1.6. Nearest Neighbors

sklearn.neighbors provides functionality for unsupervised and supervised neighbors-based learning methods. Unsupervised nearest neighbors is the foundation of many other learning methods, notably manifold learning and spectral clustering. Supervised neighbors-based learning comes in two flavors: classification for data with discrete labels, and regression for data with continuous labels.

The principle behind nearest neighbor methods is to find a predefined number of training samples closest in distance to the new point, and predict the label from these. The number of samples can be a user-defined constant (k-nearest neighbor learning), or vary based on the local density of points (radius-based neighbor learning). The distance can, in general, be any metric measure: standard Euclidean distance is the most common choice. Neighbors-based methods are known as *non-generalizing* machine learning methods, since they simply "remember" all of its training data (possibly transformed into a fast indexing structure such as a Ball Tree or KD Tree).

Despite its simplicity, nearest neighbors has been successful in a large number of classification and regression problems, including handwritten digits and satellite image scenes. Being a non-parametric method, it is often successful in classification situations where the decision boundary is very irregular.

The classes in **sklearn.neighbors** can handle either NumPy arrays or `scipy.sparse` matrices as input. For dense matrices, a large number of possible distance metrics are supported. For sparse matrices, arbitrary Minkowski metrics are supported for searches.

There are many learning routines which rely on nearest neighbors at their core. One example is kernel density estimation, discussed in the density estimation section.

1.6.1. Unsupervised Nearest Neighbors

NearestNeighbors implements unsupervised nearest neighbors learning. It acts as a uniform interface to three different nearest neighbors algorithms: **BallTree**, **KDTree**, and a brute-force algorithm based on routines in **sklearn.metrics.pairwise**. The choice of neighbors search algorithm is controlled through the keyword `'algorithm'`, which must be one of `['auto', 'ball_tree', 'kd_tree', 'brute']`. When the default value `'auto'` is passed, the algorithm attempts to determine the best approach from the training data. For a discussion of the strengths and weaknesses of each option, see Nearest Neighbor Algorithms.

> **Warning:** Regarding the Nearest Neighbors algorithms, if two neighbors $k+1$ and k have identical distances but different labels, the result will depend on the ordering of the training data.

1.6.1.1. Finding the Nearest Neighbors

For the simple task of finding the nearest neighbors between two sets of data, the unsupervised algorithms within **sklearn.neighbors** can be used:

```
>>> from sklearn.neighbors import NearestNeighbors
>>> import numpy as np
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> nbrs = NearestNeighbors(n_neighbors=2, algorithm='ball_tree').fit(X)
>>> distances, indices = nbrs.kneighbors(X)
>>> indices
array([[0, 1],
       [1, 0],
       [2, 1],
       [3, 4],
       [4, 3],
       [5, 4]]...)
>>> distances
array([[0.        , 1.        ],
       [0.        , 1.        ],
       [0.        , 1.41421356],
       [0.        , 1.        ],
       [0.        , 1.        ],
       [0.        , 1.41421356]])
```

Because the query set matches the training set, the nearest neighbor of each point is the point itself, at a distance of zero.

It is also possible to efficiently produce a sparse graph showing the connections between neighboring points:

```
>>> nbrs.kneighbors_graph(X).toarray()
array([[1., 1., 0., 0., 0., 0.],
       [1., 1., 0., 0., 0., 0.],
       [0., 1., 1., 0., 0., 0.],
       [0., 0., 0., 1., 1., 0.],
       [0., 0., 0., 1., 1., 0.],
       [0., 0., 0., 0., 1., 1.]])
```

The dataset is structured such that points nearby in index order are nearby in parameter space, leading to an approximately block-diagonal matrix of K-nearest neighbors. Such a sparse graph is useful in a variety of circumstances which make use of spatial relationships between points for unsupervised learning: in particular, see `sklearn.manifold.Isomap`, `sklearn.manifold.LocallyLinearEmbedding`, and `sklearn.cluster.SpectralClustering`.

1.6.1.2. KDTree and BallTree Classes

Alternatively, one can use the `KDTree` or `BallTree` classes directly to find nearest neighbors. This is the functionality wrapped by the `NearestNeighbors` class used above. The Ball Tree and KD Tree have the same interface; we'll show an example of using the KD Tree here:

```
>>> from sklearn.neighbors import KDTree
>>> import numpy as np
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> kdt = KDTree(X, leaf_size=30, metric='euclidean')
>>> kdt.query(X, k=2, return_distance=False)
array([[0, 1],
       [1, 0],
       [2, 1],
       [3, 4],
       [4, 3],
       [5, 4]]...)
```

Refer to the `KDTree` and `BallTree` class documentation for more information on the options available for nearest neighbors searches, including specification of query strategies, distance metrics, etc. For a list of available metrics, see the documentation of the `DistanceMetric` class.

1.6.2. Nearest Neighbors Classification

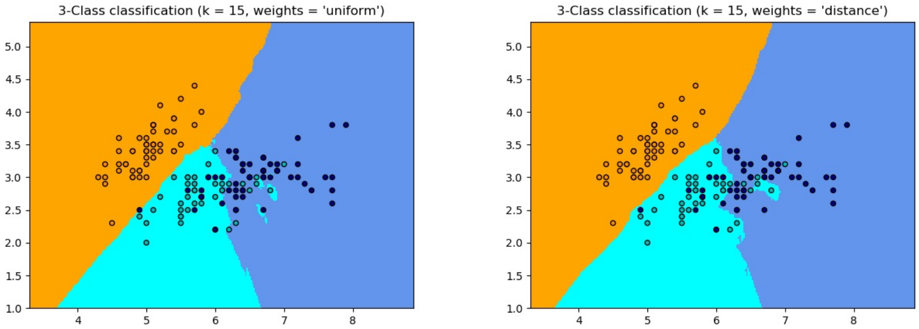
Neighbors-based classification is a type of *instance-based learning* or *non-generalizing learning*: it does not attempt to construct a general internal model, but simply stores instances of the training data. Classification is computed from a simple majority vote of the nearest neighbors of each point: a query point is assigned the data class which has the most representatives within the nearest neighbors of the point.

scikit-learn implements two different nearest neighbors classifiers: `KNeighborsClassifier` implements learning based on the k nearest neighbors of each query point, where k is an integer value specified by the user. `RadiusNeighborsClassifier` implements learning based on the number of neighbors within a fixed radius r of each training point, where r is a floating-point value specified by the user.

The k-neighbors classification in `KNeighborsClassifier` is the most commonly used technique. The optimal choice of the value k is highly data-dependent: in general a larger k suppresses the effects of noise, but makes the classification boundaries less distinct.

In cases where the data is not uniformly sampled, radius-based neighbors classification in `RadiusNeighborsClassifier` can be a better choice. The user specifies a fixed radius r, such that points in sparser neighborhoods use fewer nearest neighbors for the classification. For high-dimensional parameter spaces, this method becomes less effective due to the so-called "curse of dimensionality".

The basic nearest neighbors classification uses uniform weights: that is, the value assigned to a query point is computed from a simple majority vote of the nearest neighbors. Under some circumstances, it is better to weight the neighbors such that nearer neighbors contribute more to the fit. This can be accomplished through the `weights` keyword. The default value, `weights = 'uniform'`, assigns uniform weights to each neighbor. `weights = 'distance'` assigns weights proportional to the inverse of the distance from the query point. Alternatively, a user-defined function of the distance can be supplied to compute the weights.



Examples:

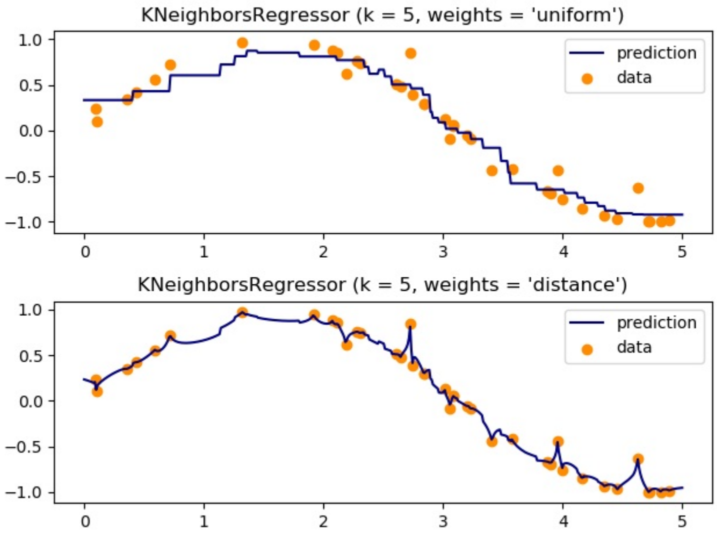
- Nearest Neighbors Classification: an example of classification using nearest neighbors.

1.6.3. Nearest Neighbors Regression

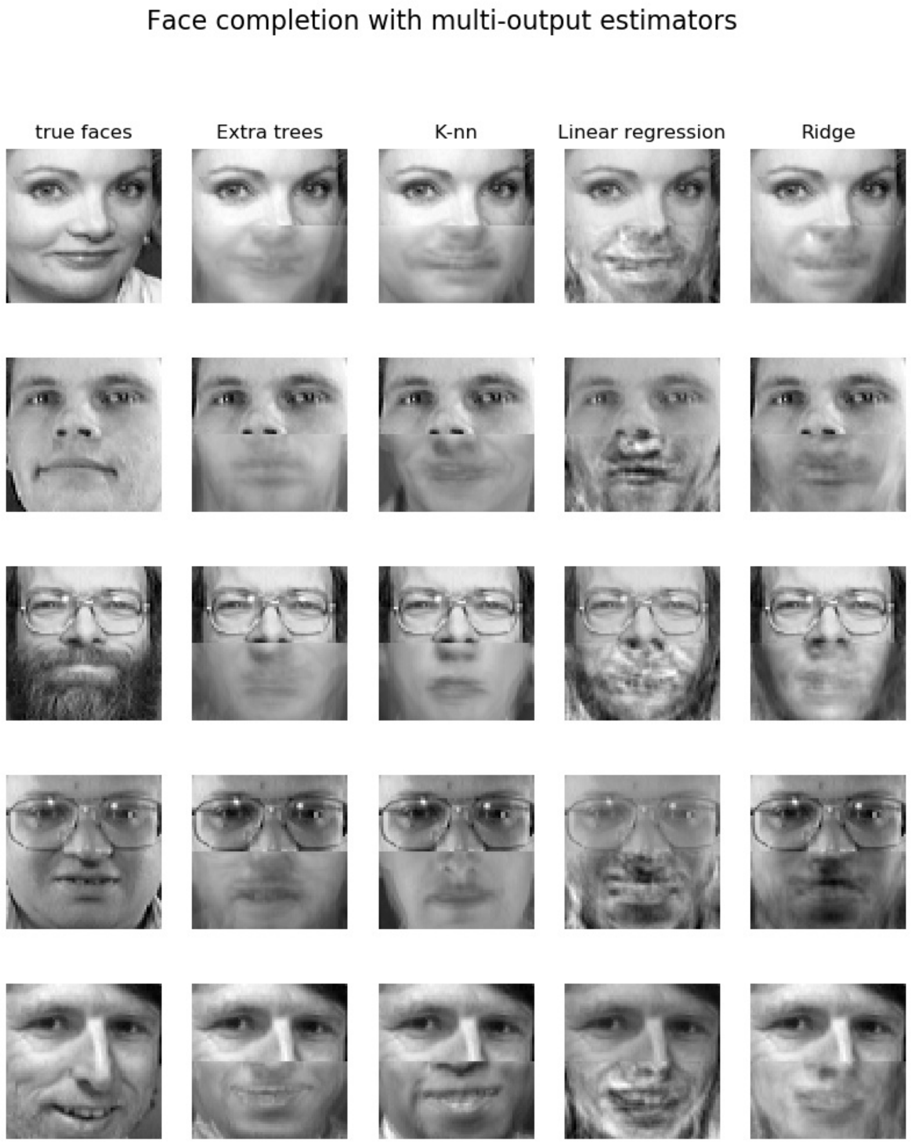
Neighbors-based regression can be used in cases where the data labels are continuous rather than discrete variables. The label assigned to a query point is computed based on the mean of the labels of its nearest neighbors.

scikit-learn implements two different neighbors regressors: **`KNeighborsRegressor`** implements learning based on the k nearest neighbors of each query point, where k is an integer value specified by the user. **`RadiusNeighborsRegressor`** implements learning based on the neighbors within a fixed radius r of the query point, where r is a floating-point value specified by the user.

The basic nearest neighbors regression uses uniform weights: that is, each point in the local neighborhood contributes uniformly to the classification of a query point. Under some circumstances, it can be advantageous to weight points such that nearby points contribute more to the regression than faraway points. This can be accomplished through the `weights` keyword. The default value, `weights = 'uniform'`, assigns equal weights to all points. `weights = 'distance'` assigns weights proportional to the inverse of the distance from the query point. Alternatively, a user-defined function of the distance can be supplied, which will be used to compute the weights.



The use of multi-output nearest neighbors for regression 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:

- Nearest Neighbors regression: an example of regression using nearest neighbors.
- Face completion with a multi-output estimators: an example of multi-output regression using nearest neighbors.

1.6.4. Nearest Neighbor Algorithms

1.6.4.1. Brute Force

Fast computation of nearest neighbors is an active area of research in machine learning. The most naive neighbor search implementation involves the brute-force computation of distances between all pairs of points in the dataset: for N samples in D dimensions, this approach scales as $O[DN^2]$. Efficient brute-force neighbors searches can be very competitive for small data samples. However, as the number of samples N grows, the brute-force approach quickly becomes infeasible. In the classes within `sklearn.neighbors`, brute-force neighbors searches are specified using the keyword `algorithm = 'brute'`, and are computed using the routines available in `sklearn.metrics.pairwise`.

1.6.4.2. K-D Tree

To address the computational inefficiencies of the brute-force approach, a variety of tree-based data structures have been invented. In general, these structures attempt to reduce the required number of distance calculations by efficiently encoding aggregate distance information for the sample. The basic idea is that if point A is very distant from point B, and point B is very close to point C, then we know that points A and C are very distant, *without having to explicitly calculate their distance*. In this way, the computational cost of a nearest neighbors search can be reduced to $O[DN\log(N)]$ or better. This is a significant improvement over brute-force for large N.

An early approach to taking advantage of this aggregate information was the *KD tree* data structure (short for *K-dimensional tree*), which generalizes two-dimensional *Quad-trees* and 3-dimensional *Oct-trees* to an arbitrary number of dimensions. The KD tree is a binary tree structure which recursively partitions the parameter space along the data axes, dividing it into nested orthotropic regions into which data points are filed. The construction of a KD tree is very fast: because partitioning is performed only along the data axes, no D-dimensional distances need to be computed. Once constructed, the nearest neighbor of a query point can be determined with only $O[\log(N)]$ distance computations. Though the KD tree approach is very fast for low-dimensional ($D < 20$) neighbors searches, it becomes inefficient as D grows very large: this is one manifestation of the so-called "curse of dimensionality". In scikit-learn, KD tree neighbors searches are specified using the keyword `algorithm = 'kd_tree'`, and are computed using the class `KDTree`.

References:

- "Multidimensional binary search trees used for associative searching", Bentley, J.L., Communications of the ACM (1975)

1.6.4.3. Ball Tree

To address the inefficiencies of KD Trees in higher dimensions, the *ball tree* data structure was developed. Where KD trees partition data along Cartesian axes, ball trees partition data in a series of nesting hyper-spheres. This makes tree construction more costly than that of the KD tree, but results in a data structure which can be very efficient on highly structured data, even in very high dimensions.

A ball tree recursively divides the data into nodes defined by a centroid C and radius r, such that each point in the node lies within the hyper-sphere defined by r and C. The number of candidate points for a neighbor search is reduced through use of the *triangle inequality*:

$$|x + y| \leq |x| + |y|$$

With this setup, a single distance calculation between a test point and the centroid is sufficient to determine a lower and upper bound on the distance to all points within the node. Because of the spherical geometry of the ball tree nodes, it can out-perform a *KD-tree* in high dimensions, though the actual performance is highly dependent on the structure of the training data. In scikit-learn, ball-tree-based neighbors searches are specified using the keyword `algorithm = 'ball_tree'`, and are computed using the class `sklearn.neighbors.BallTree`. Alternatively, the user can work with the `BallTree` class directly.

References:

- "Five balltree construction algorithms", Omohundro, S.M., International Computer Science Institute Technical Report (1989)

1.6.4.4. Choice of Nearest Neighbors Algorithm

The optimal algorithm for a given dataset is a complicated choice, and depends on a number of factors:

- number of samples N (i.e. `n_samples`) and dimensionality D (i.e. `n_features`).

  - *Brute force* query time grows as $O[DN]$
  - *Ball tree* query time grows as approximately $O[D\log(N)]$
  - *KD tree* query time changes with D in a way that is difficult to precisely characterise. For small D (less than 20 or so) the cost is approximately $O[D\log(N)]$, and the KD tree query can be very efficient. For larger D, the cost increases to nearly $O[DN]$, and the overhead due to the tree structure can lead to queries which are slower than brute force.

  For small data sets (N less than 30 or so), $\log(N)$ is comparable to N, and brute force algorithms can be more efficient than a tree-based approach. Both `KDTree` and `BallTree` address this through providing a *leaf size* parameter: this controls the number of samples at which a query switches to brute-force. This allows both algorithms to approach the efficiency of a brute-force computation for small N.

- data structure: *intrinsic dimensionality* of the data and/or *sparsity* of the data. Intrinsic dimensionality refers to the dimension $d \leq D$ of a manifold on which the data lies, which can be linearly or non-linearly embedded in the parameter space. Sparsity refers to the degree to which the data fills the parameter space (this is to be distinguished from the concept as used in "sparse" matrices. The data matrix may have no zero entries, but the **structure** can still be "sparse" in this sense).

  - *Brute force* query time is unchanged by data structure.
  - *Ball tree* and *KD tree* query times can be greatly influenced by data structure. In general, sparser data with a smaller intrinsic dimensionality leads to faster query times. Because the KD tree internal representation is aligned with the parameter axes, it will not generally show as much improvement as ball tree for arbitrarily structured data.

  Datasets used in machine learning tend to be very structured, and are very well-suited for tree-based queries.

- number of neighbors k requested for a query point.

  - *Brute force* query time is largely unaffected by the value of k
  - *Ball tree* and *KD tree* query time will become slower as k increases. This is due to two effects: first, a larger k leads to the necessity to search a larger portion of the parameter space. Second, using $k > 1$ requires internal queueing of results as the tree is traversed.

  As k becomes large compared to N, the ability to prune branches in a tree-based query is reduced. In this situation, Brute force queries can be more efficient.

- number of query points. Both the ball tree and the KD Tree require a construction phase. The cost of this construction becomes negligible when amortized over many queries. If only a small number of queries will be performed, however, the construction can make up a significant fraction of the total cost. If very few query points will be required, brute force is better than a tree-based method.

Currently, `algorithm = 'auto'` selects `'brute'` if $k >= N/2$, the input data is sparse, or `effective_metric_` isn't in the `VALID_METRICS` list for either `'kd_tree'` or `'ball_tree'`. Otherwise, it selects the first out of `'kd_tree'` and `'ball_tree'` that has `effective_metric_` in its `VALID_METRICS` list. This choice is based on the assumption that the number of query points is at least the same order as the number of training points, and that `leaf_size` is close to its default value of `30`.

1.6.4.5. Effect of `leaf_size`

As noted above, for small sample sizes a brute force search can be more efficient than a tree-based query. This fact is accounted for in the ball tree and KD tree by internally switching to brute force searches within leaf nodes. The level of this switch can be specified with the parameter `leaf_size`. This parameter choice has many effects:

construction time

A larger `leaf_size` leads to a faster tree construction time, because fewer nodes need to be created

query time

Both a large or small `leaf_size` can lead to suboptimal query cost. For `leaf_size` approaching 1, the overhead involved in traversing nodes can significantly slow query times. For `leaf_size` approaching the size of the training set, queries become essentially brute force. A good compromise between these is `leaf_size = 30`, the default value of the parameter.

memory

As `leaf_size` increases, the memory required to store a tree structure decreases. This is especially important in the case of ball tree, which stores a D-dimensional centroid for each node. The required storage space for `BallTree` is approximately `1 / leaf_size` times the size of the training set.

`leaf_size` is not referenced for brute force queries.

1.6.5. Nearest Centroid Classifier

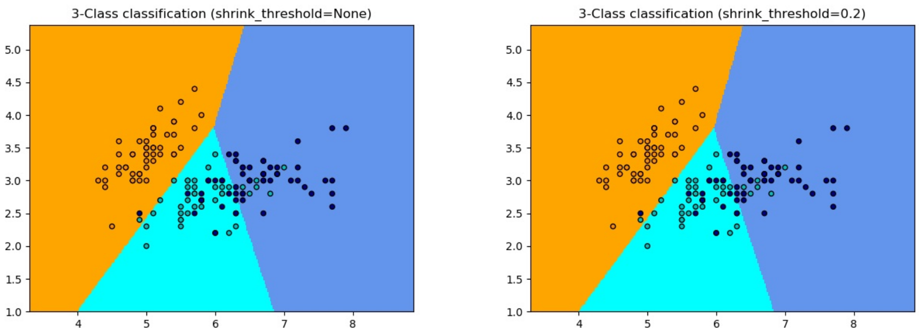
The `NearestCentroid` classifier is a simple algorithm that represents each class by the centroid of its members. In effect, this makes it similar to the label updating phase of the `sklearn.cluster.KMeans` algorithm. It also has no parameters to choose, making it a good baseline classifier. It does, however, suffer on non-convex classes, as well as when classes have drastically different variances, as equal variance in all dimensions is assumed. See Linear Discriminant Analysis (`sklearn.discriminant_analysis.LinearDiscriminantAnalysis`) and Quadratic Discriminant Analysis (`sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis`) for more complex methods that do not make this assumption. Usage of the default `NearestCentroid` is simple:

```
>>> from sklearn.neighbors import NearestCentroid
>>> import numpy as np
>>> X = np.array([[-1, -1], [-2, -1], [-3, -2], [1, 1], [2, 1], [3, 2]])
>>> y = np.array([1, 1, 1, 2, 2, 2])
>>> clf = NearestCentroid()
>>> clf.fit(X, y)
NearestCentroid()
>>> print(clf.predict([[-0.8, -1]]))
[1]
```

1.6.5.1. Nearest Shrunken Centroid

The `NearestCentroid` classifier has a `shrink_threshold` parameter, which implements the nearest shrunken centroid classifier. In effect, the value of each feature for each centroid is divided by the within-class variance of that feature. The feature values are then reduced by `shrink_threshold`. Most notably, if a particular feature value crosses zero, it is set to zero. In effect, this removes the feature from affecting the classification. This is useful, for example, for removing noisy features.

In the example below, using a small shrink threshold increases the accuracy of the model from 0.81 to 0.82.



Examples:

- Nearest Centroid Classification: an example of classification using nearest centroid with different shrink thresholds.

1.6.6. Nearest Neighbors Transformer

Many scikit-learn estimators rely on nearest neighbors: Several classifiers and regressors such as `KNeighborsClassifier` and `KNeighborsRegressor`, but also some clustering methods such as `DBSCAN` and `SpectralClustering`, and some manifold embeddings such as `TSNE` and `Isomap`.

All these estimators can compute internally the nearest neighbors, but most of them also accept precomputed nearest neighbors sparse graph, as given by `kneighbors_graph` and `radius_neighbors_graph`. With mode `mode='connectivity'`, these functions return a binary adjacency sparse graph as required, for instance, in `SpectralClustering`. Whereas with `mode='distance'`, they return a distance sparse graph as required, for instance, in `DBSCAN`. To include these functions in a scikit-learn pipeline, one can also use the corresponding classes `KNeighborsTransformer` and `RadiusNeighborsTransformer`. The benefits of this sparse graph API are multiple.

First, the precomputed graph can be re-used multiple times, for instance while varying a parameter of the estimator. This can be done manually by the user, or using the caching properties of the scikit-learn pipeline:

```
>>> from sklearn.manifold import Isomap
>>> from sklearn.neighbors import KNeighborsTransformer
>>> from sklearn.pipeline import make_pipeline
>>> estimator = make_pipeline(
...     KNeighborsTransformer(n_neighbors=5, mode='distance'),
...     Isomap(neighbors_algorithm='precomputed'),
...     memory='/path/to/cache')
```

Second, precomputing the graph can give finer control on the nearest neighbors estimation, for instance enabling multiprocessing though the parameter `n_jobs`, which might not be available in all estimators.

Finally, the precomputation can be performed by custom estimators to use different implementations, such as approximate nearest neighbors methods, or implementation with special data types. The precomputed neighbors sparse graph needs to be formatted as in `radius_neighbors_graph` output:

- a CSR matrix (although COO, CSC or LIL will be accepted).
- only explicitly store nearest neighborhoods of each sample with respect to the training data. This should include those at 0 distance from a query point, including the matrix diagonal when computing the nearest neighborhoods between the training data and itself.
- each row's `data` should store the distance in increasing order (optional. Unsorted data will be stable-sorted, adding a computational overhead).
- all values in data should be non-negative.
- there should be no duplicate `indices` in any row (see https://github.com/scipy/scipy/issues/5807).
- if the algorithm being passed the precomputed matrix uses k nearest neighbors (as opposed to radius neighborhood), at least k neighbors must be stored in each row (or k+1, as explained in the following note).

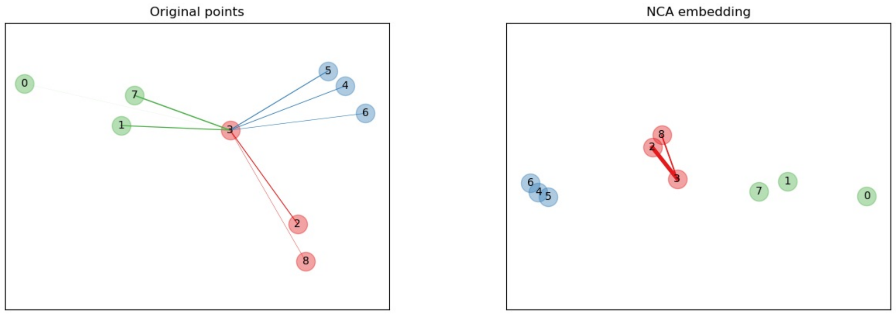
Note: When a specific number of neighbors is queried (using `KNeighborsTransformer`), the definition of `n_neighbors` is ambiguous since it can either include each training point as its own neighbor, or exclude them. Neither choice is perfect, since including them leads to a different number of non-self neighbors during training and testing, while excluding them leads to a difference between `fit(X).transform(X)` and `fit_transform(X)`, which is against scikit-learn API. In `KNeighborsTransformer` we use the definition which includes each training point as its own neighbor in the count of `n_neighbors`. However, for compatibility reasons with other estimators which use the other definition, one extra neighbor will be computed when `mode == 'distance'`. To maximise compatibility with all estimators, a safe choice is to always include one extra neighbor in a custom nearest neighbors estimator, since unnecessary neighbors will be filtered by following estimators.

Examples:

- Approximate nearest neighbors in TSNE: an example of pipelining **`KNeighborsTransformer`** and **`TSNE`**. Also proposes two custom nearest neighbors estimators based on external packages.
- Caching nearest neighbors: an example of pipelining **`KNeighborsTransformer`** and **`KNeighborsClassifier`** to enable caching of the neighbors graph during a hyper-parameter grid-search.

1.6.7. Neighborhood Components Analysis

Neighborhood Components Analysis (NCA, **`NeighborhoodComponentsAnalysis`**) is a distance metric learning algorithm which aims to improve the accuracy of nearest neighbors classification compared to the standard Euclidean distance. The algorithm directly maximizes a stochastic variant of the leave-one-out k-nearest neighbors (KNN) score on the training set. It can also learn a low-dimensional linear projection of data that can be used for data visualization and fast classification.


Original points

NCA embedding

In the above illustrating figure, we consider some points from a randomly generated dataset. We focus on the stochastic KNN classification of point no. 3. The thickness of a link between sample 3 and another point is proportional to their distance, and can be seen as the relative weight (or probability) that a stochastic nearest neighbor prediction rule would assign to this point. In the original space, sample 3 has many stochastic neighbors from various classes, so the right class is not very likely. However, in the projected space learned by NCA, the only stochastic neighbors with non-negligible weight are from the same class as sample 3, guaranteeing that the latter will be well classified. See the mathematical formulation for more details.

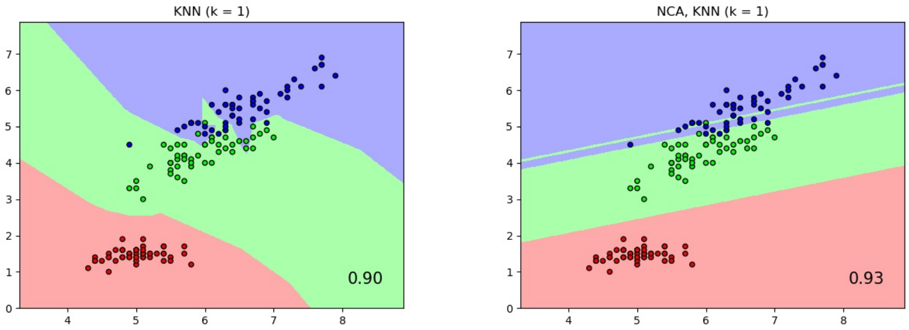
1.6.7.1. Classification

Combined with a nearest neighbors classifier (**`KNeighborsClassifier`**), NCA is attractive for classification because it can naturally handle multi-class problems without any increase in the model size, and does not introduce additional parameters that require fine-tuning by the user.

NCA classification has been shown to work well in practice for data sets of varying size and difficulty. In contrast to related methods such as Linear Discriminant Analysis, NCA does not make any assumptions about the class distributions. The nearest neighbor classification can naturally produce highly irregular decision boundaries.

To use this model for classification, one needs to combine a **`NeighborhoodComponentsAnalysis`** instance that learns the optimal transformation with a **`KNeighborsClassifier`** instance that performs the classification in the projected space. Here is an example using the two classes:

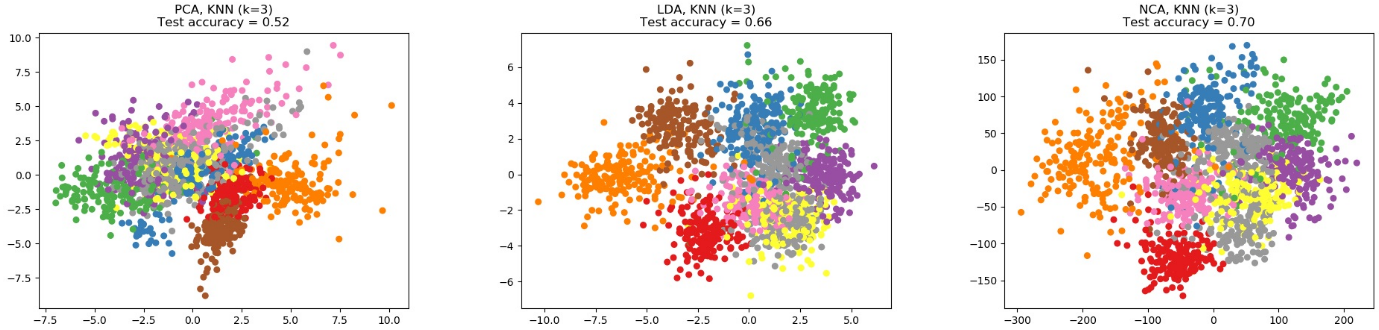
```
>>> from sklearn.neighbors import (NeighborhoodComponentsAnalysis,
... KNeighborsClassifier)
>>> from sklearn.datasets import load_iris
>>> from sklearn.model_selection import train_test_split
>>> from sklearn.pipeline import Pipeline
>>> X, y = load_iris(return_X_y=True)
>>> X_train, X_test, y_train, y_test = train_test_split(X, y,
... stratify=y, test_size=0.7, random_state=42)
>>> nca = NeighborhoodComponentsAnalysis(random_state=42)
>>> knn = KNeighborsClassifier(n_neighbors=3)
>>> nca_pipe = Pipeline([('nca', nca), ('knn', knn)])
>>> nca_pipe.fit(X_train, y_train)
Pipeline(...)
>>> print(nca_pipe.score(X_test, y_test))
0.96190476...
```



The plot shows decision boundaries for Nearest Neighbor Classification and Neighborhood Components Analysis classification on the iris dataset, when training and scoring on only two features, for visualisation purposes.

1.6.7.2. Dimensionality reduction

NCA can be used to perform supervised dimensionality reduction. The input data are projected onto a linear subspace consisting of the directions which minimize the NCA objective. The desired dimensionality can be set using the parameter `n_components`. For instance, the following figure shows a comparison of dimensionality reduction with Principal Component Analysis (`sklearn.decomposition.PCA`), Linear Discriminant Analysis (`sklearn.discriminant_analysis.LinearDiscriminantAnalysis`) and Neighborhood Component Analysis (`NeighborhoodComponentsAnalysis`) on the Digits dataset, a dataset with size $n_{samples} = 1797$ and $n_{features} = 64$. The data set is split into a training and a test set of equal size, then standardized. For evaluation the 3-nearest neighbor classification accuracy is computed on the 2-dimensional projected points found by each method. Each data sample belongs to one of 10 classes.



Examples:

- Comparing Nearest Neighbors with and without Neighborhood Components Analysis
- Dimensionality Reduction with Neighborhood Components Analysis
- Manifold learning on handwritten digits: Locally Linear Embedding, Isomap…

1.6.7.3. Mathematical formulation

The goal of NCA is to learn an optimal linear transformation matrix of size `(n_components, n_features)`, which maximises the sum over all samples i of the probability p_i that i is correctly classified, i.e.:

$$\arg\max_L \sum_{i=0}^{N-1} p_i$$

with N = `n_samples` and p_i the probability of sample i being correctly classified according to a stochastic nearest neighbors rule in the learned embedded space:

$$p_i = \sum_{j \in C_i} p_{ij}$$

where C_i is the set of points in the same class as sample i, and p_{ij} is the softmax over Euclidean distances in the embedded space:

$$p_{ij} = \frac{\exp(-||Lx_i - Lx_j||^2)}{\sum\limits_{k \neq i} \exp -(||Lx_i - Lx_k||^2)}, \quad p_{ii} = 0$$

1.6.7.3.1. Mahalanobis distance

NCA can be seen as learning a (squared) Mahalanobis distance metric:

$$||L(x_i - x_j)||^2 = (x_i - x_j)^T M (x_i - x_j),$$

where $M = L^T L$ is a symmetric positive semi-definite matrix of size `(n_features, n_features)`.

1.6.7.4. Implementation

This implementation follows what is explained in the original paper [1]. For the optimisation method, it currently uses scipy's L-BFGS-B with a full gradient computation at each iteration, to avoid to tune the learning rate and provide stable learning.

See the examples below and the docstring of **`NeighborhoodComponentsAnalysis.fit`** for further information.

1.6.7.5. Complexity

1.6.7.5.1. Training

NCA stores a matrix of pairwise distances, taking `n_samples ** 2` memory. Time complexity depends on the number of iterations done by the optimisation algorithm. However, one can set the maximum number of iterations with the argument `max_iter`. For each iteration, time complexity is `O(n_components x n_samples x min(n_samples, n_features))`.

1.6.7.5.2. Transform

Here the `transform` operation returns LX^T, therefore its time complexity equals `n_components * n_features * n_samples_test`. There is no added space complexity in the operation.

References:

[1] "Neighbourhood Components Analysis", J. Goldberger, S. Roweis, G. Hinton, R. Salakhutdinov, Advances in Neural Information Processing Systems, Vol. 17, May 2005, pp. 513-520.

Wikipedia entry on Neighborhood Components Analysis

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