Each bootstrap sample is then used to fit a classifier, C_j, which is most typically an unpruned decision tree:

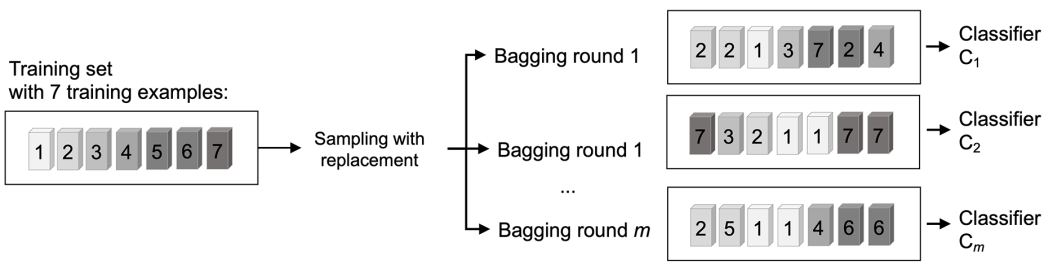


Figure 7.7: An example of bagging

As you can see from *Figure 7.7*, each classifier receives a random subset of examples from the training dataset. We denote these random samples obtained via bagging as *Bagging round 1*, *Bagging round 2*, and so on. Each subset contains a certain portion of duplicates and some of the original examples don't appear in a resampled dataset at all due to sampling with replacement. Once the individual classifiers are fit to the bootstrap samples, the predictions are combined using majority voting.

Note that bagging is also related to the random forest classifier that we introduced in *Chapter 3*. In fact, random forests are a special case of bagging where we also use random feature subsets when fitting the individual decision trees.

Model ensembles using bagging

Bagging was first proposed by Leo Breiman in a technical report in 1994; he also showed that bagging can improve the accuracy of unstable models and decrease the degree of overfitting. We highly recommend that you read about his research in *Bagging predictors* by *L. Breiman*, *Machine Learning*, 24(2):123–140, 1996, which is freely available online, to learn more details about bagging.

Applying bagging to classify examples in the Wine dataset

To see bagging in action, let's create a more complex classification problem using the Wine dataset that was introduced in *Chapter 4*, *Building Good Training Datasets – Data Preprocessing*. Here, we will only consider the Wine classes 2 and 3, and we will select two features – `Alcohol` and `OD280/OD315 of diluted wines`:

```
>>> import pandas as pd
>>> df_wine = pd.read_csv('https://archive.ics.uci.edu/ml/'
...                       'machine-learning-databases/'
...                       'wine/wine.data',
...                       header=None)
>>> df_wine.columns = ['Class label', 'Alcohol',
...                    'Malic acid', 'Ash',
...                    'Alcalinity of ash',
...                    'Magnesium', 'Total phenols',
...                    'Flavanoids', 'Nonflavanoid phenols',
...                    'Proanthocyanins',
...                    'Color intensity', 'Hue',
...                    'OD280/OD315 of diluted wines',
...                    'Proline']
>>> # drop 1 class
>>> df_wine = df_wine[df_wine['Class label'] != 1]
>>> y = df_wine['Class label'].values
>>> X = df_wine[['Alcohol',
...              'OD280/OD315 of diluted wines']].values
```

Next, we will encode the class labels into binary format and split the dataset into 80 percent training and 20 percent test datasets:

```
>>> from sklearn.preprocessing import LabelEncoder
>>> from sklearn.model_selection import train_test_split
>>> le = LabelEncoder()
>>> y = le.fit_transform(y)
>>> X_train, X_test, y_train, y_test =\
...            train_test_split(X, y,
...                             test_size=0.2,
...                             random_state=1,
...                             stratify=y)
```

Obtaining the Wine dataset

You can find a copy of the Wine dataset (and all other datasets used in this book) in the code bundle of this book, which you can use if you are working offline or the UCI server at `https://archive.ics.uci.edu/ml/machine-learning-databases/wine/wine.data` is temporarily unavailable. For instance, to load the Wine dataset from a local directory, take the following lines:

```
df = pd.read_csv('https://archive.ics.uci.edu/ml/'
                 'machine-learning-databases'
                 '/wine/wine.data',
                 header=None)
```

and replace them with these:

```
df = pd.read_csv('your/local/path/to/wine.data',
                 header=None)
```

A `BaggingClassifier` algorithm is already implemented in scikit-learn, which we can import from the `ensemble` submodule. Here, we will use an unpruned decision tree as the base classifier and create an ensemble of 500 decision trees fit on different bootstrap samples of the training dataset:

```
>>> from sklearn.ensemble import BaggingClassifier
>>> tree = DecisionTreeClassifier(criterion='entropy',
...                               random_state=1,
...                               max_depth=None)
>>> bag = BaggingClassifier(base_estimator=tree,
...                         n_estimators=500,
...                         max_samples=1.0,
...                         max_features=1.0,
...                         bootstrap=True,
```

```
...                         bootstrap_features=False,
...                         n_jobs=1,
...                         random_state=1)
```

Next, we will calculate the accuracy score of the prediction on the training and test datasets to compare the performance of the bagging classifier to the performance of a single unpruned decision tree:

```
>>> from sklearn.metrics import accuracy_score
>>> tree = tree.fit(X_train, y_train)
>>> y_train_pred = tree.predict(X_train)
>>> y_test_pred = tree.predict(X_test)
>>> tree_train = accuracy_score(y_train, y_train_pred)
>>> tree_test = accuracy_score(y_test, y_test_pred)
>>> print(f'Decision tree train/test accuracies '
...       f'{tree_train:.3f}/{tree_test:.3f}')
Decision tree train/test accuracies 1.000/0.833
```

Based on the accuracy values that we printed here, the unpruned decision tree predicts all the class labels of the training examples correctly; however, the substantially lower test accuracy indicates high variance (overfitting) of the model:

```
>>> bag = bag.fit(X_train, y_train)
>>> y_train_pred = bag.predict(X_train)
>>> y_test_pred = bag.predict(X_test)
>>> bag_train = accuracy_score(y_train, y_train_pred)
>>> bag_test = accuracy_score(y_test, y_test_pred)
>>> print(f'Bagging train/test accuracies '
...       f'{bag_train:.3f}/{bag_test:.3f}')
Bagging train/test accuracies 1.000/0.917
```

Although the training accuracies of the decision tree and bagging classifier are similar on the training dataset (both 100 percent), we can see that the bagging classifier has a slightly better generalization performance, as estimated on the test dataset. Next, let's compare the decision regions between the decision tree and the bagging classifier:

```
>>> x_min = X_train[:, 0].min() - 1
>>> x_max = X_train[:, 0].max() + 1
>>> y_min = X_train[:, 1].min() - 1
>>> y_max = X_train[:, 1].max() + 1
>>> xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.1),
...                      np.arange(y_min, y_max, 0.1))
>>> f, axarr = plt.subplots(nrows=1, ncols=2,
...                         sharex='col',
...                         sharey='row',
```

```
...                          figsize=(8, 3))
>>> for idx, clf, tt in zip([0, 1],
...                         [tree, bag],
...                         ['Decision tree', 'Bagging']):
...     clf.fit(X_train, y_train)
...
...     Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
...     Z = Z.reshape(xx.shape)
...     axarr[idx].contourf(xx, yy, Z, alpha=0.3)
...     axarr[idx].scatter(X_train[y_train==0, 0],
...                        X_train[y_train==0, 1],
...                        c='blue', marker='^')
...     axarr[idx].scatter(X_train[y_train==1, 0],
...                        X_train[y_train==1, 1],
...                        c='green', marker='o')
...     axarr[idx].set_title(tt)
>>> axarr[0].set_ylabel('OD280/OD315 of diluted wines', fontsize=12)
>>> plt.tight_layout()
>>> plt.text(0, -0.2,
...          s='Alcohol',
...          ha='center',
...          va='center',
...          fontsize=12,
...          transform=axarr[1].transAxes)
>>> plt.show()
```

As we can see in the resulting plot, the piece-wise linear decision boundary of the three-node deep decision tree looks smoother in the bagging ensemble:

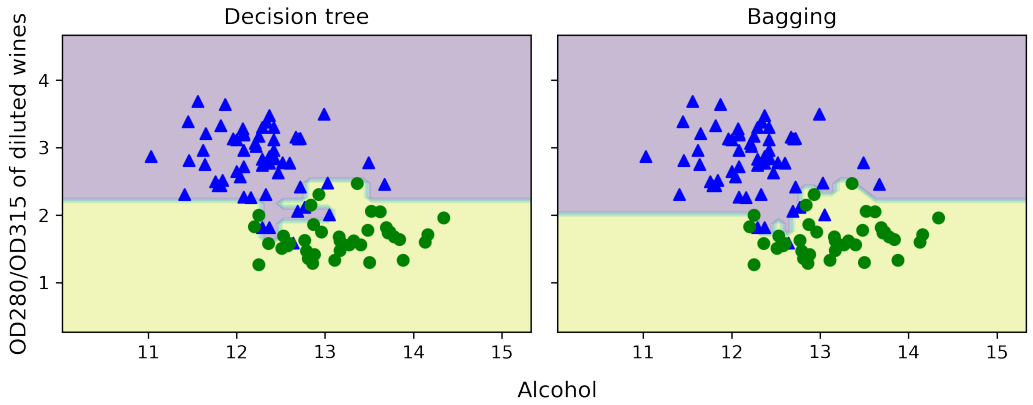


Figure 7.8: The piece-wise linear decision boundary of a decision tree versus bagging

We only looked at a very simple bagging example in this section. In practice, more complex classification tasks and a dataset's high dimensionality can easily lead to overfitting in single decision trees, and this is where the bagging algorithm can really play to its strengths. Finally, we must note that the bagging algorithm can be an effective approach to reducing the variance of a model. However, bagging is ineffective in reducing model bias, that is, models that are too simple to capture the trends in the data well. This is why we want to perform bagging on an ensemble of classifiers with low bias, for example, unpruned decision trees.

Leveraging weak learners via adaptive boosting

In this last section about ensemble methods, we will discuss **boosting**, with a special focus on its most common implementation: **Adaptive Boosting** (**AdaBoost**).

AdaBoost recognition

The original idea behind AdaBoost was formulated by Robert E. Schapire in 1990 in *The Strength of Weak Learnability*, *Machine Learning*, 5(2): 197-227, 1990, URL: `http://rob.schapire.net/papers/strengthofweak.pdf`. After Robert Schapire and Yoav Freund presented the AdaBoost algorithm in the *Proceedings of the Thirteenth International Conference* (ICML 1996), AdaBoost became one of the most widely used ensemble methods in the years that followed (*Experiments with a New Boosting Algorithm* by *Y. Freund*, *R. E. Schapire*, and others, *ICML*, volume 96, 148-156, 1996). In 2003, Freund and Schapire received the Gödel Prize for their groundbreaking work, which is a prestigious prize for the most outstanding publications in the field of computer science.

In boosting, the ensemble consists of very simple base classifiers, also often referred to as **weak learners**, which often only have a slight performance advantage over random guessing—a typical example of a weak learner is a decision tree stump. The key concept behind boosting is to focus on training examples that are hard to classify, that is, to let the weak learners subsequently learn from misclassified training examples to improve the performance of the ensemble.

The following subsections will introduce the algorithmic procedure behind the general concept of boosting and AdaBoost. Lastly, we will use scikit-learn for a practical classification example.

How adaptive boosting works

In contrast to bagging, the initial formulation of the boosting algorithm uses random subsets of training examples drawn from the training dataset without replacement; the original boosting procedure can be summarized in the following four key steps:

1. Draw a random subset (sample) of training examples, d_1, without replacement from the training dataset, D, to train a weak learner, C_1.
2. Draw a second random training subset, d_2, without replacement from the training dataset and add 50 percent of the examples that were previously misclassified to train a weak learner, C_2.

3. Find the training examples, d_3, in the training dataset, D, which C_1 and C_2 disagree upon, to train a third weak learner, C_3.
4. Combine the weak learners C_1, C_2, and C_3 via majority voting.

As discussed by Leo Breiman (*Bias, variance, and arcing classifiers*, 1996), boosting can lead to a decrease in bias as well as variance compared to bagging models. In practice, however, boosting algorithms such as AdaBoost are also known for their high variance, that is, the tendency to overfit the training data (*An improvement of AdaBoost to avoid overfitting* by *G. Raetsch*, *T. Onoda*, and *K. R. Mueller*. *Proceedings of the International Conference on Neural Information Processing*, *CiteSeer*, 1998).

In contrast to the original boosting procedure described here, AdaBoost uses the complete training dataset to train the weak learners, where the training examples are reweighted in each iteration to build a strong classifier that learns from the mistakes of the previous weak learners in the ensemble.

Before we dive deeper into the specific details of the AdaBoost algorithm, let's take a look at *Figure 7.9* to get a better grasp of the basic concept behind AdaBoost:

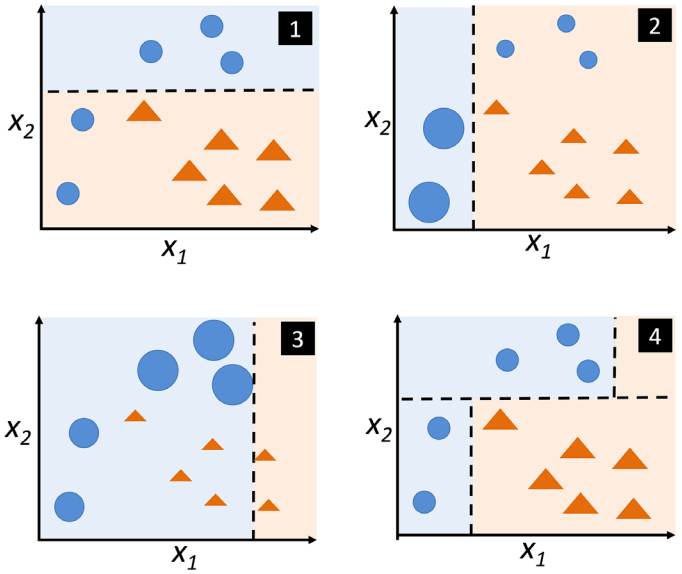


Figure 7.9: The concept of AdaBoost to improve weak learners

To walk through the AdaBoost illustration step by step, we will start with subfigure **1**, which represents a training dataset for binary classification where all training examples are assigned equal weights. Based on this training dataset, we train a decision stump (shown as a dashed line) that tries to classify the examples of the two classes (triangles and circles), as well as possibly minimizing the loss function (or the impurity score in the special case of decision tree ensembles).

For the next round (subfigure **2**), we assign a larger weight to the two previously misclassified examples (circles). Furthermore, we lower the weight of the correctly classified examples. The next decision stump will now be more focused on the training examples that have the largest weights—the training examples that are supposedly hard to classify.

The weak learner shown in subfigure **2** misclassifies three different examples from the circle class, which are then assigned a larger weight, as shown in subfigure **3**.

Assuming that our AdaBoost ensemble only consists of three rounds of boosting, we then combine the three weak learners trained on different reweighted training subsets by a weighted majority vote, as shown in subfigure **4**.

Now that we have a better understanding of the basic concept of AdaBoost, let's take a more detailed look at the algorithm using pseudo code. For clarity, we will denote element-wise multiplication by the cross symbol (×) and the dot-product between two vectors by a dot symbol (·):

1. Set the weight vector, $\boldsymbol{w}$, to uniform weights, where $\sum_i w_i = 1$.
2. For j in m boosting rounds, do the following:
    a. Train a weighted weak learner: $C_j = \text{train}(\boldsymbol{X}, \boldsymbol{y}, \boldsymbol{w})$.
    b. Predict class labels: $\hat{\boldsymbol{y}} = \text{predict}(C_j, \boldsymbol{X})$.
    c. Compute the weighted error rate: $\varepsilon = \boldsymbol{w} \cdot (\hat{\boldsymbol{y}} \neq \boldsymbol{y})$.
    d. Compute the coefficient: $\alpha_j = 0.5 \log \frac{1-\varepsilon}{\varepsilon}$.
    e. Update the weights: $\boldsymbol{w} := \boldsymbol{w} \times \exp(-\alpha_j \times \hat{\boldsymbol{y}} \times \boldsymbol{y})$.
    f. Normalize the weights to sum to 1: $\boldsymbol{w} := \boldsymbol{w} / \sum_i w_i$.
3. Compute the final prediction: $\hat{\boldsymbol{y}} = \left(\sum_{j=1}^{m} (\alpha_j \times \text{predict}(C_j, \boldsymbol{X})) > 0\right)$.

Note that the expression $(\hat{\boldsymbol{y}} \neq \boldsymbol{y})$ in *step 2c* refers to a binary vector consisting of 1s and 0s, where a 1 is assigned if the prediction is incorrect and 0 is assigned otherwise.

Although the AdaBoost algorithm seems to be pretty straightforward, let's walk through a more concrete example using a training dataset consisting of 10 training examples, as illustrated in *Figure 7.10*:

Index	x	y	Weights	$\hat{y}$(x <= 3.0)?	Correct?	Updated weights
1	1.0	1	0.1	1	Yes	0.072
2	2.0	1	0.1	1	Yes	0.072
3	3.0	1	0.1	1	Yes	0.072
4	4.0	-1	0.1	-1	Yes	0.072
5	5.0	-1	0.1	-1	Yes	0.072
6	6.0	-1	0.1	-1	Yes	0.072
7	7.0	1	0.1	-1	No	0.167
8	8.0	1	0.1	-1	No	0.167
9	9.0	1	0.1	-1	No	0.167
10	10.0	-1	0.1	-1	Yes	0.072

Figure 7.10: Running 10 training examples through the AdaBoost algorithm

The first column of the table depicts the indices of training examples 1 to 10. In the second column, you can see the feature values of the individual samples, assuming this is a one-dimensional dataset. The third column shows the true class label, y_i, for each training sample, x_i, where $y_i \in \{1, -1\}$. The initial weights are shown in the fourth column; we initialize the weights uniformly (assigning the same constant value) and normalize them to sum to 1. In the case of the 10-sample training dataset, we therefore assign 0.1 to each weight, w_i, in the weight vector, $\boldsymbol{w}$. The predicted class labels, $\hat{\boldsymbol{y}}$, are shown in the fifth column, assuming that our splitting criterion is $x \leq 3.0$. The last column of the table then shows the updated weights based on the update rules that we defined in the pseudo code.

Since the computation of the weight updates may look a little bit complicated at first, we will now follow the calculation step by step. We will start by computing the weighted error rate, ε (`epsilon`), as described in *step 2c*:

```
>>> y = np.array([1, 1, 1, -1, -1, -1,  1,  1,  1, -1])
>>> yhat = np.array([1, 1, 1, -1, -1, -1, -1, -1, -1, -1])
>>> correct = (y == yhat)
>>> weights = np.full(10, 0.1)
>>> print(weights)
[0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1 0.1]
>>> epsilon = np.mean(~correct)
>>> print(epsilon)
0.3
```

Note that `correct` is a Boolean array consisting of `True` and `False` values where `True` indicates that a prediction is correct. Via `~correct`, we invert the array such that `np.mean(~correct)` computes the proportion of incorrect predictions (`True` counts as the value 1 and `False` as 0), that is, the classification error.

Next, we will compute the coefficient, α_j—shown in *step 2d*—which will later be used in *step 2e* to update the weights, as well as for the weights in the majority vote prediction (*step 3*):

```
>>> alpha_j = 0.5 * np.log((1-epsilon) / epsilon)
>>> print(alpha_j)
0.42364893019360184
```

After we have computed the coefficient, α_j (`alpha_j`), we can now update the weight vector using the following equation:

$$\boldsymbol{w} := \boldsymbol{w} \times \exp(-\alpha_j \times \hat{\boldsymbol{y}} \times \boldsymbol{y})$$

Here, $\hat{\boldsymbol{y}} \times \boldsymbol{y}$ is an element-wise multiplication between the vectors of the predicted and true class labels, respectively. Thus, if a prediction, $\hat{y}_i$, is correct, $\hat{y}_i \times y_i$ will have a positive sign so that we decrease the ith weight, since α_j is a positive number as well:

```
>>> update_if_correct = 0.1 * np.exp(-alpha_j * 1 * 1)
>>> print(update_if_correct)
0.06546536707079771
```

Similarly, we will increase the ith weight if $\hat{y}_i$ predicted the label incorrectly, like this:

```
>>> update_if_wrong_1 = 0.1 * np.exp(-alpha_j * 1 * -1)
>>> print(update_if_wrong_1)
0.1527525231651947
```

Alternatively, it's like this:

```
>>> update_if_wrong_2 = 0.1 * np.exp(-alpha_j * -1 * 1)
>>> print(update_if_wrong_2)
0.1527525231651947
```

We can use these values to update the weights as follows:

```
>>> weights = np.where(correct == 1,
...                    update_if_correct,
...                    update_if_wrong_1)
>>> print(weights)
array([0.06546537, 0.06546537, 0.06546537, 0.06546537, 0.06546537,
       0.06546537, 0.15275252, 0.15275252, 0.15275252, 0.06546537])
```

The code above assigned the `update_if_correct` value to all correct predictions and the `update_if_wrong_1` value to all wrong predictions. We omitted using `update_if_wrong_2` for simplicity, since it is similar to `update_if_wrong_1` anyway.

After we have updated each weight in the weight vector, we normalize the weights so that they sum up to 1 (*step 2f*):

$$\boldsymbol{w} := \frac{\boldsymbol{w}}{\sum_i w_i}$$

In code, we can accomplish that as follows:

```
>>> normalized_weights = weights / np.sum(weights)
>>> print(normalized_weights)
[0.07142857 0.07142857 0.07142857 0.07142857 0.07142857 0.07142857
 0.16666667 0.16666667 0.16666667 0.07142857]
```

Thus, each weight that corresponds to a correctly classified example will be reduced from the initial value of 0.1 to 0.0714 for the next round of boosting. Similarly, the weights of the incorrectly classified examples will increase from 0.1 to 0.1667.

Applying AdaBoost using scikit-learn

The previous subsection introduced AdaBoost in a nutshell. Skipping to the more practical part, let's now train an AdaBoost ensemble classifier via scikit-learn. We will use the same Wine subset that we used in the previous section to train the bagging meta-classifier.

Via the `base_estimator` attribute, we will train the `AdaBoostClassifier` on 500 decision tree stumps:

```
>>> from sklearn.ensemble import AdaBoostClassifier
>>> tree = DecisionTreeClassifier(criterion='entropy',
...                               random_state=1,
...                               max_depth=1)
>>> ada = AdaBoostClassifier(base_estimator=tree,
...                          n_estimators=500,
...                          learning_rate=0.1,
...                          random_state=1)
>>> tree = tree.fit(X_train, y_train)
>>> y_train_pred = tree.predict(X_train)
>>> y_test_pred = tree.predict(X_test)
>>> tree_train = accuracy_score(y_train, y_train_pred)
>>> tree_test = accuracy_score(y_test, y_test_pred)
>>> print(f'Decision tree train/test accuracies '
...       f'{tree_train:.3f}/{tree_test:.3f}')
Decision tree train/test accuracies 0.916/0.875
```

As you can see, the decision tree stump seems to underfit the training data in contrast to the unpruned decision tree that we saw in the previous section:

```
>>> ada = ada.fit(X_train, y_train)
>>> y_train_pred = ada.predict(X_train)
>>> y_test_pred = ada.predict(X_test)
>>> ada_train = accuracy_score(y_train, y_train_pred)
>>> ada_test = accuracy_score(y_test, y_test_pred)
>>> print(f'AdaBoost train/test accuracies '
...       f'{ada_train:.3f}/{ada_test:.3f}')
AdaBoost train/test accuracies 1.000/0.917
```

Here, you can see that the AdaBoost model predicts all class labels of the training dataset correctly and also shows a slightly improved test dataset performance compared to the decision tree stump. However, you can also see that we introduced additional variance with our attempt to reduce the model bias—a greater gap between training and test performance.

Although we used another simple example for demonstration purposes, we can see that the performance of the AdaBoost classifier is slightly improved compared to the decision stump and achieved very similar accuracy scores as the bagging classifier that we trained in the previous section. However, we must note that it is considered bad practice to select a model based on the repeated usage of the test dataset. The estimate of the generalization performance may be overoptimistic, which we discussed in more detail in *Chapter 6*, *Learning Best Practices for Model Evaluation and Hyperparameter Tuning*.

Lastly, let's check what the decision regions look like:

```
>>> x_min = X_train[:, 0].min() - 1
>>> x_max = X_train[:, 0].max() + 1
>>> y_min = X_train[:, 1].min() - 1
>>> y_max = X_train[:, 1].max() + 1
>>> xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.1),
...                      np.arange(y_min, y_max, 0.1))
>>> f, axarr = plt.subplots(1, 2,
...                         sharex='col',
...                         sharey='row',
...                         figsize=(8, 3))
>>> for idx, clf, tt in zip([0, 1],
...                         [tree, ada],
...                         ['Decision tree', 'AdaBoost']):
...     clf.fit(X_train, y_train)
...     Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
...     Z = Z.reshape(xx.shape)
...     axarr[idx].contourf(xx, yy, Z, alpha=0.3)
...     axarr[idx].scatter(X_train[y_train==0, 0],
...                        X_train[y_train==0, 1],
...                        c='blue',
...                        marker='^')
...     axarr[idx].scatter(X_train[y_train==1, 0],
...                        X_train[y_train==1, 1],
...                        c='green',
...                        marker='o')
...     axarr[idx].set_title(tt)
...     axarr[0].set_ylabel('OD280/OD315 of diluted wines', fontsize=12)
>>> plt.tight_layout()
>>> plt.text(0, -0.2,
...          s='Alcohol',
...          ha='center',
...          va='center',
...          fontsize=12,
...          transform=axarr[1].transAxes)
>>> plt.show()
```

By looking at the decision regions, you can see that the decision boundary of the AdaBoost model is substantially more complex than the decision boundary of the decision stump. In addition, note that the AdaBoost model separates the feature space very similarly to the bagging classifier that we trained in the previous section:

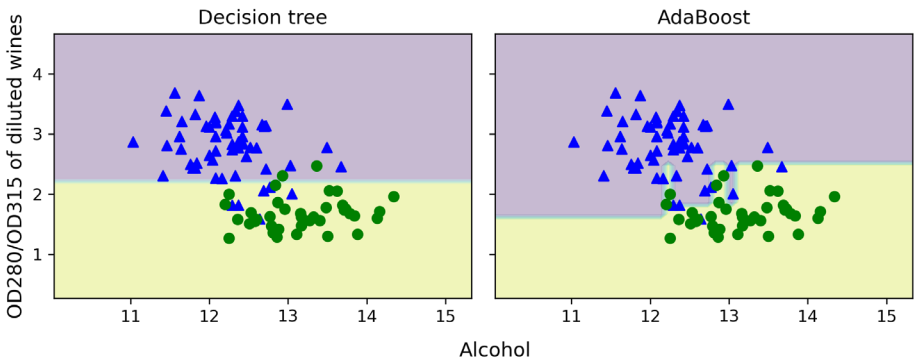


Figure 7.11: The decision boundaries of the decision tree versus AdaBoost

As concluding remarks about ensemble techniques, it is worth noting that ensemble learning increases the computational complexity compared to individual classifiers. In practice, we need to think carefully about whether we want to pay the price of increased computational costs for an often relatively modest improvement in predictive performance.

An often-cited example of this tradeoff is the famous $1 million *Netflix Prize*, which was won using ensemble techniques. The details about the algorithm were published in *The BigChaos Solution to the Netflix Grand Prize* by *A. Toescher*, *M. Jahrer*, and *R. M. Bell*, *Netflix Prize documentation*, 2009, which is available at `http://www.stat.osu.edu/~dmsl/GrandPrize2009_BPC_BigChaos.pdf`. The winning team received the $1 million grand prize money; however, Netflix never implemented their model due to its complexity, which made it infeasible for a real-world application:

> *"We evaluated some of the new methods offline but the additional accuracy gains that we measured did not seem to justify the engineering effort needed to bring them into a production environment."*
>
> `http://techblog.netflix.com/2012/04/netflix-recommendations-beyond-5-stars.html`

Gradient boosting — training an ensemble based on loss gradients

Gradient boosting is another variant of the boosting concept introduced in the previous section, that is, successively training weak learners to create a strong ensemble. Gradient boosting is an extremely important topic because it forms the basis of popular machine learning algorithms such as XGBoost, which is well-known for winning Kaggle competitions.

The gradient boosting algorithm may appear a bit daunting at first. So, in the following subsections, we will cover it step by step, starting with a general overview. Then, we will see how gradient boosting is used for classification and walk through an example. Finally, after we've introduced the fundamental concepts of gradient boosting, we will take a brief look at popular implementations, such as XGBoost, and we will see how we can use gradient boosting in practice.

Comparing AdaBoost with gradient boosting

Fundamentally, gradient boosting is very similar to AdaBoost, which we discussed previously in this chapter. AdaBoost trains decision tree stumps based on errors of the previous decision tree stump. In particular, the errors are used to compute sample weights in each round as well as for computing a classifier weight for each decision tree stump when combining the individual stumps into an ensemble. We stop training once a maximum number of iterations (decision tree stumps) is reached. Like AdaBoost, gradient boosting fits decision trees in an iterative fashion using prediction errors. However, gradient boosting trees are usually deeper than decision tree stumps and have typically a maximum depth of 3 to 6 (or a maximum number of 8 to 64 leaf nodes). Also, in contrast to AdaBoost, gradient boosting does not use the prediction errors for assigning sample weights; they are used directly to form the target variable for fitting the next tree. Moreover, instead of having an individual weighting term for each tree, like in AdaBoost, gradient boosting uses a global learning rate that is the same for each tree.

As you can see, AdaBoost and gradient boosting share several similarities but differ in certain key aspects. In the following subsection, we will sketch the general outline of the gradient boosting algorithm.

Outlining the general gradient boosting algorithm

In this section, we will look at gradient boosting for classification. For simplicity, we will look at a binary classification example. Interested readers can find the generalization to the multi-class setting with logistic loss in *Section 4.6. Multiclass logistic regression and classification* of the original gradient boosting paper written by Friedman in 2001, *Greedy function approximation: A gradient boosting machine*, `https://projecteuclid.org/journals/annals-of-statistics/volume-29/issue-5/Greedy-function-approximation-A-gradient-boostingmachine/10.1214/aos/1013203451.full`.

Gradient boosting for regression

Note that the procedure behind gradient boosting is a bit more complicated than AdaBoost. We omit a simpler regression example, which was given in Friedman's paper, for brevity, but interested readers are encouraged to also consider my complementary video tutorial on gradient boosting for regression, which is available at: `https://www.youtube.com/watch?v=zblsrxc7XpM`.

In essence, gradient boosting builds a series of trees, where each tree is fit on the error—the difference between the label and the predicted value—of the previous tree. In each round, the tree ensemble improves as we are nudging each tree more in the right direction via small updates. These updates are based on a loss gradient, which is how gradient boosting got its name.

The following steps will introduce the general algorithm behind gradient boosting. After illustrating the main steps, we will dive into some of its parts in more detail and walk through a hands-on example in the next subsections.

1. Initialize a model to return a constant prediction value. For this, we use a decision tree root node; that is, a decision tree with a single leaf node. We denote the value returned by the tree as $\hat{y}$, and we find this value by minimizing a differentiable loss function L that we will define later:

$$F_0(x) = \arg\min_{\hat{y}} \sum_{i=1}^{n} L(y_i, \hat{y})$$

   Here, n refers to the n training examples in our dataset.

2. For each tree $m = 1, \ldots, M$, where M is a user-specified total number of trees, we carry out the following computations outlined in *steps 2a* to *2d* below:

   a. Compute the difference between a predicted value $F(x_i) = \hat{y}_i$ and the class label y_i. This value is sometimes called the *pseudo-response* or *pseudo-residual*. More formally, we can write this pseudo-residual as the negative gradient of the loss function with respect to the predicted values:

$$r_{im} = -\left[\frac{\partial\, L(y_i, F(x_i))}{\partial\, F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, \ldots, n$$

   Note that in the notation above $F(x)$ is the prediction of the previous tree, $F_{m-1}(x)$. So, in the first round, this refers to the constant value from the tree (single leaf node) from step 1.

   b. Fit a tree to the pseudo-residuals r_{im}. We use the notation R_{jm} to denote the $j = 1 \ldots J_m$ leaf nodes of the resulting tree in iteration m.

c. For each leaf node R_{jm}, we compute the following output value:

$$\gamma_{jm} = \arg\min_{\gamma} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma)$$

In the next subsection, we will dive deeper into how this γ_{jm} is computed by minimizing the loss function. At this point, we can already note that leaf nodes R_{jm} may contain more than one training example, hence the summation.

d. Update the model by adding the output values γ_m to the previous tree:

$$F_m(x) = F_{m-1}(x) + \eta\gamma_m$$

However, instead of adding the full predicted values of the current tree γ_m to the previous tree F_{m-1}, we scale γ_m by a learning rate η, which is typically a small value between 0.01 and 1. In other words, we update the model incrementally by taking small steps, which helps avoid overfitting.

Now, after looking at the general structure of gradient boosting, we will adopt these mechanics to look at gradient boosting for classification.

Explaining the gradient boosting algorithm for classification

In this subsection, we will go over the details for implementing the gradient boosting algorithm for binary classification. In this context, we will be using the logistic loss function that we introduced for logistic regression in *Chapter 3*, *A Tour of Machine Learning Classifiers Using Scikit-Learn*. For a single training example, we can specify the logistic loss as follows:

$$L_i = -y_i \log p_i + (1 - y_i) \log(1 - p_i)$$

In *Chapter 3*, we also introduced the log(odds):

$$\hat{y} = \log(\text{odds}) = \log\left(\frac{p}{1-p}\right)$$

For reasons that will make sense later, we will use these log(odds) to rewrite the logistic function as follows (omitting intermediate steps here):

$$L_i = \log\left(1 + e^{\hat{y}_i}\right) - y_i\hat{y}_i$$

Now, we can define the partial derivative of the loss function with respect to these log(odds), $\hat{y}$. The derivative of this loss function with respect to the log(odds) is:

$$\frac{\partial L_i}{\partial \hat{y}_i} = \frac{e^{\hat{y}_i}}{1 + e^{\hat{y}_i}} - y_i = p_i - y_i$$

After specifying these mathematical definitions, let us now revisit the general gradient boosting *steps 1* to *2d* from the previous section and reformulate them for this binary classification scenario.

1. Create a root node that minimizes the logistic loss. It turns out that the loss is minimized if the root node returns the log(odds), $\hat{y}$.
2. For each tree $m = 1, ..., M$, where M is a user-specified number of total trees, we carry out the following computations outlined in *steps 2a* to *2d*:

    a. We convert the log(odds) into a probability using the familiar logistic function that we used in logistic regression (in *Chapter 3*):

    $$p = \frac{1}{1 + e^{-\hat{y}}}$$

    Then, we compute the pseudo-residual, which is the negative partial derivative of the loss with respect to the log(odds), which turns out to be the difference between the class label and the predicted probability:

    $$-\frac{\partial L_i}{\partial \hat{y}_i} = y_i - p_i$$

    b. Fit a new tree to the pseudo-residuals.

    c. For each leaf node R_{jm}, compute a value γ_{jm} that minimizes the logistic loss function. This includes a summarization step for dealing with leaf nodes that contain multiple training examples:

    $$\begin{aligned}\gamma_{jm} &= \arg\min_{\gamma} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma) \\ &= \log\left(1 + e^{\hat{y}_i + \gamma}\right) - y_i(\hat{y}_i + \gamma)\end{aligned}$$

    Skipping over intermediate mathematical details, this results in the following:

    $$\gamma_{jm} = \frac{\sum_i y_i - p_i}{\sum_i p_i(i - p_i)}$$

    Note that the summation here is only over the examples at the node corresponding to the leaf node R_{jm} and not the complete training set.

    d. Update the model by adding the gamma value from *step 2c* with learning rate η:

    $$F_m(x) = F_{m-1}(x) + \eta\gamma_m$$

Outputting log(odds) vs probabilities

Why do the trees return log(odds) values and not probabilities? This is because we cannot just add up probability values and arrive at a meaningful result. (So, technically speaking, gradient boosting for classification uses regression trees.)

In this section, we adopted the general gradient boosting algorithm and specified it for binary classification, for instance, by replacing the generic loss function with the logistic loss and the predicted values with the log(odds). However, many of the individual steps may still seem very abstract, and in the next section, we will apply these steps to a concrete example.

Illustrating gradient boosting for classification

The previous two subsections went over the condensed mathematical details of the gradient boosting algorithm for binary classification. To make these concepts clearer, let's apply it to a small toy example, that is, a training dataset of the following three examples shown in *Figure 7.12*:

	Feature x_1	Feature x_2	Class label y
1	1.12	1.4	1
2	2.45	2.1	0
3	3.54	1.2	1

Figure 7.12: Toy dataset for explaining gradient boosting

Let's start with *step 1*, constructing the root node and computing the log(odds), and *step 2a*, converting the log(odds) into class-membership probabilities and computing the pseudo-residuals. Note that based on what we have learned in *Chapter 3*, the odds can be computed as the number of successes divided by the number of failures. Here, we regard label 1 as success and label 0 as failure, so the odds are computed as: odds = 2/1. Carrying out steps *1* and *2a*, we get the following results shown in *Figure 7.13*:

	Feature x_1	Feature x_2	Class label y	Step 1: $\hat{y} = \log(\text{odds})$	Step 2a: $p = \frac{1}{1+e^{-\hat{y}}}$	Step 2a: $r = y - p$
1	1.12	1.4	1	0.69	0.67	0.33
2	2.45	2.1	0	0.69	0.67	-0.67
3	3.54	1.2	1	0.69	0.67	0.33

Figure 7.13: Results from the first round of applying step 1 and step 2a

Next, in *step 2b*, we fit a new tree on the pseudo-residuals r. Then, in *step 2c*, we compute the output values, γ, for this tree as shown in *Figure 7.14*:

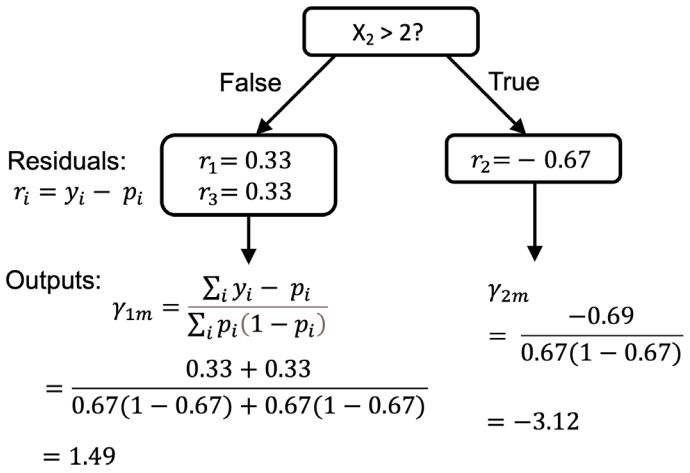
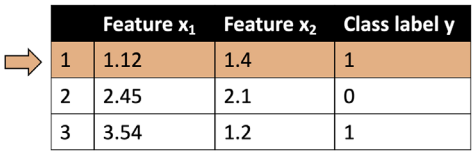


Figure 7.14: An illustration of steps 2b and 2c, which fits a tree to the residuals and computes the output values for each leaf node

(Note that we artificially limit the tree to have only two leaf nodes, which helps illustrate what happens if a leaf node contains more than one example.)

Then, in the final *step 2d*, we update the previous model and the current model. Assuming a learning rate of $\eta = 0.1$, the resulting prediction for the first training example is shown in *Figure 7.15*:



	Feature x_1	Feature x_2	Class label y
1	1.12	1.4	1
2	2.45	2.1	0
3	3.54	1.2	1

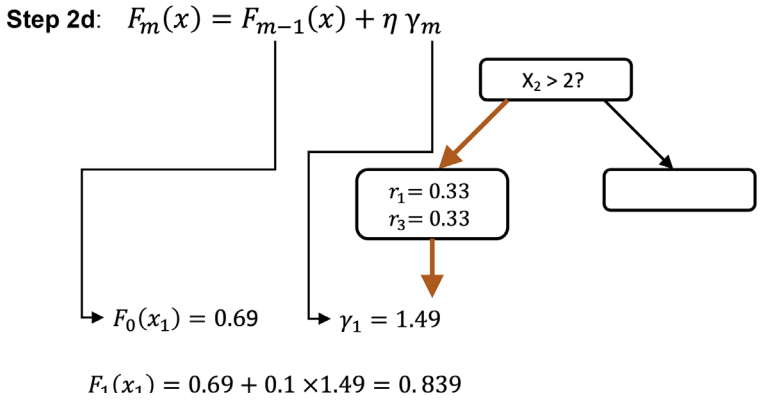


Figure 7.15: The update of the previous model shown in the context of the first training example

Now that we have completed *steps 2a* to *2d* of the first round, $m = 1$, we can proceed to execute *steps 2a* to *2d* for the second round, $m = 2$. In the second round, we use the log(odds) returned by the updated model, for example, $F_1(x_1) = 0.839$, as input to *step 2A*. The new values we obtain in the second round are shown in *Figure 7.16*:

	x_1	x_2	y	Step 1: $F_0(x) = \hat{y}$ = log(odds)	Step 2a: $p = \frac{1}{1+e^{-\hat{y}}}$	Step 2a: $r = y - p$	New log(odds) $\hat{y} = F_1(x)$	Step 2a: p	Step 2a: r
1	1.12	1.4	1	0.69	0.67	0.33	0.839	0.698	0.302
2	2.45	2.1	0	0.69	0.67	-0.67	0.378	0.593	-0.593
3	3.54	1.2	1	0.69	0.67	0.33	0.839	0.698	0.302

Round $m = 1$ Round $m = 2$

Figure 7.16: Values from the second round next to the values from the first round

We can already see that the predicted probabilities are higher for the positive class and lower for the negative class. Consequently, the residuals are getting smaller, too. Note that the process of *steps 2a* to *2d* is repeated until we have fit M trees or the residuals are smaller than a user-specified threshold value. Then, once the gradient boosting algorithm has completed, we can use it to predict the class labels by thresholding the probability values of the final model, $F_M(x)$ at 0.5, like logistic regression in *Chapter 3*. However, in contrast to logistic regression, gradient boosting consists of multiple trees and produces nonlinear decision boundaries. In the next section, we will look at how gradient boosting looks in action.

Using XGBoost

After covering the nitty-gritty details behind gradient boosting, let's finally look at how we can use gradient boosting code implementations.

In scikit-learn, gradient boosting is implemented as `sklearn.ensemble.GradientBoostingClassifier` (see `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.GradientBoostingClassifier.html` for more details). It is important to note that gradient boosting is a sequential process that can be slow to train. However, in recent years a more popular implementation of gradient boosting has emerged, namely, XGBoost.

XGBoost proposed several tricks and approximations that speed up the training process substantially. Hence, the name XGBoost, which stands for extreme gradient boosting. Moreover, these approximations and tricks result in very good predictive performances. In fact, XGBoost gained popularity as it has been the winning solution for many Kaggle competitions.

Next to XGBoost, there are also other popular implementations of gradient boosting, for example, LightGBM and CatBoost. Inspired by LightGBM, scikit-learn now also implements a `HistGradientBoostingClassifier`, which is more performant than the original gradient boosting classifier (`GradientBoostingClassifier`).

You can find more details about these methods via the resources below:

- **XGBoost**: `https://xgboost.readthedocs.io/en/stable/`
- **LightGBM**: `https://lightgbm.readthedocs.io/en/latest/`
- **CatBoost**: `https://catboost.ai`
- **HistGradientBoostingClassifier**: `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.HistGradientBoostingClassifier.html`

However, since XGBoost is still among the most popular gradient boosting implementations, we will see how we can use it in practice. First, we need to install it, for example via `pip`:

```
pip install xgboost
```

Installing XGBoost

For this chapter, we used XGBoost version 1.5.0, which can be installed via:

```
pip install XGBoost==1.5.0
```

You can find more information about the installation details at `https://xgboost.readthedocs.io/en/stable/install.html`

Fortunately, XGBoost's `XGBClassifier` follows the scikit-learn API. So, using it is relatively straightforward:

```
>>> import xgboost as xgb
>>> model = xgb.XGBClassifier(n_estimators=1000, learning_rate=0.01,
...                           max_depth=4, random_state=1,
...                           use_label_encoder=False)

>>> gbm = model.fit(X_train, y_train)
>>> y_train_pred = gbm.predict(X_train)
>>> y_test_pred = gbm.predict(X_test)

>>> gbm_train = accuracy_score(y_train, y_train_pred)
>>> gbm_test = accuracy_score(y_test, y_test_pred)
>>> print(f'XGboost train/test accuracies '
...       f'{gbm_train:.3f}/{gbm_test:.3f}')
XGboost train/test accuracies 0.968/0.917
```

Here, we fit the gradient boosting classifier with 1,000 trees (rounds) and a learning rate of 0.01. Typically, a learning rate between 0.01 and 0.1 is recommended. However, remember that the learning rate is used for scaling the predictions from the individual rounds. So, intuitively, the lower the learning rate, the more estimators are required to achieve accurate predictions.

Next, we have the `max_depth` for the individual decision trees, which we set to 4. Since we are still boosting weak learners, a value between 2 and 6 is reasonable, but larger values may also work well depending on the dataset.

Finally, `use_label_encoder=False` disables a warning message which informs users that XGBoost is not converting labels by default anymore, and it expects users to provide labels in an integer format starting with label 0. (There is nothing to worry about here, since we have been following this format throughout this book.)

There are many more settings available, and a detailed discussion is out of the scope of this book. However, interested readers can find more details in the original documentation at `https://xgboost.readthedocs.io/en/latest/python/python_api.html#xgboost.XGBClassifier`.

Summary

In this chapter, we looked at some of the most popular and widely used techniques for ensemble learning. Ensemble methods combine different classification models to cancel out their individual weaknesses, which often results in stable and well-performing models that are very attractive for industrial applications as well as machine learning competitions.

At the beginning of this chapter, we implemented `MajorityVoteClassifier` in Python, which allows us to combine different algorithms for classification. We then looked at bagging, a useful technique for reducing the variance of a model by drawing random bootstrap samples from the training dataset and combining the individually trained classifiers via majority vote. Lastly, we learned about boosting in the form of AdaBoost and gradient boosting, which are algorithms based on training weak learners that subsequently learn from mistakes.

Throughout the previous chapters, we learned a lot about different learning algorithms, tuning, and evaluation techniques. In the next chapter, we will look at a particular application of machine learning, sentiment analysis, which has become an interesting topic in the internet and social media era.

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`https://packt.link/MLwPyTorch`