3.3. Metrics and scoring: 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 `sklearn.metrics` module implements functions assessing prediction error for specific purposes. These metrics are detailed in sections on Classification metrics, Multilabel 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`	
'balanced_accuracy'	`metrics.balanced_accuracy_score`	
'top_k_accuracy'	`metrics.top_k_accuracy_score`	
'average_precision'	`metrics.average_precision_score`	
'neg_brier_score'	`metrics.brier_score_loss`	
'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'
'jaccard' etc.	`metrics.jaccard_score`	suffixes apply as with 'f1'
'roc_auc'	`metrics.roc_auc_score`	
'roc_auc_ovr'	`metrics.roc_auc_score`	
'roc_auc_ovo'	`metrics.roc_auc_score`	
'roc_auc_ovr_weighted'	`metrics.roc_auc_score`	
'roc_auc_ovo_weighted'	`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`	
'rand_score'	`metrics.rand_score`	
'v_measure_score'	`metrics.v_measure_score`	

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Scoring	Function	Comment
'explained_variance'	metrics.explained_variance_score	
'max_error'	metrics.max_error	
'neg_mean_absolute_error'	metrics.mean_absolute_error	
'neg_mean_squared_error'	metrics.mean_squared_error	
'neg_root_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	
'neg_mean_poisson_deviance'	metrics.mean_poisson_deviance	
'neg_mean_gamma_deviance'	metrics.mean_gamma_deviance	
'neg_mean_absolute_percentage_error'	metrics.mean_absolute_percentage_error	
'd2_absolute_error_score'	metrics.d2_absolute_error_score	
'd2_pinball_score'	metrics.d2_pinball_score	
'd2_tweedie_score'	metrics.d2_tweedie_score	

Usage examples:

```
>>> from sklearn import svm, datasets
>>> from sklearn.model_selection import cross_val_score
>>> X, y = datasets.load_iris(return_X_y=True)
>>> clf = svm.SVC(random_state=0)
>>> cross_val_score(clf, X, y, cv=5, scoring='recall_macro')
array([0.96..., 0.96..., 0.96..., 0.93..., 1.        ])
```

Note: If a wrong scoring name is passed, an `InvalidParameterError` is raised. You can retrieve the names of all available scorers by calling `get_scorer_names`.

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(dual="auto"), param_grid={'C': [1, 10]},
...                     scoring=ftwo_scorer, cv=5)
```

▶ **Custom scorer objects**

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.

▶ **How to build a scorer from scratch**

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3.3.1.4. Using multiple metric evaluation

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

There are three 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.

- As a callable that returns a dictionary of scores:

```
>>> 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(dual="auto", random_state=0)
>>> def confusion_matrix_scorer(clf, X, y):
...     y_pred = clf.predict(X)
...     cm = confusion_matrix(y, y_pred)
...     return {'tn': cm[0, 0], 'fp': cm[0, 1],
...             'fn': cm[1, 0], 'tp': cm[1, 1]}
>>> cv_results = cross_validate(svm, X, y, cv=5,
...                             scoring=confusion_matrix_scorer)
>>> # Getting the test set true positive scores
>>> print(cv_results['test_tp'])
[10  9  8  7  8]
>>> # Getting the test set false negative scores
>>> print(cv_results['test_fn'])
[0 1 2 3 2]
```

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).
class_likelihood_ratios(y_true, y_pred, *[, ...])	Compute binary classification positive and negative likelihood ratios.
det_curve(y_true, y_score[, pos_label, ...])	Compute error rates for different probability thresholds.

Others also work in the multiclass case:

balanced_accuracy_score(y_true, y_pred, *[, ...])	Compute the balanced accuracy.
cohen_kappa_score(y1, y2, *[, labels, ...])	Compute Cohen's kappa: a statistic that measures inter-annotator agreement.
confusion_matrix(y_true, y_pred, *[, ...])	Compute confusion matrix to evaluate the accuracy of a classification.
hinge_loss(y_true, pred_decision, *[, ...])	Average hinge loss (non-regularized).
matthews_corrcoef(y_true, y_pred, *[, ...])	Compute the Matthews correlation coefficient (MCC).
roc_auc_score(y_true, y_score, *[, average, ...])	Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.
top_k_accuracy_score(y_true, y_score, *[, ...])	Top-k Accuracy classification score.

Some also work in the multilabel case:

accuracy_score(y_true, y_pred, *[, ...])	Accuracy classification score.
classification_report(y_true, y_pred, *[, ...])	Build a text report showing the main classification metrics.
...e, y_pred, *[, labels, ...])	Compute the F1 score, also known as balanced F-score or F-measure.

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`fbeta_score`(y_true, y_pred, *, beta[, ...])	Compute the F-beta score.
`hamming_loss`(y_true, y_pred, *[, sample_weight])	Compute the average Hamming loss.
`jaccard_score`(y_true, y_pred, *[, labels, ...])	Jaccard similarity coefficient score.
`log_loss`(y_true, y_pred, *[, eps, ...])	Log loss, aka logistic loss or cross-entropy loss.
`multilabel_confusion_matrix`(y_true, y_pred, *)	Compute a confusion matrix for each class or sample.
`precision_recall_fscore_support`(y_true, ...)	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.
`roc_auc_score`(y_true, y_score, *[, average, ...])	Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.
`zero_one_loss`(y_true, y_pred, *[, ...])	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.

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.

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```
>>> 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. Top-k accuracy score

The `top_k_accuracy_score` function is a generalization of `accuracy_score`. The difference is that a prediction is considered correct as long as the true label is associated with one of the `k` highest predicted scores. `accuracy_score` is the special case of `k = 1`.

The function covers the binary and multiclass classification cases but not the multilabel case.

If $\hat{f}_{i,j}$ is the predicted class for the i-th sample corresponding to the j-th largest predicted score and y_i is the corresponding true value, then the fraction of correct predictions over n_{samples} is defined as

$$\texttt{top-k accuracy}(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \sum_{j=1}^{k} 1(\hat{f}_{i,j} = y_i)$$

where k is the number of guesses allowed and $1(x)$ is the indicator function.

```
>>> import numpy as np
>>> from sklearn.metrics import top_k_accuracy_score
>>> y_true = np.array([0, 1, 2, 2])
>>> y_score = np.array([[0.5, 0.2, 0.2],
...                     [0.3, 0.4, 0.2],
...                     [0.2, 0.4, 0.3],
...                     [0.7, 0.2, 0.1]])
>>> top_k_accuracy_score(y_true, y_score, k=2)
0.75
>>> # Not normalizing gives the number of "correctly" classified samples
>>> top_k_accuracy_score(y_true, y_score, k=2, normalize=False)
3
```

3.3.2.4. Balanced accuracy score

The `balanced_accuracy_score` function computes the balanced accuracy, which avoids inflated performance estimates on imbalanced datasets. It is the macro-average of recall scores per class or, equivalently, raw accuracy where each sample is weighted according to the inverse prevalence of its true class. Thus for balanced datasets, the score is equal to accuracy.

In the binary case, balanced accuracy is equal to the arithmetic mean of sensitivity (true positive rate) and specificity (true negative rate), or the area under the ROC curve with binary predictions rather than scores:

$$\texttt{balanced-accuracy} = \frac{1}{2}\left(\frac{TP}{TP + FN} + \frac{TN}{TN + FP}\right)$$

If the classifier performs equally well on either class, this term reduces to the conventional accuracy (i.e., the number of correct predictions divided by the total number of predictions).

In contrast, if the conventional accuracy is above chance only because the classifier takes advantage of an imbalanced test set, then the balanced accuracy, as appropriate, will drop to $\frac{1}{n\_classes}$.

The score ranges from 0 to 1, or when `adjusted=True` is used, it rescaled to the range $\frac{1}{1-n\_classes}$ to 1, inclusive, with performance at random scoring 0.

If y_i is the true value of the i-th sample, and w_i is the corresponding sample weight, then we adjust the sample weight to:

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$$\hat{w}_i = \frac{w_i}{\sum_j 1(y_j = y_i) w_j}$$

where $1(x)$ is the indicator function. Given predicted $\hat{y}_i$ for sample i, balanced accuracy is defined as:

$$\texttt{balanced-accuracy}(y, \hat{y}, w) = \frac{1}{\sum \hat{w}_i} \sum_i 1(\hat{y}_i = y_i) \hat{w}_i$$

With `adjusted=True`, balanced accuracy reports the relative increase from $\texttt{balanced-accuracy}(y, \mathbf{0}, w) = \frac{1}{n\_classes}$. In the binary case, this is also known as *Youden's J statistic*, or *informedness*.

Note: The multiclass definition here seems the most reasonable extension of the metric used in binary classification, though there is no certain consensus in the literature:

- Our definition: [Mosley2013], [Kelleher2015] and [Guyon2015], where [Guyon2015] adopt the adjusted version to ensure that random predictions have a score of 0 and perfect predictions have a score of 1..
- Class balanced accuracy as described in [Mosley2013]: the minimum between the precision and the recall for each class is computed. Those values are then averaged over the total number of classes to get the balanced accuracy.
- Balanced Accuracy as described in [Urbanowicz2015]: the average of sensitivity and specificity is computed for each class and then averaged over total number of classes.

References:

[Guyon2015] (1,2)
I. Guyon, K. Bennett, G. Cawley, H.J. Escalante, S. Escalera, T.K. Ho, N. Macià, B. Ray, M. Saeed, A.R. Statnikov, E. Viegas, Design of the 2015 ChaLearn AutoML Challenge, IJCNN 2015.

[Mosley2013] (1,2)
L. Mosley, A balanced approach to the multi-class imbalance problem, IJCV 2010.

[Kelleher2015]
John. D. Kelleher, Brian Mac Namee, Aoife D'Arcy, Fundamentals of Machine Learning for Predictive Data Analytics: Algorithms, Worked Examples, and Case Studies, 2015.

[Urbanowicz2015]
Urbanowicz R.J., Moore, J.H. ExSTraCS 2.0: description and evaluation of a scalable learning classifier system, Evol. Intel. (2015) 8: 89.

3.3.2.5. 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
```

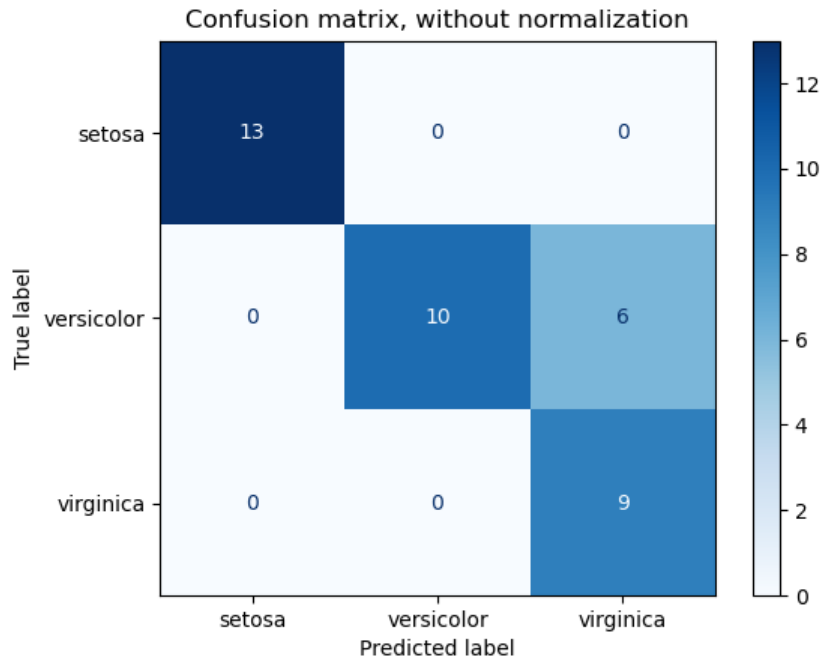
3.3.2.6. Confusion matrix

The `confusion_matrix` function evaluates classification accuracy by computing the confusion matrix with each row corresponding to the true class (Wikipedia and other references may use different convention for axes).

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]])
```

`ConfusionMatrixDisplay` can be used to visually represent a confusion matrix as shown in the Confusion matrix example, which creates the following figure:



The parameter `normalize` allows to report ratios instead of counts. The confusion matrix can be normalized in 3 different ways: `'pred'`, `'true'`, and `'all'` which will divide the counts by the sum of each columns, rows, or the entire matrix, respectively.

```
>>> y_true = [0, 0, 0, 1, 1, 1, 1, 1]
>>> y_pred = [0, 1, 0, 1, 0, 1, 0, 1]
>>> confusion_matrix(y_true, y_pred, normalize='all')
array([[0.25 , 0.125],
       [0.25 , 0.375]])
```

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.

3.3.2.7. 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

    accuracy                           0.60         5
   macro avg       0.56      0.50      0.49         5
weighted avg       0.67      0.60      0.59         5
```

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- See Recognizing hand-written digits for an example of classification report usage for hand-written digits.
- See Custom refit strategy of a grid search with cross-validation for an example of classification report usage for grid search with nested cross-validation.

3.3.2.8. Hamming loss

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

If $\hat{y}_{i,j}$ is the predicted value for the j-th label of a given sample i, $y_{i,j}$ is the corresponding true value, n_{samples} is the number of samples and n_{labels} is the number of labels, then the Hamming loss $L_{Hamming}$ is defined as:

$$L_{Hamming}(y, \hat{y}) = \frac{1}{n_{\text{samples}} * n_{\text{labels}}} \sum_{i=0}^{n_{\text{samples}}-1} \sum_{j=0}^{n_{\text{labels}}-1} 1(\hat{y}_{i,j} \neq y_{i,j})$$

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

The equation above does not hold true in the case of multiclass classification. Please refer to the note below for more information.

```
>>> 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.

3.3.2.9. 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[, ...])	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, ...)	Compute precision, recall, F-measure and support for each class.
precision_score(y_true, y_pred, *[, labels, ...])	Compute the precision.

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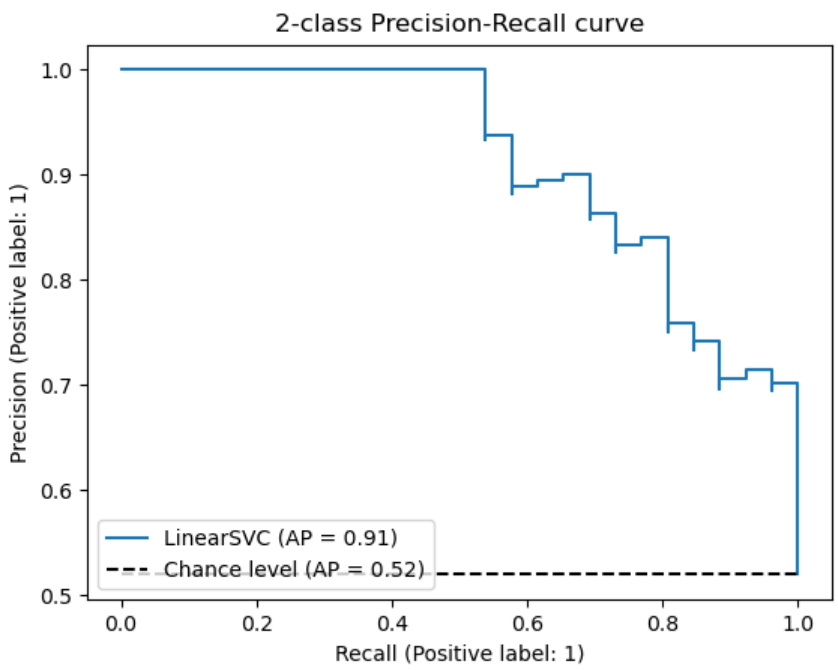
recall_score(y_true, y_pred, *[, labels, ...])	Compute the recall.

Note that the precision_recall_curve function is restricted to the binary case. The average_precision_score function supports multiclass and multilabel formats by computing each class score in a One-vs-the-rest (OvR) fashion and averaging them or not depending of its `average` argument value.

The PrecisionRecallDisplay.from_estimator and PrecisionRecallDisplay.from_predictions functions will plot the precision-recall curve as follows.



Examples:

- See Custom refit strategy of a 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.

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:

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

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

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

Toggle Menu all is also called ''sensitivity''.

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...]), array([2, 2]))


>>> 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([0.5       , 0.66..., 0.5       , 1.        , 1.        ])
>>> recall
array([1. , 1. , 0.5, 0.5, 0. ])
>>> threshold
array([0.1 , 0.35, 0.4 , 0.8 ])
>>> average_precision_score(y_true, y_scores)
0.83...
```

Multiclass and multilabel classification

In a 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`**, **`f1_score`**, **`fbeta_score`**, **`precision_recall_fscore_support`**, **`precision_score`** and **`recall_score`** functions, as described above. Note that if all labels are included, "micro"-averaging in a multiclass setting will produce precision, recall and F that are all identical to accuracy. Also note that "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 *true* $(sample, label)$ pairs
- $\hat{y}$ the set of *predicted* $(sample, label)$ pairs
- L the set of labels
- S the set of samples
- y_s the subset of y with sample s, i.e. $y_s := \{(s', l) \in y | s' = s\}$
- y_l the subset of y with label l
- similarly, $\hat{y}_s$ and $\hat{y}_l$ are subsets of $\hat{y}$
- $P(A, B) := \frac{|A \cap B|}{|B|}$ for some sets A and B
- $R(A, B) := \frac{|A \cap B|}{|A|}$ (Conventions vary on handling $A = \emptyset$; this implementation uses $R(A, B) := 0$, and similar for P.)
- $F_\beta(A, B) := \left(1 + \beta^2\right) \frac{P(A,B) \times R(A,B)}{\beta^2 P(A,B) + R(A,B)}$

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"`	$\frac{1}{\sum_{l \in L} \lvert y_l \rvert} \sum_{l \in L} \lvert y_l \rvert P(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \lvert y_l \rvert} \sum_{l \in L} \lvert y_l \rvert R(y_l, \hat{y}_l)$	$\frac{1}{\sum_{l \in L} \lvert y_l \rvert} \sum_{l \in L} \lvert y_l \rvert F_\beta(y_l, \hat{y}_l)$
`None`	$\langle P(y_l, \hat{y}_l) \mid l \in L \rangle$	$\langle R(y_l, \hat{y}_l) \mid l \in L \rangle$	$\langle F_\beta(y_l, \hat{y}_l) \mid l \in L \rangle$

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```
>>> 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..., 0.        , 0.        ]), array([2, 2, 2]...))
```

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...
```

3.3.2.10. Jaccard similarity coefficient score

The `jaccard_score` function computes the average of Jaccard similarity coefficients, also called the Jaccard index, between pairs of label sets.

The Jaccard similarity coefficient with a ground truth label set y and predicted label set $\hat{y}$, is defined as

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

The `jaccard_score` (like `precision_recall_fscore_support`) applies natively to binary targets. By computing it set-wise it can be extended to apply to multilabel and multiclass through the use of `average` (see above).

In the binary case:

```
>>> import numpy as np
>>> from sklearn.metrics import jaccard_score
>>> y_true = np.array([[0, 1, 1],
...                    [1, 1, 0]])
>>> y_pred = np.array([[1, 1, 1],
...                    [1, 0, 0]])
>>> jaccard_score(y_true[0], y_pred[0])
0.6666...
```

In the 2D comparison case (e.g. image similarity):

```
>>> jaccard_score(y_true, y_pred, average="micro")
0.6
```

In the multilabel case with binary label indicators:

```
>>> jaccard_score(y_true, y_pred, average='samples')
0.5833...
>>> jaccard_score(y_true, y_pred, average='macro')
0.6666...
>>> jaccard_score(y_true, y_pred, average=None)
array([0.5, 0.5, 1. ])
```

Multiclass problems are binarized and treated like the corresponding multilabel problem:

```
>>> y_pred = [0, 2, 1, 2]
>>> y_true = [0, 1, 2, 2]
>>> jaccard_score(y_true, y_pred, average=None)
array([1. , 0. , 0.33...])
>>> jaccard_score(y_true, y_pred, average='macro')
0.44...
>>> jaccard_score(y_true, y_pred, average='micro')
0.33...
```

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3.3.2.11. 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 true label y_i of a binary classification task is encoded as $y_i = \{-1, +1\}$ for every sample i; and w_i is the corresponding predicted decision (an array of shape `(n_samples,)` as output by the `decision_function` method), then the hinge loss is defined as:

$$L_{\text{Hinge}}(y, w) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \max\{1 - w_i y_i, 0\}$$

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

In this case the predicted decision is an array of shape `(n_samples, n_labels)`. If w_{i,y_i} is the predicted decision for the true label y_i of the i-th sample; and $\hat{w}_{i,y_i} = \max\{w_{i,y_j} \mid y_j \neq y_i\}$ is the maximum of the predicted decisions for all the other labels, then the multi-class hinge loss is defined by:

$$L_{\text{Hinge}}(y, w) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \max\{1 + \hat{w}_{i,y_i} - w_{i,y_i}, 0\}$$

Here is 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(dual="auto", random_state=0)
>>> est.fit(X, y)
LinearSVC(dual='auto', random_state=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(dual="auto")
>>> est.fit(X, Y)
LinearSVC(dual='auto')
>>> pred_decision = est.decision_function([[-1], [2], [3]])
>>> y_true = [0, 2, 3]
>>> hinge_loss(y_true, pred_decision, labels=labels)
0.56...
```

3.3.2.12. 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 $p = \Pr(y = 1)$, the log loss per sample is the negative log-likelihood of the classifier given the true label:

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

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 $p_{i,k} = \Pr(y_{i,k} = 1)$. 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.

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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.

3.3.2.13. 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...
```

3.3.2.14. Multi-label confusion matrix

The `multilabel_confusion_matrix` function computes class-wise (default) or sample-wise (samplewise=True) multilabel confusion matrix to evaluate the accuracy of a classification. multilabel_confusion_matrix also treats multiclass data as if it were multilabel, as this is a transformation commonly applied to evaluate multiclass problems with binary classification metrics (such as precision, recall, etc.).

When calculating class-wise multilabel confusion matrix C, the count of true negatives for class i is $C_{i,0,0}$, false negatives is $C_{i,1,0}$, true positives is $C_{i,1,1}$ and false positives is $C_{i,0,1}$.

Here is an example demonstrating the use of the `multilabel_confusion_matrix` function with multilabel indicator matrix input:

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```
>>> import numpy as np
>>> from sklearn.metrics import multilabel_confusion_matrix
>>> y_true = np.array([[1, 0, 1],
...                    [0, 1, 0]])
>>> y_pred = np.array([[1, 0, 0],
...                    [0, 1, 1]])
>>> multilabel_confusion_matrix(y_true, y_pred)
array([[[1, 0],
        [0, 1]],

       [[1, 0],
        [0, 1]],

       [[0, 1],
        [1, 0]]])
```

Or a confusion matrix can be constructed for each sample's labels:

```
>>> multilabel_confusion_matrix(y_true, y_pred, samplewise=True)
array([[[1, 0],
        [1, 1]],

       [[1, 1],
        [0, 1]]])
```

Here is an example demonstrating the use of the **multilabel_confusion_matrix** function with multiclass input:

```
>>> y_true = ["cat", "ant", "cat", "cat", "ant", "bird"]
>>> y_pred = ["ant", "ant", "cat", "cat", "ant", "cat"]
>>> multilabel_confusion_matrix(y_true, y_pred,
...                             labels=["ant", "bird", "cat"])
array([[[3, 1],
        [0, 2]],

       [[5, 0],
        [1, 0]],

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

Here are some examples demonstrating the use of the **multilabel_confusion_matrix** function to calculate recall (or sensitivity), specificity, fall out and miss rate for each class in a problem with multilabel indicator matrix input.

Calculating recall (also called the true positive rate or the sensitivity) for each class:

```
>>> y_true = np.array([[0, 0, 1],
...                    [0, 1, 0],
...                    [1, 1, 0]])
>>> y_pred = np.array([[0, 1, 0],
...                    [0, 0, 1],
...                    [1, 1, 0]])
>>> mcm = multilabel_confusion_matrix(y_true, y_pred)
>>> tn = mcm[:, 0, 0]
>>> tp = mcm[:, 1, 1]
>>> fn = mcm[:, 1, 0]
>>> fp = mcm[:, 0, 1]
>>> tp / (tp + fn)
array([1. , 0.5, 0. ])
```

Calculating specificity (also called the true negative rate) for each class:

```
>>> tn / (tn + fp)
array([1. , 0. , 0.5])
```

Calculating fall out (also called the false positive rate) for each class:

```
>>> fp / (fp + tn)
array([0. , 1. , 0.5])
```

Calculating miss rate (also called the false negative rate) for each class:

```
>>> fn / (fn + tp)
array([0. , 0.5, 1. ])
```

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3.3.2.15. 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."

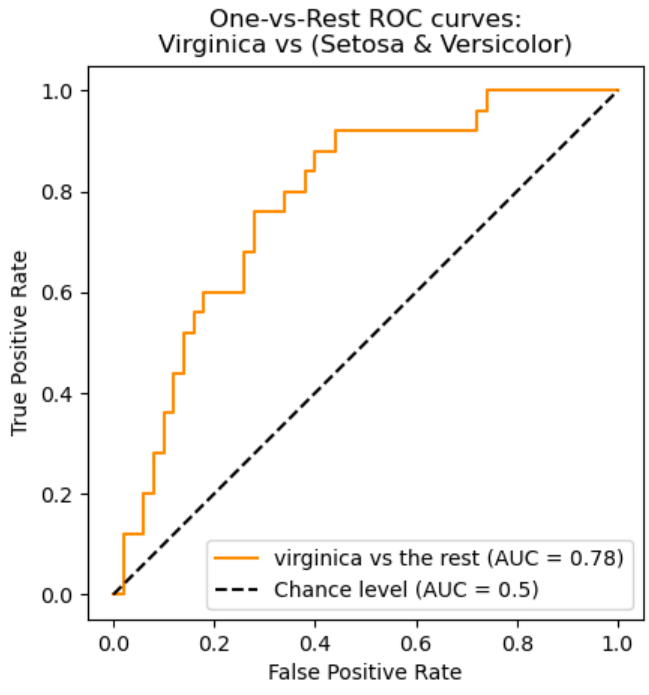
This function requires the true binary value and the target scores, which can either be probability estimates of the positive class, confidence values, or binary decisions. Here is a small example of how to use the **roc_curve** function:

```
>>> 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. , 0.5, 0.5, 1. ])
>>> tpr
array([0. , 0.5, 0.5, 1. , 1. ])
>>> thresholds
array([ inf, 0.8 , 0.4 , 0.35, 0.1 ])
```

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, denoted by ROC-AUC or AUROC, computes the area under the ROC curve. By doing so, the curve information is summarized in one number.

The following figure shows the ROC curve and ROC-AUC score for a classifier aimed to distinguish the virginica flower from the rest of the species in the Iris plants dataset:



For more information see the Wikipedia article on AUC.

Binary case

In the **binary case**, you can either provide the probability estimates, using the `classifier.predict_proba()` method, or the non-thresholded decision values given by the `classifier.decision_function()` method. In the case of providing the probability estimates, the probability of the class with the "greater label" should be provided. The "greater label" corresponds to `classifier.classes_[1]` and thus `classifier.predict_proba(X)[:, 1]`. Therefore, the `y_score` parameter is of size (n_samples,).

```
>>> from sklearn.datasets import load_breast_cancer
>>> from sklearn.linear_model import LogisticRegression
>>> from sklearn.metrics import roc_auc_score
>>> X, y = load_breast_cancer(return_X_y=True)
>>> clf = LogisticRegression(solver="liblinear").fit(X, y)
>>> clf.classes_
array([0, 1])
```

We can use the probability estimates corresponding to `clf.classes_[1]`.

```
>>> y_score = clf.predict_proba(X)[:, 1]
>>> roc_auc_score(y, y_score)
0.99...
```

Otherwise, we can use the non-thresholded decision values

```
>>> roc_auc_score(y, clf.decision_function(X))
0.99...
```

Multi-class case

The `roc_auc_score` function can also be used in **multi-class classification**. Two averaging strategies are currently supported: the one-vs-one algorithm computes the average of the pairwise ROC AUC scores, and the one-vs-rest algorithm computes the average of the ROC AUC scores for each class against all other classes. In both cases, the predicted labels are provided in an array with values from 0 to `n_classes`, and the scores correspond to the probability estimates that a sample belongs to a particular class. The OvO and OvR algorithms support weighting uniformly (`average='macro'`) and by prevalence (`average='weighted'`).

One-vs-one Algorithm: Computes the average AUC of all possible pairwise combinations of classes. [HT2001] defines a multiclass AUC metric weighted uniformly:

$$\frac{1}{c(c-1)}\sum_{j=1}^{c}\sum_{k>j}^{c}(\mathrm{AUC}(j|k)+\mathrm{AUC}(k|j))$$

where c is the number of classes and $\mathrm{AUC}(j|k)$ is the AUC with class j as the positive class and class k as the negative class. In general, $\mathrm{AUC}(j|k) \neq \mathrm{AUC}(k|j))$ in the multiclass case. This algorithm is used by setting the keyword argument `multiclass` to `'ovo'` and `average` to `'macro'`.

The [HT2001] multiclass AUC metric can be extended to be weighted by the prevalence:

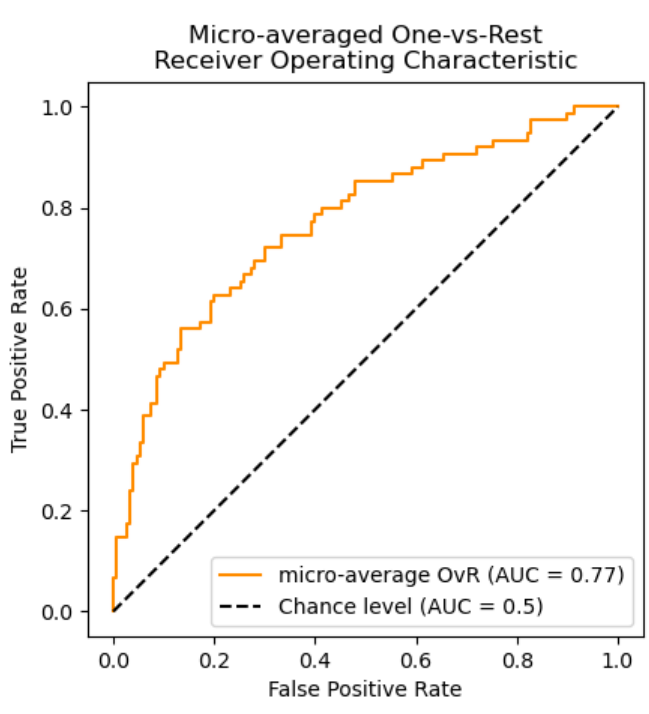
$$\frac{1}{c(c-1)}\sum_{j=1}^{c}\sum_{k>j}^{c}p(j\cup k)(\mathrm{AUC}(j|k)+\mathrm{AUC}(k|j))$$

where c is the number of classes. This algorithm is used by setting the keyword argument `multiclass` to `'ovo'` and `average` to `'weighted'`. The `'weighted'` option returns a prevalence-weighted average as described in [FC2009].

One-vs-rest Algorithm: Computes the AUC of each class against the rest [PD2000]. The algorithm is functionally the same as the multilabel case. To enable this algorithm set the keyword argument `multiclass` to `'ovr'`. Additionally to `'macro'` [F2006] and `'weighted'` [F2001] averaging, OvR supports `'micro'` averaging.

In applications where a high false positive rate is not tolerable the parameter `max_fpr` of `roc_auc_score` can be used to summarize the ROC curve up to the given limit.

The following figure shows the micro-averaged ROC curve and its corresponding ROC-AUC score for a classifier aimed to distinguish the the different species in the Iris plants dataset:



Multi-label case

In **multi-label classification**, the `roc_auc_score` function is extended by averaging over the labels as above. In this case, you should provide a `y_score` of shape `(n_samples, n_classes)`. Thus, when using the probability estimates, one needs to select the probability of the class with the greater label for each output.

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```
>>> from sklearn.datasets import make_multilabel_classification
>>> from sklearn.multioutput import MultiOutputClassifier
>>> X, y = make_multilabel_classification(random_state=0)
>>> inner_clf = LogisticRegression(solver="liblinear", random_state=0)
>>> clf = MultiOutputClassifier(inner_clf).fit(X, y)
>>> y_score = np.transpose([y_pred[:, 1] for y_pred in clf.predict_proba(X)])
>>> roc_auc_score(y, y_score, average=None)
array([0.82..., 0.86..., 0.94..., 0.85... , 0.94...])
```

And the decision values do not require such processing.

```
>>> from sklearn.linear_model import RidgeClassifierCV
>>> clf = RidgeClassifierCV().fit(X, y)
>>> y_score = clf.decision_function(X)
>>> roc_auc_score(y, y_score, average=None)
array([0.81..., 0.84... , 0.93..., 0.87..., 0.94...])
```

Examples:

- See Multiclass 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.

References:

[HT2001] (1,2)
Hand, D.J. and Till, R.J., (2001). A simple generalisation of the area under the ROC curve for multiple class classification problems. Machine learning, 45(2), pp. 171-186.

[FC2009]
Ferri, Cèsar & Hernandez-Orallo, Jose & Modroiu, R. (2009). An Experimental Comparison of Performance Measures for Classification. Pattern Recognition Letters. 30. 27-38.

[PD2000]
Provost, F., Domingos, P. (2000). Well-trained PETs: Improving probability estimation trees (Section 6.2), CeDER Working Paper #IS-00-04, Stern School of Business, New York University.

[F2006]
Fawcett, T., 2006. An introduction to ROC analysis. Pattern Recognition Letters, 27(8), pp. 861-874.

[F2001]
Fawcett, T., 2001. Using rule sets to maximize ROC performance In Data Mining, 2001. Proceedings IEEE International Conference, pp. 131-138.

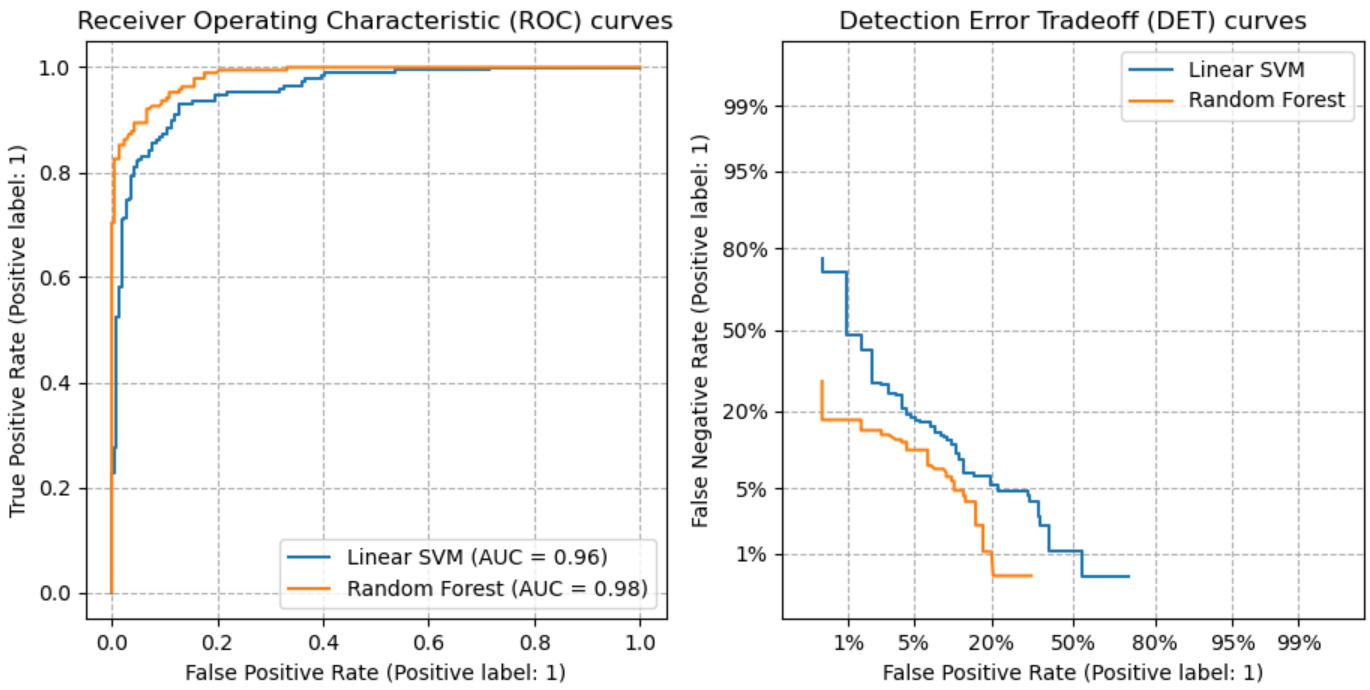
3.3.2.16. Detection error tradeoff (DET)

The function **`det_curve`** computes the detection error tradeoff curve (DET) curve [WikipediaDET2017]. Quoting Wikipedia:

> "A detection error tradeoff (DET) graph is a graphical plot of error rates for binary classification systems, plotting false reject rate vs. false accept rate. The x- and y-axes are scaled non-linearly by their standard normal deviates (or just by logarithmic transformation), yielding tradeoff curves that are more linear than ROC curves, and use most of the image area to highlight the differences of importance in the critical operating region."

DET curves are a variation of receiver operating characteristic (ROC) curves where False Negative Rate is plotted on the y-axis instead of True Positive Rate. DET curves are commonly plotted in normal deviate scale by transformation with ϕ^{-1} (with ϕ being the cumulative distribution function). The resulting performance curves explicitly visualize the tradeoff of error types for given classification algorithms. See [Martin1997] for examples and further motivation.

This figure compares the ROC and DET curves of two example classifiers on the same classification task:



Properties:

- DET curves form a linear curve in normal deviate scale if the detection scores are normally (or close-to normally) distributed. It was shown by [Navratil2007] that the reverse is not necessarily true and even more general distributions are able to produce linear DET curves.
- The normal deviate scale transformation spreads out the points such that a comparatively larger space of plot is occupied. Therefore curves with similar classification performance might be easier to distinguish on a DET plot.
- With False Negative Rate being “inverse” to True Positive Rate the point of perfection for DET curves is the origin (in contrast to the top left corner for ROC curves).

Applications and limitations:

DET curves are intuitive to read and hence allow quick visual assessment of a classifier’s performance. Additionally DET curves can be consulted for threshold analysis and operating point selection. This is particularly helpful if a comparison of error types is required.

On the other hand DET curves do not provide their metric as a single number. Therefore for either automated evaluation or comparison to other classification tasks metrics like the derived area under ROC curve might be better suited.

Examples:

- See Detection error tradeoff (DET) curve for an example comparison between receiver operating characteristic (ROC) curves and Detection error tradeoff (DET) curves.

References:

[WikipediaDET2017]
Wikipedia contributors. Detection error tradeoff. Wikipedia, The Free Encyclopedia. September 4, 2017, 23:33 UTC. Available at: https://en.wikipedia.org/w/index.php?title=Detection_error_tradeoff&oldid=798982054. Accessed February 19, 2018.

[Martin1997]
A. Martin, G. Doddington, T. Kamm, M. Ordowski, and M. Przybocki, The DET Curve in Assessment of Detection Task Performance, NIST 1997.

[Navratil2007]
J. Navractil and D. Klusacek, “On Linear DETs,” 2007 IEEE International Conference on Acoustics, Speech and Signal Processing - ICASSP ’07, Honolulu, HI, 2007, pp. IV-229-IV-232.

3.3.2.17. 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:

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

where $1(x)$ is the indicator function. The zero one loss can also be computed as $zero - oneloss = 1 - accuracy$.

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```
>>> 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.

3.3.2.18. Brier score loss

The `brier_score_loss` function computes the Brier score for binary classes [Brier1950]. 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 the mean squared error of the actual outcome $y \in \{0, 1\}$ and the predicted probability estimate $p = \mathrm{Pr}(y = 1)$ (predict_proba) as outputted by:

$$BS = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} (y_i - p_i)^2$$

The Brier score loss is also between 0 to 1 and the lower the value (the mean square difference is smaller), the more accurate the prediction is.

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
```

The Brier score can be used to assess how well a classifier is calibrated. However, a lower Brier score loss does not always mean a better calibration. This is because, by analogy with the bias-variance decomposition of the mean squared error, the Brier score loss can be decomposed as the sum of calibration loss and refinement loss [Bella2012]. Calibration loss is defined as the mean squared deviation from empirical probabilities derived from the slope of ROC segments. Refinement loss can be defined as the expected optimal loss as measured by the area under the optimal cost curve. Refinement loss can change independently from calibration loss, thus a lower Brier score loss does not necessarily mean a better calibrated model. "Only when refinement loss remains the same does a lower Brier score loss always mean better calibration" [Bella2012], [Flach2008].

Example:

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

References:

[Brier1950]
G. Brier, Verification of forecasts expressed in terms of probability, Monthly weather review 78.1 (1950)

[Bella2012] (1,2)

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Bella, Ferri, Hernández-Orallo, and Ramírez-Quintana "Calibration of Machine Learning Models" in Khosrow-Pour, M. "Machine learning: concepts, methodologies, tools and applications." Hershey, PA: Information Science Reference (2012).
[Flach2008]
Flach, Peter, and Edson Matsubara. "On classification, ranking, and probability estimation." Dagstuhl Seminar Proceedings. Schloss Dagstuhl-Leibniz-Zentrum fr Informatik (2008).

3.3.2.19. Class likelihood ratios

The `class_likelihood_ratios` function computes the positive and negative likelihood ratios $LR_{\pm}$ for binary classes, which can be interpreted as the ratio of post-test to pre-test odds as explained below. As a consequence, this metric is invariant w.r.t. the class prevalence (the number of samples in the positive class divided by the total number of samples) and **can be extrapolated between populations regardless of any possible class imbalance.**

The $LR_{\pm}$ metrics are therefore very useful in settings where the data available to learn and evaluate a classifier is a study population with nearly balanced classes, such as a case-control study, while the target application, i.e. the general population, has very low prevalence.

The positive likelihood ratio LR_{+} is the probability of a classifier to correctly predict that a sample belongs to the positive class divided by the probability of predicting the positive class for a sample belonging to the negative class:

$$LR_{+} = \frac{\mathrm{PR}(P+|T+)}{\mathrm{PR}(P+|T-)}.$$

The notation here refers to predicted (P) or true (T) label and the sign $+$ and $-$ refer to the positive and negative class, respectively, e.g. $P+$ stands for "predicted positive".

Analogously, the negative likelihood ratio LR_{-} is the probability of a sample of the positive class being classified as belonging to the negative class divided by the probability of a sample of the negative class being correctly classified:

$$LR_{-} = \frac{\mathrm{PR}(P-|T+)}{\mathrm{PR}(P-|T-)}.$$

For classifiers above chance LR_{+} above 1 **higher is better**, while LR_{-} ranges from 0 to 1 and **lower is better**. Values of $LR_{\pm} \approx 1$ correspond to chance level.

Notice that probabilities differ from counts, for instance $\mathrm{PR}(P+|T+)$ is not equal to the number of true positive counts `tp` (see the wikipedia page for the actual formulas).

Interpretation across varying prevalence:

Both class likelihood ratios are interpretable in terms of an odds ratio (pre-test and post-tests):

$$\text{post-test odds} = \text{Likelihood ratio} \times \text{pre-test odds}.$$

Odds are in general related to probabilities via

$$\text{odds} = \frac{\text{probability}}{1 - \text{probability}},$$

or equivalently

$$\text{probability} = \frac{\text{odds}}{1 + \text{odds}}.$$

On a given population, the pre-test probability is given by the prevalence. By converting odds to probabilities, the likelihood ratios can be translated into a probability of truly belonging to either class before and after a classifier prediction:

$$\text{post-test odds} = \text{Likelihood ratio} \times \frac{\text{pre-test probability}}{1 - \text{pre-test probability}},$$

$$\text{post-test probability} = \frac{\text{post-test odds}}{1 + \text{post-test odds}}.$$

Mathematical divergences:

The positive likelihood ratio is undefined when $fp = 0$, which can be interpreted as the classifier perfectly identifying positive cases. If $fp = 0$ and additionally $tp = 0$, this leads to a zero/zero division. This happens, for instance, when using a `DummyClassifier` that always predicts the negative class and therefore the interpretation as a perfect classifier is lost.

The negative likelihood ratio is undefined when $tn = 0$. Such divergence is invalid, as $LR_{-} > 1$ would indicate an increase in the odds of a sample belonging to the positive class after being classified as negative, as if the act of classifying caused the positive condition. This includes the `DummyClassifier` that always predicts the positive class (i.e. when $tn = fn = 0$).

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Both class likelihood ratios are undefined when $tp = fn = 0$, which means that no samples of the positive class were present in the testing set. This can also happen when cross-validating highly imbalanced data.

In all the previous cases the `class_likelihood_ratios` function raises by default an appropriate warning message and returns `nan` to avoid pollution when averaging over cross-validation folds.

For a worked-out demonstration of the `class_likelihood_ratios` function, see the example below.

Examples:

- Class Likelihood Ratios to measure classification performance

References:

- Wikipedia entry for Likelihood ratios in diagnostic testing
- Brenner, H., & Gefeller, O. (1997). Variation of sensitivity, specificity, likelihood ratios and predictive values with disease prevalence. Statistics in medicine, 16(9), 981-991.

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) averages over the samples the answer to the following question: for each ground truth label, what fraction of higher-ranked labels were true labels? This performance measure will be higher 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 $y \in \{0, 1\}^{n_{\text{samples}} \times n_{\text{labels}}}$ and the score associated with each label $\hat{f} \in \mathbb{R}^{n_{\text{samples}} \times n_{\text{labels}}}$, the average precision is defined as

$$LRAP(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \frac{1}{||y_i||_0} \sum_{j:y_{ij}=1} \frac{|\mathcal{L}_{ij}|}{\text{rank}_{ij}}$$

where $\mathcal{L}_{ij} = \left\{k : y_{ik} = 1, \hat{f}_{ik} \geq \hat{f}_{ij} \right\}$, $\text{rank}_{ij} = \left|\left\{k : \hat{f}_{ik} \geq \hat{f}_{ij} \right\}\right|$, $|\cdot|$ computes the cardinality of the set (i.e., the number of elements in the set), and $||\cdot||_0$ is the ℓ_0 "norm" (which computes the number of nonzero elements in a vector).

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 of the number of ordered pairs of false and true labels. The lowest achievable ranking loss is zero.

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

$$ranking\_loss(y, \hat{f}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \frac{1}{||y_i||_0(n_{\text{labels}} - ||y_i||_0)} \left|\left\{(k, l) : \hat{f}_{ik} \leq \hat{f}_{il}, y_{ik} = 1, y_{il} = 0\right\}\right|$$

where $|\cdot|$ computes the cardinality of the set (i.e., the number of elements in the set) and $||\cdot||_0$ is the ℓ_0 "norm" (which computes the number of nonzero elements in a vector).

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.

3.3.3.4. Normalized Discounted Cumulative Gain

Discounted Cumulative Gain (DCG) and Normalized Discounted Cumulative Gain (NDCG) are ranking metrics implemented in `dcg_score` and `ndcg_score` ; they compare a predicted order to ground-truth scores, such as the relevance of answers to a query.

From the Wikipedia page for Discounted Cumulative Gain:

"Discounted cumulative gain (DCG) is a measure of ranking quality. In information retrieval, it is often used to measure effectiveness of web search engine algorithms or related applications. Using a graded relevance scale of documents in a search-engine result set, DCG measures the usefulness, or gain, of a document based on its position in the result list. The gain is accumulated from the top of the result list to the bottom, with the gain of each result discounted at lower ranks"

DCG orders the true targets (e.g. relevance of query answers) in the predicted order, then multiplies them by a logarithmic decay and sums the result. The sum can be truncated after the first K results, in which case we call it DCG@K. NDCG, or NDCG@K is DCG divided by the DCG obtained by a perfect prediction, so that it is always between 0 and 1. Usually, NDCG is preferred to DCG.

Compared with the ranking loss, NDCG can take into account relevance scores, rather than a ground-truth ranking. So if the ground-truth consists only of an ordering, the ranking loss should be preferred; if the ground-truth consists of actual usefulness scores (e.g. 0 for irrelevant, 1 for relevant, 2 for very relevant), NDCG can be used.

For one sample, given the vector of continuous ground-truth values for each target $y \in \mathbb{R}^M$, where M is the number of outputs, and the prediction $\hat{y}$, which induces the ranking function f, the DCG score is

$$\sum_{r=1}^{\min(K,M)} \frac{y_{f(r)}}{\log(1+r)}$$

and the NDCG score is the DCG score divided by the DCG score obtained for y.

References:

- Wikipedia entry for Discounted Cumulative Gain
- Jarvelin, K., & Kekalainen, J. (2002). Cumulated gain-based evaluation of IR techniques. ACM Transactions on Information Systems (TOIS), 20(4), 422-446.
- Wang, Y., Wang, L., Li, Y., He, D., Chen, W., & Liu, T. Y. (2013, May). A theoretical analysis of NDCG ranking measures. In Proceedings of the 26th Annual Conference on Learning Theory (COLT 2013)
- McSherry, F., & Najork, M. (2008, March). Computing information retrieval performance measures efficiently in the presence of tied scores. In European conference on information retrieval (pp. 414-421). Springer, Berlin, Heidelberg.

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`, `r2_score`, `explained_variance_score`, `mean_pinball_loss`, `d2_pinball_score` and `d2_absolute_error_score`.

These functions have a `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'`, 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 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. R^2 score, the coefficient of determination

The `r2_score` function computes the coefficient of determination, usually denoted as R^2.

It represents the proportion of variance (of y) that has been explained by the independent variables in the model. It provides an indication of goodness of fit and therefore a measure of how well unseen samples are likely to be predicted by the model, through the proportion of explained variance.

As such variance is dataset dependent, R^2 may not be meaningfully comparable across different datasets. 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 (average) value of y, disregarding the input features, would get an R^2 score of 0.0.

Note: when the prediction residuals have zero mean, the R^2 score and the Explained variance score are identical.

If $\hat{y}_i$ is the predicted value of the i-th sample and y_i is the corresponding true value for total n samples, the estimated R^2 is defined as:

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

where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$ and $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \epsilon_i^2$.

Note that `r2_score` calculates unadjusted R^2 without correcting for bias in sample variance of y.

In the particular case where the true target is constant, the R^2 score is not finite: it is either `NaN` (perfect predictions) or `-Inf` (imperfect predictions). Such non-finite scores may prevent correct model optimization such as grid-search cross-validation to be performed correctly. For this reason the default behaviour of `r2_score` is to replace them with 1.0 (perfect predictions) or 0.0 (imperfect predictions). If `force_finite` is set to `False`, this score falls back on the original R^2 definition.

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...
>>> y_true = [-2, -2, -2]
>>> y_pred = [-2, -2, -2]
>>> r2_score(y_true, y_pred)
1.0
>>> r2_score(y_true, y_pred, force_finite=False)
nan
>>> y_true = [-2, -2, -2]
>>> y_pred = [-2, -2, -2 + 1e-8]
>>> r2_score(y_true, y_pred)
0.0
>>> r2_score(y_true, y_pred, force_finite=False)
-inf
```

Example:

- See L1-based models for Sparse Signals for an example of R^2 score usage to evaluate Lasso and Elastic Net on sparse signals.

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])
0.85...
```

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

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

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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. Mean absolute percentage error

The `mean_absolute_percentage_error` (MAPE), also known as mean absolute percentage deviation (MAPD), is an evaluation metric for regression problems. The idea of this metric is to be sensitive to relative errors. It is for example not changed by a global scaling of the target variable.

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 percentage error (MAPE) estimated over n_{samples} is defined as

$$\text{MAPE}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \frac{|y_i - \hat{y}_i|}{\max(\epsilon, |y_i|)}$$

where ϵ is an arbitrary small yet strictly positive number to avoid undefined results when y is zero.

The `mean_absolute_percentage_error` function supports multioutput.

Here is a small example of usage of the `mean_absolute_percentage_error` function:

```
>>> from sklearn.metrics import mean_absolute_percentage_error
>>> y_true = [1, 10, 1e6]
>>> y_pred = [0.9, 15, 1.2e6]
>>> mean_absolute_percentage_error(y_true, y_pred)
0.2666...
```

In above example, if we had used `mean_absolute_error`, it would have ignored the small magnitude values and only reflected the error in prediction of highest magnitude value. But that problem is resolved in case of MAPE because it calculates relative percentage error with respect to actual output.

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3.3.4.6. 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
```

3.3.4.7. Max error

The `max_error` function computes the maximum residual error , a metric that captures the worst case error between the predicted value and the true value. In a perfectly fitted single output regression model, `max_error` would be `0` on the training set and though this would be highly unlikely in the real world, this metric shows the extent of error that the model had when it was fitted.

If $\hat{y}_i$ is the predicted value of the i-th sample, and y_i is the corresponding true value, then the max error is defined as

$$\text{Max Error}(y, \hat{y}) = \max(|y_i - \hat{y}_i|)$$

Here is a small example of usage of the `max_error` function:

```
>>> from sklearn.metrics import max_error
>>> y_true = [3, 2, 7, 1]
>>> y_pred = [9, 2, 7, 1]
>>> max_error(y_true, y_pred)
6
```

The `max_error` does not support multioutput.

3.3.4.8. 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:

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

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

Link to R^2 score, the coefficient of determination

The difference between the explained variance score and the R^2 score, the coefficient of determination is that when the explained variance score does not account for systematic offset in the prediction. For this reason, the R^2 score, the coefficient of determination should be preferred in general.

In the particular case where the true target is constant, the Explained Variance score is not finite: it is either `NaN` (perfect predictions) or `-Inf` (imperfect predictions). Such non-finite scores may prevent correct model optimization such as grid-search cross-validation to be performed correctly. For this reason the default behaviour of `explained_variance_score` is to replace them with 1.0 (perfect predictions) or 0.0 (imperfect predictions). You can set the `force_finite` parameter to `False` to prevent this fix from happening and fallback on the original Explained Variance score.

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...
>>> y_true = [-2, -2, -2]
>>> y_pred = [-2, -2, -2]
>>> explained_variance_score(y_true, y_pred)
1.0
>>> explained_variance_score(y_true, y_pred, force_finite=False)
nan
>>> y_true = [-2, -2, -2]
>>> y_pred = [-2, -2, -2 + 1e-8]
>>> explained_variance_score(y_true, y_pred)
0.0
>>> explained_variance_score(y_true, y_pred, force_finite=False)
-inf
```

3.3.4.9. Mean Poisson, Gamma, and Tweedie deviances

The `mean_tweedie_deviance` function computes the mean Tweedie deviance error with a `power` parameter (p). This is a metric that elicits predicted expectation values of regression targets.

Following special cases exist,

- when `power=0` it is equivalent to `mean_squared_error`.
- when `power=1` it is equivalent to `mean_poisson_deviance`.
- when `power=2` it is equivalent to `mean_gamma_deviance`.

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

$$\text{D}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \begin{cases} (y_i - \hat{y}_i)^2, & \text{for } p = 0 \text{ (Normal)} \\ 2(y_i \log(y_i/\hat{y}_i) + \hat{y}_i - y_i), & \text{for } p = 1 \text{ (Poisson)} \\ 2(\log(\hat{y}_i/y_i) + y_i/\hat{y}_i - 1), & \text{for } p = 2 \text{ (Gamma)} \\ 2\left(\frac{\max(y_i,0)^{2-p}}{(1-p)(2-p)} - \frac{y_i\,\hat{y}_i^{1-p}}{1-p} + \frac{\hat{y}_i^{2-p}}{2-p}\right), & \text{otherwise} \end{cases}$$

Tweedie deviance is a homogeneous function of degree `2-power`. Thus, Gamma distribution with `power=2` means that simultaneously scaling `y_true` and `y_pred` has no effect on the deviance. For Poisson distribution `power=1` the deviance scales linearly, and for Normal distribution (`power=0`), quadratically. In general, the higher `power` the less weight is given to extreme deviations between true and predicted targets.

For instance, let's compare the two predictions 1.5 and 150 that are both 50% larger than their corresponding true value.

The mean squared error (`power=0`) is very sensitive to the prediction difference of the second point,:

```
>>> from sklearn.metrics import mean_tweedie_deviance
>>> mean_tweedie_deviance([1.0], [1.5], power=0)
0.25
>>> mean_tweedie_deviance([100.], [150.], power=0)
2500.0
```

If we increase `power` to 1,:

```
>>> mean_tweedie_deviance([1.0], [1.5], power=1)
0.18...
>>> mean_tweedie_deviance([100.], [150.], power=1)
18.9...
```

the difference in errors decreases. Finally, by setting, `power=2`:

```
>>> mean_tweedie_deviance([1.0], [1.5], power=2)
0.14...
>>> mean_tweedie_deviance([100.], [150.], power=2)
0.14...
```

Toggle Menu dentical errors. The deviance when `power=2` is thus only sensitive to relative errors.

3.3.4.10. Pinball loss

The `mean_pinball_loss` function is used to evaluate the predictive performance of quantile regression models.

$$\text{pinball}(y, \hat{y}) = \frac{1}{n_{\text{samples}}} \sum_{i=0}^{n_{\text{samples}}-1} \alpha \max(y_i - \hat{y}_i, 0) + (1 - \alpha) \max(\hat{y}_i - y_i, 0)$$

The value of pinball loss is equivalent to half of `mean_absolute_error` when the quantile parameter `alpha` is set to 0.5.

Here is a small example of usage of the `mean_pinball_loss` function:

```
>>> from sklearn.metrics import mean_pinball_loss
>>> y_true = [1, 2, 3]
>>> mean_pinball_loss(y_true, [0, 2, 3], alpha=0.1)
0.03...
>>> mean_pinball_loss(y_true, [1, 2, 4], alpha=0.1)
0.3...
>>> mean_pinball_loss(y_true, [0, 2, 3], alpha=0.9)
0.3...
>>> mean_pinball_loss(y_true, [1, 2, 4], alpha=0.9)
0.03...
>>> mean_pinball_loss(y_true, y_true, alpha=0.1)
0.0
>>> mean_pinball_loss(y_true, y_true, alpha=0.9)
0.0
```

It is possible to build a scorer object with a specific choice of `alpha`:

```
>>> from sklearn.metrics import make_scorer
>>> mean_pinball_loss_95p = make_scorer(mean_pinball_loss, alpha=0.95)
```

Such a scorer can be used to evaluate the generalization performance of a quantile regressor via cross-validation:

```
>>> from sklearn.datasets import make_regression
>>> from sklearn.model_selection import cross_val_score
>>> from sklearn.ensemble import GradientBoostingRegressor
>>>
>>> X, y = make_regression(n_samples=100, random_state=0)
>>> estimator = GradientBoostingRegressor(
...     loss="quantile",
...     alpha=0.95,
...     random_state=0,
... )
>>> cross_val_score(estimator, X, y, cv=5, scoring=mean_pinball_loss_95p)
array([13.6..., 9.7..., 23.3..., 9.5..., 10.4...])
```

It is also possible to build scorer objects for hyper-parameter tuning. The sign of the loss must be switched to ensure that greater means better as explained in the example linked below.

Example:

- See Prediction Intervals for Gradient Boosting Regression for an example of using the pinball loss to evaluate and tune the hyper-parameters of quantile regression models on data with non-symmetric noise and outliers.

3.3.4.11. D^2 score

The D^2 score computes the fraction of deviance explained. It is a generalization of R^2, where the squared error is generalized and replaced by a deviance of choice $\text{dev}(y, \hat{y})$ (e.g., Tweedie, pinball or mean absolute error). D^2 is a form of a *skill score*. It is calculated as

$$D^2(y, \hat{y}) = 1 - \frac{\text{dev}(y, \hat{y})}{\text{dev}(y, y_{\text{null}})} .$$

Where y_{null} is the optimal prediction of an intercept-only model (e.g., the mean of `y_true` for the Tweedie case, the median for absolute error and the alpha-quantile for pinball loss).

Like R^2, the best possible score is 1.0 and it can be negative (because the model can be arbitrarily worse). A constant model that always predicts y_{null}, disregarding the input features, would get a D^2 score of 0.0.

D^2 Tweedie score

The `d2_tweedie_score` function implements the special case of D^2 where $\text{dev}(y, \hat{y})$ is the Tweedie deviance, see Mean Poisson, Gamma, and Tweedie deviances. It is also known as D^2 Tweedie and is related to McFadden's likelihood ratio index.

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The argument `power` defines the Tweedie power as for `mean_tweedie_deviance`. Note that for `power=0`, `d2_tweedie_score` equals `r2_score` (for single targets).

A scorer object with a specific choice of `power` can be built by:

```
>>> from sklearn.metrics import d2_tweedie_score, make_scorer
>>> d2_tweedie_score_15 = make_scorer(d2_tweedie_score, power=1.5)
```

D^2 pinball score

The `d2_pinball_score` function implements the special case of D^2 with the pinball loss, see Pinball loss, i.e.:

$$\text{dev}(y, \hat{y}) = \text{pinball}(y, \hat{y}).$$

The argument `alpha` defines the slope of the pinball loss as for `mean_pinball_loss` (Pinball loss). It determines the quantile level `alpha` for which the pinball loss and also D^2 are optimal. Note that for `alpha=0.5` (the default) `d2_pinball_score` equals `d2_absolute_error_score`.

A scorer object with a specific choice of `alpha` can be built by:

```
>>> from sklearn.metrics import d2_pinball_score, make_scorer
>>> d2_pinball_score_08 = make_scorer(d2_pinball_score, alpha=0.8)
```

D^2 absolute error score

The `d2_absolute_error_score` function implements the special case of the Mean absolute error:

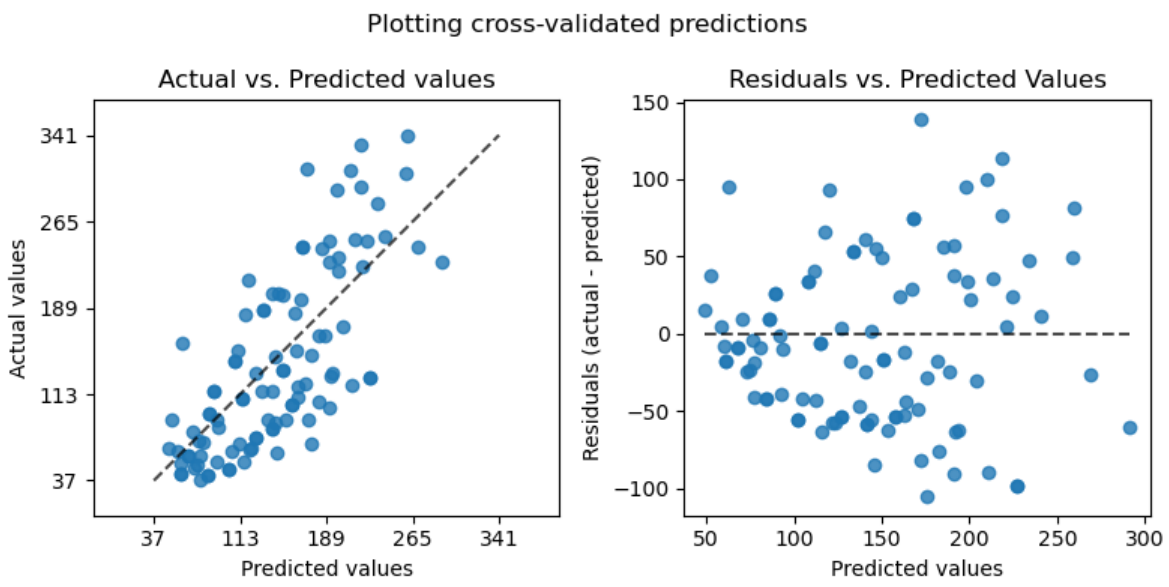
$$\text{dev}(y, \hat{y}) = \text{MAE}(y, \hat{y}).$$

Here are some usage examples of the `d2_absolute_error_score` function:

```
>>> from sklearn.metrics import d2_absolute_error_score
>>> y_true = [3, -0.5, 2, 7]
>>> y_pred = [2.5, 0.0, 2, 8]
>>> d2_absolute_error_score(y_true, y_pred)
0.764...
>>> y_true = [1, 2, 3]
>>> y_pred = [1, 2, 3]
>>> d2_absolute_error_score(y_true, y_pred)
1.0
>>> y_true = [1, 2, 3]
>>> y_pred = [2, 2, 2]
>>> d2_absolute_error_score(y_true, y_pred)
0.0
```

3.3.4.12. Visual evaluation of regression models

Among methods to assess the quality of regression models, scikit-learn provides the `PredictionErrorDisplay` class. It allows to visually inspect the prediction errors of a model in two different manners.



The plot on the left shows the actual values vs predicted values. For a noise-free regression task aiming to predict the (conditional) expectation of `y`, a perfect regression model would display data points on the diagonal defined by predicted equal to actual values. The further away from this optimal line, the larger the error of the model. In a more realistic setting with irreducible noise, that is, when not all the variations of `y` can be explained by features in `X`, then the best model would lead to a cloud of points densely arranged around the diagonal.

Note that the above only holds when the predicted values is the expected value of `y` given `X`. This is typically the case for regression models that minimize the mean squared error objective function or more generally the mean Tweedie deviance for any value of its "power" parameter.

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When plotting the predictions of an estimator that predicts a quantile of `y` given `X`, e.g. **`QuantileRegressor`** or any other model minimizing the pinball loss, a fraction of the points are either expected to lie above or below the diagonal depending on the estimated quantile level.

All in all, while intuitive to read, this plot does not really inform us on what to do to obtain a better model.

The right-hand side plot shows the residuals (i.e. the difference between the actual and the predicted values) vs. the predicted values.

This plot makes it easier to visualize if the residuals follow and homoscedastic or heteroschedastic distribution.

In particular, if the true distribution of `y|X` is Poisson or Gamma distributed, it is expected that the variance of the residuals of the optimal model would grow with the predicted value of `E[y|X]` (either linearly for Poisson or quadratically for Gamma).

When fitting a linear least squares regression model (see **`LinearRegression`** and **`Ridge`**), we can use this plot to check if some of the model assumptions are met, in particular that the residuals should be uncorrelated, their expected value should be null and that their variance should be constant (homoschedasticity).

If this is not the case, and in particular if the residuals plot show some banana-shaped structure, this is a hint that the model is likely mis-specified and that non-linear feature engineering or switching to a non-linear regression model might be useful.

Refer to the example below to see a model evaluation that makes use of this display.

Example:

- See Effect of transforming the targets in regression model for an example on how to use **`PredictionErrorDisplay`** to visualize the prediction quality improvement of a regression model obtained by transforming the target before learning.

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
>>> X, y = load_iris(return_X_y=True)
>>> 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(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:

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```
>>> clf = SVC(kernel='rbf', C=1).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.94...
```

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.

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