3.3. Model evaluation: quantifying the quality of predictions

There are 3 different APIs for evaluating the quality of a model's predictions:

- **Estimator score method**: Estimators have a `score` method providing a default evaluation criterion for the problem they are designed to solve. This is not discussed on this page, but in each estimator's documentation.
- **Scoring parameter**: Model-evaluation tools using cross-validation (such as `model_selection.cross_val_score` and `model_selection.GridSearchCV`) rely on an internal *scoring* strategy. This is discussed in the section The scoring parameter: defining model evaluation rules.
- **Metric functions**: The `metrics` module implements functions assessing prediction error for specific purposes. These metrics are detailed in sections on Classification metrics, Multi-label ranking metrics, Regression metrics and Clustering metrics.

Finally, Dummy estimators are useful to get a baseline value of those metrics for random predictions.

See also: For "pairwise" metrics, between *samples* and not estimators or predictions, see the Pairwise metrics, Affinities and Kernels section.

3.3.1. The `scoring` parameter: defining model evaluation rules

Model selection and evaluation using tools, such as `model_selection.GridSearchCV` and `model_selection.cross_val_score`, take a `scoring` parameter that controls what metric they apply to the estimators evaluated.

3.3.1.1. Common cases: predefined values

For the most common use cases, you can designate a scorer object with the `scoring` parameter; the table below shows all possible values. All scorer objects follow the convention that **higher return values are better than lower return values**. Thus metrics which measure the distance between the model and the data, like `metrics.mean_squared_error`, are available as neg_mean_squared_error which return the negated value of the metric.

Scoring	Function	Comment
Classification		
'accuracy'	`metrics.accuracy_score`	
'average_precision'	`metrics.average_precision_score`	

‘f1’	`metrics.f1_score`	for binary targets
‘f1_micro’	`metrics.f1_score`	micro-averaged
‘f1_macro’	`metrics.f1_score`	macro-averaged
‘f1_weighted’	`metrics.f1_score`	weighted average
‘f1_samples’	`metrics.f1_score`	by multilabel sample
‘neg_log_loss’	`metrics.log_loss`	requires `predict_proba` support
‘precision’ etc.	`metrics.precision_score`	suffixes apply as with ‘f1’
‘recall’ etc.	`metrics.recall_score`	suffixes apply as with ‘f1’
‘roc_auc’	`metrics.roc_auc_score`	
Clustering		
‘adjusted_mutual_info_score’	`metrics.adjusted_mutual_info_score`	
‘adjusted_rand_score’	`metrics.adjusted_rand_score`	
‘completeness_score’	`metrics.completeness_score`	
‘fowlkes_mallows_score’	`metrics.fowlkes_mallows_score`	
‘homogeneity_score’	`metrics.homogeneity_score`	
‘mutual_info_score’	`metrics.mutual_info_score`	
‘normalized_mutual_info_score’	`metrics.normalized_mutual_info_score`	
‘v_measure_score’	`metrics.v_measure_score`	
Regression		
‘explained_variance’	`metrics.explained_variance_score`	
‘neg_mean_absolute_error’	`metrics.mean_absolute_error`	
‘neg_mean_squared_error’	`metrics.mean_squared_error`	
‘neg_mean_squared_log_error’	`metrics.mean_squared_log_error`	
‘neg_median_absolute_error’	`metrics.median_absolute_error`	
‘r2’	`metrics.r2_score`	

Usage examples:

```
>>> from sklearn import svm, datasets
>>> from sklearn.model_selection import cross_val_score
>>> iris = datasets.load_iris()
>>> X, y = iris.data, iris.target
>>> clf = svm.SVC(probability=True, random_state=0)
>>> cross_val_score(clf, X, y, scoring='neg_log_loss')
array([-0.07..., -0.16..., -0.06...])
>>> model = svm.SVC()
>>> cross_val_score(model, X, y, scoring='wrong_choice')
Traceback (most recent call last):
ValueError: 'wrong_choice' is not a valid scoring value. Valid options are ['accura
```

Note: The values listed by the ValueError exception correspond to the functions measuring prediction accuracy described in the following sections. The scorer objects for those functions are stored in the dictionary `sklearn.metrics.SCORERS`.

3.3.1.2. Defining your scoring strategy from metric functions

The module **`sklearn.metrics`** also exposes a set of simple functions measuring a prediction error given ground truth and prediction:

- functions ending with `_score` return a value to maximize, the higher the better.
- functions ending with `_error` or `_loss` return a value to minimize, the lower the better. When converting into a scorer object using **`make_scorer`**, set the `greater_is_better` parameter to False (True by default; see the parameter description below).

Metrics available for various machine learning tasks are detailed in sections below.

Many metrics are not given names to be used as `scoring` values, sometimes because they require additional parameters, such as **`fbeta_score`**. In such cases, you need to generate an appropriate scoring object. The simplest way to generate a callable object for scoring is by using **`make_scorer`**. That function converts metrics into callables that can be used for model evaluation.

One typical use case is to wrap an existing metric function from the library with non-default values for its parameters, such as the `beta` parameter for the **`fbeta_score`** function:

```
>>> from sklearn.metrics import fbeta_score, make_scorer
>>> ftwo_scorer = make_scorer(fbeta_score, beta=2)
>>> from sklearn.model_selection import GridSearchCV
>>> from sklearn.svm import LinearSVC
>>> grid = GridSearchCV(LinearSVC(), param_grid={'C': [1, 10]}, scoring=ftwo_scorer
```

The second use case is to build a completely custom scorer object from a simple python function using **`make_scorer`**, which can take several parameters:

- the python function you want to use (`my_custom_loss_func` in the example below)
- whether the python function returns a score (`greater_is_better=True`, the default) or a loss (`greater_is_better=False`). If a loss, the output of the python function is negated by the scorer object, conforming to the cross validation convention that scorers return higher values for better models.
- for classification metrics only: whether the python function you provided requires continuous decision certainties (`needs_threshold=True`). The default value is False.
- any additional parameters, such as `beta` or `labels` in **`f1_score`**.

Here is an example of building custom scorers, and of using the `greater_is_better` parameter:

```
>>> import numpy as np
>>> def my_custom_loss_func(ground_truth, predictions):
...     diff = np.abs(ground_truth - predictions).max()
...     return np.log(1 + diff)
...
>>> # loss_func will negate the return value of my_custom_loss_func,
>>> #  which will be np.log(2), 0.693, given the values for ground_truth
>>> #  and predictions defined below.
>>> loss  = make_scorer(my_custom_loss_func, greater_is_better=False)
>>> score = make_scorer(my_custom_loss_func, greater_is_better=True)
>>> ground_truth = [[1], [1]]
>>> predictions  = [0, 1]
>>> from sklearn.dummy import DummyClassifier
>>> clf = DummyClassifier(strategy='most_frequent', random_state=0)
>>> clf = clf.fit(ground_truth, predictions)
>>> loss(clf,ground_truth, predictions)
-0.69...
>>> score(clf,ground_truth, predictions)
0.69...
```

3.3.1.3. Implementing your own scoring object

You can generate even more flexible model scorers by constructing your own scoring object from scratch, without using the **make_scorer** factory. For a callable to be a scorer, it needs to meet the protocol specified by the following two rules:

- It can be called with parameters `(estimator, X, y)`, where `estimator` is the model that should be evaluated, `X` is validation data, and `y` is the ground truth target for `X` (in the supervised case) or `None` (in the unsupervised case).
- It returns a floating point number that quantifies the `estimator` prediction quality on `X`, with reference to `y`. Again, by convention higher numbers are better, so if your scorer returns loss, that value should be negated.

3.3.1.4. Using multiple metric evaluation

Scikit-learn also permits evaluation of multiple metrics in `GridSearchCV`, `RandomizedSearchCV` and `cross_validate`.

There are two ways to specify multiple scoring metrics for the `scoring` parameter:

- As an iterable of string metrics::

```
>>> scoring = ['accuracy', 'precision']
```

- As a `dict` mapping the scorer name to the scoring function::

```
>>> from sklearn.metrics import accuracy_score
>>> from sklearn.metrics import make_scorer
>>> scoring = {'accuracy': make_scorer(accuracy_score),
...            'prec': 'precision'}
```

Note that the dict values can either be scorer functions or one of the predefined metric strings.

Currently only those scorer functions that return a single score can be passed inside the dict. Scorer functions that return multiple values are not permitted and will require a wrapper to return a single metric:

```
>>> from sklearn.model_selection import cross_validate
>>> from sklearn.metrics import confusion_matrix
>>> # A sample toy binary classification dataset
>>> X, y = datasets.make_classification(n_classes=2, random_state=0)
>>> svm = LinearSVC(random_state=0)
>>> def tp(y_true, y_pred): return confusion_matrix(y_true, y_pred)[0, 0]
>>> def tn(y_true, y_pred): return confusion_matrix(y_true, y_pred)[0, 0]
>>> def fp(y_true, y_pred): return confusion_matrix(y_true, y_pred)[1, 0]
>>> def fn(y_true, y_pred): return confusion_matrix(y_true, y_pred)[0, 1]
>>> scoring = {'tp' : make_scorer(tp), 'tn' : make_scorer(tn),
...            'fp' : make_scorer(fp), 'fn' : make_scorer(fn)}
>>> cv_results = cross_validate(svm.fit(X, y), X, y, scoring=scoring)
>>> # Getting the test set true positive scores
>>> print(cv_results['test_tp'])
[12 13 15]
>>> # Getting the test set false negative scores
>>> print(cv_results['test_fn'])
[5 4 1]
```

3.3.2. Classification metrics

The **`sklearn.metrics`** module implements several loss, score, and utility functions to measure classification performance. Some metrics might require probability estimates of the positive class, confidence values, or binary decisions values. Most implementations allow each sample to provide a weighted contribution to the overall score, through the `sample_weight` parameter.

Some of these are restricted to the binary classification case:

`precision_recall_curve`(y_true, probas_pred)	Compute precision-recall pairs for different probability thresholds
`roc_curve`(y_true, y_score[, pos_label, …])	Compute Receiver operating characteristic (ROC)

Others also work in the multiclass case:

`cohen_kappa_score`(y1, y2[, labels, weights, …])	Cohen's kappa: a statistic that measures inter-annotator agreement.
`confusion_matrix`(y_true, y_pred[, labels, …])	Compute confusion matrix to evaluate the accuracy of a classification
`hinge_loss`(y_true, pred_decision[, labels, …])	Average hinge loss (non-regularized)
`matthews_corrcoef`(y_true, y_pred[, …])	Compute the Matthews correlation coefficient (MCC)

Some also work in the multilabel case:

`accuracy_score`(y_true, y_pred[, normalize, …])	Accuracy classification score.
`classification_report`(y_true, y_pred[, …])	Build a text report showing the main classification metrics
`f1_score`(y_true, y_pred[, labels, …])	Compute the F1 score, also known as balanced F-score or F-measure
`fbeta_score`(y_true, y_pred, beta[, labels, …])	Compute the F-beta score
`hamming_loss`(y_true, y_pred[, labels, …])	Compute the average Hamming loss.
`jaccard_similarity_score`(y_true, y_pred[, …])	Jaccard similarity coefficient score
`log_loss`(y_true, y_pred[, eps, normalize, …])	Log loss, aka logistic loss or cross-entropy loss.
`precision_recall_fscore_support`(y_true, y_pred)	Compute precision, recall, F-measure and support for each class
`precision_score`(y_true, y_pred[, labels, …])	Compute the precision
`recall_score`(y_true, y_pred[, labels, …])	Compute the recall
`zero_one_loss`(y_true, y_pred[, normalize, …])	Zero-one classification loss.

And some work with binary and multilabel (but not multiclass) problems:

`average_precision_score`(y_true, y_score[, …])	Compute average precision (AP) from prediction scores
`roc_auc_score`(y_true, y_score[, average, …])	Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.

In the following sub-sections, we will describe each of those functions, preceded by some notes on common API and metric definition.

3.3.2.1. From binary to multiclass and multilabel

Some metrics are essentially defined for binary classification tasks (e.g. **`f1_score`**, **`roc_auc_score`**). In these cases, by default only the positive label is evaluated, assuming by default that the positive class is labelled `1` (though this may be configurable through the `pos_label` parameter).

In extending a binary metric to multiclass or multilabel problems, the data is treated as a collection of binary problems, one for each class. There are then a number of ways to average binary metric calculations across the set of classes, each of which may be useful in some scenario. Where available, you should select among these using the `average` parameter.

- `"macro"` simply calculates the mean of the binary metrics, giving equal weight to each class. In problems where infrequent classes are nonetheless important, macro-averaging may be a means of highlighting their performance. On the other hand, the assumption that all classes are equally important is often untrue, such that macro-averaging will over-emphasize the typically low performance on an infrequent class.
- `"weighted"` accounts for class imbalance by computing 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 (except as a result of sample-weight). Rather than summing the metric per class, this sums the dividends and divisors that make up the per-class metrics to calculate an overall quotient. Micro-averaging may be preferred in multilabel settings, including multiclass classification where a majority class is to be ignored.
- `"samples"` applies only to multilabel problems. It does not calculate a per-class measure, instead calculating the metric over the true and predicted classes for each sample in the evaluation data, and returning their (`sample_weight`-weighted) average.
- Selecting `average=None` will return an array with the score for each class.

While multiclass data is provided to the metric, like binary targets, as an array of class labels, multilabel data is specified as an indicator matrix, in which cell `[i, j]` has value 1 if sample `i` has label `j` and value 0 otherwise.

3.3.2.2. Accuracy score

The **`accuracy_score`** function computes the accuracy, either the fraction (default) or the count (normalize=False) of correct predictions.

In multilabel classification, the function returns the subset accuracy. If the entire set of predicted labels for a sample strictly match with the true set of labels, then the subset accuracy is 1.0; otherwise it is 0.0.

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value, then the fraction of correct predictions over n_samples is defined as

$$\texttt{accuracy}(y, \hat{y}) = \frac{1}{n_\text{samples}} \sum_{i=0}^{n_\text{samples}-1} 1(\hat{y}_i = y_i)$$

where $1(x)$ is the indicator function.

```
>>> import numpy as np
>>> from sklearn.metrics import accuracy_score
>>> y_pred = [0, 2, 1, 3]
>>> y_true = [0, 1, 2, 3]
>>> accuracy_score(y_true, y_pred)
0.5
```

```
>>> accuracy_score(y_true, y_pred, normalize=False)
2
```

In the multilabel case with binary label indicators:

```
>>> accuracy_score(np.array([[0, 1], [1, 1]]), np.ones((2, 2)))
0.5
```

Example:

- See Test with permutations the significance of a classification score for an example of accuracy score usage using permutations of the dataset.

3.3.2.3. Cohen's kappa

The function **`cohen_kappa_score`** computes Cohen's kappa statistic. This measure is intended to compare labelings by different human annotators, not a classifier versus a ground truth.

The kappa score (see docstring) is a number between -1 and 1. Scores above .8 are generally considered good agreement; zero or lower means no agreement (practically random labels).

Kappa scores can be computed for binary or multiclass problems, but not for multilabel problems (except by manually computing a per-label score) and not for more than two annotators.

```
>>> from sklearn.metrics import cohen_kappa_score
>>> y_true = [2, 0, 2, 2, 0, 1]
>>> y_pred = [0, 0, 2, 2, 0, 2]
>>> cohen_kappa_score(y_true, y_pred)
0.4285714285714286
```

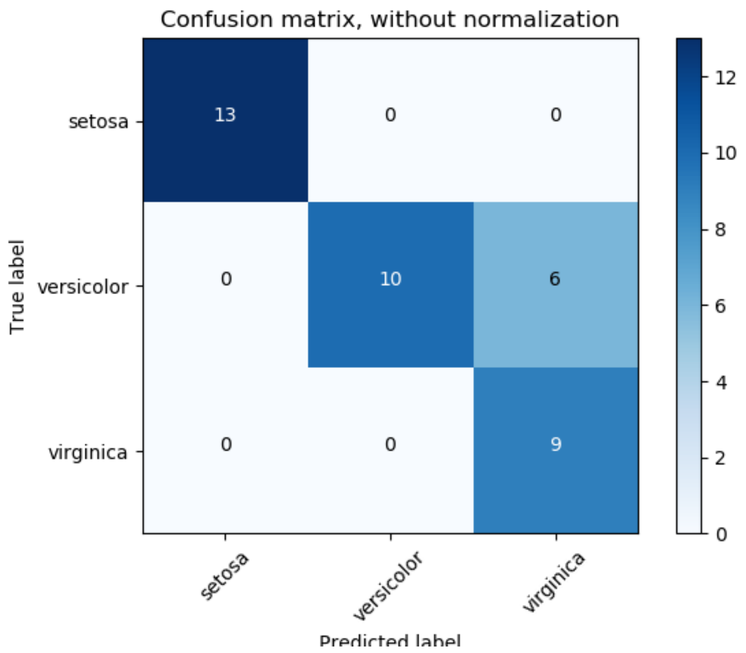
3.3.2.4. Confusion matrix

The **`confusion_matrix`** function evaluates classification accuracy by computing the confusion matrix.

By definition, entry i, j in a confusion matrix is the number of observations actually in group i, but predicted to be in group j. Here is an example:

```
>>> from sklearn.metrics import confusion_matrix
>>> y_true = [2, 0, 2, 2, 0, 1]
>>> y_pred = [0, 0, 2, 2, 0, 2]
>>> confusion_matrix(y_true, y_pred)
array([[2, 0, 0],
       [0, 0, 1],
       [1, 0, 2]])
```

Here is a visual representation of such a confusion matrix (this figure comes from the Confusion matrix example):



For binary problems, we can get counts of true negatives, false positives, false negatives and true positives as follows:

```
>>> y_true = [0, 0, 0, 1, 1, 1, 1, 1]
>>> y_pred = [0, 1, 0, 1, 0, 1, 0, 1]
>>> tn, fp, fn, tp = confusion_matrix(y_true, y_pred).ravel()
>>> tn, fp, fn, tp
(2, 1, 2, 3)
```

Example:

- See Confusion matrix for an example of using a confusion matrix to evaluate classifier output quality.
- See Recognizing hand-written digits for an example of using a confusion matrix to classify hand-written digits.
- See Classification of text documents using sparse features for an example of using a confusion matrix to classify text documents.

3.3.2.5. Classification report

The **`classification_report`** function builds a text report showing the main classification metrics. Here is a small example with custom `target_names` and inferred labels:

```
>>> from sklearn.metrics import classification_report
>>> y_true = [0, 1, 2, 2, 0]
>>> y_pred = [0, 0, 2, 1, 0]
>>> target_names = ['class 0', 'class 1', 'class 2']
>>> print(classification_report(y_true, y_pred, target_names=target_names))
             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

avg / total       0.67      0.60      0.59         5
```

Example:

- See Recognizing hand-written digits for an example of classification report usage for hand-written digits.
- See Classification of text documents using sparse features for an example of classification report usage for text documents.
- See Parameter estimation using grid search with cross-validation for an example of classification report usage for grid search with nested cross-validation.

3.3.2.6. Hamming loss

The **`hamming_loss`** computes the average Hamming loss or Hamming distance between two sets of samples.

If $\hat{y}_j$ is the predicted value for the j-th label of a given sample, y_j is the corresponding true value, and n_labels is the number of classes or labels, then the Hamming loss $L_{Hamming}$ between two samples is defined as:

$$L_{Hamming}(y, \hat{y}) = \frac{1}{n_\text{labels}} \sum_{j=0}^{n_\text{labels} - 1} 1(\hat{y}_j \not= y_j)$$

where $1(x)$ is the indicator function.

```
>>> from sklearn.metrics import hamming_loss
>>> y_pred = [1, 2, 3, 4]
>>> y_true = [2, 2, 3, 4]
>>> hamming_loss(y_true, y_pred)
0.25
```

In the multilabel case with binary label indicators:

```
>>> hamming_loss(np.array([[0, 1], [1, 1]]), np.zeros((2, 2)))
0.75
```

Note: In multiclass classification, the Hamming loss corresponds to the Hamming distance between `y_true` and `y_pred` which is similar to the Zero one loss function. However, while zero-one loss penalizes prediction sets that do not strictly match true sets, the Hamming loss penalizes individual labels. Thus the Hamming loss, upper bounded by the zero-one loss, is always between zero and one, inclusive; and predicting a proper subset or superset of the true labels will give a Hamming loss between zero and one, exclusive.

3.3.2.7. Jaccard similarity coefficient score

The **`jaccard_similarity_score`** function computes the average (default) or sum of Jaccard similarity coefficients, also called the Jaccard index, between pairs of label sets.

The Jaccard similarity coefficient of the i-th samples, with a ground truth label set y_i and predicted label set $\hat{y}_i$, is defined as

$$J(y_i, \hat{y}_i) = \frac{|y_i \cap \hat{y}_i|}{|y_i \cup \hat{y}_i|}.$$

In binary and multiclass classification, the Jaccard similarity coefficient score is equal to the classification accuracy.

```
>>> import numpy as np
>>> from sklearn.metrics import jaccard_similarity_score
>>> y_pred = [0, 2, 1, 3]
>>> y_true = [0, 1, 2, 3]
>>> jaccard_similarity_score(y_true, y_pred)
0.5
>>> jaccard_similarity_score(y_true, y_pred, normalize=False)
2
```

In the multilabel case with binary label indicators:

```
>>> jaccard_similarity_score(np.array([[0, 1], [1, 1]]), np.ones((2, 2)))
0.75
```

3.3.2.8. Precision, recall and F-measures

Intuitively, precision is the ability of the classifier not to label as positive a sample that is negative, and recall is the ability of the classifier to find all the positive samples.

The F-measure (F_β and F_1 measures) can be interpreted as a weighted harmonic mean of the precision and recall. A F_β measure reaches its best value at 1 and its worst score at 0. With $\beta = 1$, F_β and F_1 are equivalent, and the recall and the precision are equally important.

The **precision_recall_curve** computes a precision-recall curve from the ground truth label and a score given by the classifier by varying a decision threshold.

The **average_precision_score** function computes the average precision (AP) from prediction scores. The value is between 0 and 1 and higher is better. AP is defined as

$$\text{AP} = \sum_n (R_n - R_{n-1}) P_n$$

where P_n and R_n are the precision and recall at the nth threshold. With random predictions, the AP is the fraction of positive samples.

References [Manning2008] and [Everingham2010] present alternative variants of AP that interpolate the precision-recall curve. Currently, **average_precision_score** does not implement any interpolated variant. References [Davis2006] and [Flach2015] describe why a linear interpolation of points on the precision-recall curve provides an overly-optimistic measure of classifier performance. This linear interpolation is used when computing area under the curve with the trapezoidal rule in **auc**.

Several functions allow you to analyze the precision, recall and F-measures score:

average_precision_score(y_true, y_score[, …])	Compute average precision (AP) from prediction scores
f1_score(y_true, y_pred[, labels, …])	Compute the F1 score, also known as balanced F-score or F-measure

fbeta_score(y_true, y_pred, beta[, labels, …])	Compute the F-beta score
precision_recall_curve(y_true, probas_pred)	Compute precision-recall pairs for different probability thresholds
precision_recall_fscore_support(y_true, y_pred)	Compute precision, recall, F-measure and support for each class
precision_score(y_true, y_pred[, labels, …])	Compute the precision
recall_score(y_true, y_pred[, labels, …])	Compute the recall

Note that the **precision_recall_curve** function is restricted to the binary case. The **average_precision_score** function works only in binary classification and multilabel indicator format.

Examples:

- See Classification of text documents using sparse features for an example of **f1_score** usage to classify text documents.
- See Parameter estimation using grid search with cross-validation for an example of **precision_score** and **recall_score** usage to estimate parameters using grid search with nested cross-validation.
- See Precision-Recall for an example of **precision_recall_curve** usage to evaluate classifier output quality.

References:

[Manning2008] C.D. Manning, P. Raghavan, H. Schütze, Introduction to Information Retrieval, 2008.

[Everingham2010] M. Everingham, L. Van Gool, C.K.I. Williams, J. Winn, A. Zisserman, The Pascal Visual Object Classes (VOC) Challenge, IJCV 2010.

[Davis2006] J. Davis, M. Goadrich, The Relationship Between Precision-Recall and ROC Curves, ICML 2006.

[Flach2015] P.A. Flach, M. Kull, Precision-Recall-Gain Curves: PR Analysis Done Right, NIPS 2015.

3.3.2.8.1. Binary classification

In a binary classification task, the terms ''positive'' and ''negative'' refer to the classifier's prediction, and the terms ''true'' and ''false'' refer to whether that prediction corresponds to the external judgment (sometimes known as the ''observation''). Given these definitions, we can formulate the following table:

	Actual class (observation)	
Predicted class (expectation)	tp (true positive) Correct result	fp (false positive) Unexpected result
	fn (false negative) Missing result	tn (true negative) Correct absence of result

In this context, we can define the notions of precision, recall and F-measure:

$$\text{precision} = \frac{tp}{tp + fp},$$

$$\text{recall} = \frac{tp}{tp + fn},$$

$$F_\beta = (1 + \beta^2) \frac{\text{precision} \times \text{recall}}{\beta^2 \text{precision} + \text{recall}}.$$

Here are some small examples in binary classification:

```
>>> from sklearn import metrics
>>> y_pred = [0, 1, 0, 0]
>>> y_true = [0, 1, 0, 1]
>>> metrics.precision_score(y_true, y_pred)
1.0
>>> metrics.recall_score(y_true, y_pred)
0.5
>>> metrics.f1_score(y_true, y_pred)
0.66...
>>> metrics.fbeta_score(y_true, y_pred, beta=0.5)
0.83...
>>> metrics.fbeta_score(y_true, y_pred, beta=1)
0.66...
>>> metrics.fbeta_score(y_true, y_pred, beta=2)
0.55...
>>> metrics.precision_recall_fscore_support(y_true, y_pred, beta=0.5)
(array([ 0.66...,  1.        ]), array([ 1. ,  0.5]), array([ 0.71...,  0.83...]),


>>> import numpy as np
>>> from sklearn.metrics import precision_recall_curve
>>> from sklearn.metrics import average_precision_score
>>> y_true = np.array([0, 0, 1, 1])
>>> y_scores = np.array([0.1, 0.4, 0.35, 0.8])
>>> precision, recall, threshold = precision_recall_curve(y_true, y_scores)
>>> precision
array([ 0.66...,  0.5       ,  1.        ,  1.        ])
>>> recall
array([ 1. ,  0.5,  0.5,  0. ])
>>> threshold
array([ 0.35,  0.4 ,  0.8 ])
>>> average_precision_score(y_true, y_scores)
0.83...
```

3.3.2.8.2. Multiclass and multilabel classification

In multiclass and multilabel classification task, the notions of precision, recall, and F-measures can be applied to each label independently. There are a few ways to combine results across labels, specified by the `average` argument to the **`average_precision_score`** (multilabel only), **`f1_score`**, **`fbeta_score`**, **`precision_recall_fscore_support`**, **`precision_score`** and **`recall_score`** functions, as described above. Note that for "micro"-averaging in a multiclass setting with all labels included will produce equal precision, recall and F, while "weighted" averaging may produce an F-score that is not between precision and recall.

To make this more explicit, consider the following notation:

- y the set of *predicted* $(sample, label)$ pairs
- $\hat{y}$ the set of *true* $(sample, label)$ pairs
- L the set of labels
- S the set of samples
- y_s the subset of y with sample s, i.e. $y_s := \left\{(s', l) \in y | s' = s\right\}$
- y_l the subset of y with label l
- similarly, $\hat{y}_s$ and $\hat{y}_l$ are subsets of $\hat{y}$
- $P(A, B) := \frac{\left| A \cap B \right|}{\left|A\right|}$

- $R(A, B) := \frac{|A \cap B|}{|B|}$ (Conventions vary on handling $B = \emptyset$; this implementation uses $R(A, B) := 0$, and similar for P.)
- $F_\beta(A, B) := (1 + \beta^2) \frac{P(A,B) \times R(A,B)}{\beta^2 P(A,B) + R(A,B)}$

Then the metrics are defined as:

`average`	**Precision**	**Recall**	**F_beta**
`"micro"`	$P(y, \hat{y})$	$R(y, \hat{y})$	$F_\beta(y, \hat{y})$
`"samples"`	$\frac{1}{\lvert S\rvert} \sum_{s \in S} P(y_s, \hat{y}_s)$	$\frac{1}{\lvert S\rvert} \sum_{s \in S} R(y_s, \hat{y}_s)$	$\frac{1}{\lvert S\rvert} \sum_{s \in S} F_\beta(y_s, \hat{y}_s)$
`"macro"`	$\frac{1}{\lvert L\rvert} \sum_{l \in L} P(y_l, \hat{y}_l)$	$\frac{1}{\lvert L\rvert} \sum_{l \in L} R(y_l, \hat{y}_l)$	$\frac{1}{\lvert L\rvert} \sum_{l \in L} F_\beta(y_l, \hat{y}_l)$
`"weighted"`	$\frac{1}{\sum_{l \in L} \lvert\hat{y}_l\rvert} \sum_{l \in L} \lvert\hat{y}_l\rvert P(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \lvert\hat{y}_l\rvert} \sum_{l \in L} \lvert\hat{y}_l\rvert R(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \lvert\hat{y}_l\rvert} \sum_{l \in L} \lvert\hat{y}_l\rvert F_\beta(y_l, \hat{y}_l)$
`None`	$\langle P(y_l, \hat{y}_l) \mid l \in L\rangle$	$\langle R(y_l, \hat{y}_l) \mid l \in L\rangle$	$\langle F_\beta(y_l, \hat{y}_l) \mid l \in L\rangle$

```
>>> from sklearn import metrics
>>> y_true = [0, 1, 2, 0, 1, 2]
>>> y_pred = [0, 2, 1, 0, 0, 1]
>>> metrics.precision_score(y_true, y_pred, average='macro')
0.22...
>>> metrics.recall_score(y_true, y_pred, average='micro')
...
0.33...
>>> metrics.f1_score(y_true, y_pred, average='weighted')
0.26...
>>> metrics.fbeta_score(y_true, y_pred, average='macro', beta=0.5)
0.23...
>>> metrics.precision_recall_fscore_support(y_true, y_pred, beta=0.5, average=None)
...
(array([ 0.66...,  0.        ,  0.        ]), array([ 1.,  0.,  0.]), array([ 0.71.
```

For multiclass classification with a “negative class”, it is possible to exclude some labels:

```
>>> metrics.recall_score(y_true, y_pred, labels=[1, 2], average='micro')
... # excluding 0, no labels were correctly recalled
0.0
```

Similarly, labels not present in the data sample may be accounted for in macro-averaging.

```
>>> metrics.precision_score(y_true, y_pred, labels=[0, 1, 2, 3], average='macro')
...
0.166...
```

3.3.2.9. Hinge loss

The **`hinge_loss`** function computes the average distance between the model and the data using hinge loss, a one-sided metric that considers only prediction errors. (Hinge loss is used in maximal margin classifiers such as support vector machines.)

If the labels are encoded with +1 and -1, y: is the true value, and w is the predicted decisions as output by `decision_function`, then the hinge loss is defined as:

$$L_{\text{Hinge}}(y, w) = \max\left\{1 - wy, 0\right\} = \left|1 - wy\right|_+$$

If there are more than two labels, **`hinge_loss`** uses a multiclass variant due to Crammer & Singer. Here is the paper describing it.

If y_w is the predicted decision for true label and y_t is the maximum of the predicted decisions for all other labels, where predicted decisions are output by decision function, then multiclass hinge loss is defined by:

$$L_{\text{Hinge}}(y_w, y_t) = \max\left\{1 + y_t - y_w, 0\right\}$$

Here a small example demonstrating the use of the **hinge_loss** function with a svm classifier in a binary class problem:

```
>>> from sklearn import svm
>>> from sklearn.metrics import hinge_loss
>>> X = [[0], [1]]
>>> y = [-1, 1]
>>> est = svm.LinearSVC(random_state=0)
>>> est.fit(X, y)
LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l2', random_state=0, tol=0.0001,
     verbose=0)
>>> pred_decision = est.decision_function([[-2], [3], [0.5]])
>>> pred_decision
array([-2.18...,  2.36...,  0.09...])
>>> hinge_loss([-1, 1, 1], pred_decision)
0.3...
```

Here is an example demonstrating the use of the **hinge_loss** function with a svm classifier in a multiclass problem:

```
>>> X = np.array([[0], [1], [2], [3]])
>>> Y = np.array([0, 1, 2, 3])
>>> labels = np.array([0, 1, 2, 3])
>>> est = svm.LinearSVC()
>>> est.fit(X, Y)
LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
     intercept_scaling=1, loss='squared_hinge', max_iter=1000,
     multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
     verbose=0)
>>> pred_decision = est.decision_function([[-1], [2], [3]])
>>> y_true = [0, 2, 3]
>>> hinge_loss(y_true, pred_decision, labels)
0.56...
```

3.3.2.10. Log loss

Log loss, also called logistic regression loss or cross-entropy loss, is defined on probability estimates. It is commonly used in (multinomial) logistic regression and neural networks, as well as in some variants of expectation-maximization, and can be used to evaluate the probability outputs (`predict_proba`) of a classifier instead of its discrete predictions.

For binary classification with a true label $y \in \{0, 1\}$ and a probability estimate $p = \operatorname{Pr}(y = 1)$, the log loss per sample is the negative log-likelihood of the classifier given the true label:

$$L_{\log}(y, p) = -\log \operatorname{Pr}(y|p) = -(y \log(p) + (1 - y) \log(1 - p))$$

This extends to the multiclass case as follows. Let the true labels for a set of samples be encoded as a 1-of-K binary indicator matrix Y, i.e., $y_{i,k} = 1$ if sample i has label k taken from a set of K labels. Let P be a matrix of probability estimates, with $p_{i,k} = \operatorname{Pr}(t_{i,k} = 1)$. Then the log loss of the whole set is

$$L_{\log}(Y, P) = -\log \Pr(Y|P) = -\frac{1}{N} \sum_{i=0}^{N-1} \sum_{k=0}^{K-1} y_{i,k} \log p_{i,k}$$

To see how this generalizes the binary log loss given above, note that in the binary case, $p_{i,0} = 1 - p_{i,1}$ and $y_{i,0} = 1 - y_{i,1}$, so expanding the inner sum over $y_{i,k} \in \{0, 1\}$ gives the binary log loss.

The **log_loss** function computes log loss given a list of ground-truth labels and a probability matrix, as returned by an estimator's `predict_proba` method.

```
>>> from sklearn.metrics import log_loss
>>> y_true = [0, 0, 1, 1]
>>> y_pred = [[.9, .1], [.8, .2], [.3, .7], [.01, .99]]
>>> log_loss(y_true, y_pred)
0.1738...
```

The first `[.9, .1]` in `y_pred` denotes 90% probability that the first sample has label 0. The log loss is non-negative.

3.3.2.11. Matthews correlation coefficient

The **matthews_corrcoef** function computes the Matthew's correlation coefficient (MCC) for binary classes. Quoting Wikipedia:

> "The Matthews correlation coefficient is used in machine learning as a measure of the quality of binary (two-class) classifications. It takes into account true and false positives and negatives and is generally regarded as a balanced measure which can be used even if the classes are of very different sizes. The MCC is in essence a correlation coefficient value between -1 and +1. A coefficient of +1 represents a perfect prediction, 0 an average random prediction and -1 an inverse prediction. The statistic is also known as the phi coefficient."

In the binary (two-class) case, tp, tn, fp and fn are respectively the number of true positives, true negatives, false positives and false negatives, the MCC is defined as

$$MCC = \frac{tp \times tn - fp \times fn}{\sqrt{(tp + fp)(tp + fn)(tn + fp)(tn + fn)}}.$$

In the multiclass case, the Matthews correlation coefficient can be defined in terms of a **confusion_matrix** C for K classes. To simplify the definition consider the following intermediate variables:

- $t_k = \sum_i^K C_{ik}$ the number of times class k truly occurred,
- $p_k = \sum_i^K C_{ki}$ the number of times class k was predicted,
- $c = \sum_k^K C_{kk}$ the total number of samples correctly predicted,
- $s = \sum_i^K \sum_j^K C_{ij}$ the total number of samples.

Then the multiclass MCC is defined as:

$$MCC = \frac{c \times s - \sum_k^K p_k \times t_k}{\sqrt{(s^2 - \sum_k^K p_k^2) \times (s^2 - \sum_k^K t_k^2)}}$$

When there are more than two labels, the value of the MCC will no longer range between -1 and +1. Instead the minimum value will be somewhere between -1 and 0 depending on the number and distribution of ground true labels. The maximum value is always +1.

Here is a small example illustrating the usage of the **matthews_corrcoef** function:

```
>>> from sklearn.metrics import matthews_corrcoef
>>> y_true = [+1, +1, +1, -1]
>>> y_pred = [+1, -1, +1, +1]
>>> matthews_corrcoef(y_true, y_pred)
-0.33...
```

3.3.2.12. Receiver operating characteristic (ROC)

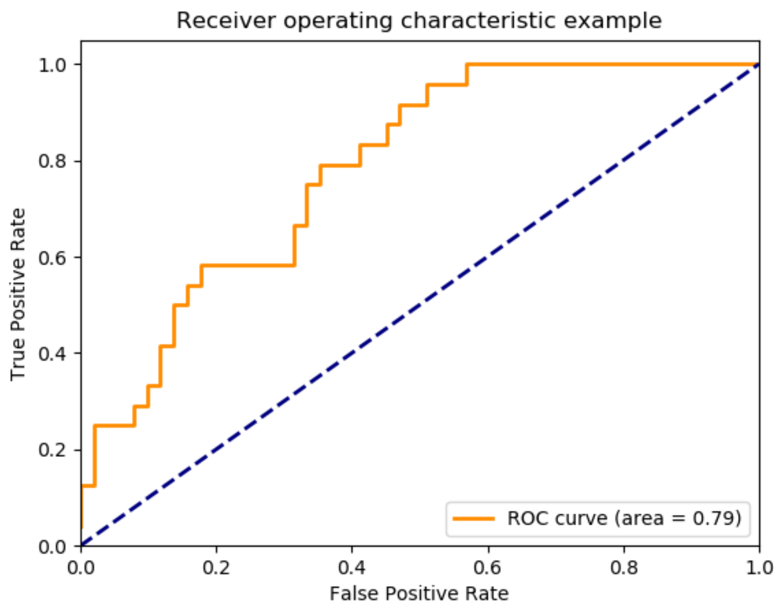
The function **roc_curve** computes the receiver operating characteristic curve, or ROC curve. Quoting Wikipedia :

> "A receiver operating characteristic (ROC), or simply ROC curve, is a graphical plot which illustrates the performance of a binary classifier system as its discrimination threshold is varied. It is created by plotting the fraction of true positives out of the positives (TPR = true positive rate) vs. the fraction of false positives out of the negatives (FPR = false positive rate), at various threshold settings. TPR is also known as sensitivity, and FPR is one minus the specificity or true negative rate."

This function requires the true binary value and the target scores, which can either be probability estimates of the positive class, confidence values, or binary decisions. Here is a small example of how to use the **roc_curve** function:

```
>>> import numpy as np
>>> from sklearn.metrics import roc_curve
>>> y = np.array([1, 1, 2, 2])
>>> scores = np.array([0.1, 0.4, 0.35, 0.8])
>>> fpr, tpr, thresholds = roc_curve(y, scores, pos_label=2)
>>> fpr
array([ 0. ,  0.5,  0.5,  1. ])
>>> tpr
array([ 0.5,  0.5,  1. ,  1. ])
>>> thresholds
array([ 0.8 ,  0.4 ,  0.35,  0.1 ])
```

This figure shows an example of such an ROC curve:

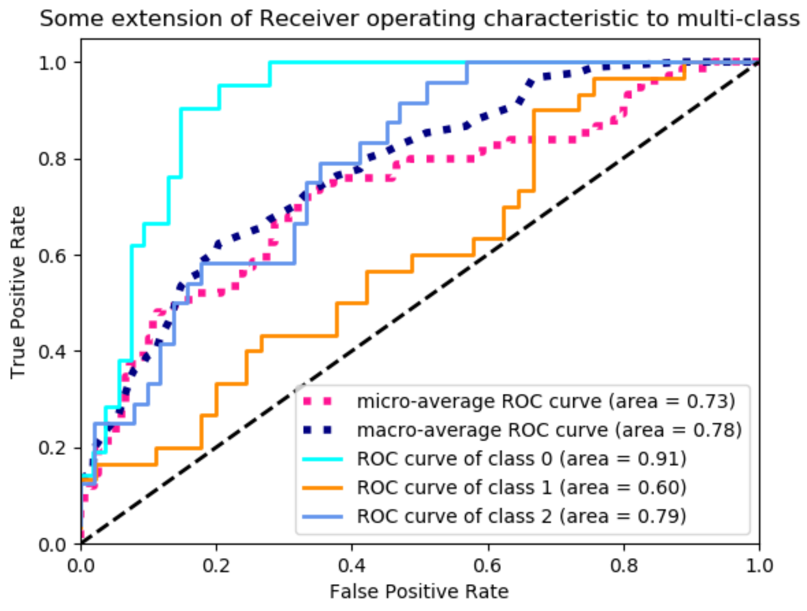


The **roc_auc_score** function computes the area under the receiver operating characteristic (ROC) curve, which is also denoted by AUC or AUROC. By computing the area under the roc curve, the curve information is summarized in one number. For more information see the Wikipedia article on AUC.

```
>>> import numpy as np
>>> from sklearn.metrics import roc_auc_score
>>> y_true = np.array([0, 0, 1, 1])
>>> y_scores = np.array([0.1, 0.4, 0.35, 0.8])
>>> roc_auc_score(y_true, y_scores)
0.75
```

In multi-label classification, the **roc_auc_score** function is extended by averaging over the labels as above.

Compared to metrics such as the subset accuracy, the Hamming loss, or the F1 score, ROC doesn't require optimizing a threshold for each label. The **roc_auc_score** function can also be used in multi-class classification, if the predicted outputs have been binarized.



Examples:

- See Receiver Operating Characteristic (ROC) for an example of using ROC to evaluate the quality of the output of a classifier.
- See Receiver Operating Characteristic (ROC) with cross validation for an example of using ROC to evaluate classifier output quality, using cross-validation.
- See Species distribution modeling for an example of using ROC to model species distribution.

3.3.2.13. Zero one loss

The `zero_one_loss` function computes the sum or the average of the 0-1 classification loss (L_{0-1}) over n_{samples}. By default, the function normalizes over the sample. To get the sum of the L_{0-1}, set `normalize` to `False`.

In multilabel classification, the `zero_one_loss` scores a subset as one if its labels strictly match the predictions, and as a zero if there are any errors. By default, the function returns the percentage of imperfectly predicted subsets. To get the count of such subsets instead, set `normalize` to `False`

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value, then the 0-1 loss L_{0-1} is defined as:

$$L_{0-1}(y_i, \hat{y}_i) = 1(\hat{y}_i \neq y_i)$$

where $1(x)$ is the indicator function.

```
>>> from sklearn.metrics import zero_one_loss
>>> y_pred = [1, 2, 3, 4]
>>> y_true = [2, 2, 3, 4]
>>> zero_one_loss(y_true, y_pred)
0.25
```

```
>>> zero_one_loss(y_true, y_pred, normalize=False)
1
```

In the multilabel case with binary label indicators, where the first label set [0,1] has an error:

```
>>> zero_one_loss(np.array([[0, 1], [1, 1]]), np.ones((2, 2)))
0.5

>>> zero_one_loss(np.array([[0, 1], [1, 1]]), np.ones((2, 2)),  normalize=False)
1
```

Example:

- See Recursive feature elimination with cross-validation for an example of zero one loss usage to perform recursive feature elimination with cross-validation.

3.3.2.14. Brier score loss

The **`brier_score_loss`** function computes the Brier score for binary classes. Quoting Wikipedia:

> "The Brier score is a proper score function that measures the accuracy of probabilistic predictions. It is applicable to tasks in which predictions must assign probabilities to a set of mutually exclusive discrete outcomes."

This function returns a score of the mean square difference between the actual outcome and the predicted probability of the possible outcome. The actual outcome has to be 1 or 0 (true or false), while the predicted probability of the actual outcome can be a value between 0 and 1.

The brier score loss is also between 0 to 1 and the lower the score (the mean square difference is smaller), the more accurate the prediction is. It can be thought of as a measure of the "calibration" of a set of probabilistic predictions.

$$BS = \frac{1}{N} \sum_{t=1}^{N}(f_t - o_t)^2$$

where : N is the total number of predictions, f_t is the predicted probability of the actual outcome o_t.

Here is a small example of usage of this function::

```
>>> import numpy as np
>>> from sklearn.metrics import brier_score_loss
>>> y_true = np.array([0, 1, 1, 0])
>>> y_true_categorical = np.array(["spam", "ham", "ham", "spam"])
>>> y_prob = np.array([0.1, 0.9, 0.8, 0.4])
>>> y_pred = np.array([0, 1, 1, 0])
>>> brier_score_loss(y_true, y_prob)
0.055
>>> brier_score_loss(y_true, 1-y_prob, pos_label=0)
0.055
>>> brier_score_loss(y_true_categorical, y_prob, pos_label="ham")
0.055
>>> brier_score_loss(y_true, y_prob > 0.5)
0.0
```

Example:

- See Probability calibration of classifiers for an example of Brier score loss usage to perform probability calibration of classifiers.

References:

- G. Brier, Verification of forecasts expressed in terms of probability, Monthly weather review 78.1 (1950)

3.3.3. Multilabel ranking metrics

In multilabel learning, each sample can have any number of ground truth labels associated with it. The goal is to give high scores and better rank to the ground truth labels.

3.3.3.1. Coverage error

« The **`coverage_error`** function computes the average number of labels that have to be included in the final prediction such that all true labels are predicted. This is useful if you want to know how many top-scored-labels you have to predict in average without missing any true one. The best value of this metrics is thus the average number of true labels.

Note: Our implementation's score is 1 greater than the one given in Tsoumakas et al., 2010. This extends it to handle the degenerate case in which an instance has 0 true labels.

Formally, given a binary indicator matrix of the ground truth labels $y \in \{0, 1\}^{n_\text{samples} \times n_\text{labels}}$ and the score associated with each label $\hat{f} \in \mathbb{R}^{n_\text{samples} \times n_\text{labels}}$, the coverage is defined as

$$coverage(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}} - 1} \max_{j:y_{ij} = 1} \text{rank}_{ij}$$

with $\text{rank}_{ij} = \left|\left\{k: \hat{f}_{ik} \geq \hat{f}_{ij} \right\}\right|$. Given the rank definition, ties in `y_scores` are broken by giving the maximal rank that would have been assigned to all tied values.

Here is a small example of usage of this function:

```
>>> import numpy as np
>>> from sklearn.metrics import coverage_error
>>> y_true = np.array([[1, 0, 0], [0, 0, 1]])
>>> y_score = np.array([[0.75, 0.5, 1], [1, 0.2, 0.1]])
>>> coverage_error(y_true, y_score)
2.5
```

3.3.3.2. Label ranking average precision

The **`label_ranking_average_precision_score`** function implements label ranking average precision (LRAP). This metric is linked to the **`average_precision_score`** function, but is based on the notion of label ranking instead of precision and recall.

Label ranking average precision (LRAP) is the average over each ground truth label assigned to each sample, of the ratio of true vs. total labels with lower score. This metric will yield better scores if you are able to give better rank to the labels associated with each sample. The obtained score is always strictly greater than 0, and the best value is 1. If there is exactly one relevant label per sample, label ranking average precision is equivalent to the mean reciprocal rank.

Formally, given a binary indicator matrix of the ground truth labels $y \in \mathcal{R}^{n_\text{samples} \times n_\text{labels}}$ and the score associated with each label $\hat{f} \in \mathcal{R}^{n_\text{samples} \times n_\text{labels}}$, the average precision is defined as

$$LRAP(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}} - 1} \frac{1}{|y_i|} \sum_{j:y_{ij} = 1} \frac{|\mathcal{L}_{ij}|}{\text{rank}_{ij}}$$

with $\mathcal{L}_{ij} = \left\{k: y_{ik} = 1, \hat{f}_{ik} \geq \hat{f}_{ij} \right\}$, $\text{rank}_{ij} = \left|\left\{k: \hat{f}_{ik} \geq \hat{f}_{ij} \right\}\right|$ and $|\cdot|$ is the l0 norm or the cardinality of the set.

Here is a small example of usage of this function:

```
>>> import numpy as np
>>> from sklearn.metrics import label_ranking_average_precision_score
>>> y_true = np.array([[1, 0, 0], [0, 0, 1]])
>>> y_score = np.array([[0.75, 0.5, 1], [1, 0.2, 0.1]])
>>> label_ranking_average_precision_score(y_true, y_score)
0.416...
```

3.3.3.3. Ranking loss

The `label_ranking_loss` function computes the ranking loss which averages over the samples the number of label pairs that are incorrectly ordered, i.e. true labels have a lower score than false labels, weighted by the inverse number of false and true labels. The lowest achievable ranking loss is zero.

Formally, given a binary indicator matrix of the ground truth labels $y \in \left\{0, 1\right\}^{n_\text{samples} \times n_\text{labels}}$ and the score associated with each label $\hat{f} \in \mathbb{R}^{n_\text{samples} \times n_\text{labels}}$, the ranking loss is defined as

$$\text{ranking\_loss}(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}} - 1} \frac{1}{|y_i|(n_\text{labels} - |y_i|)} \left|\left\{(k, l): \hat{f}_{ik} < \hat{f}_{il}, y_{ik} = 1, y_{il} = 0 \right\}\right|$$

where $|\cdot|$ is the ℓ_0 norm or the cardinality of the set.

Here is a small example of usage of this function:

```
>>> import numpy as np
>>> from sklearn.metrics import label_ranking_loss
>>> y_true = np.array([[1, 0, 0], [0, 0, 1]])
>>> y_score = np.array([[0.75, 0.5, 1], [1, 0.2, 0.1]])
>>> label_ranking_loss(y_true, y_score)
0.75...
>>> # With the following prediction, we have perfect and minimal loss
>>> y_score = np.array([[1.0, 0.1, 0.2], [0.1, 0.2, 0.9]])
>>> label_ranking_loss(y_true, y_score)
0.0
```

References:

- Tsoumakas, G., Katakis, I., & Vlahavas, I. (2010). Mining multi-label data. In Data mining and knowledge discovery handbook (pp. 667-685). Springer US.

3.3.4. Regression metrics

The **sklearn.metrics** module implements several loss, score, and utility functions to measure regression performance. Some of those have been enhanced to handle the multioutput case: **mean_squared_error**, **mean_absolute_error**, **explained_variance_score** and **r2_score**.

These functions have an `multioutput` keyword argument which specifies the way the scores or losses for each individual target should be averaged. The default is `'uniform_average'`, which specifies a uniformly weighted mean over outputs. If an `ndarray` of shape `(n_outputs,)` is passed, then its entries are interpreted as weights and an according weighted average is returned. If `multioutput` is `'raw_values'` is specified, then all unaltered individual scores or losses will be returned in an array of shape `(n_outputs,)`.

The **r2_score** and **explained_variance_score** accept an additional value `'variance_weighted'` for the `multioutput` parameter. This option leads to a weighting of each individual score by the variance of the corresponding target variable. This setting quantifies the globally captured unscaled variance. If the target variables are of different scale, then this score puts more importance on well explaining the higher variance variables. `multioutput='variance_weighted'` is the default value for **r2_score** for backward compatibility. This will be changed to `uniform_average` in the future.

3.3.4.1. Explained variance score

The **explained_variance_score** computes the explained variance regression score.

If $\hat{y}$ is the estimated target output, y the corresponding (correct) target output, and Var is Variance, the square of the standard deviation, then the explained variance is estimated as follow:

$$\texttt{explained\_variance}(y, \hat{y}) = 1 - \frac{Var\{y - \hat{y}\}}{Var\{y\}}$$

The best possible score is 1.0, lower values are worse.

Here is a small example of usage of the **explained_variance_score** function:

```
>>> from sklearn.metrics import explained_variance_score
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> explained_variance_score(y_true, y_pred)
0.957...
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> explained_variance_score(y_true, y_pred, multioutput='raw_values')
...
array([ 0.967...,  1.        ])
>>> explained_variance_score(y_true, y_pred, multioutput=[0.3, 0.7])
...
0.990...
```

3.3.4.2. Mean absolute error

The **mean_absolute_error** function computes mean absolute error, a risk metric corresponding to the expected value of the absolute error loss or $l1$-norm loss.

If $\hat{y}_i$ is the predicted value of the i-th sample, and y_i is the corresponding true value, then the mean absolute error (MAE) estimated over n_{samples} is defined as

$$\text{MAE}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \left| y_i - \hat{y}_i \right|.$$

Here is a small example of usage of the **mean_absolute_error** function:

```
>>> from sklearn.metrics import mean_absolute_error
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> mean_absolute_error(y_true, y_pred)
0.5
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> mean_absolute_error(y_true, y_pred)
0.75
>>> mean_absolute_error(y_true, y_pred, multioutput='raw_values')
array([ 0.5,  1. ])
>>> mean_absolute_error(y_true, y_pred, multioutput=[0.3, 0.7])
...
0.849...
```

3.3.4.3. Mean squared error

The **mean_squared_error** function computes mean square error, a risk metric corresponding to the expected value of the squared (quadratic) error or loss.

If $\hat{y}_i$ is the predicted value of the i-th sample, and y_i is the corresponding true value, then the mean squared error (MSE) estimated over n_{samples} is defined as

$$\text{MSE}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} (y_i - \hat{y}_i)^2.$$

Here is a small example of usage of the **mean_squared_error** function:

```
>>> from sklearn.metrics import mean_squared_error
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> mean_squared_error(y_true, y_pred)
0.375
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> mean_squared_error(y_true, y_pred)
0.7083...
```

Examples:

- See Gradient Boosting regression for an example of mean squared error usage to evaluate gradient boosting regression.

3.3.4.4. Mean squared logarithmic error

The **mean_squared_log_error** function computes a risk metric corresponding to the expected value of the squared logarithmic (quadratic) error or loss.

If $\hat{y}_i$ is the predicted value of the i-th sample, and y_i is the corresponding true value, then the mean squared logarithmic error (MSLE) estimated over n_{samples} is defined as

$$\text{MSLE}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} (\log_e(1 + y_i) - \log_e(1 + \hat{y}_i))^2.$$

Where $\log_e(x)$ means the natural logarithm of x. This metric is best to use when targets having exponential growth, such as population counts, average sales of a commodity over a span of years etc. Note that this metric penalizes an under-predicted estimate greater than an over-predicted estimate.

Here is a small example of usage of the **mean_squared_log_error** function:

```
>>> from sklearn.metrics import mean_squared_log_error
>>> y_true = [3, 5, 2.5, 7]
>>> y_pred = [2.5, 5, 4, 8]
>>> mean_squared_log_error(y_true, y_pred)
0.039...
>>> y_true = [[0.5, 1], [1, 2], [7, 6]]
>>> y_pred = [[0.5, 2], [1, 2.5], [8, 8]]
>>> mean_squared_log_error(y_true, y_pred)
0.044...
```

3.3.4.5. Median absolute error

The **median_absolute_error** is particularly interesting because it is robust to outliers. The loss is calculated by taking the median of all absolute differences between the target and the prediction.

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value, then the median absolute error (MedAE) estimated over n_{samples} is defined as

$$\text{MedAE}(y, \hat{y}) = \text{median}(\mid y_1 - \hat{y}_1 \mid, \ldots, \mid y_n - \hat{y}_n \mid).$$

The **median_absolute_error** does not support multioutput.

Here is a small example of usage of the **median_absolute_error** function:

```
>>> from sklearn.metrics import median_absolute_error
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> median_absolute_error(y_true, y_pred)
0.5
```

3.3.4.6. R² score, the coefficient of determination

The **r2_score** function computes R², the coefficient of determination. It provides a measure of how well future samples are likely to be predicted by the model. Best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse). A constant model that always predicts the expected value of y, disregarding the input features, would get a R^2 score of 0.0.

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value, then the score R² estimated over n_{samples} is defined as

$$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=0}^{n_{\text{samples}}-1}(y_i - \hat{y}_i)^2}{\sum_{i=0}^{n_{\text{samples}}-1}(y_i - \bar{y})^2}$$

where $\bar{y} = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} y_i$.

Here is a small example of usage of the **`r2_score`** function:

```
>>> from sklearn.metrics import r2_score
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> r2_score(y_true, y_pred)
0.948...
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> r2_score(y_true, y_pred, multioutput='variance_weighted')
...
0.938...
>>> y_true = [[0.5, 1], [-1, 1], [7, -6]]
>>> y_pred = [[0, 2], [-1, 2], [8, -5]]
>>> r2_score(y_true, y_pred, multioutput='uniform_average')
...
0.936...
>>> r2_score(y_true, y_pred, multioutput='raw_values')
...
array([ 0.965...,  0.908...])
>>> r2_score(y_true, y_pred, multioutput=[0.3, 0.7])
...
0.925...
```

Example:

- See Lasso and Elastic Net for Sparse Signals for an example of R² score usage to evaluate Lasso and Elastic Net on sparse signals.

3.3.5. Clustering metrics

The **`sklearn.metrics`** module implements several loss, score, and utility functions. For more information see the Clustering performance evaluation section for instance clustering, and Biclustering evaluation for biclustering.

3.3.6. Dummy estimators

When doing supervised learning, a simple sanity check consists of comparing one's estimator against simple rules of thumb. **`DummyClassifier`** implements several such simple strategies for classification:

- `stratified` generates random predictions by respecting the training set class distribution.
- `most_frequent` always predicts the most frequent label in the training set.
- `prior` always predicts the class that maximizes the class prior (like `most_frequent`) and ``predict_proba` returns the class prior.
- `uniform` generates predictions uniformly at random.
- `constant` always predicts a constant label that is provided by the user.

  A major motivation of this method is F1-scoring, when the positive class is in the minority.

Note that with all these strategies, the `predict` method completely ignores the input data!

To illustrate **`DummyClassifier`**, first let's create an imbalanced dataset:

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.model_selection import train_test_split
>>> iris = load_iris()
>>> X, y = iris.data, iris.target
>>> y[y != 1] = -1
>>> X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

Next, let's compare the accuracy of `SVC` and `most_frequent`:

```
>>> from sklearn.dummy import DummyClassifier
>>> from sklearn.svm import SVC
>>> clf = SVC(kernel='linear', C=1).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.63...
>>> clf = DummyClassifier(strategy='most_frequent',random_state=0)
>>> clf.fit(X_train, y_train)
DummyClassifier(constant=None, random_state=0, strategy='most_frequent')
>>> clf.score(X_test, y_test)
0.57...
```

We see that `SVC` doesn't do much better than a dummy classifier. Now, let's change the kernel:

```
>>> clf = SVC(kernel='rbf', C=1).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.97...
```

We see that the accuracy was boosted to almost 100%. A cross validation strategy is recommended for a better estimate of the accuracy, if it is not too CPU costly. For more information see the Cross-validation: evaluating estimator performance section. Moreover if you want to optimize over the parameter space, it is highly recommended to use an appropriate methodology; see the Tuning the hyper-parameters of an estimator section for details.

More generally, when the accuracy of a classifier is too close to random, it probably means that something went wrong: features are not helpful, a hyperparameter is not correctly tuned, the classifier is suffering from class imbalance, etc…

`DummyRegressor` also implements four simple rules of thumb for regression:

- `mean` always predicts the mean of the training targets.
- `median` always predicts the median of the training targets.
- `quantile` always predicts a user provided quantile of the training targets.
- `constant` always predicts a constant value that is provided by the user.

In all these strategies, the `predict` method completely ignores the input data.