



3.10. Multiclass and multilabel algorithms

This module implements multiclass and multilabel learning algorithms:

- one-vs-the-rest / one-vs-all
- one-vs-one
- error correcting output codes

Multiclass classification means classification with more than two classes. Multilabel classification is a different task, where a classifier is used to predict a set of target labels for each instance; i.e., the set of target classes is not assumed to be disjoint as in ordinary (binary or multiclass) classification. This is also called any-of classification.

The estimators provided in this module are meta-estimators: they require a base estimator to be provided in their constructor. For example, it is possible to use these estimators to turn a binary classifier or a regressor into a multiclass classifier. It is also possible to use these estimators with multiclass estimators in the hope that their accuracy or runtime performance improves.

Note: You don't need to use these estimators unless you want to experiment with different multiclass strategies: all classifiers in scikit-learn support multiclass classification out-of-the-box. Below is a summary of the classifiers supported in scikit-learn grouped by the strategy used.

- Inherently multiclass: *Naive Bayes*, `sklearn.lda.LDA`, *Decision Trees*, *Random Forests*
- One-Vs-One: `sklearn.svm.SVC`.
- One-Vs-All: `sklearn.svm.LinearSVC`,
`sklearn.linear_model.LogisticRegression`,
`sklearn.linear_model.SGDClassifier`,
`sklearn.linear_model.RidgeClassifier`.

Note: At the moment there are no evaluation metrics implemented for multilabel learnings.

3.10.1. One-Vs-The-Rest

This strategy, also known as **one-vs-all**, is implemented in `OneVsRestClassifier`. The strategy consists in fitting one classifier per class. For each classifier, the class is fitted against all the other classes. In addition to its computational efficiency (only $n_{classes}$ classifiers are needed), one advantage of this approach is its interpretability. Since each class is represented by one and one classifier only, it is possible to gain knowledge about the class by inspecting its corresponding classifier. This is the most commonly used strategy and is a fair default choice. Below is an example:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OneVsRestClassifier
>>> from sklearn.svm import LinearSVC
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
```

3.10.1.1. Multilabel learning with OvR

The figure consists of four scatter plots arranged in a 2x2 grid, illustrating the effect of unlabeled samples on dimensionality reduction results.

- Top Left: With unlabeled samples + CCA**
 - Y-axis: Second principal component
 - X-axis: First principal component
 - Legend:
 - Boundary for class 1 (dashed line)
 - Boundary for class 2 (dotted line)
 - Class 1 (blue circles)
 - Class 2 (orange circles)
 - Observation: The boundaries for Class 1 and Class 2 are well-separated and distinct.
- Top Right: With unlabeled samples + PCA**
 - Y-axis: Second principal component
 - X-axis: First principal component
 - Legend:
 - Boundary for class 1 (dashed line)
 - Boundary for class 2 (dotted line)
 - Class 1 (blue circles)
 - Class 2 (orange circles)
 - Observation: The boundaries for Class 1 and Class 2 are well-separated and distinct.
- Bottom Left: Without unlabeled samples + CCA**
 - Y-axis: Second principal component
 - X-axis: First principal component
 - Legend:
 - Boundary for class 1 (dashed line)
 - Boundary for class 2 (dotted line)
 - Class 1 (blue circles)
 - Class 2 (orange circles)
 - Observation: The boundaries for Class 1 and Class 2 are well-separated and distinct.
- Bottom Right: Without unlabeled samples + PCA**
 - Y-axis: Second principal component
 - X-axis: First principal component
 - Legend:
 - Boundary for class 1 (dashed line)
 - Boundary for class 2 (dotted line)
 - Class 1 (blue circles)
 - Class 2 (orange circles)
 - Observation: The boundaries for Class 1 and Class 2 are well-separated and distinct.

3.10.2. One-Vs-One

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OneVsOneClassifier
>>> from sklearn.svm import LinearSVC
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> OneVsOneClassifier(LinearSVC()).fit(X, y).predict(X)
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1])
```

```
1, 2, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1,
1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

3.10.3. Error-Correcting Output-Codes

Output-code based strategies are fairly different from one-vs-the-rest and one-vs-one. With these strategies, each class is represented in a euclidean space, where each dimension can only be 0 or 1. Another way to put it is that each class is represented by a binary code (an array of 0 and 1). The matrix which keeps track of the location/code of each class is called the code book. The code size is the dimensionality of the aforementioned space. Intuitively, each class should be represented by a code as unique as possible and a good code book should be designed to optimize classification accuracy. In this implementation, we simply use a randomly-generated code book as advocated in [2] although more elaborate methods may be added in the future.

At fitting time, one binary classifier per bit in the code book is fitted. At prediction time, the classifiers are used to project new points in the class space and the class closest to the points is chosen.

In **OutputCodeClassifier**, the *code_size* attribute allows the user to control the number of classifiers which will be used. It is a percentage of the total number of classes.

A number between 0 and 1 will require fewer classifiers than one-vs-the-rest. In theory, $\log_2(n_classes) / n_classes$ is sufficient to represent each class unambiguously. However, in practice, it may not lead to good accuracy since $\log_2(n_classes)$ is much smaller than $n_classes$.

A number greater than 1 will require more classifiers than one-vs-the-rest. In this case, some classifiers will in theory correct for the mistakes made by other classifiers, hence the name “error-correcting”. In practice, however, this may not happen as classifier mistakes will typically be correlated. The error-correcting output codes have a similar effect to bagging.

Example:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OutputCodeClassifier
>>> from sklearn.svm import LinearSVC
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> OutputCodeClassifier(LinearSVC(), code_size=2, random_state=0).fit(X, y)
array([[0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
        0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
        1, 2, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 2, 2, 2, 1, 1, 1, 1, 1, 1,
        1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,
        2, 2, 2, 2, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 1, 1, 2, 2, 2,
        2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

References:

- [1] “Solving multiclass learning problems via error-correcting output codes”, Dietterich T., Bakiri G., Journal of Artificial Intelligence Research 2, 1995.
- [2] “The error coding method and PICTs”, James G., Hastie T., Journal of Computational and Graphical statistics 7, 1998.
- [3] “The Elements of Statistical Learning”, Hastie T., Tibshirani R., Friedman J., page 606 (second-edition) 2008.