7. Ensemble Learning

COMP3314
Machine Learning

Outline

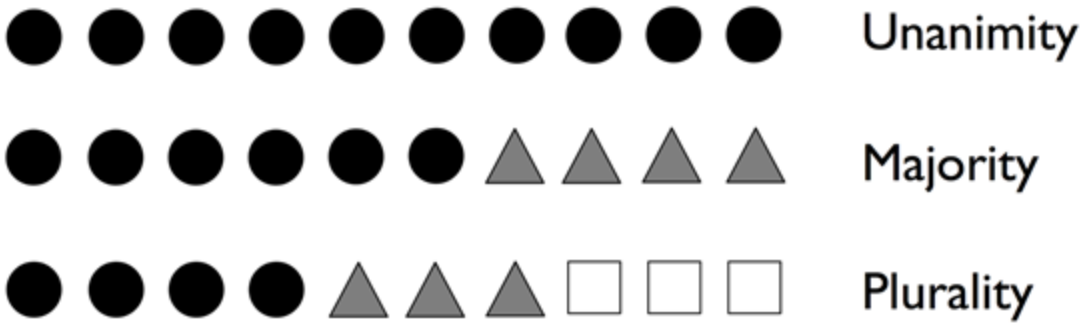
- A set of classifiers can often have a better predictive performance than any of its individual members
- We will learn how to do the following
  - Make predictions based on majority voting
  - Use bagging to reduce overfitting by drawing random combinations of the training set with repetition
  - Apply boosting to build powerful models from weak learners that learn from their mistakes

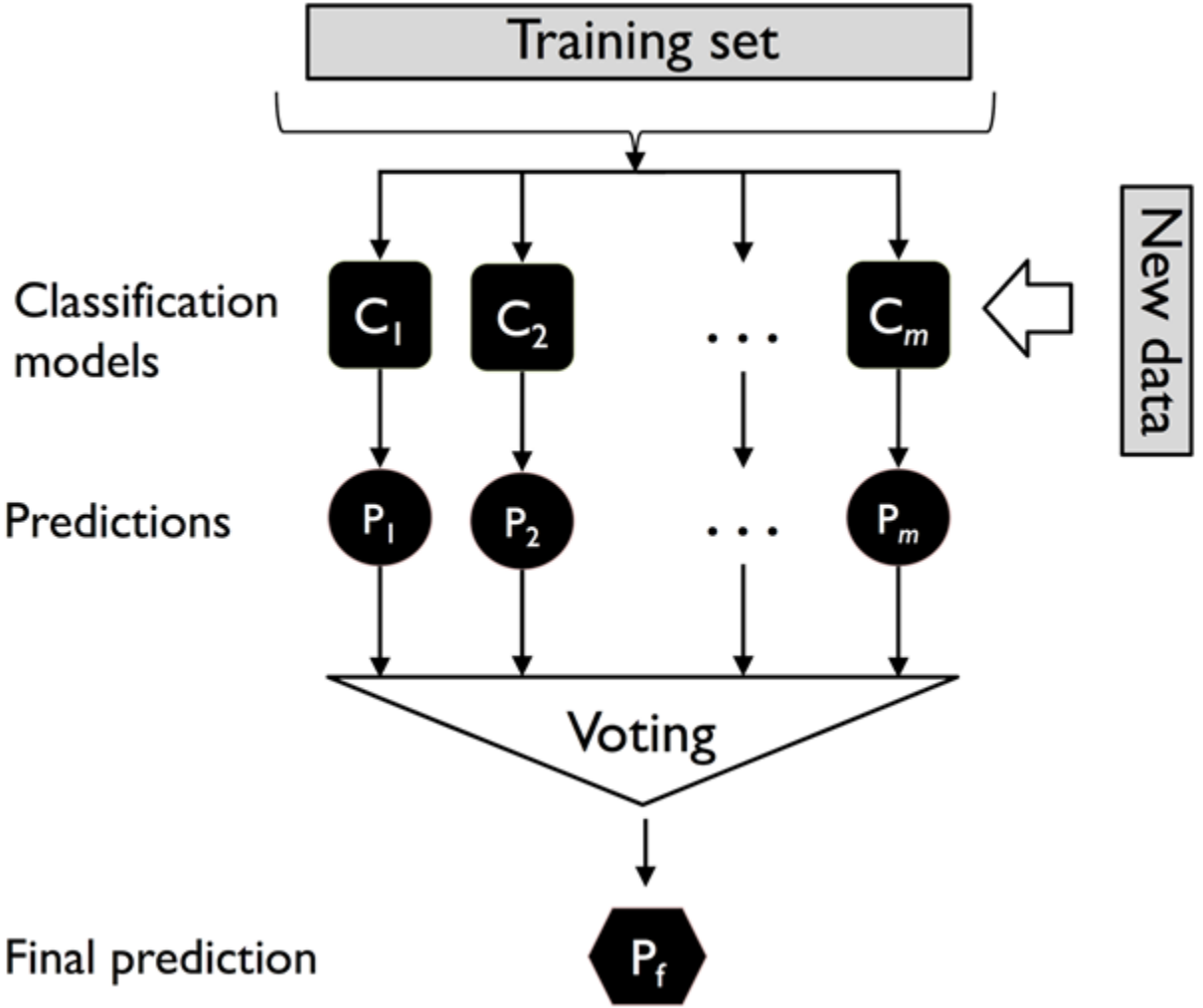
Learning with Ensembles

- Goal
  - Combine different classifiers into a meta-classifier that has better generalization performance than each individual classifier alone
- E.g., assuming that we collected predictions from 10 experts
  - Ensemble methods would allow us to strategically combine these predictions by the 10 experts to come up with a prediction that is more accurate and robust than the predictions by each individual expert

Majority/Plurality Voting

- 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
- Majority vote refers to binary class settings only
  - However, it is easy to generalize the majority voting principle to multi-class settings, which is called plurality voting
    - Select the class label that received the most votes (mode)




Training set
Classification models
C_1
C_2
C_m
New data
Predictions
P_1
P_2
P_m
Voting
Final prediction
P_f

Majority/Plurality Voting

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

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

- E.g., in a binary classification task where class_1 = −1 and class_2 = +1, we can write the majority vote prediction as follows

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

Does an ensemble method work better than an individual classifier?

Task 1

- Suppose we have 5 completely independent binary classifiers, each with an accuracy of 70%
- Calculate the majority vote accuracy

Task 2

- Suppose we have 100 completely independent binary classifiers, each with an error rate of $\varepsilon = 30\%$
- Calculate the majority vote error

Code - EnsembleLearning.ipynb

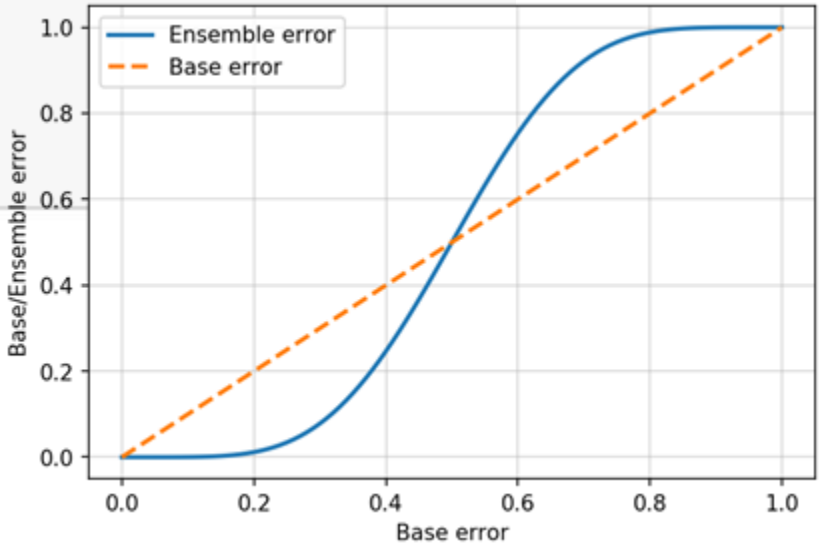
- Available here on CoLab

```
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)
```

Does an ensemble method work better than an individual classifier?

```
import numpy as np
error_range = np.arange(0.0, 1.01, 0.01)
ens_errors = [ensemble_error(n_classifier=11, error=error)
              for error in error_range]
```

```
import matplotlib.pyplot as plt
import matplotlib as mpl
mpl.rcParams['figure.dpi'] = 150
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()
```



Ensemble Methods vs. Individual Classifier

- Let's apply the simple concepts of combinatorics and assume
  - All n-base classifiers for a binary classification task have an equal error rate, ε
  - Classifiers are independent
  - Error rates are not correlated
- Probability that the prediction of the ensemble is wrong

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

Weighted Majority Vote Classifier

- Consider the following simple weighted majority vote classifier

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

- Here,
  - w_j is a weight associated with a base classifier C_j ,
  - $\hat{y}$ is the predicted class label of the ensemble,
  - χ_A (Greek chi) is a function that gives you the prediction $[C_j(x) = i \in A]$
  - A is the set of unique class labels
- For equal weights, we can simplify this equation and write it as follows

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

Example

- Consider an ensemble of three base classifiers, C_j ($j \in \{1, 2, 3\}$)
  - Two classifiers predict the class label 0, and one classifier C_3 predicts that the sample belongs to class 1
- If we weight the predictions of each base classifier equally, the majority vote would predict that the sample belongs to class 0

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

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

- Now, let us assign a weight of 0.6 to C_3 and a weight of 0.2 to C_1 and C_2

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

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

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

```
1
```

Probabilities

- Recall that certain classifiers can return the probability of a predicted class label
  - In scikit-learn: 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

Example

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

- We have a binary classification problem with class labels $i \in \{0, 1\}$ and an ensemble of three classifiers C_j ($j \in \{1,2,3\}$)
- The classifiers C_j return the following class membership probabilities for a particular sample x

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

- We can then calculate the individual class probabilities as follows

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

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

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

```
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])
```

MajorityVoteClassifier

- Let's implement our own 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
```

MajorityVoteClassifier

```
def fit(self, X, y):
    if self.vote not in ('probability', 'classlabel'):
        raise ValueError("vote must be 'probability' or 'classlabel' ; got (vote=%r)" % self.vote)
    if self.weights and len(self.weights) != len(self.classifiers):
        raise ValueError('Number of classifiers and weights must be equal'
                         '; got %d weights, %d classifiers' % (len(self.weights), len(self.classifiers)))
    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
```

MajorityVoteClassifier

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

VotingClassifier

- We showed the MajorityVoteClassifier implementation for demonstration purposes
  - A more sophisticated version of this majority vote classifier is available in scikit-learn as sklearn.ensemble.VotingClassifier

MajorityVoteClassifier

- Let's prepare a dataset that we can test the MajorityVoteClassifier on

```
from sklearn import datasets
from sklearn.preprocessing import StandardScaler
from sklearn.preprocessing import LabelEncoder
from sklearn.model_selection import train_test_split
iris = datasets.load_iris()
X, y = iris.data[50:, [1, 2]], iris.target[50:]
le = LabelEncoder()
y = le.fit_transform(y)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.5, random_state=1, stratify=y)
```

```
import numpy as np
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.pipeline import Pipeline
from sklearn.model_selection import cross_val_score
clf1 = LogisticRegression(penalty='l2', solver='lbfgs', C=0.001, random_state=0)
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("ROC AUC: %0.2f (+/- %0.2f) [%s]" % (scores.mean(), scores.std(), label))
```

```
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]
```

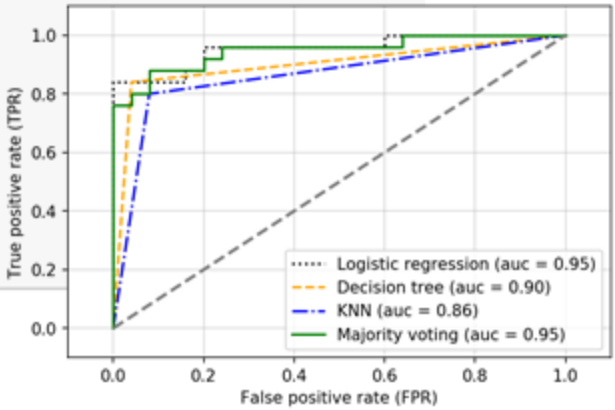
```
mv_clf = MajorityVoteClassifier(classifiers=[pipe1, clf2, pipe3])
clf_labels += ['Majority voting']
all_clf = [pipe1, clf2, pipe3, mv_clf]
for clf, label in zip(all_clf, clf_labels):
    scores = cross_val_score(estimator=clf, X=X_train, y=y_train, cv=10, scoring='roc_auc')
    print("ROC AUC: %0.2f (+/- %0.2f) [%s]" % (scores.mean(), scores.std(), 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]
```

Plotting ROC Curves

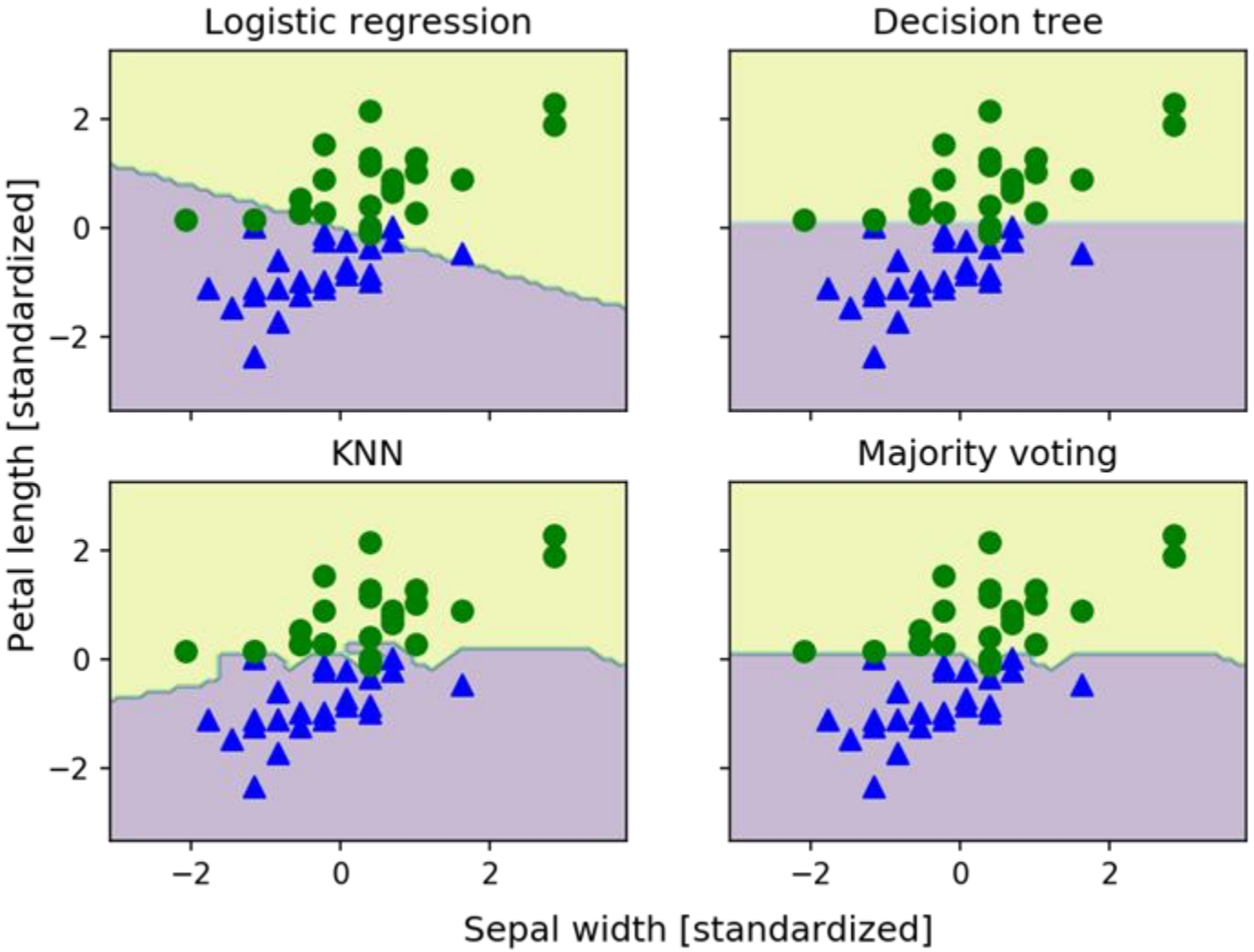
- Let's compute the ROC curves from the test set

```
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):
    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='%s (auc = %0.2f)' % (label, roc_auc))
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()
```



Decision Region Plotting

```
from itertools import product
sc = StandardScaler()
X_train_std = sc.fit_transform(X_train)
all_clf = [pipe1, clf2, pipe3, mv_clf]
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()
```


Logistic regression
Decision tree
KNN
Majority voting
Petal length [standardized]
Sepal width [standardized]
2
0
−2
−2
0
2

How to perform tuning ?

BaseEstimator

- Recall that our MajorityVoteClassifier inherited all methods from BaseEstimator

`get_params` (*deep=True*) [source]

Get parameters for this estimator.

Parameters:	**deep : *boolean, optional*** If True, will return the parameters for this estimator and contained subobjects that are estimators.
Returns:	**params : *mapping of string to any*** Parameter names mapped to their values.

```
type(mv_clf.get_params())
```

```
dict
```

```
for k,v in mv_clf.get_params().items():
    print(k)
    print('',v)
```

```
classifiers
 [Pipeline(memory=None,
     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='warn',
          n_jobs=None, penalty='l2', random_state=0, solver='lbfgs',
          tol=0.0001, verbose=0, warm_start=False)]]), DecisionTreeClassifier(class_weight=None, criterion='entropy', max_depth
=1,
            max_features=None, max_leaf_nodes=None,
            min_impurity_decrease=0.0, min_impurity_split=None,
            min_samples_leaf=1, min_samples_split=2,
            min_weight_fraction_leaf=0.0, presort=False, random_state=0,
            splitter='best'), Pipeline(memory=None,
     steps=[('sc', StandardScaler(copy=True, with_mean=True, with_std=True)), ['clf', KNeighborsClassifier(algorithm='auto', le
af_size=30, metric='minkowski',
           metric_params=None, n_jobs=None, n_neighbors=1, p=2,
           weights='uniform')]])]
vote
 classlabel
weights
 None
```

MajorityVoteClassifier.get_params()

- Let's override the get_params method with ‘deep’ support.

```
def get_params(self, deep=True):
    if not deep:
        return super(MajorityVoteClassifier, self).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['%s__%s' % (name, key)] = value
        return out
```

```
for k,v in mv_clf.get_params().items():
    print(k)
    print('',v)
```

```
pipeline-1__clf__C
 0.001

decisiontreeclassifier__max_depth
 1
```

Tuning via Grid Search

- Let's tune the inverse regularization parameter C of the logistic regression classifier and the decision tree depth using GridSearchCV

```
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', iid=True)
grid.fit(X_train, y_train)
for r, _ in enumerate(grid.cv_results_['mean_test_score']):
    print("%0.3f +/- %0.2f %r"
          % (grid.cv_results_['mean_test_score'][r],
             grid.cv_results_['std_test_score'][r] / 2.0,
             grid.cv_results_['params'][r]))
```

```
0.933 +/- 0.07 {'decisiontreeclassifier__max_depth': 1, 'pipeline-1__clf__C': 0.001}
0.947 +/- 0.07 {'decisiontreeclassifier__max_depth': 1, 'pipeline-1__clf__C': 0.1}
0.973 +/- 0.04 {'decisiontreeclassifier__max_depth': 1, 'pipeline-1__clf__C': 100.0}
0.947 +/- 0.07 {'decisiontreeclassifier__max_depth': 2, 'pipeline-1__clf__C': 0.001}
0.947 +/- 0.07 {'decisiontreeclassifier__max_depth': 2, 'pipeline-1__clf__C': 0.1}
0.973 +/- 0.04 {'decisiontreeclassifier__max_depth': 2, 'pipeline-1__clf__C': 100.0}
```

Tuning via Grid Search

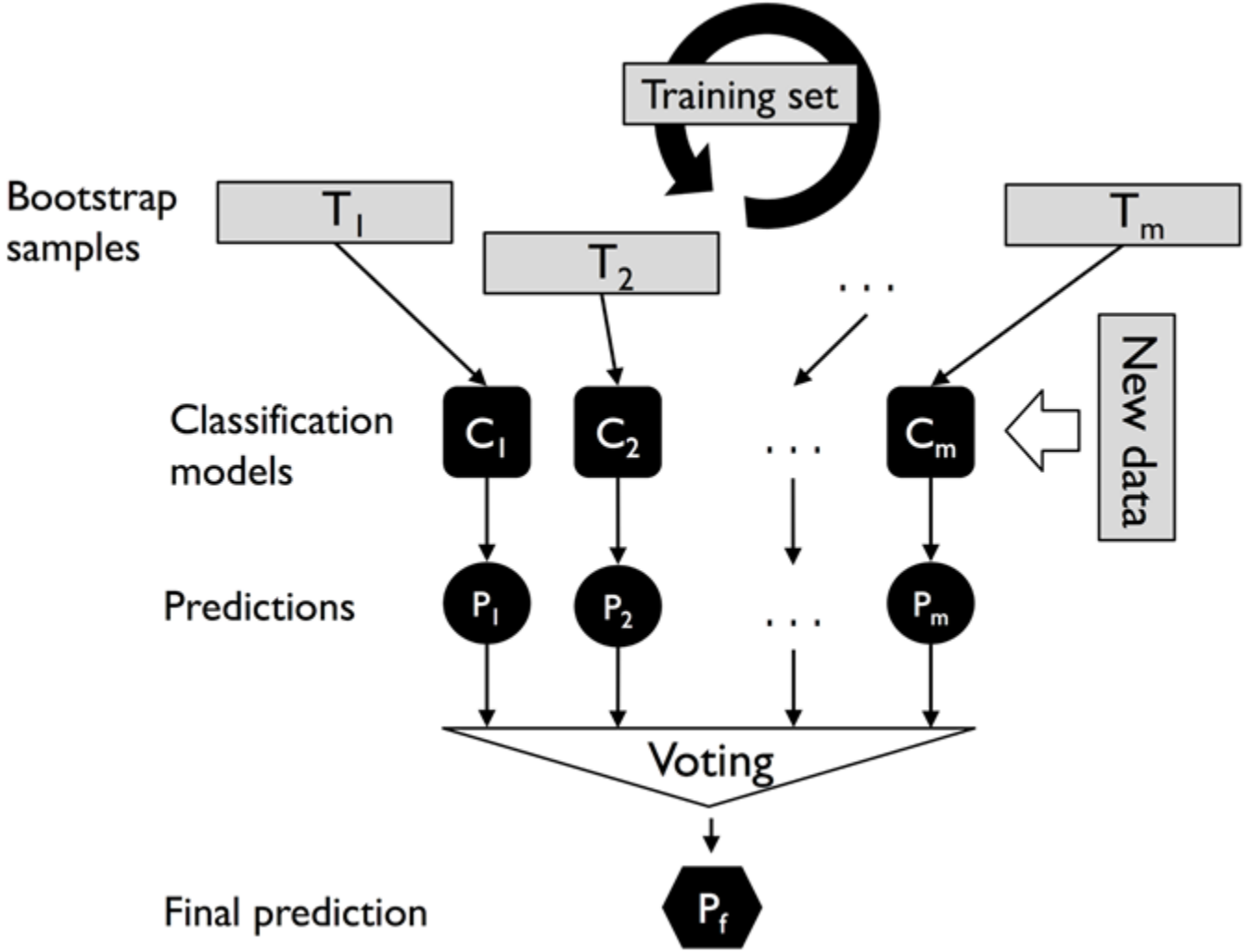
- We get the best cross-validation results when we choose a lower regularization strength (C=100.0)
- The tree depth does not seem to affect the performance much

```
print('Best parameters: %s' % grid.best_params_)
print('Accuracy: %.2f' % grid.best_score_)
```

```
Best parameters: {'decisiontreeclassifier__max_depth': 1, 'pipeline-1__clf__C': 100.0}
Accuracy: 0.97
```

Outline

- In this chapter, we will construct 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 set with repetition
  - Apply boosting to build powerful models from weak learners that learn from their mistakes


Training set
Bootstrap samples
T_1
T_2
. . .
T_m
New data
Classification models
C_1
C_2
. . .
C_m
Predictions
P_1
P_2
. . .
P_m
Voting
Final prediction
P_f

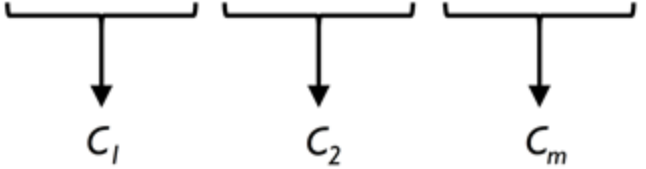
Bagging

- Bagging is an ensemble learning technique that is closely related to the MajorityVoteClassifier implemented previously
- Instead of using the same training set to fit the individual classifiers in the ensemble, we draw bootstrap samples (random samples with replacement) from the initial training set
- Bagging is also known as bootstrap aggregating
- Bagging was first proposed by Leo Breiman in 1994
  - He showed that bagging can improve the accuracy of unstable models and decrease the degree of overfitting
  - Recommend reading:
    Bagging predictors, L. Breiman, Technical Report
    - > 30 000 citations

Bagging in a Nutshell

- Seven different training instances
  - 1 to 7
- Sampled randomly with replacement in each round of bagging
- Each bootstrap sample is then used to fit a classifier C_j
- Note that each subset contains a certain portion of duplicates and some of the original samples don't appear in a resampled dataset at all
- Once the individual classifiers are fit to the bootstrap samples, the predictions are combined using majority voting

Sample indices	Bagging round 1	Bagging round 2	…
1	2	7	…
2	2	3	…
3	1	2	…
4	3	1	…
5	7	1	…
6	2	7	…
7	4	7	…



Wine Bagging

- Wine Dataset
  - Let's only consider the wine classes 2 and 3 and only two features

```
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']
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
```

  - Encode class labels into binary format and split the dataset into 80:20; training:testing

```
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)
```

BaggingClassifier

- A bagging classifier algorithm is already implemented in scikit-learn
  - Imported from ensemble submodule
- 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
from sklearn.tree import DecisionTreeClassifier
tree = DecisionTreeClassifier(criterion='entropy', max_depth=None, random_state=1)
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)
```

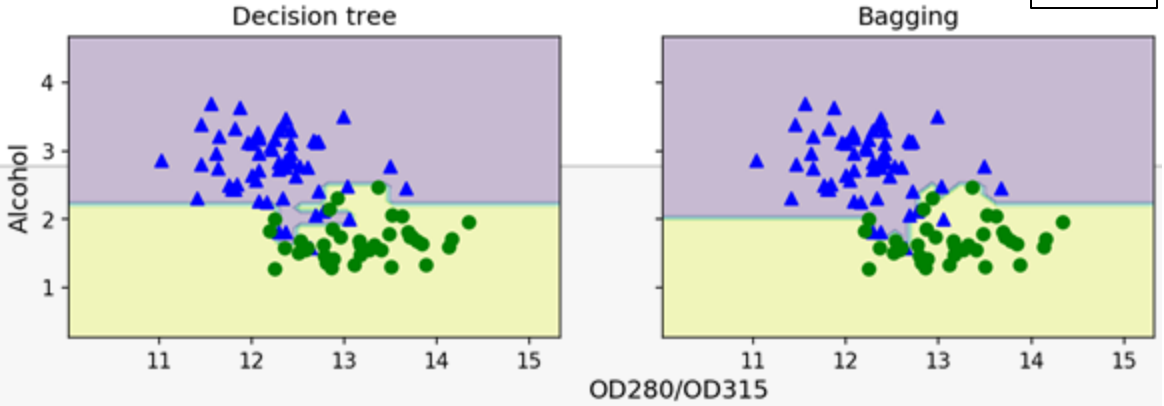
Bagging in Action

- Calculate the accuracy score of the prediction on the training and test dataset 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('Decision tree train/test accuracies %.3f/%.3f' % (tree_train, tree_test))
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('Bagging train/test accuracies %.3f/%.3f' % (bag_train, bag_test))
```

```
Decision tree train/test accuracies 1.000/0.833
Bagging train/test accuracies 1.000/0.917
```

Decision Regions




```
import numpy as np
import matplotlib.pyplot as plt
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('Alcohol', fontsize=12)
plt.text(10.2, -0.5, s='OD280/OD315', ha='center', va='center', fontsize=12)
plt.tight_layout()
plt.show()
```

Bagging - Conclusion

- In practice, more complex classification tasks and a dataset's high dimensionality can often lead to overfitting in single decision tree
- This is where the bagging algorithm can really play to its strengths
  - It can be an effective approach to reduce the variance of a model
- However, bagging is ineffective in reducing model bias, that is, models that are too simple to capture the trend in the data well
- This is why we want to perform bagging on an ensemble of classifiers with low bias
  - E.g., unpruned decision trees

Outline

- In this chapter, we will construct 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 set with repetition
  - Apply boosting to build powerful models from weak learners that learn from their mistakes

AdaBoost (Adaptive Boosting)

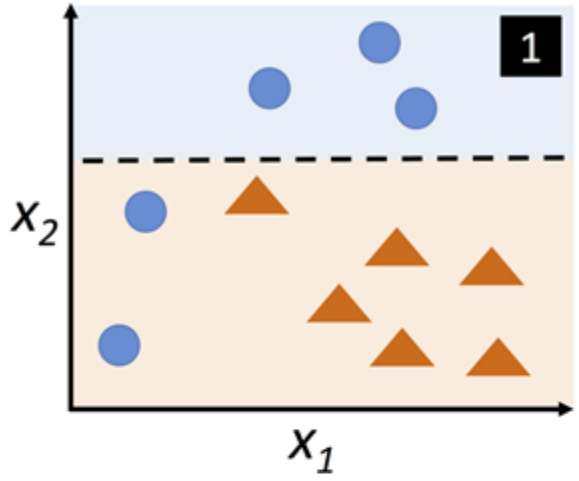
- The original idea behind AdaBoost was formulated by Robert E. Schapire in 1990
  - The Strength of Weak Learnability, R. E. Schapire, Machine Learning, 5(2): 197-227, 1990
  - Experiments with a New Boosting Algorithm, Yoav Freund and Robert E. Schapire
- In 2003, Freund and Schapire received the Goedel Prize for their groundbreaking work
  - A prestigious prize for outstanding publications in the field of computer science

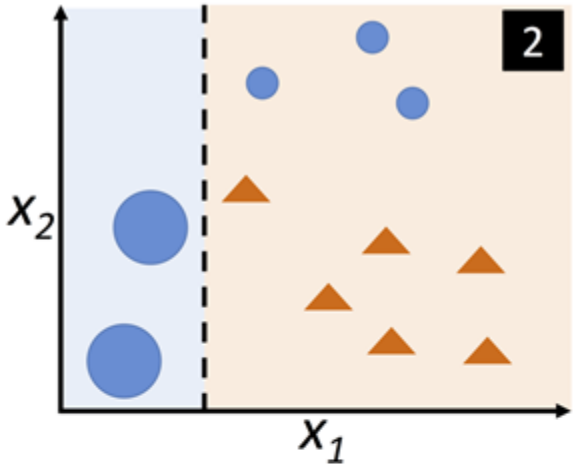
Idea

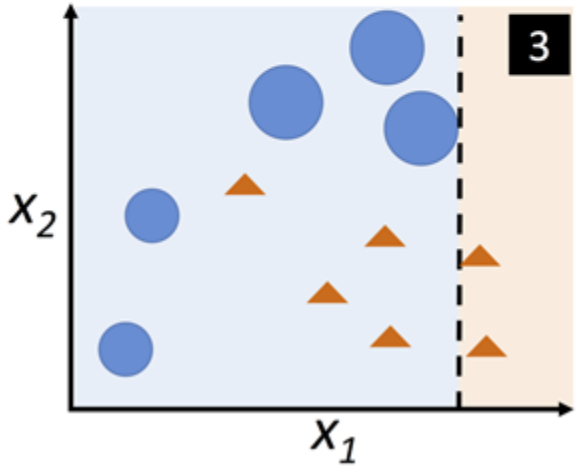
- In boosting, the ensemble consists of simple base classifiers
  - Often referred to as weak learners
- The weak learners may only have a slight performance advantage over random guessing
- The key concept behind boosting is to focus on training samples that are hard to classify
- The weak learners subsequently learn from misclassified training samples to improve the performance of the ensemble

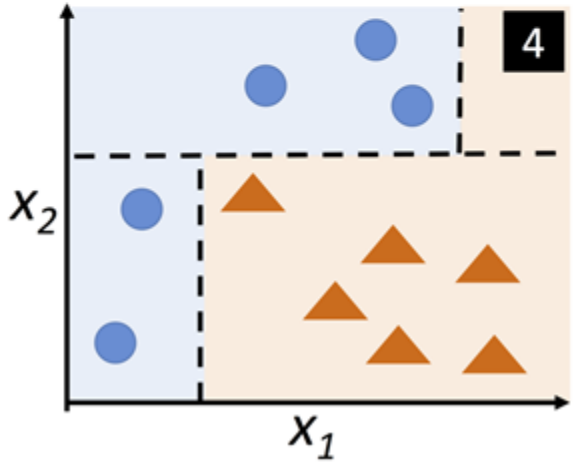
Original Boosting Procedure

- Draw a random subset of training samples d_1 without replacement from training set D to train a weak learner C_1
- Draw a second random training subset d_2 without replacement from the training set and add 50 percent of the samples that were previously misclassified to train a weak learner C_2
- Find the training samples d_3 in training set D, which C_1 and C_2 disagree upon, to train a third weak learner C_3
- Combine the weak learners C_1, C_2, and C_3 via majority voting


1
x_2
x_1


2
x_2
x_1


3
x_2
x_1


4
x_2
x_1

AdaBoost Pseudocode

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

Note: We denote element-wise multiplication by the cross symbol (×) and the dot-product between two vectors by a dot symbol (·)

Example

Sample indices	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

Example: Weight Update

Sample indices	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

- We start by computing the weighted error rate

$$\varepsilon = 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 0 + 0.1\times 1 + 0.1\times 1 + 0.1\times 1 + 0.1\times 0 = \frac{3}{10} = 0.3$$

- Next, we compute the coefficient α_j

$$\alpha_j = 0.5 \log\left(\frac{1-\varepsilon}{\varepsilon}\right) \approx 0.424$$

- After we have computed the coefficient α_j, we can now update the weight vector using the equation $\mathbf{w} = \mathbf{w} \times \exp(-\boldsymbol{\alpha}_j \times \hat{\mathbf{y}} \times \mathbf{y})$
- Here $\hat{\mathbf{y}} \times \mathbf{y}$ 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

Example: Weight Update

Sample indices	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

$$0.1 \times \exp\left(-0.424 \times 1 \times 1\right) \approx 0.065$$

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

$$0.1 \times \exp\left(-0.424 \times 1 \times \left(-1\right)\right) \approx 0.153$$

Alternatively, it's like this:

$$0.1 \times \exp\left(-0.424 \times \left(-1\right) \times \left(1\right)\right) \approx 0.153$$

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

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

Here, $\sum_i w_i = 7 \times 0.065 + 3 \times 0.153 = 0.914$.

Thus, each weight that corresponds to a correctly classified sample will be reduced from the initial value of 0.1 to $0.065 / 0.914 \approx 0.071$ for the next round of boosting. Similarly, the weights of the incorrectly classified samples will increase from 0.1 to $0.153 / 0.914 \approx 0.167$.

AdaBoost in scikit-learn

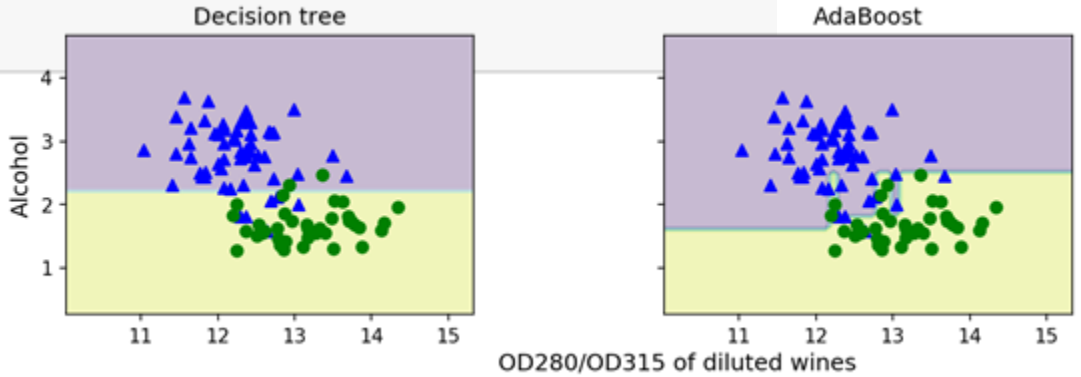
```
from sklearn.ensemble import AdaBoostClassifier
tree = DecisionTreeClassifier(criterion='entropy', max_depth=1, random_state=1)
ada = AdaBoostClassifier(base_estimator=tree, n_estimators=500, learning_rate=0.1, random_state=1)
```

```
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('Decision tree train/test accuracies %.3f/%.3f' % (tree_train, tree_test))
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('AdaBoost train/test accuracies %.3f/%.3f' % (ada_train, ada_test))
```

```
Decision tree train/test accuracies 0.916/0.875
AdaBoost train/test accuracies 1.000/0.917
```

Decision Region Plotting

```
x_min, x_max = X_train[:, 0].min() - 1, X_train[:, 0].max() + 1
y_min, y_max = X_train[:, 1].min() - 1, 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('Alcohol', fontsize=12)
plt.text(10.2, -0.5, s='OD280/OD315 of diluted wines', ha='center', va='center', fontsize=12)
plt.tight_layout()
plt.show()
```



AdaBoost: Conclusion

- 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

References

- Most materials in this chapter are based on
  - Book
  - Code