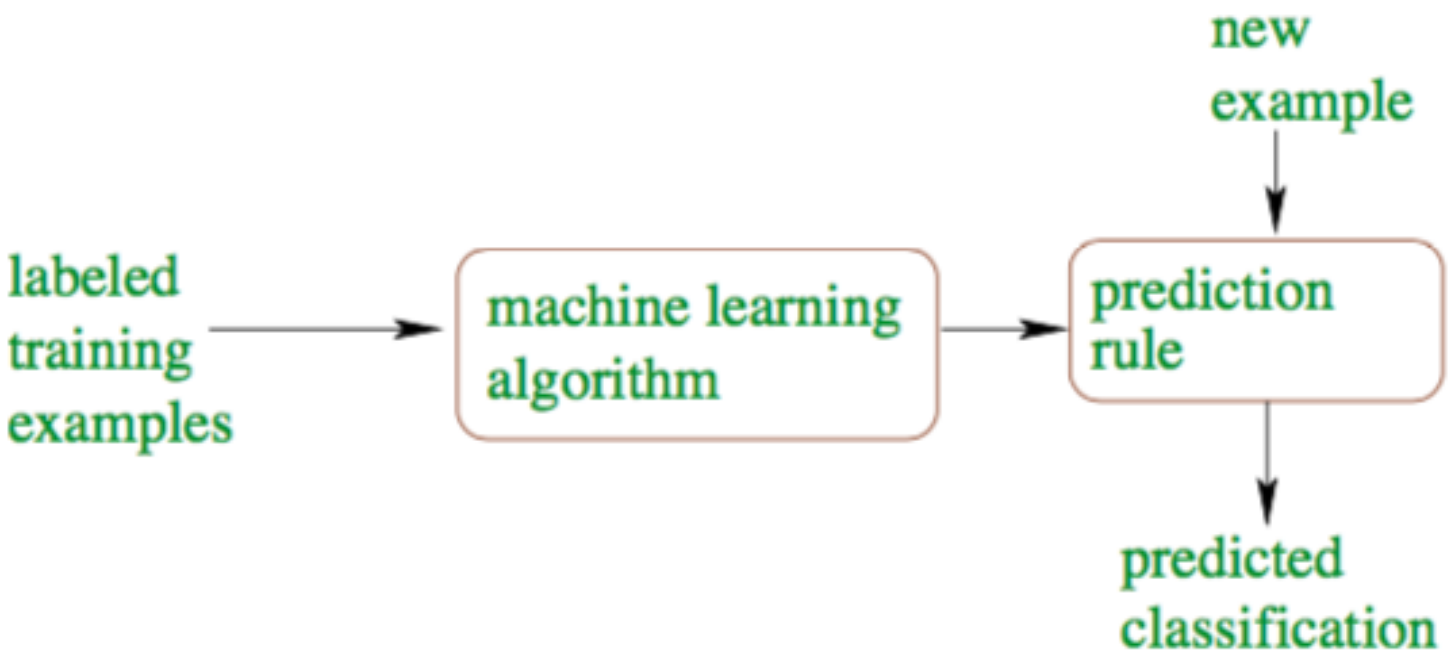
Mathematical techniques in data science

Lecture 3: Nearest neighbors

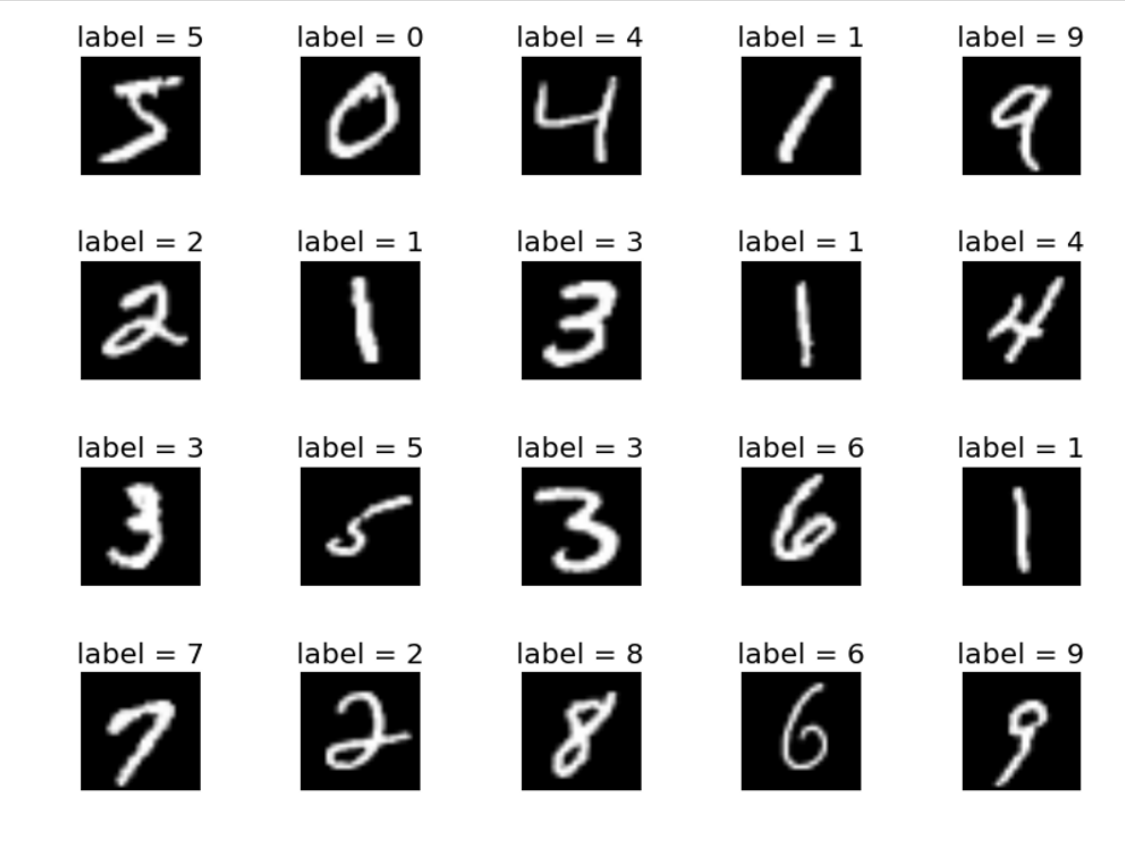
Supervised learning



Learning a function that maps an input to an output based on example input-output pairs

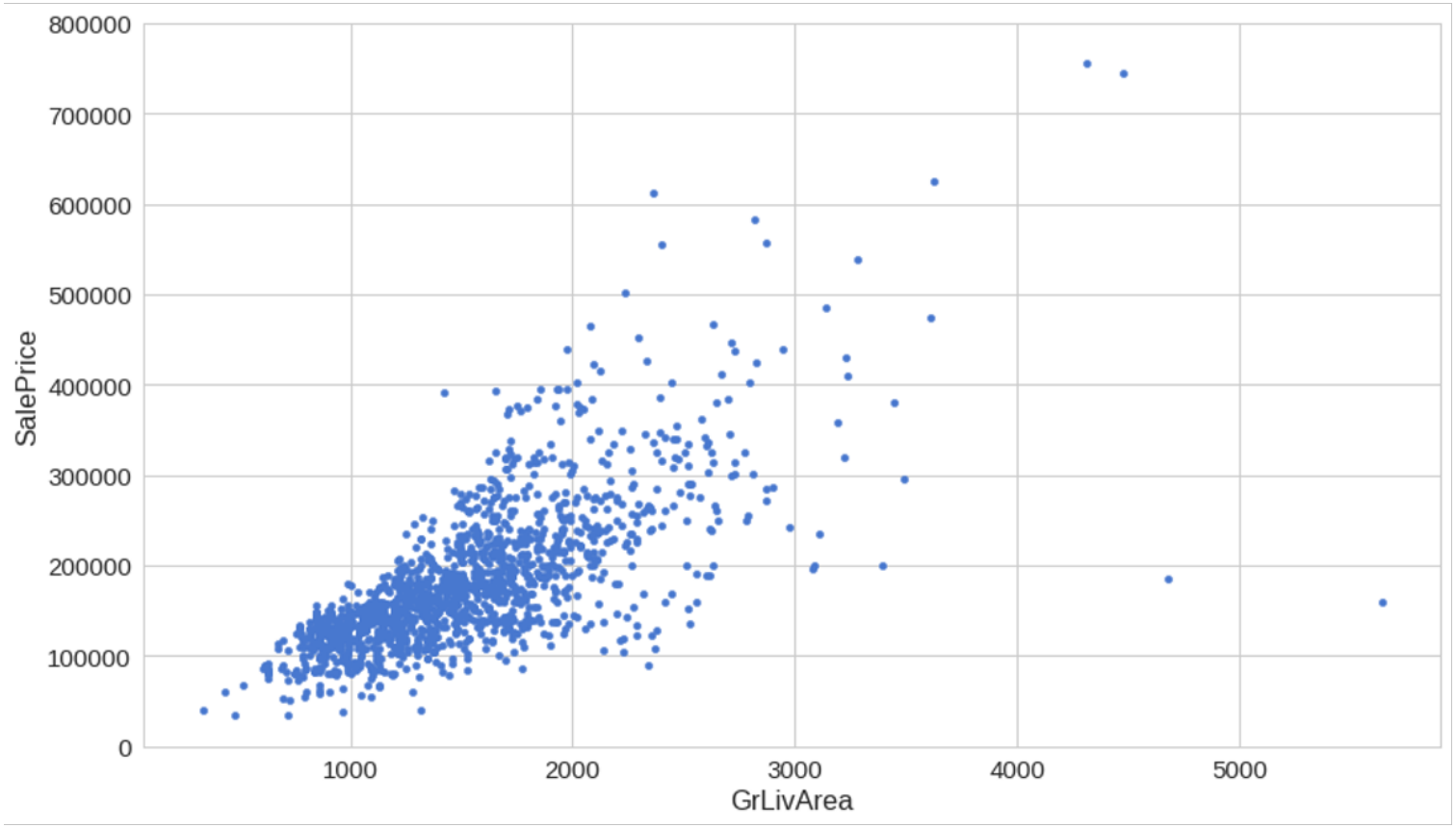
Supervised learning: Classification

Hand-written digit recognition



Supervised learning: Regression

Predict house price by living area

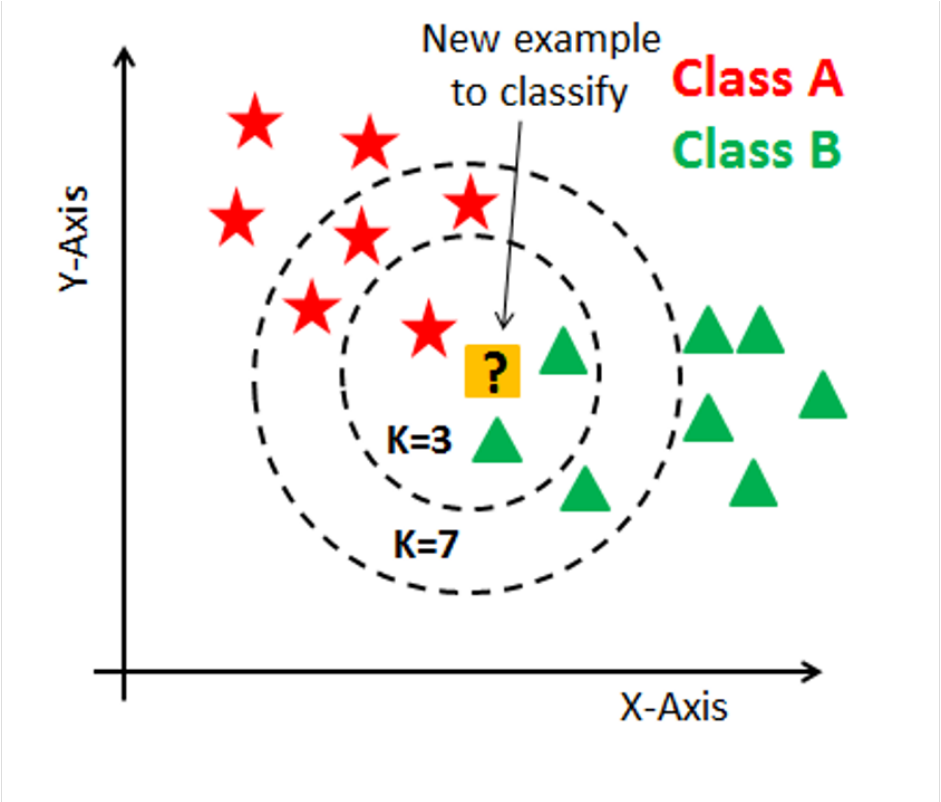


Nearest Neighbors

- Very simple idea: Make predictions based on labels of the nearest training examples
- Applicable to both classification and regression

K-nearest neighbor (K-NN) for classification

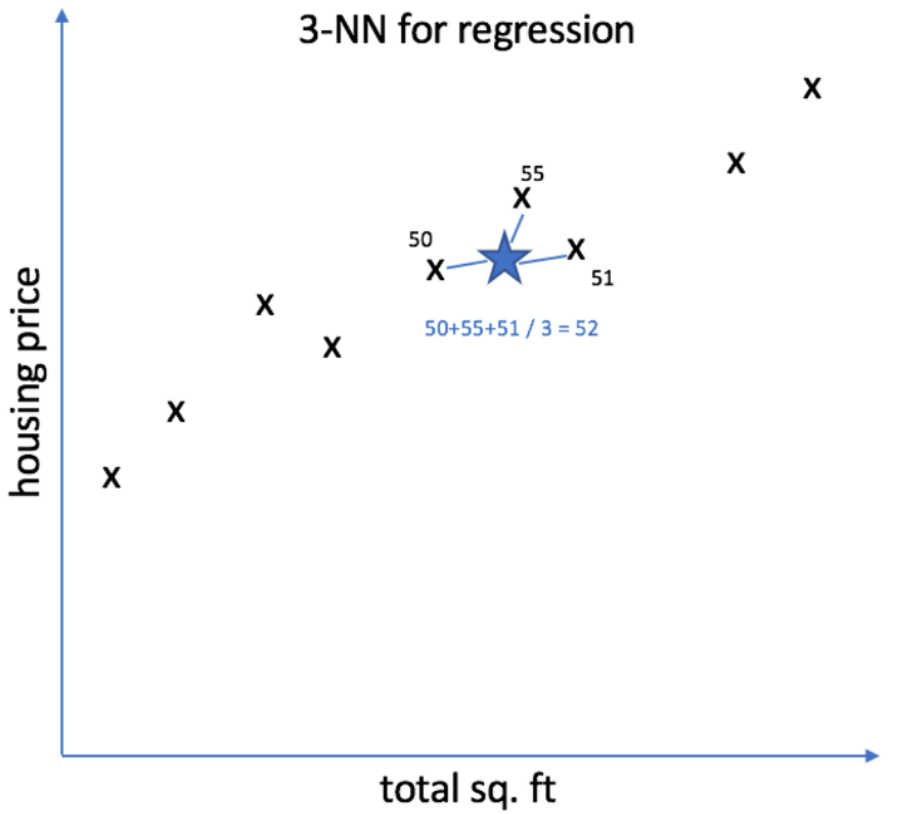
- Learning: Store all training examples
- Predict label of x:
  - Find the nearest K training examples to x
  - Assign the most frequent label to x



(Source: kdnuggets.com)

K-nearest neighbor (K-NN) for regression

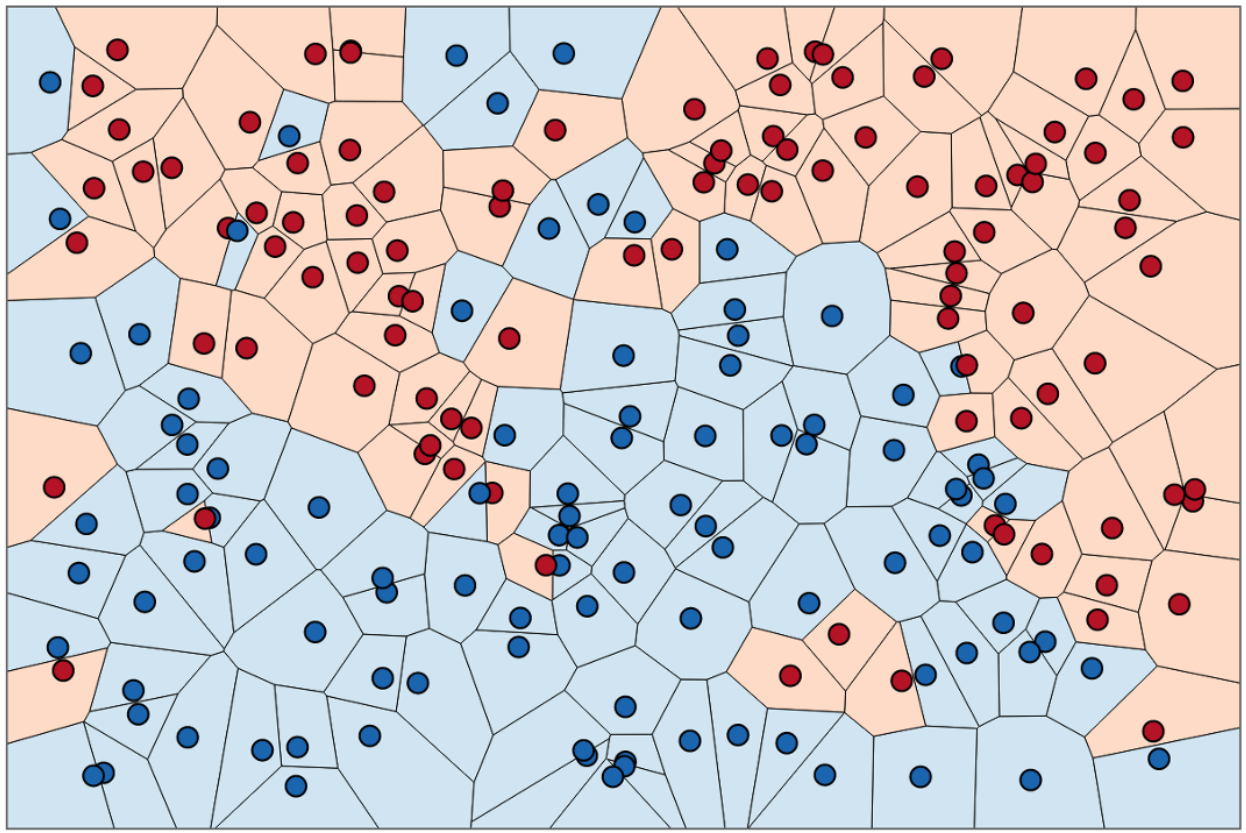
- Learning: Store all training examples
- Predict label of x:
  - Find the nearest K training examples to x
  - Assign the average of the K nearest labels to x



(Source: Jeremy Jordan)

Decision boundary for K-NN (classification)

- Divide feature space into Voronoi cells
- Decision boundaries are linear



(Source: Kevin Zakka)

How to define "near-ness"?

- Need to define a distance metric between data points
- Common metric: Euclidean distance (L2 distance)

$$d(x, x') = \sqrt{\sum_{i=1}^{n} (x_i - x_i')^2}$$

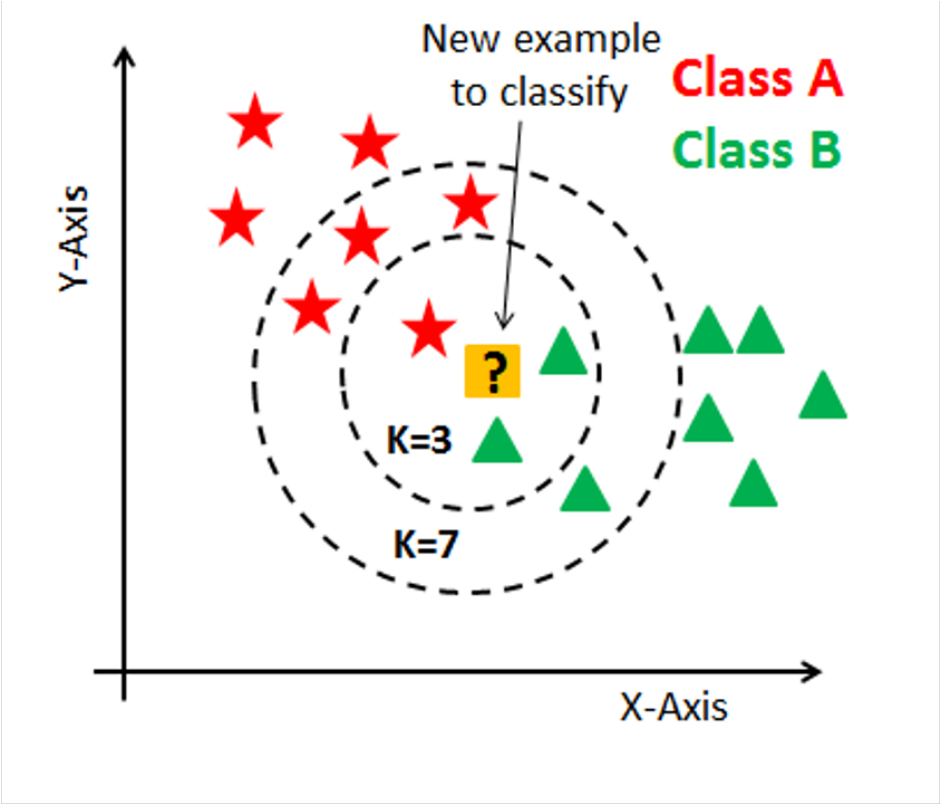
- Other metrics: Manhattan distance, Minkowski distance, etc.

How to find the nearest neighbors?

- Simplest algorithm: brute-force search
  - Compute distance between every training data point to the test point
  - Pick K points with the smallest distances
- Space partitioning algorithms: arrange data points into some data structure (such as a binary tree) for faster search
  - Ball tree (`https://en.wikipedia.org/wiki/Ball_tree`)
  - k-d tree (`https://en.wikipedia.org/wiki/K-d_tree`)
- Approximate algorithms

Variant: Prediction with non-uniform weights

Nearer neighbors have more weights when making predictions



Machine learning models from scikit-learn

Keys to read the documentations

- Parameters (to set up the model)
- Methods (what we can do with the model)
- Attributes (components we can extract from the model)

Nearest Neighbors on scikit-learn

sklearn.neighbors.KNeighborsClassifier

class `sklearn.neighbors.` **`KNeighborsClassifier`**(*n_neighbors=5, *, weights='uniform', algorithm='auto', leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None, **kwargs*) [source]

Classifier implementing the k-nearest neighbors vote.

Read more in the User Guide.

Parameters:

n_neighbors : *int, default=5*
Number of neighbors to use by default for `kneighbors` queries.

weights : *{'uniform', 'distance'} or callable, default='uniform'*
weight function used in prediction. Possible values:

- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

algorithm : *{'auto', 'ball_tree', 'kd_tree', 'brute'}, default='auto'*
Algorithm used to compute the nearest neighbors:

- 'ball_tree' will use `BallTree`
- 'kd_tree' will use `KDTree`
- 'brute' will use a brute-force search.
- 'auto' will attempt to decide the most appropriate algorithm based on the values passed to `fit` method.

Nearest Neighbors on scikit-learn

sklearn.neighbors.KNeighborsRegressor

class `sklearn.neighbors.` **`KNeighborsRegressor`**(*n_neighbors=5, *, weights='uniform', algorithm='auto', leaf_size=30, p=2, metric='minkowski', metric_params=None, n_jobs=None, **kwargs*) ¶ [source]

Regression based on k-nearest neighbors.

The target is predicted by local interpolation of the targets associated of the nearest neighbors in the training set.

Read more in the User Guide.

New in version 0.9.

Parameters:

n_neighbors : *int, default=5*
Number of neighbors to use by default for `kneighbors` queries.

weights : *{'uniform', 'distance'} or callable, default='uniform'*
weight function used in prediction. Possible values:

- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

Uniform weights are used by default.

algorithm : *{'auto', 'ball_tree', 'kd_tree', 'brute'}, default='auto'*
Algorithm used to compute the nearest neighbors:

- 'ball_tree' will use `BallTree`
- 'kd_tree' will use `KDTree`
- 'brute' will use a brute-force search.
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Nearest Neighbors on scikit-learn

`sklearn.neighbors`: Nearest Neighbors

The `sklearn.neighbors` module implements the k-nearest neighbors algorithm.

User guide: See the Nearest Neighbors section for further details.

`neighbors.BallTree`(X[, leaf_size, metric])	BallTree for fast generalized N-point problems
`neighbors.DistanceMetric`	DistanceMetric class
`neighbors.KDTree`(X[, leaf_size, metric])	KDTree for fast generalized N-point problems
`neighbors.KernelDensity`(*[, bandwidth, ...])	Kernel Density Estimation.
`neighbors.KNeighborsClassifier`([...])	Classifier implementing the k-nearest neighbors vote.
`neighbors.KNeighborsRegressor`([n_neighbors, ...])	Regression based on k-nearest neighbors.
`neighbors.KNeighborsTransformer`(*[, mode, ...])	Transform X into a (weighted) graph of k nearest neighbors
`neighbors.LocalOutlierFactor`([n_neighbors, ...])	Unsupervised Outlier Detection using Local Outlier Factor (LOF)
`neighbors.RadiusNeighborsClassifier`([...])	Classifier implementing a vote among neighbors within a given radius
`neighbors.RadiusNeighborsRegressor`([radius, ...])	Regression based on neighbors within a fixed radius.
`neighbors.RadiusNeighborsTransformer`(*[, ...])	Transform X into a (weighted) graph of neighbors nearer than a radius
`neighbors.NearestCentroid`([metric, ...])	Nearest centroid classifier.
`neighbors.NearestNeighbors`(*[, n_neighbors, ...])	Unsupervised learner for implementing neighbor searches.
`neighbors.NeighborhoodComponentsAnalysis`([...])	Neighborhood Components Analysis

`neighbors.kneighbors_graph`(X, n_neighbors, *)	Computes the (weighted) graph of k-Neighbors for points in X
`neighbors.radius_neighbors_graph`(X, radius, *)	Computes the (weighted) graph of Neighbors for points in X

General steps to build ML models

- Get and pre-process data
- Visualize the data (optional)
- Split data into training/test sets
- Create a model
- Train the model on training set; i.e. call model.fit()
- Predict on test data
- Compute evaluation metrics (accuracy, mean squared error, etc.)
- Visualize the trained model (optional)

Review: Evaluate a learned model

- How effective the model makes predictions on new (unseen) data
- Classification: accuracy or error rate
- Regression: average (squared) distance between predicted and true values (mean squared error)

Review: Data splitting practices