

# Classification functions in sci-kit learn

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Machine Learning Practice

- In this week, we will study **sklearn functionality** for implementing **classification** algorithms.

- We will cover sklearn APIs for
  - Specific classification algorithms for **least square classification, perceptron**, and **logistic regression** classifier.
    - with regularization
    - multiclass, multilabel and multi-output setting
  - Various classification metrics.

- **Cross validation** and **hyper parameter search** for classification works exactly like how it works in regression setting.
  - However there are a couple of CV strategies that are specific to classification

# Part I: sklearn API for classification

There are broadly two types of APIs based on their functionality:

### Generic

- SGD classifier

Uses **gradient descent** for opt

Need to specify **loss function**

### Specific

- Logistic regression
- Perceptron
- Ridge classifier (for LSC)
- K-nearest neighbours (KNNs)
- Support vector machines (SVMs)
- Naive Bayes

**Specialized solvers** for opt

All sklearn estimators for classification implement a few common methods for **model training, prediction and evaluation**.

## Model training

```
fit(X, y[, coef_init, intercept_init, ...])
```

## Prediction

```
predict(X)
```

 predicts **class label** for samples

```
decision_function(X)
```

 predicts **confidence score** for samples.

## Evaluation

```
score(X, y[, sample_weight])
```

Return the **mean accuracy** on the given test data and labels.

There are a few common **miscellaneous methods** as follows:

`get_params([deep])` gets parameter for this estimator.

`set_params(**params)` sets the parameters of this estimator.

`densify()` converts coefficient matrix to dense array format.

`sparsify()` converts coefficient matrix to sparse format.

Now let's study how to implement different classifiers with sklearn APIs.



Let's start with implementation of **least square classification** (LSC) with **RidgeClassifier** API.

# Ridge classifier

- `RidgeClassifier` is a classifier variant of the `Ridge` regressor.

## Binary classification:

- classifier first converts binary targets to  $\{-1, 1\}$  and then treats the problem as a regression task, optimizing the objective of regressor:
  - minimize a penalized residual sum of squares
    - $\min_{\mathbf{w}} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \alpha ||\mathbf{w}||_2^2$ 
      - `sklearn` provides different solvers for this optimization
      - `sklearn` uses  $\alpha$  to denote regularization rate
    - predicted class corresponds to the sign of the regressor's prediction

## Multiclass classification:

- treated as multi-output regression
- predicted class corresponds to the output with the highest value

# How to train a least square classifier?

**Step 1:** Instantiate a **classification estimator** without passing any arguments to it. This creates a ridge classifier object.

```
1 from sklearn.linear_model import RidgeClassifier
2 ridge_classifier = RidgeClassifier()
```

**Step 2:** Call **fit** method on **ridge classifier object** with **training feature matrix** and **label vector** as arguments.

**Note:** The model is fitted using **X\_train** and **y\_train**.

```
1 # Model training with feature matrix X_train and
2 # label vector or matrix y_train
3 ridge_classifier.fit(X_train, y_train)
```

# How to set regularization rate in RidgeClassifier?

Set **alpha** to float value. The default value is 0.1.

```
1 from sklearn.linear_model import RidgeClassifier
2 ridge_classifier = RidgeClassifier(alpha=0.001)
```

- **alpha** should be positive.
- Larger alpha values specify stronger regularization.

# How to solve **optimization** problem in RidgeClassifier?

Using one of the following **solvers**

**svd**

uses a Singular Value Decomposition of the feature matrix to compute the Ridge coefficients.

**cholesky**

uses `scipy.linalg.solve` function to obtain the closed-form solution

**sparse\_cg**

uses the conjugate gradient solver of `scipy.sparse.linalg.cg`.

**lsqr**

uses the dedicated regularized least-squares routine `scipy.sparse.linalg.lsqr` and it is fastest.

**sag , saga**

uses a Stochastic Average Gradient descent iterative procedure  
'saga' is unbiased and more flexible version of 'sag'

**lbfgs**

uses L-BFGS-B algorithm implemented in

`scipy.optimize.minimize`.

can be used only when coefficients are forced to be positive.

# Uses of **solver** in RidgeClassifier

- For large scale data, use '**sparse\_cg**' solver.
- When both **n\_samples** and **n\_features** are large, use '**sag**' or '**saga**' solvers.
  - Note that fast convergence is only guaranteed on features with approximately the same scale.

# How to make RidgeClassifier select the solver automatically?

```
1 ridge_classifier = RidgeClassifier(solver=auto)
```

**auto**

chooses the solver automatically based on the type of data

```
1 if solver == 'auto':
2     if return_intercept:
3         # only sag supports fitting intercept directly
4         solver = "sag"
5     elif not sparse.issparse(X):
6         solver = "cholesky"
7     else:
8         solver = "sparse_cg"
```

Default choice for solver is **auto** .

# Is `intercept` estimation necessary for RidgeClassifier?

If data is already centered, set `fit_intercept` as false, so that no intercept will be used in calculations.

Default:

```
1 ridge_classifier = RidgeClassifier(fit_intercept=True)
```



# How to make **predictions** on new data samples?

Use `predict` method to predict class labels for samples

**Step 1:** Arrange data for prediction in a feature matrix of shape (#samples, #features) or in sparse matrix format.

**Step 2:** Call `predict` method on **classifier object** with **feature matrix** as an argument.

```
1 # Predict labels for feature matrix X_test
2 y_pred = ridge_classifier.predict(X_test)
```

Other classifiers also use the same `predict` method.

RidgeClassifierCV implements  
RidgeClassifier with built-in cross validation.

Let's implement **perceptron classifier** with  
**Perceptron API**.

# Perceptron classification

- It is a simple classification algorithm suitable for **large-scale learning**.
- Shares the same underlying implementation with **SGDClassifier**

`Perceptron()`



```
SGDClassifier(loss="perceptron", eta0=1,  
learning_rate="constant", penalty=None)
```

Perceptron uses SGD for training.

# How to implement perceptron classifier?

**Step 1:** Instantiate a **Perceptron** estimator without passing any arguments to it to create a classifier object.

```
1 from sklearn.linear_model import Perceptron
2 perceptron_classifier = Perceptron()
```

**Step 2:** Call **fit** method on **perceptron estimator object** with **training feature matrix** and **label vector** as arguments.

```
1 # Model training with feature matrix X_train and
2 # label vector or matrix y_train
3 perceptron_classifier.fit(X_train, y_train)
```

Perceptron can be further customized with the following parameters:

**penalty**

(default = 'l2')

**l1\_ratio**

(default = 0.15)

**alpha**

(default = 0.0001)

**early\_stopping**

(default = False)

**fit\_intercept**

(default = True)

**max\_iter**

(default = 1000)

**n\_iter\_no\_change**

(default = 5)

**tol**

(default = 1e-3)

**eta0**

(default = 1)

**validation\_fraction**

(default = 0.1)

- Perceptron classifier can be trained in an **iterative manner** with **partial\_fit** method
- Perceptron classifier can be initialized to the weights of the previous run by specifying **warm\_start = True** in the constructor.

Let's implement logistic regression classifier  
with `LogisticRegression` API.



# LogisticRegression API

- Implements **logistic regression classifier**, which is also known by a few different names like **logit regression**, **maximum entropy classifier** (**maxent**) and **log-linear** classifier.

$$\arg \min_{\mathbf{w}, C} \text{ regularization penalty } + C \text{ cross entropy loss}$$

- This implementation can fit
  - binary classification
  - one-vs-rest (OVR)
  - multinomial logistic regression
- Provision for  $\ell_1, \ell_2$  or **elastic-net** regularization

# How to train a **LogisticRegression** classifier?

**Step 1:** Instantiate a **classifier estimator** without passing any arguments to it. This creates a logistic regression object.

```
1 from sklearn.linear_model import LogisticRegression
2 logit_classifier = LogisticRegression()
```

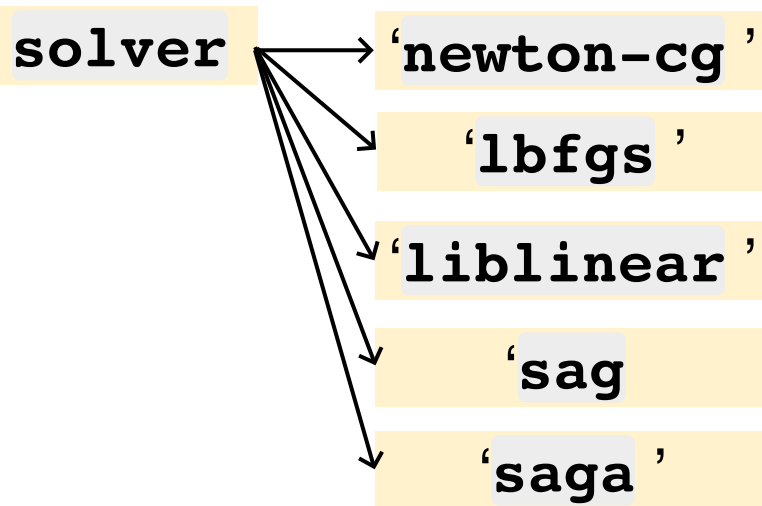
**Step 2:** Call **fit** method on **logistic regression classifier object** with **training feature matrix** and **label vector** as arguments

```
1 # Model training with feature matrix X_train and
2 # label vector or matrix y_train
3 logit_classifier.fit(X_train, y_train)
```

Logistic regression uses **specific algorithms** for solving the optimization problem in training. These algorithms are known as **solvers**.

The **choice** of the solver depends on the **classification problem set up** such as **size of the dataset**, **number of features** and **labels**.

# How to select **solvers** for Logistic Regression classifier?



- For **small datasets**, **'liblinear'** is a good choice, whereas **'sag'** and **'saga'** are faster for **large** ones.

- For **unscaled datasets**, **'liblinear'**, **'lbfgs'** and **'newton-cg'** are robust.

- For **multiclass problems**, only **'newton-cg'**, **'sag'**, **'saga'** and **'lbfgs'** handle multinomial loss.
- **'liblinear'** is limited to one-versus-rest schemes

By default, logistic regression uses **lbfgs** solver.

```
1 logit_classifier = LogisticRegression(solver='lbfgs')
```

# How to add **regularization** in Logistic Regression classifier?

- **l2** - adds a L2 penalty term

- **l1** - adds a L1 penalty term

**penalty**



- **elasticnet** - both L1 and L2 penalty terms are added

- **none** - no penalty is added

Regularization is applied by default because it improves numerical stability.

By default, it uses **L2 penalty**.

```
1 logit_classifier = LogisticRegression(penalty='l2')
```

- Not all the solvers supports all the penalties.
- Select appropriate solver for the desired penalty.
  - L2 penalty is supported by all solvers
  - L1 penalty is supported only by a few solvers.

Solver	Penalty
<code>'newton-cg'</code>	<code>['l2', 'none']</code>
<code>'lbfgs'</code>	<code>['l2', 'none']</code>
<code>'liblinear'</code>	<code>['l1', 'l2']</code>
<code>'sag'</code>	<code>['l2', 'none']</code>
<code>'saga'</code>	<code>['elasticnet', 'l1', 'l2', 'none']</code>

# How to control amount of regularization in logistic regression?

- sklearn implementation uses parameter **C**, which is **inverse of regularization rate** to control regularization.

- Recall

$$\arg \min_{\mathbf{w}, C} \text{regularization penalty} + C \text{ cross entropy loss}$$

- C is specified in the constructor and must be positive
  - **Smaller value** leads to **stronger** regularization.
  - **Larger value** leads to **weaker** regularization.

LogisticRegression classifier has a `class_weight` parameter in its constructor.

What purpose does it serve?

- Handles `class imbalance` with `differential class weights`.
- Mistakes in a class are `penalized by the class weight`.
  - `Higher value` here would mean `higher emphasis` on the class.

This parameter is available in classifier estimators in sklearn.

Exercise: Read [stack overflow discussion](#) on this parameter.



`LogisticRegressionCV` implements logistic regression with in built cross validation support to find the best values of `C` and `l1_ratio` parameters according to the specified `scoring` attribute.

These classifiers can also be implemented with a generic `SGDClassifier` API by setting the `loss` `parameter` appropriately.

Let's study `SGDClassifier` API.

# SGDClassifier

- **SGD** is a simple yet very efficient **approach to fitting linear classifiers** under convex loss functions
- This API uses SGD as an **optimization technique** and can be applied to build a variety of linear classifiers by adjusting the loss parameter.
- It supports **multi-class classification** by combining multiple binary classifiers in a “**one versus all**” (OVA) scheme.
- **Easily scales up to large scale problems** with more than  $10^5$  training examples and  $10^5$  features. It also works with **sparse** machine learning problems
  - Text classification and natural language processing

We need to set **loss parameter** appropriately to build train classifier of our interest with **SGDClassifier**

**loss  
parameter**

'hinge' - (soft-margin) linear Support Vector Machine

'log' - logistic regression

'modified\_huber' - smoothed hinge loss brings tolerance to outliers as well as probability estimates

'squared\_hinge' - like hinge but is quadratically penalized

'perceptron' - linear loss used by the perceptron algorithm

'squared\_error', 'huber', 'epsilon\_insensitive', or 'squared\_epsilon\_insensitive' - regression losses

By default **SGDClassifier** uses **hinge loss** and hence trains **linear support vector machine classifier**.

- An instance of **SGDClassifier** might have an **equivalent estimator** in the scikit-learn API.

```
SGDClassifier(loss='log')
```



```
LogisticRegression(solver='sgd')
```

```
SGDClassifier(loss='hinge')
```



```
Linear Support vector machine
```

# How does **SGDClassifier** work?

- SGDClassifier implements a **plain stochastic gradient descent learning routine**.
  - the gradient of the loss is estimated with one sample at a time and the model is updated along the way with a decreasing learning rate (or strength) schedule.

## Advantages:

- Efficiency.
- Ease of implementation

## Disadvantages:

- Requires a number of hyperparameters.
- Sensitive to feature scaling.

- It is important
  - to **permute** (shuffle) the **training data before fitting** the model.
  - to standardize the **features**.



# How to use `SGDClassifier` for training a classifier?

**Step 1:** Instantiate a `SGDClassifier` estimator by setting appropriate loss parameter to define classifier of interest. By default it uses `hinge loss`, which is used for training linear support vector machine.

```
1 from sklearn.linear_model import SGDClassifier
2 SGD_classifier = SGDClassifier(loss='log')
```

Here we have used `'log'` loss that defines a `logistic regression classifier`.

**Step 2:** Call `fit` method on `SGD classifier object` with `training feature matrix` and `label vector` as arguments.

```
1 # Model training with feature matrix X_train and
2 # label vector or matrix y_train
3 SGD_classifier.fit(X_train, y_train)
```

# How to perform **regularization** in SGD classifier?

- **l2** - adds a L2 penalty term

- **l1** - adds a L1 penalty term

**penalty**



```
graph TD; penalty[penalty] --> l2[l2]; penalty --> l1[l1]; penalty --> elasticnet[elasticnet];
```

- **elasticnet** - Convex combination of L2 and L1

$$(1 - \text{l1\_ratio}) * \text{L2} + \text{l1\_ratio} * \text{L1}$$

(**l1\_ratio** controls the convex combination of L1 and L2 penalty. default=0.15)

Default:

```
1 SGD_classifier = SGDClassifier(penalty='l2')
```

**alpha**



- Constant that multiplies the regularization term.
- Has float values and **default = 0.0001**

# How to set **maximum number of epochs** for SGD Classifier?

The maximum number of passes over the training data (aka epochs) is an integer that can be set by the `max_iter` parameter.

```
1 SGD_classifier = SGDClassifier(max_iter=100)
```

Default:

```
max_iter = 1000
```

# Some common parameters between SGDClassifier and SGDRegressor

## learning\_rate

- 'constant'
- 'optimal'
- 'invscaling'
- 'adaptive'

## warm\_start

- 'True'
- 'False'

## average

- SGDClassifier also supports averaged SGD (ASGD)

## Stopping criteria

- tol
- n\_iter\_no\_change
- max\_iter
- early\_stopping
- validation\_fraction

# Summary

We learnt how to implement the following classifiers with sklearn APIs:

- Least square classification ([RidgeClassifier](#))
- Perceptron ([Perceptron](#))
- Logistic regression ([LogisticRegression](#))

Alternatively we can use [SGDClassifier](#) with appropriate [loss](#) setting for implementing these classifiers:

- [loss = `log`](#) for [logistic regression](#)
- [loss = `perceptron`](#) for [perceptron](#)
- [loss = `squared\\_error`](#) for [least square classification](#)

Classification estimators implements a few common methods like [fit](#), [score](#), [decision\\_function](#), and [predict](#).

- These estimators can be readily used in **multiclass setting**.
- They support **regularized loss function** optimization.
- All classification estimators have ability to deal with **class imbalance** through **class\_weight** parameter in the constructor.

## Part II: Multi-learning classification set up

Let's extend these classifiers to multi-learning (multi-class, multi-label & multi-output) settings.



# Basics of multiclass, multilabel and multioutput classification

- **Multiclass classification** has **exactly one output label** and the total **number of labels**  $> 2$ .
- For **more than one output**, there are **two types** of classification models:

**Multilabel**

**total #labels**  $= 2$

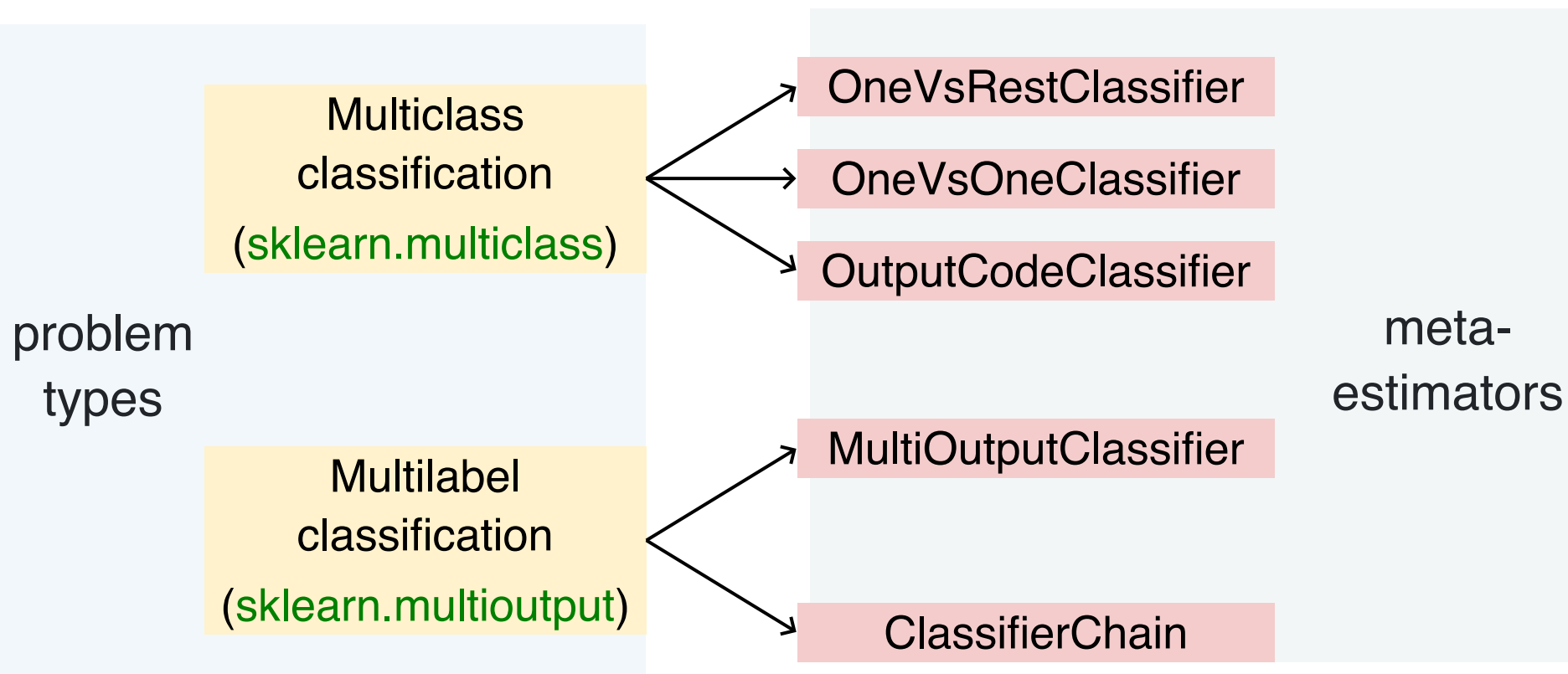
**Multiclass multioutput**

**total #labels**  $> 2$

We will refer both these models as **multi-label classification** models, where **# of output labels**  $> 1$ .

**Multiclass, multilabel, multioutput** problems are referred to as **multi-learning problems**.

- sklearn provides a bunch of **meta-estimators**, which **extend** the functionality of **base estimators** to support multi-learning problems.
- The meta-estimators **transform** the multi-learning problem into **a set of simpler problems** and **fit one estimator per problem**.



- Many sklearn estimators have **built-in support** for multi-learning problems.
  - Meta-estimators are not needed for such estimators, however meta-estimators can be used in case we want to use these base estimators with **strategies** beyond the built-in ones.

Inherently  
multiclass

Multiclass as  
OVO

Multiclass as  
OVR

Multilabel

Inherently  
multiclass

LogisticRegression (`multi_class = 'multinomial'`)

LogisticRegressionCV (`multi_class = 'multinomial'`)

RidgeClassifier

RidgeClassifierCV

Multiclass as  
OVR

LogisticRegression (`multi_class = 'ovr'`)

LogisticRegressionCV (`multi_class = 'ovr'`)

SGDClassifier

Perceptron

Multilabel

RidgeClassifier

RidgeClassifierCV

First we will study **multiclass APIs** in sklearn.

# Multi-class classification

- Classification task with more than two classes.
- Each example is labeled with exactly one class

In Iris dataset,

- There are three class labels: setosa, versicolor and virginica.
- Each example has exactly one label of the three available class labels.
- Thus, this is an instance of a multi-class classification.

In MNIST digit recognition dataset,

- There are 10 class labels: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9.
- Each example has exactly one label of the 10 available class labels.
- Thus, this is an instance of a multi-class classification.

# How to represent class labels in multi-class setup?

- Each example is marked with a single label out of  $k$  labels. The shape of label vector is  $(n, 1)$ .
- Use [LabelBinarizer](#) transformation to convert the class label to multi-class format.

```
1 from sklearn.preprocessing import LabelBinarizer
2 y = np.array(['apple', 'pear', 'apple', 'orange'])
3 y_dense = LabelBinarizer().fit_transform(y)
```

- The resulting label vector has shape of  $(n, k)$ .

```
[[1 0 0]
 [0 0 1]
 [1 0 0]
 [0 1 0]]
```

Let's say, you are given labels as part of the training set, how do we check if they are suitable for multi-class classification?

- Use `type_of_target` to determine the type of the label.

```
1 from sklearn.utils.multiclass import type_of_target
2 type_of_target(y)
```

- In case,  $y$  is a vector with more than two discrete values, `type_of_target` returns `multiclass`.



`type_of_target` can determine different types  
of multi-learning targets.

## target\_type

'multiclass'

'multiclass-  
multioutput'

'multilabel-  
indicator'

'unknown'

## y

- contains more than two discrete values
- not a sequence of sequences
- 1d or a column vector

- 2d array that contains more than two discrete values
- not a sequence of sequences
- dimensions are of size  $> 1$

- label indicator matrix
- an array of two dimensions with at least two columns, and at most 2 unique values.

- array-like but none of the above, such as a 3d array,
- sequence of sequences, or an array of non-sequence objects.

# Examples

multiclass

```
1 >>> type_of_target([1, 0, 2])
2 'multiclass'
3 >>> type_of_target([1.0, 0.0, 3.0])
4 'multiclass'
5 >>> type_of_target(['a', 'b', 'c'])
6 'multiclass'
```

multiclass-multioutput

```
1 >>> type_of_target(np.array([[1, 2], [3, 1]]))
2 'multiclass-multioutput'
```

multilabel-indicator

```
1 type_of_target(np.array([[0, 1], [1, 1]]))
2 'multilabel-indicator'
3 >>> type_of_target([[1, 2]])
4 'multilabel-indicator'
```

Apart from these, there are three more types, `type_of_target` can determine targets corresponding to `regression` and `binary classification`.

- `continuous` - regression target
- `continuous-multioutput` - multi-output target
- `binary` - classification

All classifiers in scikit-learn perform multiclass classification out-of-the-box.

- Use `sklearn.multiclass` module only when you want to experiment with different multiclass strategies.
- Using different multi-class strategy than the one implemented by default may affect performance of classifier in terms of either generalization error or computational resource requirement.

# What are different multi-class classification strategies implemented in sklearn?

- One-vs-all or one-vs-rest (OVR)
  - One-vs-One (OVA)
- 
- OVR is implemented by `OneVsRestClassifier` API.
  - OVA is implemented by `OneVsOneClassifier` API.

# OVR - OneVsRestClassifier

- Fits **one classifier per class  $c$**  -  $c$  vs **not  $c$** .
- This approach is computationally efficient and requires only  $k$  classifiers.
- The resulting model is interpretable.

```
1 from sklearn.multiclass import OneVsRestClassifier
2 OneVsRestClassifier(LinearSVC(random_state=0)).fit(X, y)
```

- We need to supply estimator as an argument in the constructor.
- Support methods like other classifiers - fit, predict, predict\_proba, partial\_fit.

OneVsRest classifier also supports **multilabel classification**. We need to supply labels as **indicator matrix** of shape  $(n, k)$ .

# OVA - OneVsOneClassifier

- Fits **one classifier per pair of classes**. **Total classifiers** =  $\binom{k}{2}$ .
- Predicts class that receives maximum votes.
  - The tie among classes is broken by selecting the class with the highest aggregate classification confidence.

```
1 from sklearn.multiclass import OneVsOneClassifier
2 OneVsOneClassifier(LinearSVC(random_state=0)).fit(X, y)
```

- We need to supply estimator as an argument in the constructor.
- Support methods like other classifiers - fit, predict, predict\_proba, partial\_fit.

OneVsOne classifier processes subset of data at a time and is useful in cases where the classifier does not scale with the data.



# What is the difference between OVR and OVA?

## OneVsRestClassifier

- Fits one classifier per class.
- For each classifier, the class is fitted against all the other classes.

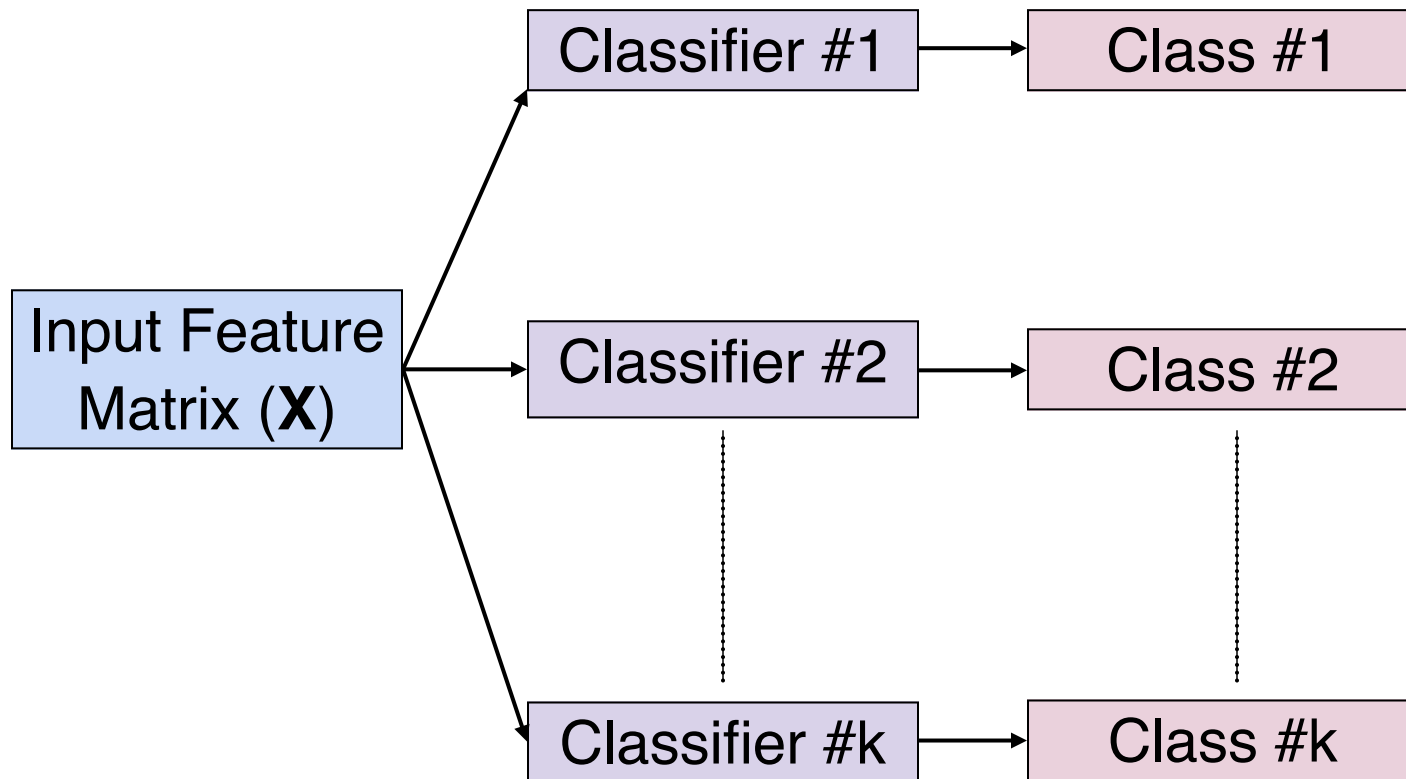
## OneVsOneClassifier

- Fits one classifier per pair of classes.
- At prediction time, the class which received the most votes is selected.

Now we will learn how to perform **multilabel**  
and **multi-output** classification.

# How MultiOutputClassifier works?

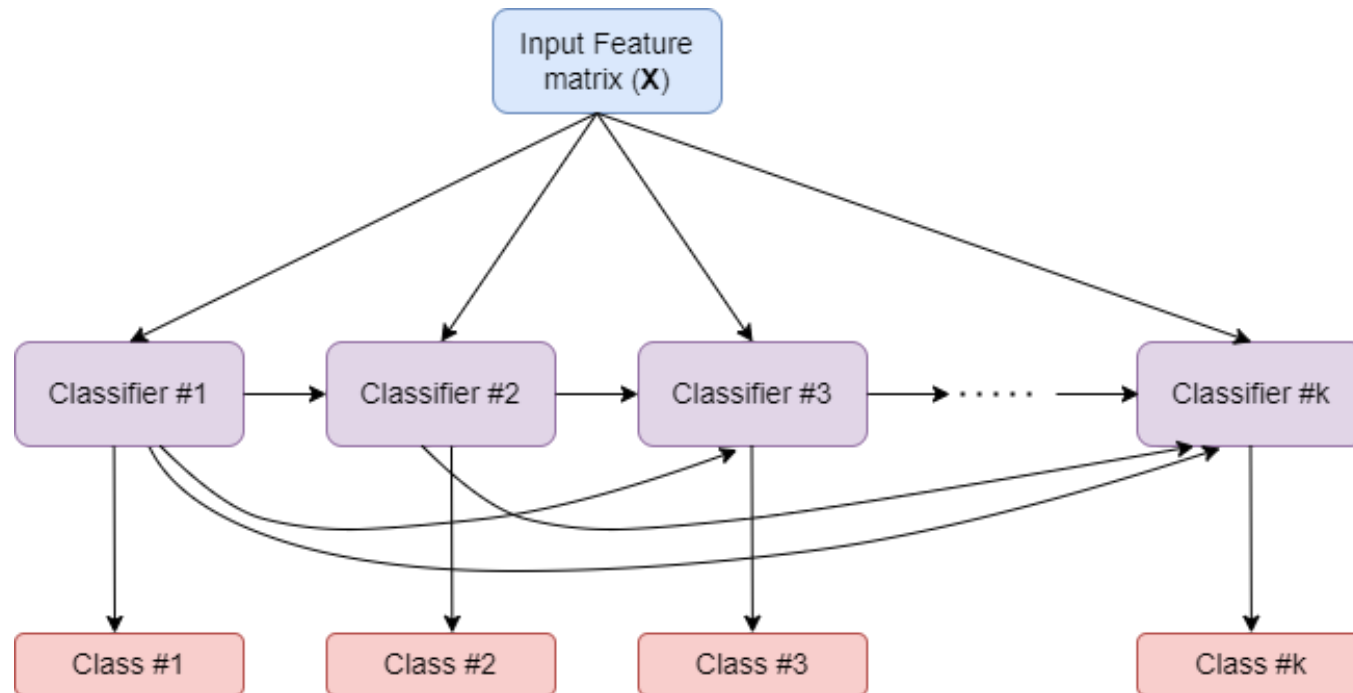
- Strategy consists of fitting **one classifier per target**.



- Allows multiple target variable classifications.

# How ClassifierChain works?

- A multi-label model that arranges binary classifiers into a chain.
- Way of combining a number of binary classifiers into a single multi-label model.



# Comparison of MultiOutputClassifier and ClassifierChain

## MultiOutputClassifier

- Able to estimate a series of target functions that are trained on a single predictor matrix to predict a series of responses.
- Allows multiple target variable classifications.

## ClassifierChain

- Capable of exploiting correlations among targets.
- For a multi-label classification problem with  $k$  classes,  $k$  binary classifiers are assigned an integer between 0 and  $k - 1$ .
- These integers define the order of models in the chain.

# Summary

- Different types of multi-learning setups: multi-class, multi-label, multi-output.
- `type_of_target` to determine the nature of supplied labels.
- Meta-estimators:
  - multi-class: One-vs-rest, one-vs-one
  - multi-label: Classifier chain and multi-output classifier

# Evaluating Classifiers

So far we learnt how to **train** classifiers for **binary, multi-class** and **multi-label/output** cases.

We will learn how to evaluate these classifiers with **different scoring functions** and with **cross-validation**.

We will also study how to set **hyper-parameters** for classifiers.

Many cross-validation and HPT methods discussed in the regression context are also applicable in classifiers.

- We will not repeat that discussion in this topic.
- Instead we will focus on only additional methods that are specific to classifiers.



# Stratified cross validation iterators

There may be issues like **class imbalance** in classification, which tend to impact the cross validation folds.

The **overall class distribution** and the ones in **folds** may be **different** and this has implications in effective model training.

**sklearn.model\_selection** module provides three **stratified APIs** to create folds such that the **overall class distribution** is replicated in individual folds.

`sklearn.model_selection` module provides the following three **stratified APIs** to create folds such that the **overall class distribution is replicated in individual folds**.

- StratifiedKFold
- RepeatedStratifiedKFold
- StratifiedShuffleSplit

**Note:** Folds obtained via StratifiedShuffleSplit may not be completely different.

# LogisticRegressionCV

- Support in-build cross validation for optimizing hyperparameters
- The following are key parameters for HPT and cross validation

**cv** specifies  
cross validation  
iterator

**scoring** specifies  
scoring function to  
use for HPT

**cs** specifies  
regularization  
strengths to  
experiment with.

- Choosing the best hyper-parameters

**refit = True**

Scores averaged across folds, values corresponding to the best score are selected and final refit with these parameters

**refit = False**

the **coefs, intercepts and C** that correspond to the best scores across folds are averaged.

Now let's look at classification metrics  
implemented in sklearn.

# Classification metrics

`sklearn.metrics` implements a bunch of **classification scoring metrics** based on **true labels** and **predicted labels** as inputs.

`accuracy_score`

`balanced_accuracy_score`

`top_k_accuracy_score`

`roc_auc_score`

`precision_score`

`recall_score`

`f1_score`

`score(actual_labels, predicted_labels)`

# Confusion matrix

- `confusion_matrix` evaluates classification accuracy by computing the confusion matrix with each row corresponding to the true class.

```
1 from sklearn.metrics import confusion_matrix
2 confusion_matrix(y_true, y_predicted)
```

Example:

```
array([[2, 0, 0],
       [0, 0, 1],
       [1, 0, 2]])
```

Entry  $i, j$  in a confusion matrix

number of observations actually in group  $i$ ,  
but predicted to be in group  $j$ .

Confusion matrix can be displayed with `ConfusionMatrixDisplay` API in `sklearn.metrics`.

- Confusion matrix

```
1 ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=clf.classes_)
```

- From estimators

```
1 ConfusionMatrixDisplay.from_estimator(clf, X_test, y_test)
```

- From predictions

```
1 ConfusionMatrixDisplay.from_predictions(y_test, y_pred)
```

The `classification_report` function builds a text report showing the main classification metrics.

```
1 from sklearn.metrics import classification_report
2 print(classification_report(y_true, y_predicted))
```

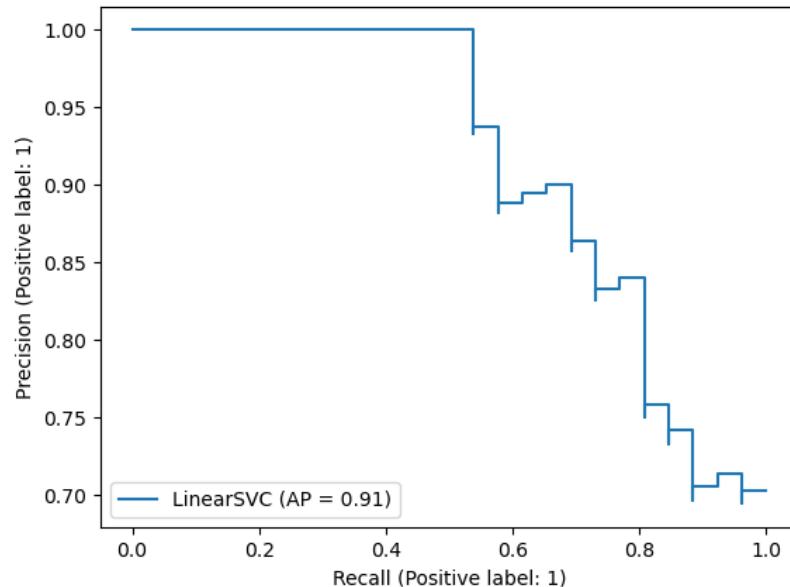
	precision	recall	f1-score	support
class 0	0.67	1.00	0.80	2
class 1	0.00	0.00	0.00	1
class 2	1.00	0.50	0.67	2
accuracy			0.60	5
macro avg	0.56	0.50	0.49	5
weighted avg	0.67	0.60	0.59	5



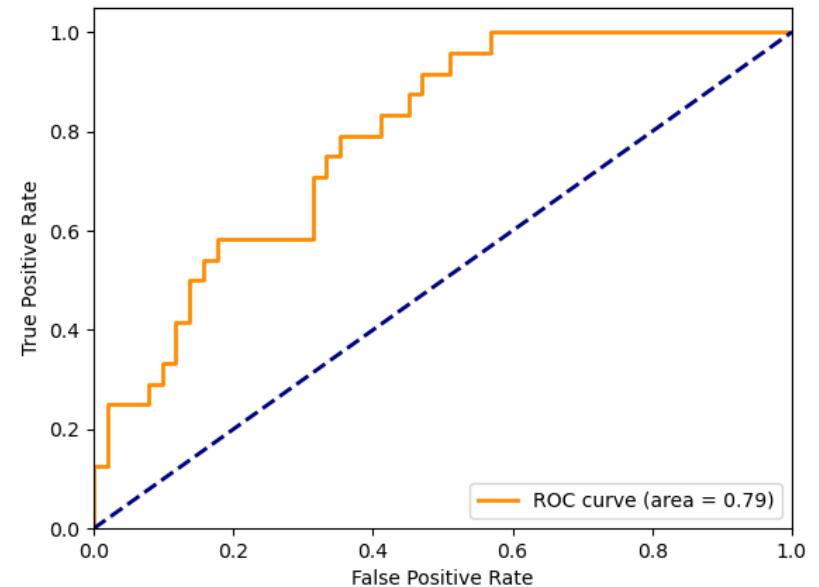
# Classifier Performance across probability thresholds

```
1 from sklearn.metrics import precision_recall_curve
2 precision, recall, thresholds = precision_recall_curve(y_true, y_predicted)
```

2-class Precision-Recall curve



Receiver operating characteristic example



```
1 from sklearn.metrics import roc_curve
2 fpr, tpr, thresholds = metrics.roc_curve(y_true, y_scores, pos_label=2)
```

# How to extend binary metric to multiclass or multilabel problems?

- Treat data as a collection of binary problems, one for each class.
  - Then, average binary metric calculations across the set of classes.
- Can be done using **average** parameter.

**macro**

calculates the mean of the binary metrics

**weighted**

computes the average of binary metrics in which each class's score is weighted by its presence in the true data sample.

**micro**

gives each sample-class pair an equal contribution to the overall metric

**samples**

calculates the metric over the true and predicted classes for each sample in the evaluation data, and returns their average

**None**

returns an array with the score for each class

# Summary

- Classification specific cross validation iterator based on stratification.
- Classification metrics
- Extending binary metrics to multi-learning set up.