1.11. Ensemble methods

The goal of **ensemble methods** is to combine the predictions of several base estimators built with a given learning algorithm in order to improve generalizability / robustness over a single estimator.

Two families of ensemble methods are usually distinguished:

- In **averaging methods**, the driving principle is to build several estimators independently and then to average their predictions. On average, the combined estimator is usually better than any of the single base estimator because its variance is reduced.

  Examples: Bagging methods, Forests of randomized trees, …

- By contrast, in **boosting methods**, base estimators are built sequentially and one tries to reduce the bias of the combined estimator. The motivation is to combine several weak models to produce a powerful ensemble.

  Examples: AdaBoost, Gradient Tree Boosting, …

1.11.1. Bagging meta-estimator

In ensemble algorithms, bagging methods form a class of algorithms which build several instances of a black-box estimator on random subsets of the original training set and then aggregate their individual predictions to form a final prediction. These methods are used as a way to reduce the variance of a base estimator (e.g., a decision tree), by introducing randomization into its construction procedure and then making an ensemble out of it. In many cases, bagging methods constitute a very simple way to improve with respect to a single model, without making it necessary to adapt the underlying base algorithm. As they provide a way to reduce overfitting, bagging methods work best with strong and complex models (e.g., fully developed decision trees), in contrast with boosting methods which usually work best with weak models (e.g., shallow decision trees).

Bagging methods come in many flavours but mostly differ from each other by the way they draw random subsets of the training set:

- When random subsets of the dataset are drawn as random subsets of the samples, then this algorithm is known as Pasting [B1999].
- When samples are drawn with replacement, then the method is known as Bagging [B1996].
- When random subsets of the dataset are drawn as random subsets of the features, then the method is known as Random Subspaces [H1998].
- Finally, when base estimators are built on subsets of both samples and features, then the method is known as Random Patches [LG2012].

In scikit-learn, bagging methods are offered as a unified **`BaggingClassifier`** meta-estimator (resp. **`BaggingRegressor`**), taking as input a user-specified base estimator along with parameters specifying the strategy to draw random subsets. In particular, `max_samples` and `max_features` control the size of the subsets (in terms of samples and features), while `bootstrap` and `bootstrap_features` control whether samples and features are drawn with or without replacement. When using a subset of the available samples the generalization accuracy can be estimated with the out-of-bag samples by setting `oob_score=True`. As an example, the snippet below illustrates how to instantiate a bagging ensemble of `KNeighborsClassifier` base estimators, each built on random subsets of 50% of the samples and 50% of the features.

```
>>> from sklearn.ensemble import BaggingClassifier
>>> from sklearn.neighbors import KNeighborsClassifier
>>> bagging = BaggingClassifier(KNeighborsClassifier(),
...                             max_samples=0.5, max_features=0.5)
```

Examples:

- Single estimator versus bagging: bias-variance decomposition

References

[B1999] L. Breiman, “Pasting small votes for classification in large databases and on-line”, Machine Learning, 36(1), 85-103, 1999.

[B1996] L. Breiman, “Bagging predictors”, Machine Learning, 24(2), 123-140, 1996.

[H1998] T. Ho, “The random subspace method for constructing decision forests”, Pattern Analysis and Machine Intelligence, 20(8), 832-844, 1998.

[LG2012] G. Louppe and P. Geurts, “Ensembles on Random Patches”, Machine Learning and Knowledge Discovery in Databases, 346-361, 2012.

1.11.2. Forests of randomized trees

The `sklearn.ensemble` module includes two averaging algorithms based on randomized decision trees: the RandomForest algorithm and the Extra-Trees method. Both algorithms are perturb-and-combine techniques [B1998] specifically designed for trees. This means a diverse set of classifiers is created by introducing randomness in the classifier construction. The prediction of the ensemble is given as the averaged prediction of the individual classifiers.

As other classifiers, forest classifiers have to be fitted with two arrays: a sparse or dense array X of size `[n_samples, n_features]` holding the training samples, and an array Y of size `[n_samples]` holding the target values (class labels) for the training samples:

```
>>> from sklearn.ensemble import RandomForestClassifier
>>> X = [[0, 0], [1, 1]]
>>> Y = [0, 1]
>>> clf = RandomForestClassifier(n_estimators=10)
>>> clf = clf.fit(X, Y)
```

Like decision trees, forests of trees also extend to multi-output problems (if Y is an array of size `[n_samples, n_outputs]`).

1.11.2.1. Random Forests

In random forests (see `RandomForestClassifier` and `RandomForestRegressor` classes), each tree in the ensemble is built from a sample drawn with replacement (i.e., a bootstrap sample) from the training set.

Furthermore, when splitting each node during the construction of a tree, the best split is found either from all input features or a random subset of size `max_features`. (See the parameter tuning guidelines for more details).

The purpose of these two sources of randomness is to decrease the variance of the forest estimator. Indeed, individual decision trees typically exhibit high variance and tend to overfit. The injected randomness in forests yield decision trees with somewhat decoupled prediction errors. By taking an average of those predictions, some errors can cancel out. Random forests achieve a reduced variance by combining diverse trees, sometimes at the cost of a slight increase in bias. In practice the variance reduction is often significant hence yielding an overall better model.

In contrast to the original publication [B2001], the scikit-learn implementation combines classifiers by averaging their probabilistic prediction, instead of letting each classifier vote for a single class.

1.11.2.2. Extremely Randomized Trees

In extremely randomized trees (see `ExtraTreesClassifier` and `ExtraTreesRegressor` classes), randomness goes one step further in the way splits are computed. As in random forests, a random subset of candidate features is used, but instead of looking for the most discriminative thresholds, thresholds are drawn at random for each candidate feature and the best of these randomly-generated thresholds is picked as the splitting rule. This usually allows to reduce the variance of the model a bit more, at the expense of a slightly greater increase in bias:

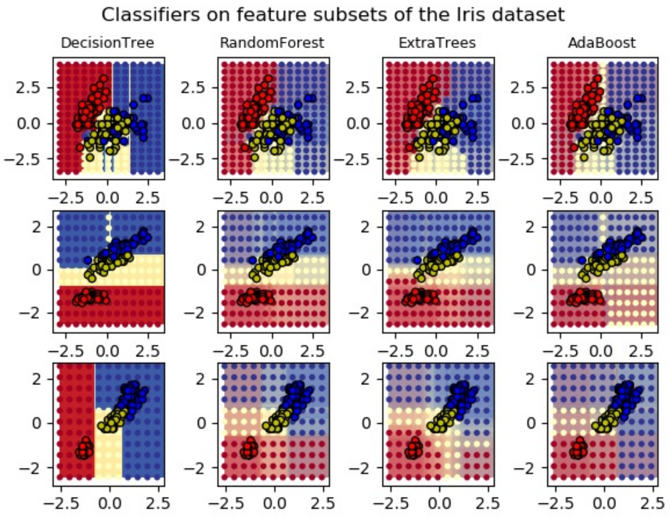
```
>>> from sklearn.model_selection import cross_val_score
>>> from sklearn.datasets import make_blobs
>>> from sklearn.ensemble import RandomForestClassifier
>>> from sklearn.ensemble import ExtraTreesClassifier
>>> from sklearn.tree import DecisionTreeClassifier

>>> X, y = make_blobs(n_samples=10000, n_features=10, centers=100,
...     random_state=0)

>>> clf = DecisionTreeClassifier(max_depth=None, min_samples_split=2,
...     random_state=0)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores.mean()
0.98...

>>> clf = RandomForestClassifier(n_estimators=10, max_depth=None,
...     min_samples_split=2, random_state=0)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores.mean()
0.999...

>>> clf = ExtraTreesClassifier(n_estimators=10, max_depth=None,
...     min_samples_split=2, random_state=0)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores.mean() > 0.999
True
```



1.11.2.3. Parameters

The main parameters to adjust when using these methods is `n_estimators` and `max_features`. The former is the number of trees in the forest. The larger the better, but also the longer it will take to compute. In addition, note that results will stop getting significantly better beyond a critical number of trees. The latter is the size of the random subsets of features to consider when splitting a node. The lower the greater the reduction of variance, but also the greater the increase in bias. Empirical good default values are `max_features=None` (always considering all features instead of a random subset) for regression problems, and `max_features="sqrt"` (using a random subset of size `sqrt(n_features)`) for classification tasks (where `n_features` is the number of features in the data). Good results are often achieved when setting `max_depth=None` in combination with `min_samples_split=2` (i.e., when fully developing the trees). Bear in mind though that these values are usually not optimal, and might result in models that consume a lot of RAM. The best parameter values should always be cross-validated. In addition, note that in random forests, bootstrap samples are used by default (`bootstrap=True`) while the default strategy for extra-trees is to use the whole dataset (`bootstrap=False`). When using bootstrap sampling the generalization accuracy can be estimated on the left out or out-of-bag samples. This can be enabled by setting `oob_score=True`.

Note: The size of the model with the default parameters is $O(M * N * log(N))$, where M is the number of trees and N is the number of samples. In order to reduce the size of the model, you can change these parameters: `min_samples_split`, `max_leaf_nodes`, `max_depth` and `min_samples_leaf`.

1.11.2.4. Parallelization

Finally, this module also features the parallel construction of the trees and the parallel computation of the predictions through the `n_jobs` parameter. If `n_jobs=k` then computations are partitioned into `k` jobs, and run on `k` cores of the machine. If `n_jobs=-1` then all cores available on the machine are used. Note that because of inter-process communication overhead, the speedup might not be linear (i.e., using `k` jobs will unfortunately not be `k` times as fast). Significant speedup can still be achieved though when building a large number of trees, or when building a single tree requires a fair amount of time (e.g., on large datasets).

Examples:

- Plot the decision surfaces of ensembles of trees on the iris dataset
- Pixel importances with a parallel forest of trees
- Face completion with a multi-output estimators

References

[B2001] Breiman, "Random Forests", Machine Learning, 45(1), 5-32, 2001.

[B1998] Breiman, "Arcing Classifiers", Annals of Statistics 1998.

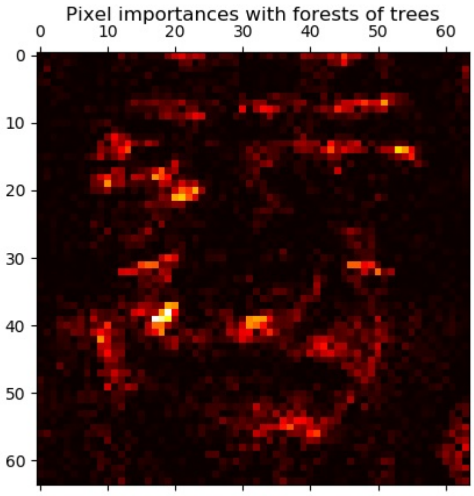
- P. Geurts, D. Ernst., and L. Wehenkel, "Extremely randomized trees", Machine Learning, 63(1), 3-42, 2006.

1.11.2.5. Feature importance evaluation

The relative rank (i.e. depth) of a feature used as a decision node in a tree can be used to assess the relative importance of that feature with respect to the predictability of the target variable. Features used at the top of the tree contribute to the final prediction decision of a larger fraction of the input samples. The **expected fraction of the samples** they contribute to can thus be used as an estimate of the **relative importance of the features**. In scikit-learn, the fraction of samples a feature contributes to is combined with the decrease in impurity from splitting them to create a normalized estimate of the predictive power of that feature.

By **averaging** the estimates of predictive ability over several randomized trees one can **reduce the variance** of such an estimate and use it for feature selection. This is known as the mean decrease in impurity, or MDI. Refer to [L2014] for more information on MDI and feature importance evaluation with Random Forests.

The following example shows a color-coded representation of the relative importances of each individual pixel for a face recognition task using a `ExtraTreesClassifier` model.



In practice those estimates are stored as an attribute named `feature_importances_` on the fitted model. This is an array with shape `(n_features,)` whose values are positive and sum to 1.0. The higher the value, the more important is the contribution of the matching feature to the prediction function.

Examples:

- Pixel importances with a parallel forest of trees
- Feature importances with forests of trees

References

[L2014] G. Louppe, "Understanding Random Forests: From Theory to Practice", PhD Thesis, U. of Liege, 2014.

1.11.2.6. Totally Random Trees Embedding

`RandomTreesEmbedding` implements an unsupervised transformation of the data. Using a forest of completely random trees, `RandomTreesEmbedding` encodes the data by the indices of the leaves a data point ends up in. This index is then encoded in a one-of-K manner, leading to a high dimensional, sparse binary coding. This coding can be computed very efficiently and can then be used as a basis for other learning tasks. The size and sparsity of the code can be influenced by choosing the number of trees and the maximum depth per tree. For each tree in the ensemble, the coding contains one entry of one. The size of the coding is at most `n_estimators * 2 ** max_depth`, the maximum number of leaves in the forest.

As neighboring data points are more likely to lie within the same leaf of a tree, the transformation performs an implicit, non-parametric density estimation.

Examples:

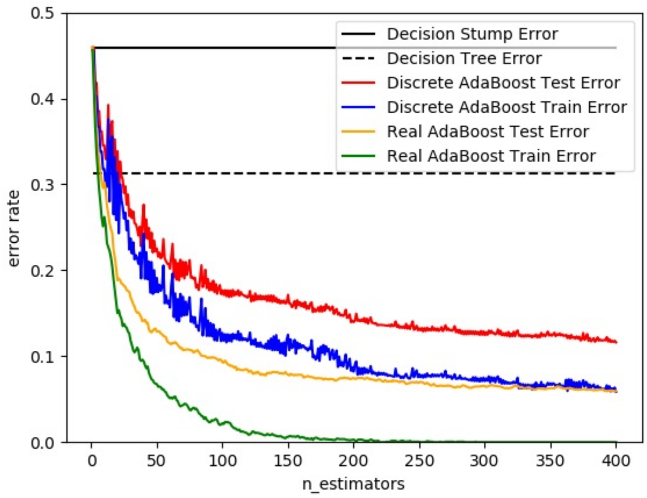
- Hashing feature transformation using Totally Random Trees
- Manifold learning on handwritten digits: Locally Linear Embedding, Isomap… compares non-linear dimensionality reduction techniques on handwritten digits.
- Feature transformations with ensembles of trees compares supervised and unsupervised tree based feature transformations.

See also: Manifold learning techniques can also be useful to derive non-linear representations of feature space, also these approaches focus also on dimensionality reduction.

1.11.3. AdaBoost

The module `sklearn.ensemble` includes the popular boosting algorithm AdaBoost, introduced in 1995 by Freund and Schapire [FS1995].

The core principle of AdaBoost is to fit a sequence of weak learners (i.e., models that are only slightly better than random guessing, such as small decision trees) on repeatedly modified versions of the data. The predictions from all of them are then combined through a weighted majority vote (or sum) to produce the final prediction. The data modifications at each so-called boosting iteration consist of applying weights w_1, w_2, …, w_N to each of the training samples. Initially, those weights are all set to $w_i = 1/N$, so that the first step simply trains a weak learner on the original data. For each successive iteration, the sample weights are individually modified and the learning algorithm is reapplied to the reweighted data. At a given step, those training examples that were incorrectly predicted by the boosted model induced at the previous step have their weights increased, whereas the weights are decreased for those that were predicted correctly. As iterations proceed, examples that are difficult to predict receive ever-increasing influence. Each subsequent weak learner is thereby forced to concentrate on the examples that are missed by the previous ones in the sequence [HTF].



AdaBoost can be used both for classification and regression problems:

- For multi-class classification, `AdaBoostClassifier` implements AdaBoost-SAMME and AdaBoost-SAMME.R [ZZRH2009].
- For regression, `AdaBoostRegressor` implements AdaBoost.R2 [D1997].

1.11.3.1. Usage

The following example shows how to fit an AdaBoost classifier with 100 weak learners:

```
>>> from sklearn.model_selection import cross_val_score
>>> from sklearn.datasets import load_iris
>>> from sklearn.ensemble import AdaBoostClassifier

>>> X, y = load_iris(return_X_y=True)
>>> clf = AdaBoostClassifier(n_estimators=100)
>>> scores = cross_val_score(clf, X, y, cv=5)
>>> scores.mean()
0.9...
```

The number of weak learners is controlled by the parameter `n_estimators`. The `learning_rate` parameter controls the contribution of the weak learners in the final combination. By default, weak learners are decision stumps. Different weak learners can be specified through the `base_estimator` parameter. The main parameters to tune to obtain good results are `n_estimators` and the complexity of the base estimators (e.g., its depth `max_depth` or minimum required number of samples to consider a split `min_samples_split`).

Examples:

- Discrete versus Real AdaBoost compares the classification error of a decision stump, decision tree, and a boosted decision stump using AdaBoost-SAMME and AdaBoost-SAMME.R.
- Multi-class AdaBoosted Decision Trees shows the performance of AdaBoost-SAMME and AdaBoost-SAMME.R on a multi-class problem.
- Two-class AdaBoost shows the decision boundary and decision function values for a non-linearly separable two-class problem using AdaBoost-SAMME.
- Decision Tree Regression with AdaBoost demonstrates regression with the AdaBoost.R2 algorithm.

References

[FS1995] Y. Freund, and R. Schapire, “A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting”, 1997.

[ZZRH2009] J. Zhu, H. Zou, S. Rosset, T. Hastie. “Multi-class AdaBoost”, 2009.

[D1997] Drucker. “Improving Regressors using Boosting Techniques”, 1997.

HTF(1,2,3) T. Hastie, R. Tibshirani and J. Friedman, “Elements of Statistical Learning Ed. 2”, Springer, 2009.

1.11.4. Gradient Tree Boosting

Gradient Tree Boosting or Gradient Boosted Decision Trees (GBDT) is a generalization of boosting to arbitrary differentiable loss functions. GBDT is an accurate and effective off-the-shelf procedure that can be used for both regression and classification problems in a variety of areas including Web search ranking and ecology.

The module **`sklearn.ensemble`** provides methods for both classification and regression via gradient boosted decision trees.

Note: Scikit-learn 0.21 introduces two new experimental implementations of gradient boosting trees, namely **`HistGradientBoostingClassifier`** and **`HistGradientBoostingRegressor`**, inspired by LightGBM (See [LightGBM]).
These histogram-based estimators can be **orders of magnitude faster** than **`GradientBoostingClassifier`** and **`GradientBoostingRegressor`** when the number of samples is larger than tens of thousands of samples.
They also have built-in support for missing values, which avoids the need for an imputer.
These estimators are described in more detail below in Histogram-Based Gradient Boosting.
The following guide focuses on **`GradientBoostingClassifier`** and **`GradientBoostingRegressor`**, which might be preferred for small sample sizes since binning may lead to split points that are too approximate in this setting.

1.11.4.1. Classification

`GradientBoostingClassifier` supports both binary and multi-class classification. The following example shows how to fit a gradient boosting classifier with 100 decision stumps as weak learners:

```
>>> from sklearn.datasets import make_hastie_10_2
>>> from sklearn.ensemble import GradientBoostingClassifier

>>> X, y = make_hastie_10_2(random_state=0)
>>> X_train, X_test = X[:2000], X[2000:]
>>> y_train, y_test = y[:2000], y[2000:]

>>> clf = GradientBoostingClassifier(n_estimators=100, learning_rate=1.0,
...     max_depth=1, random_state=0).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.913...
```

The number of weak learners (i.e. regression trees) is controlled by the parameter `n_estimators`; The size of each tree can be controlled either by setting the tree depth via `max_depth` or by setting the number of leaf nodes via `max_leaf_nodes`. The `learning_rate` is a hyper-parameter in the range (0.0, 1.0] that controls overfitting via shrinkage .

Note: Classification with more than 2 classes requires the induction of `n_classes` regression trees at each iteration, thus, the total number of induced trees equals `n_classes * n_estimators`. For datasets with a large number of classes we strongly recommend to use **`HistGradientBoostingClassifier`** as an alternative to **`GradientBoostingClassifier`** .

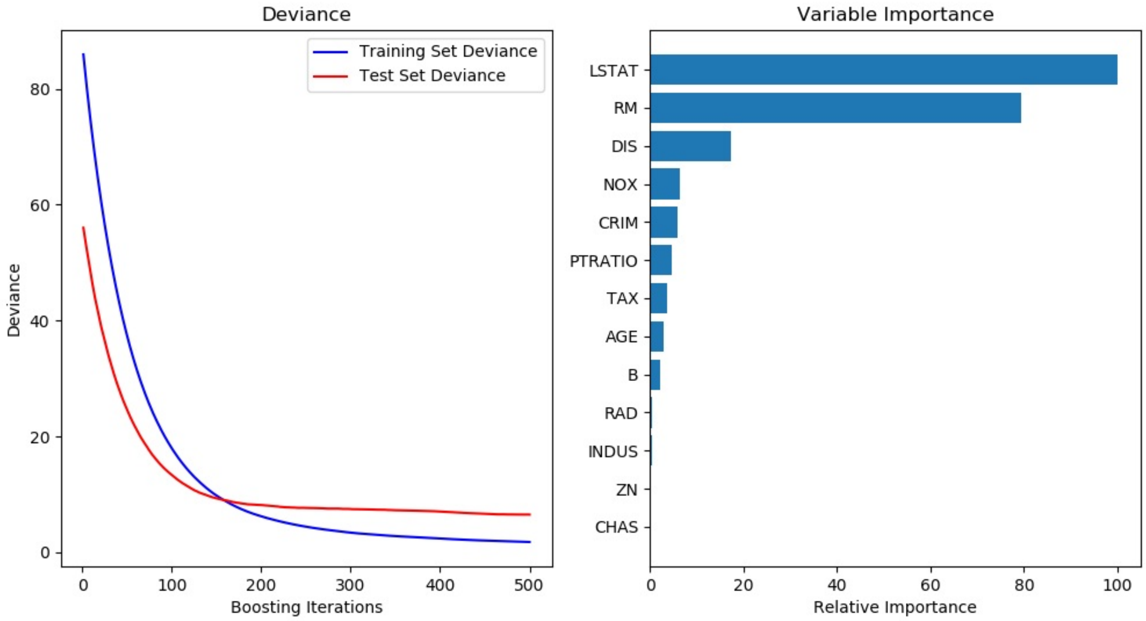
1.11.4.2. Regression

`GradientBoostingRegressor` supports a number of different loss functions for regression which can be specified via the argument `loss`; the default loss function for regression is least squares (`'ls'`).

```
>>> import numpy as np
>>> from sklearn.metrics import mean_squared_error
>>> from sklearn.datasets import make_friedman1
>>> from sklearn.ensemble import GradientBoostingRegressor

>>> X, y = make_friedman1(n_samples=1200, random_state=0, noise=1.0)
>>> X_train, X_test = X[:200], X[200:]
>>> y_train, y_test = y[:200], y[200:]
>>> est = GradientBoostingRegressor(n_estimators=100, learning_rate=0.1,
...     max_depth=1, random_state=0, loss='ls').fit(X_train, y_train)
>>> mean_squared_error(y_test, est.predict(X_test))
5.00...
```

The figure below shows the results of applying **`GradientBoostingRegressor`** with least squares loss and 500 base learners to the Boston house price dataset (**`sklearn.datasets.load_boston`**). The plot on the left shows the train and test error at each iteration. The train error at each iteration is stored in the `train_score_` attribute of the gradient boosting model. The test error at each iterations can be obtained via the **`staged_predict`** method which returns a generator that yields the predictions at each stage. Plots like these can be used to determine the optimal number of trees (i.e. `n_estimators`) by early stopping. The plot on the right shows the feature importances which can be obtained via the `feature_importances_` property.



Examples:

- Gradient Boosting regression
- Gradient Boosting Out-of-Bag estimates

1.11.4.3. Fitting additional weak-learners

Both **`GradientBoostingRegressor`** and **`GradientBoostingClassifier`** support `warm_start=True` which allows you to add more estimators to an already fitted model.

```
>>> _ = est.set_params(n_estimators=200, warm_start=True)  # set warm_start and new nr of trees
>>> _ = est.fit(X_train, y_train) # fit additional 100 trees to est
>>> mean_squared_error(y_test, est.predict(X_test))
3.84...
```

1.11.4.4. Controlling the tree size

The size of the regression tree base learners defines the level of variable interactions that can be captured by the gradient boosting model. In general, a tree of depth `h` can capture interactions of order `h` . There are two ways in which the size of the individual regression trees can be controlled.

If you specify `max_depth=h` then complete binary trees of depth `h` will be grown. Such trees will have (at most) `2**h` leaf nodes and `2**h - 1` split nodes.

Alternatively, you can control the tree size by specifying the number of leaf nodes via the parameter `max_leaf_nodes`. In this case, trees will be grown using best-first search where nodes with the highest improvement in impurity will be expanded first. A tree with `max_leaf_nodes=k` has `k - 1` split nodes and thus can model interactions of up to order `max_leaf_nodes - 1` .

We found that `max_leaf_nodes=k` gives comparable results to `max_depth=k-1` but is significantly faster to train at the expense of a slightly higher training error. The parameter `max_leaf_nodes` corresponds to the variable `J` in the chapter on gradient boosting in [F2001] and is related to the parameter `interaction.depth` in R's gbm package where `max_leaf_nodes == interaction.depth + 1` .

1.11.4.5. Mathematical formulation

GBRT considers additive models of the following form:

$$F(x) = \sum_{m=1}^{M} \gamma_m h_m(x)$$

where $h_m(x)$ are the basis functions which are usually called *weak learners* in the context of boosting. Gradient Tree Boosting uses decision trees of fixed size as weak learners. Decision trees have a number of abilities that make them valuable for boosting, namely the ability to handle data of mixed type and the ability to model complex functions.

Similar to other boosting algorithms, GBRT builds the additive model in a greedy fashion:

$$F_m(x) = F_{m-1}(x) + \gamma_m h_m(x),$$

where the newly added tree h_m tries to minimize the loss L, given the previous ensemble F_{m-1}:

$$h_m = \arg\min_{h} \sum_{i=1}^{n} L(y_i, F_{m-1}(x_i) + h(x_i)).$$

The initial model F_0 is problem specific, for least-squares regression one usually chooses the mean of the target values.

Note: The initial model can also be specified via the `init` argument. The passed object has to implement `fit` and `predict`.

Gradient Boosting attempts to solve this minimization problem numerically via steepest descent: The steepest descent direction is the negative gradient of the loss function evaluated at the current model F_{m-1} which can be calculated for any differentiable loss function:

$$F_m(x) = F_{m-1}(x) - \gamma_m \sum_{i=1}^{n} \nabla_F L(y_i, F_{m-1}(x_i))$$

Where the step length γ_m is chosen using line search:

$$\gamma_m = \arg\min_{\gamma} \sum_{i=1}^{n} L(y_i, F_{m-1}(x_i) - \gamma \frac{\partial L(y_i, F_{m-1}(x_i))}{\partial F_{m-1}(x_i)})$$

The algorithms for regression and classification only differ in the concrete loss function used.

1.11.4.5.1. Loss Functions

The following loss functions are supported and can be specified using the parameter `loss`:

- Regression
  - Least squares (`'ls'`): The natural choice for regression due to its superior computational properties. The initial model is given by the mean of the target values.
  - Least absolute deviation (`'lad'`): A robust loss function for regression. The initial model is given by the median of the target values.
  - Huber (`'huber'`): Another robust loss function that combines least squares and least absolute deviation; use `alpha` to control the sensitivity with regards to outliers (see [F2001] for more details).
  - Quantile (`'quantile'`): A loss function for quantile regression. Use `0 < alpha < 1` to specify the quantile. This loss function can be used to create prediction intervals (see Prediction Intervals for Gradient Boosting Regression).
- Classification
  - Binomial deviance (`'deviance'`): The negative binomial log-likelihood loss function for binary classification (provides probability estimates). The initial model is given by the log odds-ratio.
  - Multinomial deviance (`'deviance'`): The negative multinomial log-likelihood loss function for multi-class classification with `n_classes` mutually exclusive classes. It provides probability estimates. The initial model is given by the prior probability of each class. At each iteration `n_classes` regression trees have to be constructed which makes GBRT rather inefficient for data sets with a large number of classes.
  - Exponential loss (`'exponential'`): The same loss function as **`AdaBoostClassifier`**. Less robust to mislabeled examples than `'deviance'`; can only be used for binary classification.

1.11.4.6. Regularization

1.11.4.6.1. Shrinkage

[F2001] proposed a simple regularization strategy that scales the contribution of each weak learner by a factor ν:

$$F_m(x) = F_{m-1}(x) + \nu \gamma_m h_m(x)$$

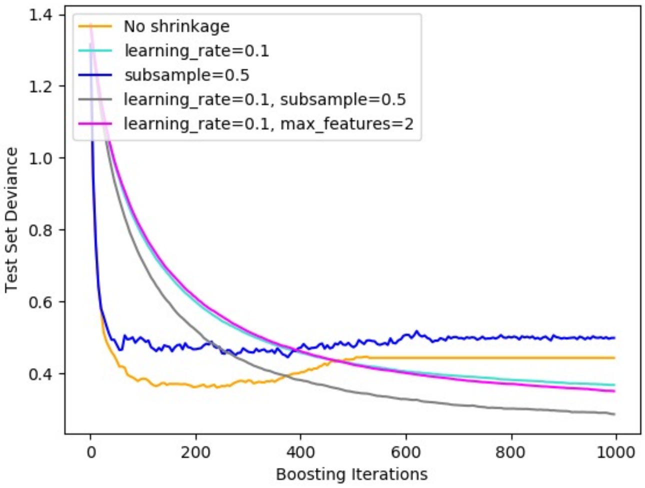
The parameter ν is also called the **learning rate** because it scales the step length the gradient descent procedure; it can be set via the `learning_rate` parameter.

The parameter `learning_rate` strongly interacts with the parameter `n_estimators`, the number of weak learners to fit. Smaller values of `learning_rate` require larger numbers of weak learners to maintain a constant training error. Empirical evidence suggests that small values of `learning_rate` favor better test error. [HTF] recommend to set the learning rate to a small constant (e.g. `learning_rate <= 0.1`) and choose `n_estimators` by early stopping. For a more detailed discussion of the interaction between `learning_rate` and `n_estimators` see [R2007].

1.11.4.6.2. Subsampling

[F1999] proposed stochastic gradient boosting, which combines gradient boosting with bootstrap averaging (bagging). At each iteration the base classifier is trained on a fraction `subsample` of the available training data. The subsample is drawn without replacement. A typical value of `subsample` is 0.5.

The figure below illustrates the effect of shrinkage and subsampling on the goodness-of-fit of the model. We can clearly see that shrinkage outperforms no-shrinkage. Subsampling with shrinkage can further increase the accuracy of the model. Subsampling without shrinkage, on the other hand, does poorly.



Another strategy to reduce the variance is by subsampling the features analogous to the random splits in `RandomForestClassifier` . The number of subsampled features can be controlled via the `max_features` parameter.

Note: Using a small `max_features` value can significantly decrease the runtime.

Stochastic gradient boosting allows to compute out-of-bag estimates of the test deviance by computing the improvement in deviance on the examples that are not included in the bootstrap sample (i.e. the out-of-bag examples). The improvements are stored in the attribute `oob_improvement_`. `oob_improvement_[i]` holds the improvement in terms of the loss on the OOB samples if you add the i-th stage to the current predictions. Out-of-bag estimates can be used for model selection, for example to determine the optimal number of iterations. OOB estimates are usually very pessimistic thus we recommend to use cross-validation instead and only use OOB if cross-validation is too time consuming.

Examples:

- Gradient Boosting regularization
- Gradient Boosting Out-of-Bag estimates
- OOB Errors for Random Forests

1.11.4.7. Interpretation

Individual decision trees can be interpreted easily by simply visualizing the tree structure. Gradient boosting models, however, comprise hundreds of regression trees thus they cannot be easily interpreted by visual inspection of the individual trees. Fortunately, a number of techniques have been proposed to summarize and interpret gradient boosting models.

1.11.4.7.1. Feature importance

Often features do not contribute equally to predict the target response; in many situations the majority of the features are in fact irrelevant. When interpreting a model, the first question usually is: what are those important features and how do they contributing in predicting the target response?

Individual decision trees intrinsically perform feature selection by selecting appropriate split points. This information can be used to measure the importance of each feature; the basic idea is: the more often a feature is used in the split points of a tree the more important that feature is. This notion of importance can be extended to decision tree ensembles by simply averaging the feature importance of each tree (see Feature importance evaluation for more details).

The feature importance scores of a fit gradient boosting model can be accessed via the `feature_importances_` property:

```
>>> from sklearn.datasets import make_hastie_10_2
>>> from sklearn.ensemble import GradientBoostingClassifier

>>> X, y = make_hastie_10_2(random_state=0)
>>> clf = GradientBoostingClassifier(n_estimators=100, learning_rate=1.0,
...     max_depth=1, random_state=0).fit(X, y)
>>> clf.feature_importances_
array([0.10..., 0.10..., 0.11..., ...
```

Examples:

- Gradient Boosting regression

1.11.5. Histogram-Based Gradient Boosting

Scikit-learn 0.21 introduces two new experimental implementations of gradient boosting trees, namely `HistGradientBoostingClassifier` and `HistGradientBoostingRegressor`, inspired by LightGBM (See [LightGBM]).

These histogram-based estimators can be **orders of magnitude faster** than `GradientBoostingClassifier` and `GradientBoostingRegressor` when the number of samples is larger than tens of thousands of samples.

They also have built-in support for missing values, which avoids the need for an imputer.

These fast estimators first bin the input samples `X` into integer-valued bins (typically 256 bins) which tremendously reduces the number of splitting points to consider, and allows the algorithm to leverage integer-based data structures (histograms) instead of relying on sorted continuous values when building the trees. The API of these estimators is slightly different, and some of the features from `GradientBoostingClassifier` and `GradientBoostingRegressor` are not yet supported: in particular sample weights, and some loss functions.

These estimators are still **experimental**: their predictions and their API might change without any deprecation cycle. To use them, you need to explicitly import `enable_hist_gradient_boosting`:

```
>>> # explicitly require this experimental feature
>>> from sklearn.experimental import enable_hist_gradient_boosting  # noqa
>>> # now you can import normally from ensemble
>>> from sklearn.ensemble import HistGradientBoostingClassifier
```

Examples:

- Partial Dependence Plots

1.11.5.1. Usage

Most of the parameters are unchanged from `GradientBoostingClassifier` and `GradientBoostingRegressor`. One exception is the `max_iter` parameter that replaces `n_estimators`, and controls the number of iterations of the boosting process:

```
>>> from sklearn.experimental import enable_hist_gradient_boosting
>>> from sklearn.ensemble import HistGradientBoostingClassifier
>>> from sklearn.datasets import make_hastie_10_2

>>> X, y = make_hastie_10_2(random_state=0)
>>> X_train, X_test = X[:2000], X[2000:]
>>> y_train, y_test = y[:2000], y[2000:]

>>> clf = HistGradientBoostingClassifier(max_iter=100).fit(X_train, y_train)
>>> clf.score(X_test, y_test)
0.8965
```

Available losses for regression are 'least_squares' and 'least_absolute_deviation', which is less sensitive to outliers. For classification, 'binary_crossentropy' is used for binary classification and 'categorical_crossentropy' is used for multiclass classification. By default the loss is 'auto' and will select the appropriate loss depending on y passed to fit.

The size of the trees can be controlled through the `max_leaf_nodes`, `max_depth`, and `min_samples_leaf` parameters.

The number of bins used to bin the data is controlled with the `max_bins` parameter. Using less bins acts as a form of regularization. It is generally recommended to use as many bins as possible, which is the default.

The `l2_regularization` parameter is a regularizer on the loss function and corresponds to λ in equation (2) of [XGBoost].

The early-stopping behaviour is controlled via the `scoring`, `validation_fraction`, `n_iter_no_change`, and `tol` parameters. It is possible to early-stop using an arbitrary scorer, or just the training or validation loss. By default, early-stopping is performed using the default scorer of the estimator on a validation set but it is also possible to perform early-stopping based on the loss value, which is significantly faster.

1.11.5.2. Missing values support

`HistGradientBoostingClassifier` and `HistGradientBoostingRegressor` have built-in support for missing values (NaNs).

During training, the tree grower learns at each split point whether samples with missing values should go to the left or right child, based on the potential gain. When predicting, samples with missing values are assigned to the left or right child consequently:

```
>>> from sklearn.experimental import enable_hist_gradient_boosting  # noqa
>>> from sklearn.ensemble import HistGradientBoostingClassifier
>>> import numpy as np

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

>>> gbdt = HistGradientBoostingClassifier(min_samples_leaf=1).fit(X, y)
>>> gbdt.predict(X)
array([0, 0, 1, 1])
```

When the missingness pattern is predictive, the splits can be done on whether the feature value is missing or not:

```
>>> X = np.array([0, np.nan, 1, 2, np.nan]).reshape(-1, 1)
>>> y = [0, 1, 0, 0, 1]
>>> gbdt = HistGradientBoostingClassifier(min_samples_leaf=1,
...                                       max_depth=2,
...                                       learning_rate=1,
...                                       max_iter=1).fit(X, y)
>>> gbdt.predict(X)
array([0, 1, 0, 0, 1])
```

If no missing values were encountered for a given feature during training, then samples with missing values are mapped to whichever child has the most samples.

1.11.5.3. Low-level parallelism

`HistGradientBoostingClassifier` and `HistGradientBoostingRegressor` have implementations that use OpenMP for parallelization through Cython. For more details on how to control the number of threads, please refer to our Parallelism notes.

The following parts are parallelized:

- mapping samples from real values to integer-valued bins (finding the bin thresholds is however sequential)
- building histograms is parallelized over features
- finding the best split point at a node is parallelized over features
- during fit, mapping samples into the left and right children is parallelized over samples
- gradient and hessians computations are parallelized over samples
- predicting is parallelized over samples

1.11.5.4. Why it's faster

The bottleneck of a gradient boosting procedure is building the decision trees. Building a traditional decision tree (as in the other GBDTs `GradientBoostingClassifier` and `GradientBoostingRegressor`) requires sorting the samples at each node (for each feature). Sorting is needed so that the potential gain of a split point can be computed efficiently. Splitting a single node has thus a complexity of $\mathcal{O}(n_\text{features} \times n \log(n))$ where n is the number of samples at the node.

`HistGradientBoostingClassifier` and `HistGradientBoostingRegressor`, in contrast, do not require sorting the feature values and instead use a data-structure called a histogram, where the samples are implicitly ordered. Building a histogram has a $\mathcal{O}(n)$ complexity, so the node splitting procedure has a $\mathcal{O}(n_\text{features} \times n)$ complexity, much smaller than the previous one. In addition, instead of considering n split points, we here consider only `max_bins` split points, which is much smaller.

In order to build histograms, the input data `X` needs to be binned into integer-valued bins. This binning procedure does require sorting the feature values, but it only happens once at the very beginning of the boosting process (not at each node, like in `GradientBoostingClassifier` and `GradientBoostingRegressor`).

Finally, many parts of the implementation of `HistGradientBoostingClassifier` and `HistGradientBoostingRegressor` are parallelized.

References

[F1999] Friedmann, Jerome H., 2007, "Stochastic Gradient Boosting"

[R2007] G. Ridgeway, "Generalized Boosted Models: A guide to the gbm package", 2007

[XGBoost] Tianqi Chen, Carlos Guestrin, "XGBoost: A Scalable Tree Boosting System"

LightGBM(1,2) Ke et. al. "LightGBM: A Highly Efficient Gradient BoostingDecision Tree"

1.11.6. Voting Classifier

The idea behind the `VotingClassifier` is to combine conceptually different machine learning classifiers and use a majority vote or the average predicted probabilities (soft vote) to predict the class labels. Such a classifier can be useful for a set of equally well performing model in order to balance out their individual weaknesses.

1.11.6.1. Majority Class Labels (Majority/Hard Voting)

In majority voting, the predicted class label for a particular sample is the class label that represents the majority (mode) of the class labels predicted by each individual classifier.

E.g., if the prediction for a given sample is

- classifier 1 -> class 1
- classifier 2 -> class 1
- classifier 3 -> class 2

the VotingClassifier (with `voting='hard'`) would classify the sample as “class 1” based on the majority class label.

In the cases of a tie, the `VotingClassifier` will select the class based on the ascending sort order. E.g., in the following scenario

- classifier 1 -> class 2
- classifier 2 -> class 1

the class label 1 will be assigned to the sample.

1.11.6.1.1. Usage

The following example shows how to fit the majority rule classifier:

```
>>> from sklearn import datasets
>>> from sklearn.model_selection import cross_val_score
>>> from sklearn.linear_model import LogisticRegression
>>> from sklearn.naive_bayes import GaussianNB
>>> from sklearn.ensemble import RandomForestClassifier
>>> from sklearn.ensemble import VotingClassifier

>>> iris = datasets.load_iris()
>>> X, y = iris.data[:, 1:3], iris.target

>>> clf1 = LogisticRegression(random_state=1)
>>> clf2 = RandomForestClassifier(n_estimators=50, random_state=1)
>>> clf3 = GaussianNB()

>>> eclf = VotingClassifier(
...     estimators=[('lr', clf1), ('rf', clf2), ('gnb', clf3)],
...     voting='hard')

>>> for clf, label in zip([clf1, clf2, clf3, eclf], ['Logistic Regression', 'Random Forest', 'naive Bayes',
'Ensemble']):
...     scores = cross_val_score(clf, X, y, scoring='accuracy', cv=5)
...     print("Accuracy: %0.2f (+/- %0.2f) [%s]" % (scores.mean(), scores.std(), label))
Accuracy: 0.95 (+/- 0.04) [Logistic Regression]
Accuracy: 0.94 (+/- 0.04) [Random Forest]
Accuracy: 0.91 (+/- 0.04) [naive Bayes]
Accuracy: 0.95 (+/- 0.04) [Ensemble]
```

1.11.6.2. Weighted Average Probabilities (Soft Voting)

In contrast to majority voting (hard voting), soft voting returns the class label as argmax of the sum of predicted probabilities.

Specific weights can be assigned to each classifier via the `weights` parameter. When weights are provided, the predicted class probabilities for each classifier are collected, multiplied by the classifier weight, and averaged. The final class label is then derived from the class label with the highest average probability.

To illustrate this with a simple example, let’s assume we have 3 classifiers and a 3-class classification problems where we assign equal weights to all classifiers: w1=1, w2=1, w3=1.

The weighted average probabilities for a sample would then be calculated as follows:

classifier	class 1	class 2	class 3
classifier 1	w1 * 0.2	w1 * 0.5	w1 * 0.3
classifier 2	w2 * 0.6	w2 * 0.3	w2 * 0.1
classifier 3	w3 * 0.3	w3 * 0.4	w3 * 0.3
weighted average	0.37	0.4	0.23

Here, the predicted class label is 2, since it has the highest average probability.

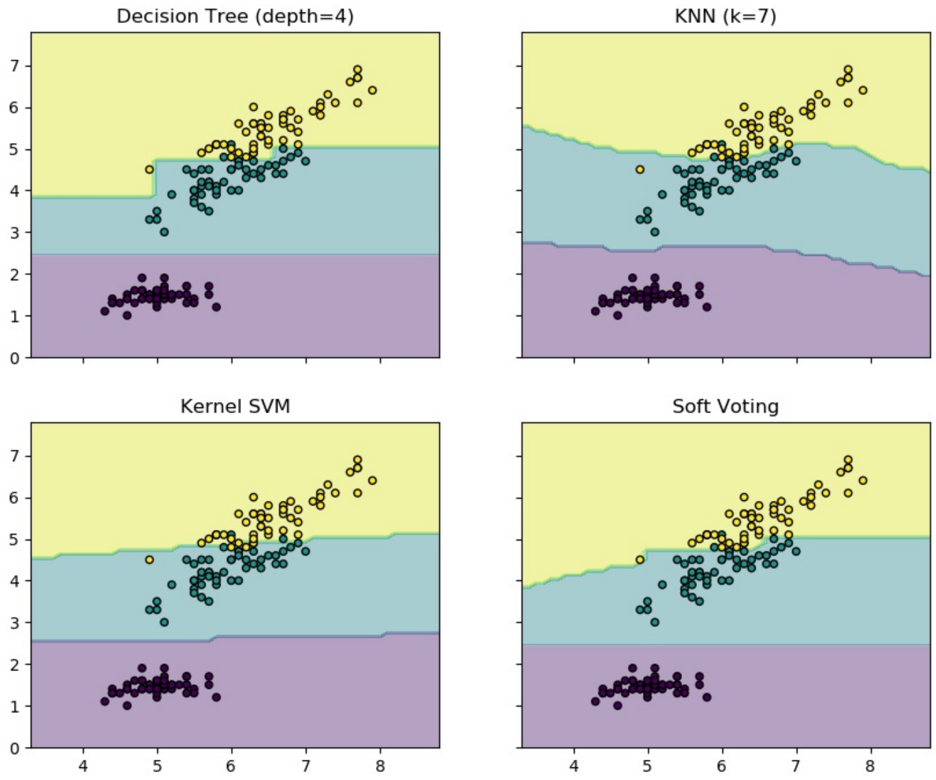
The following example illustrates how the decision regions may change when a soft `VotingClassifier` is used based on an linear Support Vector Machine, a Decision Tree, and a K-nearest neighbor classifier:

```
>>> from sklearn import datasets
>>> from sklearn.tree import DecisionTreeClassifier
>>> from sklearn.neighbors import KNeighborsClassifier
>>> from sklearn.svm import SVC
>>> from itertools import product
>>> from sklearn.ensemble import VotingClassifier

>>> # Loading some example data
>>> iris = datasets.load_iris()
>>> X = iris.data[:, [0, 2]]
>>> y = iris.target

>>> # Training classifiers
>>> clf1 = DecisionTreeClassifier(max_depth=4)
>>> clf2 = KNeighborsClassifier(n_neighbors=7)
>>> clf3 = SVC(kernel='rbf', probability=True)
>>> eclf = VotingClassifier(estimators=[('dt', clf1), ('knn', clf2), ('svc', clf3)],
...                         voting='soft', weights=[2, 1, 2])

>>> clf1 = clf1.fit(X, y)
>>> clf2 = clf2.fit(X, y)
>>> clf3 = clf3.fit(X, y)
>>> eclf = eclf.fit(X, y)
```


Decision Tree (depth=4)

KNN (k=7)

Kernel SVM

Soft Voting

1.11.6.3. Using the `VotingClassifier` with `GridSearchCV`

The `VotingClassifier` can also be used together with `GridSearchCV` in order to tune the hyperparameters of the individual estimators:

```
>>> from sklearn.model_selection import GridSearchCV
>>> clf1 = LogisticRegression(random_state=1)
>>> clf2 = RandomForestClassifier(random_state=1)
>>> clf3 = GaussianNB()
>>> eclf = VotingClassifier(
...     estimators=[('lr', clf1), ('rf', clf2), ('gnb', clf3)],
...     voting='soft'
... )

>>> params = {'lr__C': [1.0, 100.0], 'rf__n_estimators': [20, 200]}

>>> grid = GridSearchCV(estimator=eclf, param_grid=params, cv=5)
>>> grid = grid.fit(iris.data, iris.target)
```

1.11.6.3.1. Usage

In order to predict the class labels based on the predicted class-probabilities (scikit-learn estimators in the VotingClassifier must support `predict_proba` method):

```
>>> eclf = VotingClassifier(
...     estimators=[('lr', clf1), ('rf', clf2), ('gnb', clf3)],
...     voting='soft'
... )
```

Optionally, weights can be provided for the individual classifiers:

```
>>> eclf = VotingClassifier(
...     estimators=[('lr', clf1), ('rf', clf2), ('gnb', clf3)],
...     voting='soft', weights=[2,5,1]
... )
```

1.11.7. Voting Regressor

The idea behind the `VotingRegressor` is to combine conceptually different machine learning regressors and return the average predicted values. Such a regressor can be useful for a set of equally well performing models in order to balance out their individual weaknesses.

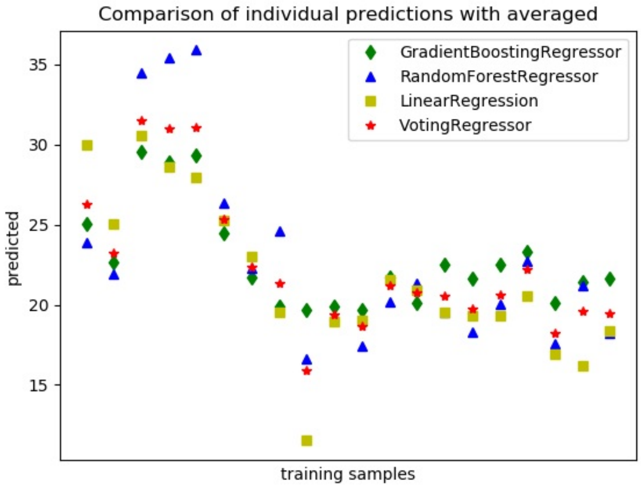
1.11.7.1. Usage

The following example shows how to fit the VotingRegressor:

```
>>> from sklearn.datasets import load_boston
>>> from sklearn.ensemble import GradientBoostingRegressor
>>> from sklearn.ensemble import RandomForestRegressor
>>> from sklearn.linear_model import LinearRegression
>>> from sklearn.ensemble import VotingRegressor

>>> # Loading some example data
>>> X, y = load_boston(return_X_y=True)

>>> # Training classifiers
>>> reg1 = GradientBoostingRegressor(random_state=1, n_estimators=10)
>>> reg2 = RandomForestRegressor(random_state=1, n_estimators=10)
>>> reg3 = LinearRegression()
>>> ereg = VotingRegressor(estimators=[('gb', reg1), ('rf', reg2), ('lr', reg3)])
>>> ereg = ereg.fit(X, y)
```



Examples:

- Plot individual and voting regression predictions

1.11.8. Stacked generalization

Stacked generalization is a method for combining estimators to reduce their biases [W1992] [HTF]. More precisely, the predictions of each individual estimator are stacked together and used as input to a final estimator to compute the prediction. This final estimator is trained through cross-validation.

The `StackingClassifier` and `StackingRegressor` provide such strategies which can be applied to classification and regression problems.

The `estimators` parameter corresponds to the list of the estimators which are stacked together in parallel on the input data. It should be given as a list of names and estimators:

```
>>> from sklearn.linear_model import RidgeCV, LassoCV
>>> from sklearn.svm import SVR
>>> estimators = [('ridge', RidgeCV()),
...               ('lasso', LassoCV(random_state=42)),
...               ('svr', SVR(C=1, gamma=1e-6))]
```

The `final_estimator` will use the predictions of the `estimators` as input. It needs to be a classifier or a regressor when using `StackingClassifier` or `StackingRegressor`, respectively:

```
>>> from sklearn.ensemble import GradientBoostingRegressor
>>> from sklearn.ensemble import StackingRegressor
>>> reg = StackingRegressor(
...     estimators=estimators,
...     final_estimator=GradientBoostingRegressor(random_state=42))
```

To train the `estimators` and `final_estimator`, the `fit` method needs to be called on the training data:

```
>>> from sklearn.datasets import load_boston
>>> X, y = load_boston(return_X_y=True)
>>> from sklearn.model_selection import train_test_split
>>> X_train, X_test, y_train, y_test = train_test_split(X, y,
...                                                     random_state=42)
>>> reg.fit(X_train, y_train)
StackingRegressor(...)
```

During training, the `estimators` are fitted on the whole training data `X_train`. They will be used when calling `predict` or `predict_proba`. To generalize and avoid over-fitting, the `final_estimator` is trained on out-samples using `sklearn.model_selection.cross_val_predict` internally.

For `StackingClassifier`, note that the output of the `estimators` is controlled by the parameter `stack_method` and it is called by each estimator. This parameter is either a string, being estimator method names, or `'auto'` which will automatically identify an available method depending on the availability, tested in the order of preference: `predict_proba`, `decision_function` and `predict`.

A `StackingRegressor` and `StackingClassifier` can be used as any other regressor or classifier, exposing a `predict`, `predict_proba`, and `decision_function` methods, e.g.:

```
>>> y_pred = reg.predict(X_test)
>>> from sklearn.metrics import r2_score
>>> print('R2 score: {:.2f}'.format(r2_score(y_test, y_pred)))
R2 score: 0.81
```

Note that it is also possible to get the output of the stacked outputs of the `estimators` using the `transform` method:

```
>>> reg.transform(X_test[:5])
array([[28.78..., 28.43...  , 22.62...],
       [35.96..., 32.58..., 23.68...],
       [14.97..., 14.05..., 16.45...],
       [25.19..., 25.54..., 22.92...],
       [18.93..., 19.26..., 17.03... ]])
```

In practise, a stacking predictor predict as good as the best predictor of the base layer and even sometimes outputperform it by combining the different strength of the these predictors. However, training a stacking predictor is computationally expensive.

Note: For `StackingClassifier`, when using `stack_method_='predict_proba'`, the first column is dropped when the problem is a binary classification problem. Indeed, both probability columns predicted by each estimator are perfectly collinear.

Note: Multiple stacking layers can be achieved by assigning `final_estimator` to a `StackingClassifier` or `StackingRegressor`:

```
>>> final_layer = StackingRegressor(
...     estimators=[('rf', RandomForestRegressor(random_state=42)),
...                 ('gbrt', GradientBoostingRegressor(random_state=42))],
...     final_estimator=RidgeCV()
...     )
>>> multi_layer_regressor = StackingRegressor(
...     estimators=[('ridge', RidgeCV()),
...                 ('lasso', LassoCV(random_state=42)),
...                 ('svr', SVR(C=1, gamma=1e-6, kernel='rbf'))],
...     final_estimator=final_layer
... )
>>> multi_layer_regressor.fit(X_train, y_train)
StackingRegressor(...)
>>> print('R2 score: {:.2f}'
...       .format(multi_layer_regressor.score(X_test, y_test)))
R2 score: 0.82
```

References

[W1992] Wolpert, David H. “Stacked generalization.” Neural networks 5.2 (1992): 241-259.

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