1.12. Multiclass and multilabel algorithms

Warning: All classifiers in scikit-learn do multiclass classification out-of-the-box. You don't need to use the `sklearn.multiclass` module unless you want to experiment with different multiclass strategies.

The `sklearn.multiclass` module implements *meta-estimators* to solve `multiclass` and `multilabel` classification problems by decomposing such problems into binary classification problems. `multioutput` regression is also supported.

- **Multiclass classification**: classification task with more than two classes. Each sample can only be labelled as one class.

  For example, classification using features extracted from a set of images of fruit, where each image may either be of an orange, an apple, or a pear. Each image is one sample and is labelled as one of the 3 possible classes. Multiclass classification makes the assumption that each sample is assigned to one and only one label - one sample cannot, for example, be both a pear and an apple.

  Valid multiclass representations for `type_of_target` (`y`) are:

  - 1d or column vector containing more than two discrete values. An example of a vector `y` for 3 samples:

    ```
    >>> import numpy as np
    >>> y = np.array(['apple', 'pear', 'apple'])
    >>> print(y)
    ['apple' 'pear' 'apple']
    ```

  - sparse binary matrix of shape `(n_samples, n_classes)` with a single element per row, where each column represents one class. An example of a sparse binary matrix `y` for 3 samples, where the columns, in order, are orange, apple and pear:

    ```
    >>> from scipy import sparse
    >>> row_ind = np.array([0, 1, 2])
    >>> col_ind = np.array([1, 2, 1])
    >>> y_sparse = sparse.csr_matrix((np.ones(3), (row_ind, col_ind)))
    >>> print(y_sparse)
      (0, 1)        1.0
      (1, 2)        1.0
      (2, 1)        1.0
    ```

- **Multilabel classification**: classification task labelling each sample with `x` labels from `n_classes` possible classes, where `x` can be 0 to `n_classes` inclusive. This can be thought of as predicting properties of a sample that are not mutually exclusive. Formally, a binary output is assigned to each class, for every sample. Positive classes are indicated with 1 and negative classes with 0 or -1. It is thus comparable to running `n_classes` binary classification tasks, for example with `sklearn.multioutput.MultiOutputClassifier`. This approach treats each label independently whereas multilabel classifiers *may* treat the multiple classes simultaneously, accounting for correlated behaviour amoung them.

  For example, prediction of the topics relevant to a text document or video. The document or video may be about one of 'religion', 'politics', 'finance' or 'education', several of the topic classes or all of the topic classes.

  Valid representation of multilabel `y` is either dense (or sparse) binary matrix of shape `(n_samples, n_classes)`. Each column represents a class. The `1`'s in each row denote the positive classes a sample has been labelled with. An example of a dense matrix `y` for 3 samples:

  ```
  >>> y = np.array([[1, 0, 0, 1], [0, 0, 1, 1], [0, 0, 0, 0]])
  >>> print(y)
  [[1 0 0 1]
   [0 0 1 1]
   [0 0 0 0]]
  ```

  An example of the same `y` in sparse matrix form:

  ```
  >>> y_sparse = sparse.csr_matrix(y)
  >>> print(y_sparse)
    (0, 0)    1
    (0, 3)    1
    (1, 2)    1
    (1, 3)    1
  ```

- **Multioutput regression**: predicts multiple numerical properties for each sample. Each property is a numerical variable and the number of properties to be predicted for each sample is greater than or equal to 2. Some estimators that support multioutput regression are faster than just running `n_output` estimators.

  For example, prediction of both wind speed and wind direction, in degrees, using data obtained at a certain location. Each sample would be data obtained at one location and both wind speed and directtion would be output for each sample.

  Valid representation of multilabel `y` is dense matrix of shape `(n_samples, n_classes)` of floats. A column wise concatenation of continuous variables. An example of `y` for 3 samples:

```
>>> y = np.array([[31.4, 94], [40.5, 109], [25.0, 30]])
>>> print(y)
[[ 31.4  94. ]
 [ 40.5 109. ]
 [ 25.   30. ]]
```

- **Multioutput-multiclass classification** (also known as **multitask classification**): classification task which labels each sample with a set of **non-binary** properties. Both the number of properties and the number of classes per property is greater than 2. A single estimator thus handles several joint classification tasks. This is both a generalization of the multi*label* classification task, which only considers binary attributes, as well as a generalization of the multi*class* classification task, where only one property is considered.

  For example, classification of the properties “type of fruit” and “colour” for a set of images of fruit. The property “type of fruit” has the possible classes: “apple”, “pear” and “orange”. The property “colour” has the possible classes: “green”, “red”, “yellow” and “orange”. Each sample is an image of a fruit, a label is output for both properties and each label is one of the possible classes of the corresponding property.

  Valid representation of multilabel `y` is dense matrix of shape `(n_samples, n_classes)` of floats. A column wise concatenation of 1d multiclass variables. An example of `y` for 3 samples:

```
>>> y = np.array([['apple', 'green'], ['orange', 'orange'], ['pear', 'green']])
>>> print(y)
[['apple' 'green']
 ['orange' 'orange']
 ['pear' 'green']]
```

  Note that any classifiers handling multioutput-multiclass (also known as multitask classification) tasks, support the multilabel classification task as a special case. Multitask classification is similar to the multioutput classification task with different model formulations. For more information, see the relevant estimator documentation.

All scikit-learn classifiers are capable of multiclass classification, but the meta-estimators offered by **`sklearn.multiclass`** permit changing the way they handle more than two classes because this may have an effect on classifier performance (either in terms of generalization error or required computational resources).

Summary

	Number of targets	Target cardinality	Valid `type_of_target`
Multiclass classification	1	>2	• ‘multiclass’
Multilabel classification	>1	2 (0 or 1)	• ‘multilabel-indicator’
Multioutput regression	>1	Continuous	• ‘continuous-multioutput’
Multioutput-multiclass classification	>1	>2	• ‘multiclass-multioutput’

Below is a summary of the classifiers supported by scikit-learn grouped by strategy; you don’t need the meta-estimators in this class if you’re using one of these, unless you want custom multiclass behavior:

- **Inherently multiclass:**
  - **`sklearn.naive_bayes.BernoulliNB`**
  - **`sklearn.tree.DecisionTreeClassifier`**
  - **`sklearn.tree.ExtraTreeClassifier`**
  - **`sklearn.ensemble.ExtraTreesClassifier`**
  - **`sklearn.naive_bayes.GaussianNB`**
  - **`sklearn.neighbors.KNeighborsClassifier`**

- `sklearn.semi_supervised.LabelPropagation`
- `sklearn.semi_supervised.LabelSpreading`
- `sklearn.discriminant_analysis.LinearDiscriminantAnalysis`
- `sklearn.svm.LinearSVC` (setting multi_class="crammer_singer")
- `sklearn.linear_model.LogisticRegression` (setting multi_class="multinomial")
- `sklearn.linear_model.LogisticRegressionCV` (setting multi_class="multinomial")
- `sklearn.neural_network.MLPClassifier`
- `sklearn.neighbors.NearestCentroid`
- `sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis`
- `sklearn.neighbors.RadiusNeighborsClassifier`
- `sklearn.ensemble.RandomForestClassifier`
- `sklearn.linear_model.RidgeClassifier`
- `sklearn.linear_model.RidgeClassifierCV`

- **Multiclass as One-Vs-One:**
  - `sklearn.svm.NuSVC`
  - `sklearn.svm.SVC`.
  - `sklearn.gaussian_process.GaussianProcessClassifier` (setting multi_class = "one_vs_one")
- **Multiclass as One-Vs-The-Rest:**
  - `sklearn.ensemble.GradientBoostingClassifier`
  - `sklearn.gaussian_process.GaussianProcessClassifier` (setting multi_class = "one_vs_rest")
  - `sklearn.svm.LinearSVC` (setting multi_class="ovr")
  - `sklearn.linear_model.LogisticRegression` (setting multi_class="ovr")
  - `sklearn.linear_model.LogisticRegressionCV` (setting multi_class="ovr")
  - `sklearn.linear_model.SGDClassifier`
  - `sklearn.linear_model.Perceptron`
  - `sklearn.linear_model.PassiveAggressiveClassifier`
- **Support multilabel:**
  - `sklearn.tree.DecisionTreeClassifier`
  - `sklearn.tree.ExtraTreeClassifier`
  - `sklearn.ensemble.ExtraTreesClassifier`
  - `sklearn.neighbors.KNeighborsClassifier`
  - `sklearn.neural_network.MLPClassifier`
  - `sklearn.neighbors.RadiusNeighborsClassifier`
  - `sklearn.ensemble.RandomForestClassifier`
  - `sklearn.linear_model.RidgeClassifierCV`
- **Support multiclass-multioutput:**
  - `sklearn.tree.DecisionTreeClassifier`
  - `sklearn.tree.ExtraTreeClassifier`
  - `sklearn.ensemble.ExtraTreesClassifier`
  - `sklearn.neighbors.KNeighborsClassifier`
  - `sklearn.neighbors.RadiusNeighborsClassifier`
  - `sklearn.ensemble.RandomForestClassifier`

Warning: At present, no metric in `sklearn.metrics` supports the multioutput-multiclass classification task.

1.12.1. Multilabel classification format

In multilabel learning, the joint set of binary classification tasks is expressed with label binary indicator array: each sample is one row of a 2d array of shape (n_samples, n_classes) with binary values: the one, i.e. the non zero elements, corresponds to the subset of labels. An array such as `np.array([[1, 0, 0], [0, 1, 1], [0, 0, 0]])` represents label 0 in the first sample, labels 1 and 2 in the second sample, and no labels in the third sample.

Producing multilabel data as a list of sets of labels may be more intuitive. The `MultiLabelBinarizer` transformer can be used to convert between a collection of collections of labels and the indicator format.

```
>>> from sklearn.preprocessing import MultiLabelBinarizer
>>> y = [[2, 3, 4], [2], [0, 1, 3], [0, 1, 2, 3, 4], [0, 1, 2]]
>>> MultiLabelBinarizer().fit_transform(y)
array([[0, 0, 1, 1, 1],
       [0, 0, 1, 0, 0],
       [1, 1, 0, 1, 0],
       [1, 1, 1, 1, 1],
       [1, 1, 1, 0, 0]])
```

1.12.2. 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 only one classifier, 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.

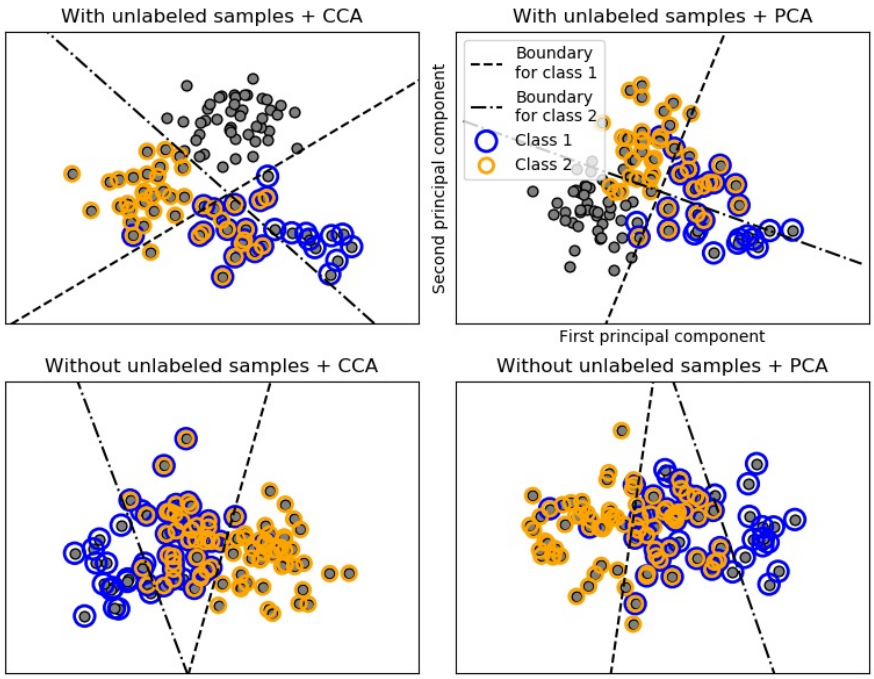
1.12.2.1. Multiclass learning

Below is an example of multiclass learning using OvR:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OneVsRestClassifier
>>> from sklearn.svm import LinearSVC
>>> X, y = datasets.load_iris(return_X_y=True)
>>> OneVsRestClassifier(LinearSVC(random_state=0)).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,
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 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, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 1, 2, 2, 2, 1, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

1.12.2.2. Multilabel learning

`OneVsRestClassifier` also supports multilabel classification. To use this feature, feed the classifier an indicator matrix, in which cell [i, j] indicates the presence of label j in sample i.



Examples:

- Multilabel classification

1.12.3. One-Vs-One

`OneVsOneClassifier` constructs one classifier per pair of classes. At prediction time, the class which received the most votes is selected. In the event of a tie (among two classes with an equal number of votes), it selects the class with the highest aggregate classification confidence by summing over the pair-wise classification confidence levels computed by the underlying binary classifiers.

Since it requires to fit `n_classes * (n_classes - 1) / 2` classifiers, this method is usually slower than one-vs-the-rest, due to its O(n_classes^2) complexity. However, this method may be advantageous for algorithms such as kernel algorithms which don't scale well with `n_samples`. This is because each individual learning problem only involves a small subset of the data whereas, with one-vs-the-rest, the complete dataset is used `n_classes` times. The decision function is the result of a monotonic transformation of the one-versus-one classification.

1.12.3.1. Multiclass learning

Below is an example of multiclass learning using OvO:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OneVsOneClassifier
>>> from sklearn.svm import LinearSVC
>>> X, y = datasets.load_iris(return_X_y=True)
>>> OneVsOneClassifier(LinearSVC(random_state=0)).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,
       0, 0, 0, 0, 1, 1, 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, 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])
```

References:

- "Pattern Recognition and Machine Learning. Springer", Christopher M. Bishop, page 183, (First Edition)

1.12.4. 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 [3] 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, `log2(n_classes) / n_classes` is sufficient to represent each class unambiguously. However, in practice, it may not lead to good accuracy since `log2(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.

1.12.4.1. Multiclass learning

Below is an example of multiclass learning using Output-Codes:

```
>>> from sklearn import datasets
>>> from sklearn.multiclass import OutputCodeClassifier
>>> from sklearn.svm import LinearSVC
>>> X, y = datasets.load_iris(return_X_y=True)
>>> clf = OutputCodeClassifier(LinearSVC(random_state=0),
...                            code_size=2, random_state=0)
>>> clf.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,
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 2, 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, 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, 1, 2, 2, 2, 1, 1, 2, 2, 2,
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

References:

- "Solving multiclass learning problems via error-correcting output codes", Dietterich T., Bakiri G., Journal of Artificial Intelligence Research 2, 1995.

[3] "The error coding method and PICTs", James G., Hastie T., Journal of Computational and Graphical statistics 7, 1998.

- "The Elements of Statistical Learning", Hastie T., Tibshirani R., Friedman J., page 606 (second-edition) 2008.

1.12.5. Multioutput regression

Multioutput regression support can be added to any regressor with `MultiOutputRegressor`. This strategy consists of fitting one regressor per target. Since each target is represented by exactly one regressor it is possible to gain knowledge about the target by inspecting its corresponding regressor. As `MultiOutputRegressor` fits one regressor per target it can not take advantage of correlations between targets.

Below is an example of multioutput regression:

```
>>> from sklearn.datasets import make_regression
>>> from sklearn.multioutput import MultiOutputRegressor
>>> from sklearn.ensemble import GradientBoostingRegressor
>>> X, y = make_regression(n_samples=10, n_targets=3, random_state=1)
>>> MultiOutputRegressor(GradientBoostingRegressor(random_state=0)).fit(X, y).predict(X)
array([[-154.75474165, -147.03498585,  -50.03812219],
       [   7.12165031,    5.12914884,  -81.46081961],
       [-187.8948621 , -100.44373091,   13.88978285],
       [-141.62745778,   95.02891072, -191.48204257],
       [  97.03260883,  165.34867495,  139.52003279],
       [ 123.92529176,   21.25719016,   -7.84253   ],
       [-122.25193977,  -85.16443186, -107.12274212],
       [ -30.170388  ,  -94.80956739,   12.16979946],
       [ 140.72667194,  176.50941682,  -17.50447799],
       [ 149.37967282,  -81.15699552,   -5.72850319]])
```

1.12.6. Multioutput classification

Multioutput classification support can be added to any classifier with `MultiOutputClassifier`. This strategy consists of fitting one classifier per target. This allows multiple target variable classifications. The purpose of this class is to extend estimators to be able to estimate a series of target functions (f1,f2,f3…,fn) that are trained on a single X predictor matrix to predict a series of responses (y1,y2,y3…,yn).

Below is an example of multioutput classification:

```
>>> from sklearn.datasets import make_classification
>>> from sklearn.multioutput import MultiOutputClassifier
>>> from sklearn.ensemble import RandomForestClassifier
>>> from sklearn.utils import shuffle
>>> import numpy as np
>>> X, y1 = make_classification(n_samples=10, n_features=100, n_informative=30, n_classes=3, random_state=1)
>>> y2 = shuffle(y1, random_state=1)
>>> y3 = shuffle(y1, random_state=2)
>>> Y = np.vstack((y1, y2, y3)).T
>>> n_samples, n_features = X.shape # 10,100
>>> n_outputs = Y.shape[1] # 3
>>> n_classes = 3
>>> forest = RandomForestClassifier(random_state=1)
>>> multi_target_forest = MultiOutputClassifier(forest, n_jobs=-1)
>>> multi_target_forest.fit(X, Y).predict(X)
array([[2, 2, 0],
       [1, 2, 1],
       [2, 1, 0],
       [0, 0, 2],
       [0, 2, 1],
       [0, 0, 2],
       [1, 1, 0],
       [1, 1, 1],
       [0, 0, 2],
       [2, 0, 0]])
```

1.12.7. Classifier Chain

Classifier chains (see `ClassifierChain`) are a way of combining a number of binary classifiers into a single multi-label model that is capable of exploiting correlations among targets.

For a multi-label classification problem with N classes, N binary classifiers are assigned an integer between 0 and N-1. These integers define the order of models in the chain. Each classifier is then fit on the available training data plus the true labels of the classes whose models were assigned a lower number.

When predicting, the true labels will not be available. Instead the predictions of each model are passed on to the subsequent models in the chain to be used as features.

Clearly the order of the chain is important. The first model in the chain has no information about the other labels while the last model in the chain has features indicating the presence of all of the other labels. In general one does not know the optimal ordering of the models in the chain so typically many randomly ordered chains are fit and their predictions are averaged together.

References:

Jesse Read, Bernhard Pfahringer, Geoff Holmes, Eibe Frank,
"Classifier Chains for Multi-label Classification", 2009.

1.12.8. Regressor Chain

Regressor chains (see `RegressorChain`) is analogous to ClassifierChain as a way of combining a number of regressions into a single multi-target model that is capable of exploiting correlations among targets.