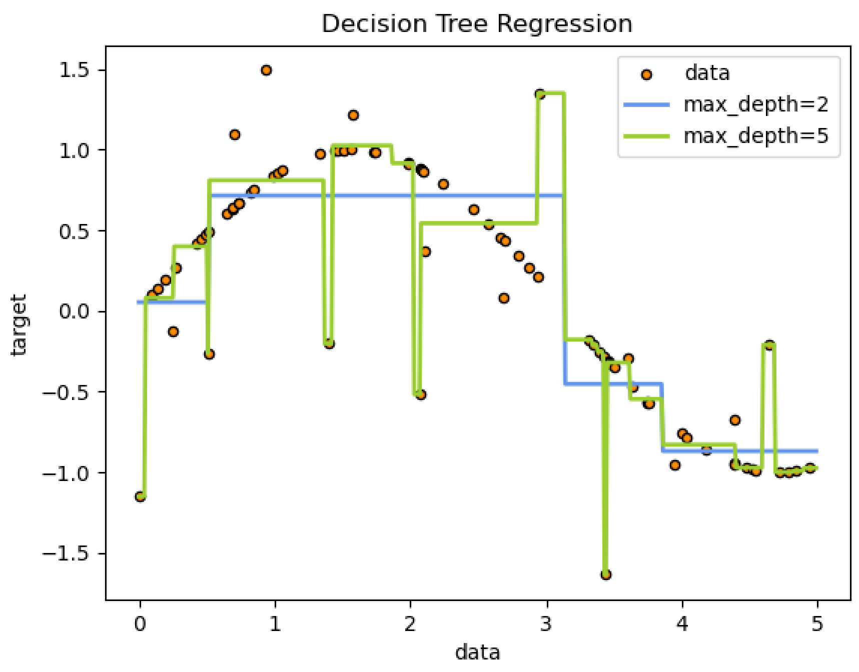
1.10. Decision Trees

Decision Trees (DTs) are a non-parametric supervised learning method used for classification and regression. The goal is to create a model that predicts the value of a target variable by learning simple decision rules inferred from the data features. A tree can be seen as a piecewise constant approximation.

For instance, in the example below, decision trees learn from data to approximate a sine curve with a set of if-then-else decision rules. The deeper the tree, the more complex the decision rules and the fitter the model.



Some advantages of decision trees are:

- Simple to understand and to interpret. Trees can be visualized.
- Requires little data preparation. Other techniques often require data normalization, dummy variables need to be created and blank values to be removed. Some tree and algorithm combinations support missing values.
- The cost of using the tree (i.e., predicting data) is logarithmic in the number of data points used to train the tree.
- Able to handle both numerical and categorical data. However, the scikit-learn implementation does not support categorical variables for now. Other techniques are usually specialized in analyzing datasets that have only one type of variable. See algorithms for more information.
- Able to handle multi-output problems.
- Uses a white box model. If a given situation is observable in a model, the explanation for the condition is easily explained by boolean logic. By contrast, in a black box model (e.g., in an artificial neural network), results may be more difficult to interpret.
- Possible to validate a model using statistical tests. That makes it possible to account for the reliability of the model.
- Performs well even if its assumptions are somewhat violated by the true model from which the data were generated.

The disadvantages of decision trees include:

- Decision-tree learners can create over-complex trees that do not generalize the data well. This is called overfitting. Mechanisms such as pruning, setting the minimum number of samples required at a leaf node or setting the maximum depth of the tree are necessary to avoid this problem.
- Decision trees can be unstable because small variations in the data might result in a completely different tree being generated. This problem is mitigated by using decision trees within an ensemble.
- Predictions of decision trees are neither smooth nor continuous, but piecewise constant approximations as seen in the above figure. Therefore, they are not good at extrapolation.
- The problem of learning an optimal decision tree is known to be NP-complete under several aspects of optimality and even for simple concepts. Consequently, practical decision-tree learning algorithms are based on heuristic algorithms such as the greedy algorithm where locally optimal decisions are made at each node. Such algorithms cannot guarantee to return the globally optimal decision tree. This can be mitigated by training multiple trees in an ensemble learner, where the features and samples are randomly sampled with replacement.
- There are concepts that are hard to learn because decision trees do not express them easily, such as XOR, parity or multiplexer problems.
- Decision tree learners create biased trees if some classes dominate. It is therefore recommended to balance the dataset prior to fitting with the decision tree.

Toggle Menu

1.10.1. Classification

`DecisionTreeClassifier` is a class capable of performing multi-class classification on a dataset.

As with other classifiers, **`DecisionTreeClassifier`** takes as input two arrays: an array X, sparse or dense, of shape `(n_samples, n_features)` holding the training samples, and an array Y of integer values, shape `(n_samples,)`, holding the class labels for the training samples:

```
>>> from sklearn import tree
>>> X = [[0, 0], [1, 1]]
>>> Y = [0, 1]
>>> clf = tree.DecisionTreeClassifier()
>>> clf = clf.fit(X, Y)
```

After being fitted, the model can then be used to predict the class of samples:

```
>>> clf.predict([[2., 2.]])
array([1])
```

In case that there are multiple classes with the same and highest probability, the classifier will predict the class with the lowest index amongst those classes.

As an alternative to outputting a specific class, the probability of each class can be predicted, which is the fraction of training samples of the class in a leaf:

```
>>> clf.predict_proba([[2., 2.]])
array([[0., 1.]])
```

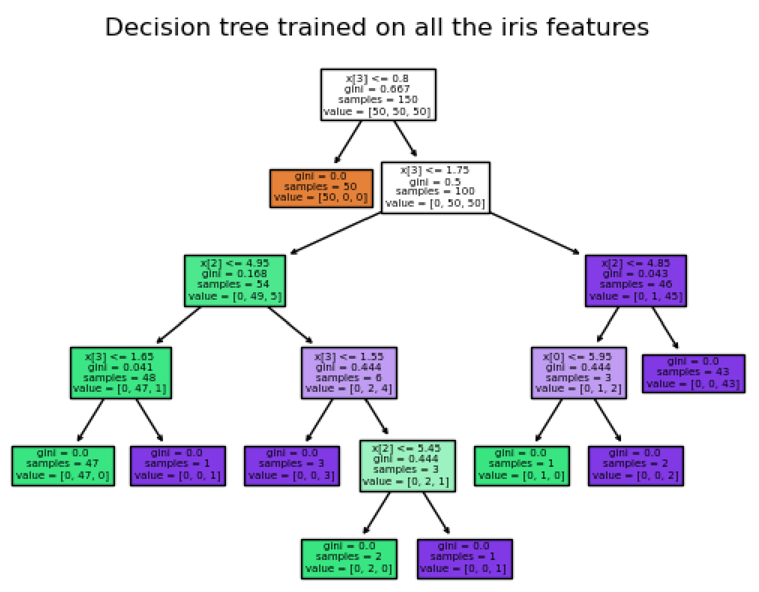
`DecisionTreeClassifier` is capable of both binary (where the labels are [-1, 1]) classification and multiclass (where the labels are [0, …, K-1]) classification.

Using the Iris dataset, we can construct a tree as follows:

```
>>> from sklearn.datasets import load_iris
>>> from sklearn import tree
>>> iris = load_iris()
>>> X, y = iris.data, iris.target
>>> clf = tree.DecisionTreeClassifier()
>>> clf = clf.fit(X, y)
```

Once trained, you can plot the tree with the **`plot_tree`** function:

```
>>> tree.plot_tree(clf)
[...]
```

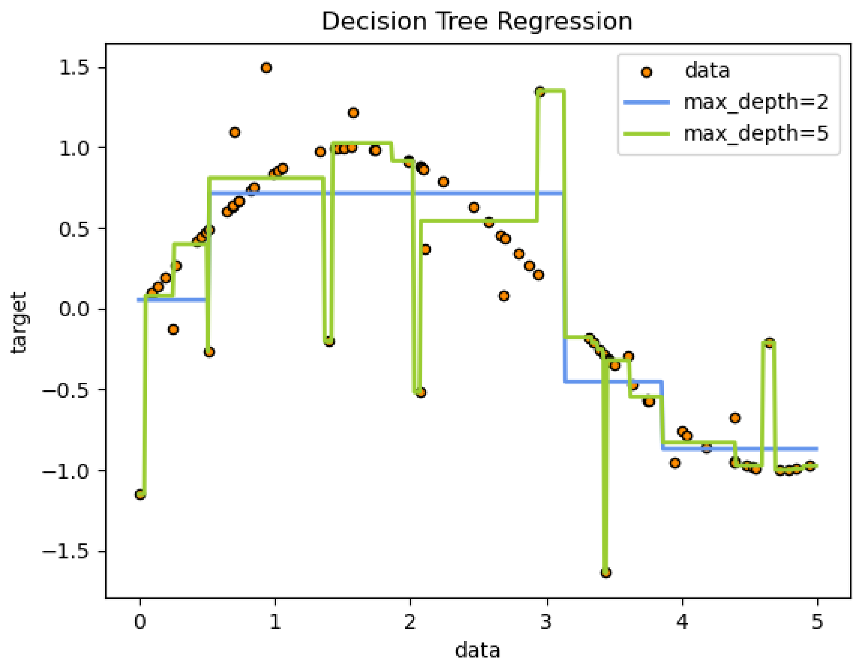


▶ **Alternative ways to export trees**

Examples:

- Plot the decision surface of decision trees trained on the iris dataset
- Toggle Menu ding the decision tree structure

1.10.2. Regression



Decision trees can also be applied to regression problems, using the [`DecisionTreeRegressor`](#) class.

As in the classification setting, the fit method will take as argument arrays X and y, only that in this case y is expected to have floating point values instead of integer values:

```
>>> from sklearn import tree
>>> X = [[0, 0], [2, 2]]
>>> y = [0.5, 2.5]
>>> clf = tree.DecisionTreeRegressor()
>>> clf = clf.fit(X, y)
>>> clf.predict([[1, 1]])
array([0.5])
```

Examples:

- Decision Tree Regression

1.10.3. Multi-output problems

A multi-output problem is a supervised learning problem with several outputs to predict, that is when Y is a 2d array of shape `(n_samples, n_outputs)`.

When there is no correlation between the outputs, a very simple way to solve this kind of problem is to build n independent models, i.e. one for each output, and then to use those models to independently predict each one of the n outputs. However, because it is likely that the output values related to the same input are themselves correlated, an often better way is to build a single model capable of predicting simultaneously all n outputs. First, it requires lower training time since only a single estimator is built. Second, the generalization accuracy of the resulting estimator may often be increased.

With regard to decision trees, this strategy can readily be used to support multi-output problems. This requires the following changes:

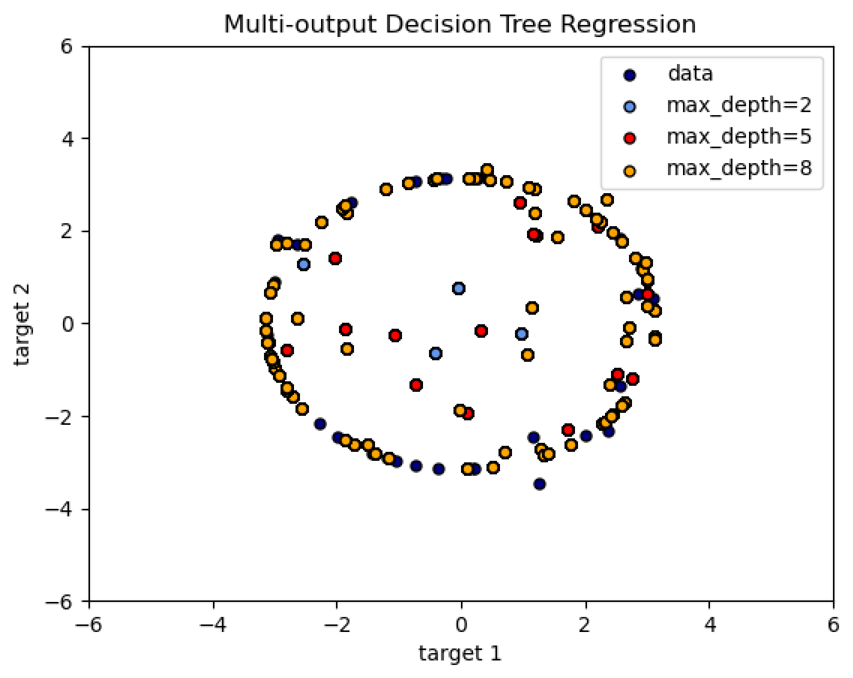
- Store n output values in leaves, instead of 1;
- Use splitting criteria that compute the average reduction across all n outputs.

This module offers support for multi-output problems by implementing this strategy in both `DecisionTreeClassifier` and `DecisionTreeRegressor`. If a decision tree is fit on an output array Y of shape `(n_samples, n_outputs)` then the resulting estimator will:

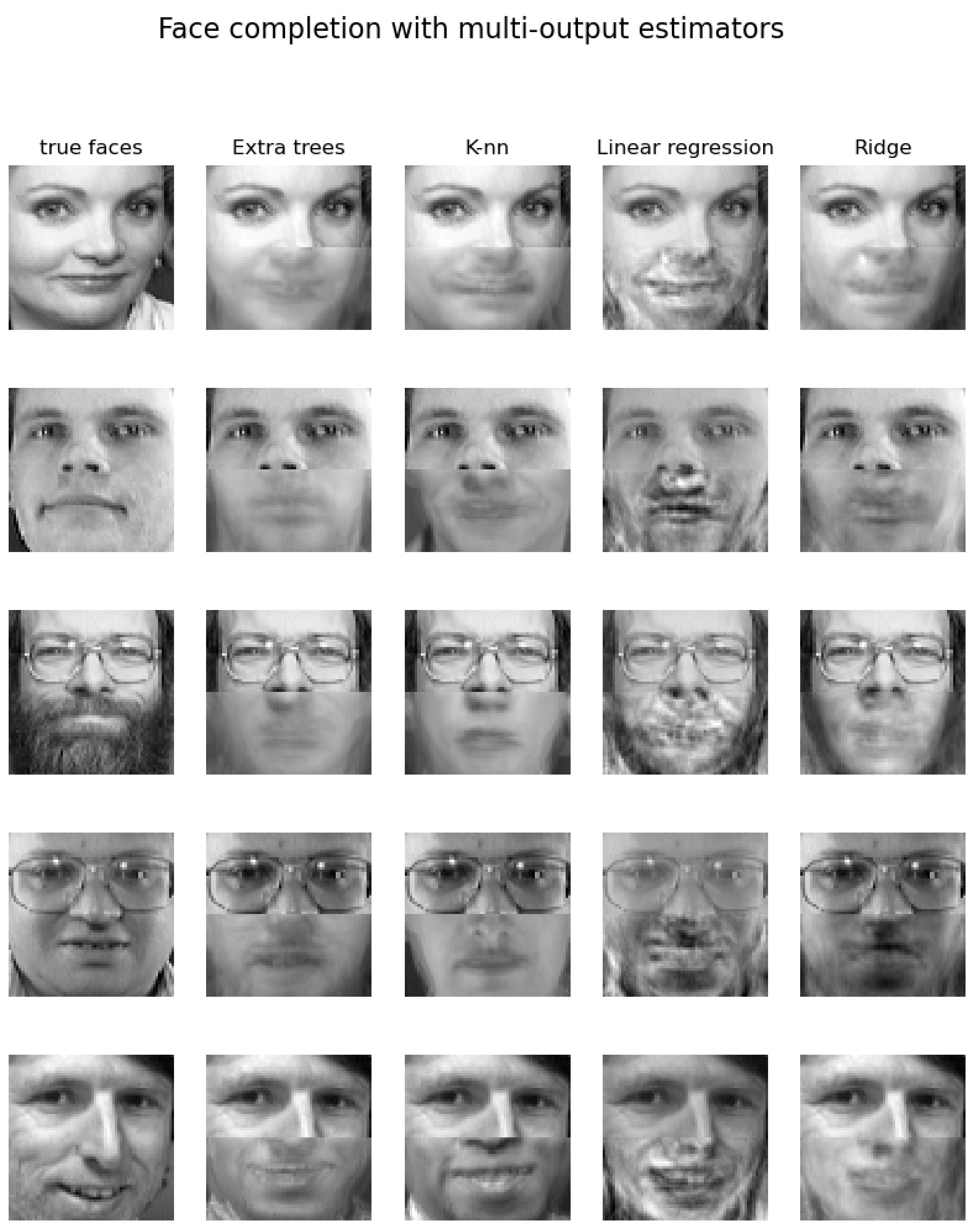
- Output n_output values upon `predict`;
- Output a list of n_output arrays of class probabilities upon `predict_proba`.

The use of multi-output trees for regression is demonstrated in Multi-output Decision Tree Regression. In this example, the input X is a single real value and the outputs Y are the sine and cosine of X.

Toggle Menu



The use of multi-output trees for classification is demonstrated in [Face completion with a multi-output estimators](). In this example, the inputs X are the pixels of the upper half of faces and the outputs Y are the pixels of the lower half of those faces.



Examples:

- [Multi-output Decision Tree Regression]()
- [Face completion with a multi-output estimators]()

▶ **References**

Toggle Menu

1.10.4. Complexity

In general, the run time cost to construct a balanced binary tree is $O(n_{samples}n_{features}\log(n_{samples}))$ and query time $O(\log(n_{samples}))$. Although the tree construction algorithm attempts to generate balanced trees, they will not always be balanced. Assuming that the subtrees remain approximately balanced, the cost at each node consists of searching through $O(n_{features})$ to find the feature that offers the largest reduction in the impurity criterion, e.g. log loss (which is equivalent to an information gain). This has a cost of $O(n_{features}n_{samples}\log(n_{samples}))$ at each node, leading to a total cost over the entire trees (by summing the cost at each node) of $O(n_{features}n_{samples}^{2}\log(n_{samples}))$.

1.10.5. Tips on practical use

- Decision trees tend to overfit on data with a large number of features. Getting the right ratio of samples to number of features is important, since a tree with few samples in high dimensional space is very likely to overfit.
- Consider performing dimensionality reduction (PCA, ICA, or Feature selection) beforehand to give your tree a better chance of finding features that are discriminative.
- Understanding the decision tree structure will help in gaining more insights about how the decision tree makes predictions, which is important for understanding the important features in the data.
- Visualize your tree as you are training by using the `export` function. Use `max_depth=3` as an initial tree depth to get a feel for how the tree is fitting to your data, and then increase the depth.
- Remember that the number of samples required to populate the tree doubles for each additional level the tree grows to. Use `max_depth` to control the size of the tree to prevent overfitting.
- Use `min_samples_split` or `min_samples_leaf` to ensure that multiple samples inform every decision in the tree, by controlling which splits will be considered. A very small number will usually mean the tree will overfit, whereas a large number will prevent the tree from learning the data. Try `min_samples_leaf=5` as an initial value. If the sample size varies greatly, a float number can be used as percentage in these two parameters. While `min_samples_split` can create arbitrarily small leaves, `min_samples_leaf` guarantees that each leaf has a minimum size, avoiding low-variance, over-fit leaf nodes in regression problems. For classification with few classes, `min_samples_leaf=1` is often the best choice.

  Note that `min_samples_split` considers samples directly and independent of `sample_weight`, if provided (e.g. a node with m weighted samples is still treated as having exactly m samples). Consider `min_weight_fraction_leaf` or `min_impurity_decrease` if accounting for sample weights is required at splits.
- Balance your dataset before training to prevent the tree from being biased toward the classes that are dominant. Class balancing can be done by sampling an equal number of samples from each class, or preferably by normalizing the sum of the sample weights (`sample_weight`) for each class to the same value. Also note that weight-based pre-pruning criteria, such as `min_weight_fraction_leaf`, will then be less biased toward dominant classes than criteria that are not aware of the sample weights, like `min_samples_leaf`.
- If the samples are weighted, it will be easier to optimize the tree structure using weight-based pre-pruning criterion such as `min_weight_fraction_leaf`, which ensure that leaf nodes contain at least a fraction of the overall sum of the sample weights.
- All decision trees use `np.float32` arrays internally. If training data is not in this format, a copy of the dataset will be made.
- If the input matrix X is very sparse, it is recommended to convert to sparse `csc_matrix` before calling fit and sparse `csr_matrix` before calling predict. Training time can be orders of magnitude faster for a sparse matrix input compared to a dense matrix when features have zero values in most of the samples.

1.10.6. Tree algorithms: ID3, C4.5, C5.0 and CART

What are all the various decision tree algorithms and how do they differ from each other? Which one is implemented in scikit-learn?

▶ **Various decision tree algorithms**

scikit-learn uses an optimized version of the CART algorithm; however, the scikit-learn implementation does not support categorical variables for now.

Toggle Menu

1.10.7. Mathematical formulation

Given training vectors $x_i \in R^n$, i=1,..., l and a label vector $y \in R^l$, a decision tree recursively partitions the feature space such that the samples with the same labels or similar target values are grouped together.

Let the data at node m be represented by Q_m with n_m samples. For each candidate split $\theta = (j, t_m)$ consisting of a feature j and threshold t_m, partition the data into $Q_m^{left}(\theta)$ and $Q_m^{right}(\theta)$ subsets

$$Q_m^{left}(\theta) = \{(x, y) | x_j \leq t_m\}$$
$$Q_m^{right}(\theta) = Q_m \setminus Q_m^{left}(\theta)$$

The quality of a candidate split of node m is then computed using an impurity function or loss function $H()$, the choice of which depends on the task being solved (classification or regression)

$$G(Q_m, \theta) = \frac{n_m^{left}}{n_m} H(Q_m^{left}(\theta)) + \frac{n_m^{right}}{n_m} H(Q_m^{right}(\theta))$$

Select the parameters that minimises the impurity

$$\theta^* = \operatorname{argmin}_\theta G(Q_m, \theta)$$

Recurse for subsets $Q_m^{left}(\theta^*)$ and $Q_m^{right}(\theta^*)$ until the maximum allowable depth is reached, $n_m < \min_{samples}$ or $n_m = 1$.

1.10.7.1. Classification criteria

If a target is a classification outcome taking on values 0,1,...,K-1, for node m, let

$$p_{mk} = \frac{1}{n_m} \sum_{y \in Q_m} I(y = k)$$

be the proportion of class k observations in node m. If m is a terminal node, `predict_proba` for this region is set to p_{mk}. Common measures of impurity are the following.

Gini:

$$H(Q_m) = \sum_k p_{mk}(1 - p_{mk})$$

Log Loss or Entropy:

$$H(Q_m) = - \sum_k p_{mk} \log(p_{mk})$$

▶ Shannon entropy:

1.10.7.2. Regression criteria

If the target is a continuous value, then for node m, common criteria to minimize as for determining locations for future splits are Mean Squared Error (MSE or L2 error), Poisson deviance as well as Mean Absolute Error (MAE or L1 error). MSE and Poisson deviance both set the predicted value of terminal nodes to the learned mean value $\bar{y}_m$ of the node whereas the MAE sets the predicted value of terminal nodes to the median $median(y)_m$.

Mean Squared Error:

$$\bar{y}_m = \frac{1}{n_m} \sum_{y \in Q_m} y$$
$$H(Q_m) = \frac{1}{n_m} \sum_{y \in Q_m} (y - \bar{y}_m)^2$$

Half Poisson deviance:

$$H(Q_m) = \frac{1}{n_m} \sum_{y \in Q_m} (y \log\frac{y}{\bar{y}_m} - y + \bar{y}_m)$$

Toggle Menu

Setting `criterion="poisson"` might be a good choice if your target is a count or a frequency (count per some unit). In any case, $y >= 0$ is a necessary condition to use this criterion. Note that it fits much slower than the MSE criterion.

Mean Absolute Error:

$$median(y)_m = \underset{y \in Q_m}{\mathrm{median}}(y)$$
$$H(Q_m) = \frac{1}{n_m} \sum_{y \in Q_m} |y - median(y)_m|$$

Note that it fits much slower than the MSE criterion.

1.10.8. Missing Values Support

`DecisionTreeClassifier` and `DecisionTreeRegressor` have built-in support for missing values when `splitter='best'` and criterion is `'gini'`, `'entropy'`, or `'log_loss'`, for classification or `'squared_error'`, `'friedman_mse'`, or `'poisson'` for regression.

For each potential threshold on the non-missing data, the splitter will evaluate the split with all the missing values going to the left node or the right node.

Decisions are made as follows:

- By default when predicting, the samples with missing values are classified with the class used in the split found during training:

```
>>> from sklearn.tree import DecisionTreeClassifier
>>> import numpy as np

>>> X = np.array([0, 1, 6, np.nan]).reshape(-1, 1)
>>> y = [0, 0, 1, 1]

>>> tree = DecisionTreeClassifier(random_state=0).fit(X, y)
>>> tree.predict(X)
array([0, 0, 1, 1])
```

- If the the criterion evaluation is the same for both nodes, then the tie for missing value at predict time is broken by going to the right node. The splitter also checks the split where all the missing values go to one child and non-missing values go to the other:

```
>>> from sklearn.tree import DecisionTreeClassifier
>>> import numpy as np

>>> X = np.array([np.nan, -1, np.nan, 1]).reshape(-1, 1)
>>> y = [0, 0, 1, 1]

>>> tree = DecisionTreeClassifier(random_state=0).fit(X, y)

>>> X_test = np.array([np.nan]).reshape(-1, 1)
>>> tree.predict(X_test)
array([1])
```

- If no missing values are seen during training for a given feature, then during prediction missing values are mapped to the child with the most samples:

```
>>> from sklearn.tree import DecisionTreeClassifier
>>> import numpy as np

>>> X = np.array([0, 1, 2, 3]).reshape(-1, 1)
>>> y = [0, 1, 1, 1]

>>> tree = DecisionTreeClassifier(random_state=0).fit(X, y)

>>> X_test = np.array([np.nan]).reshape(-1, 1)
>>> tree.predict(X_test)
array([1])
```

Toggle Menu

1.10.9. Minimal Cost-Complexity Pruning

Minimal cost-complexity pruning is an algorithm used to prune a tree to avoid over-fitting, described in Chapter 3 of [BRE]. This algorithm is parameterized by $\alpha \geq 0$ known as the complexity parameter. The complexity parameter is used to define the cost-complexity measure, $R_\alpha(T)$ of a given tree T:

$$R_\alpha(T) = R(T) + \alpha|\widetilde{T}|$$

where $|\widetilde{T}|$ is the number of terminal nodes in T and $R(T)$ is traditionally defined as the total misclassification rate of the terminal nodes. Alternatively, scikit-learn uses the total sample weighted impurity of the terminal nodes for $R(T)$. As shown above, the impurity of a node depends on the criterion. Minimal cost-complexity pruning finds the subtree of T that minimizes $R_\alpha(T)$.

The cost complexity measure of a single node is $R_\alpha(t) = R(t) + \alpha$. The branch, T_t, is defined to be a tree where node t is its root. In general, the impurity of a node is greater than the sum of impurities of its terminal nodes, $R(T_t) < R(t)$. However, the cost complexity measure of a node, t, and its branch, T_t, can be equal depending on α. We define the effective α of a node to be the value where they are equal, $R_\alpha(T_t) = R_\alpha(t)$ or $\alpha_{eff}(t) = \frac{R(t) - R(T_t)}{|T| - 1}$. A non-terminal node with the smallest value of α_{eff} is the weakest link and will be pruned. This process stops when the pruned tree's minimal α_{eff} is greater than the `ccp_alpha` parameter.

Examples:

- Post pruning decision trees with cost complexity pruning

▶ **References**

Toggle Menu