Supervised Learning – Part 2

ESM3081 Programming for Data Science

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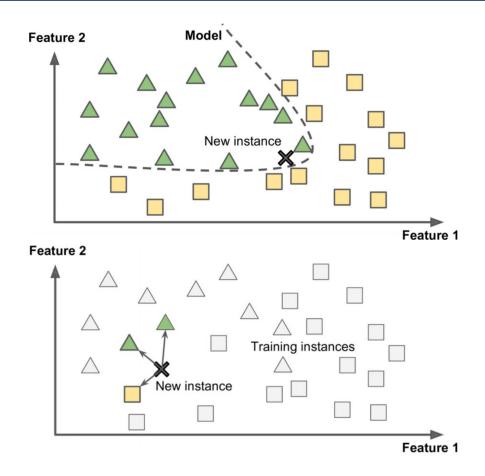


Learning algorithms covered in this course

- Supervised Learning (Classification/Regression)
 - K-Nearest Neighbors
 - Linear Models (Logistic/Linear Regression)
 - Decision Trees
 - Random Forests
 - Support Vector Machines
 - Neural Networks
 - * Many algorithms have a classification and a regression variant, and we will describe both.
 - * We will review the most popular machine learning algorithms, explain how they learn from data and how they make predictions, and examine the strengths and weaknesses of each algorithm.

Model-Based vs. Instance-Based Learning

- Model-Based Learning (Eager Learning)
 - Training phase: Build a model using training data
 - Prediction phase: Use the model to make predictions
- Instance-Based Learning (Lazy Learning)
 - **Training phase:** Do nothing
 - Prediction phase: Compare new instances with training data to make predictions



Instance-based learning takes less time in training but more time in predicting,
 and is advantageous when training data becomes available gradually over time.

- The k-NN algorithm simply stores the training dataset.
- To make a prediction for a new data point, the algorithm finds the closest data points in the training dataset—its "nearest neighbors."
- The prediction is an aggregation of the known outputs for the nearest neighbors.
 - Example:

For *classification*, the prediction is the majority class among the relevant neighbors. For *regression*, the prediction is the average of the relevant neighbors' labels.

- Given a (training) dataset $D = \{(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)\}$ such that $x_i = (x_{i1}, ..., x_{id}) \in \mathbb{R}^d$ is the *i*-th input vector of *d* features and y_i is the corresponding target label.
- For a query data point $x_{
 m new}$
 - 1. Compute distance from x_{new} to each data point in D (distance metric)
 - 2. Identify k nearest neighbors of x_{new} , $kNN(x_{\text{new}}) = \{(x_{(1)}, y_{(1)}), ..., (x_{(k)}, y_{(k)})\} \subset D$ (k)
 - 3. Use labels of the nearest neighbors to predict y_{new} (weighting scheme)
 - e.g) voting or weighted voting for classification, averaging or weighted averaging for regression.

What are parameters? What are hyperparameters?

For Classification,

Voting:
$$\hat{y} = \underset{j}{\operatorname{argmax}} \sum_{\left(x_{(i)}, y_{(i)}\right) \in kNN(x)} I(y_{(i)} = j)$$

Weighted Voting: $\hat{y} = \underset{j}{\operatorname{argmax}} \sum_{\left(x_{(i)}, y_{(i)}\right) \in kNN(x)} w(x_{(i)}, x) I(y_{(i)} = j)$

• For Regression,

Averaging:
$$\hat{y} = \frac{1}{k} \sum_{(x_{(i)}, y_{(i)}) \in kNN(x)} y_{(i)}$$

Weighted Averaging:
$$\hat{y} = \frac{1}{\sum_{\left(x_{(i)},y_{(i)}\right) \in kNN(x)} w(x_{(i)},x)} \sum_{\left(x_{(i)},y_{(i)}\right) \in kNN(x)} w(x_{(i)},x) y_{(i)}$$

 $w(x_{(i)}, x)$ is a weight function (hyperparameter, not learned) e.g., inverse of Euclidean distance $\frac{1}{\|x_{(i)}-x\|_2}$

Hyperparameters

Distance metric

- Euclidean: $\|x_{(i)} x\|_2$
- Manhattan: $\|x_{(i)} x\|_1$
- Minkowski: $\|x_{(i)} x\|_p$

https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.DistanceMetric.html

The number of nearest neighbors k

- Smaller $k \rightarrow$ capture local structure in data (but also noise)
- Larger $k \rightarrow$ provide more smoothing, less noise, but may miss local structure

^{*} Distance Metrics available in scikit-learn

Hyperparameters

Weight function

- Uniform: $w(x_{(i)}, x) = 1$
- Distance Weight (Inverse of Euclidean): $w(x_{(i)}, x) = \frac{1}{\|x_{(i)} x\|_2}$
- Distance Weight (Inverse of Manhattan): $w(x_{(i)}, x) = \frac{1}{\|x_{(i)} x\|_1}$
- Distance Weight (Inverse of Minkowski (p)): $w(x_{(i)}, x) = \frac{1}{\|x_{(i)} x\|_p}$

https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html

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.

Note: fitting on sparse input will override the setting of this parameter, using brute force.

https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html

p:int, default=2

Power parameter for the Minkowski metric. When p = 1, this is equivalent to using manhattan_distance (I1), and euclidean_distance (I2) for p = 2. For arbitrary p, minkowski_distance (I_p) is used.

metric: str or callable, default='minkowski'

the distance metric to use for the tree. The default metric is minkowski, and with p=2 is equivalent to the standard Euclidean metric. See the documentation of **DistanceMetric** for a list of available metrics. If metric is "precomputed", X is assumed to be a distance matrix and must be square during fit. X may be a sparse graph, in which case only "nonzero" elements may be considered neighbors.

metric_params: dict, default=None

Additional keyword arguments for the metric function.

Methods

fit(X, y)	Fit the k-nearest neighbors classifier from the training dataset.
get_params([deep])	Get parameters for this estimator.
${\tt kneighbors}([X,n_neighbors,return_distance])$	Finds the K-neighbors of a point.
kneighbors_graph([X, n_neighbors, mode])	Computes the (weighted) graph of k-Neighbors for points in X
predict(X)	Predict the class labels for the provided data.
predict_proba(X)	Return probability estimates for the test data X.
<pre>score(X, y[, sample_weight])</pre>	Return the mean accuracy on the given test data and labels.
set_params(**params)	Set the parameters of this estimator.

Example with the forge dataset

- The dataset consists of 26 data points with two classes (binary classification).

```
import mglearn
import matplotlib.pyplot as plt

In[1]:

    # generate dataset
    X, y = mglearn.datasets.make_forge()
    # plot dataset
    mglearn.discrete_scatter(X[:, 0], X[:, 1], y)
    plt.legend(["Class 0", "Class 1"], loc=4)
    plt.xlabel("First feature")
    plt.ylabel("Second feature")
    print("X.shape: {}".format(X.shape))

Out[1]:

    X.shape: (26, 2)
```

observed by the second of the

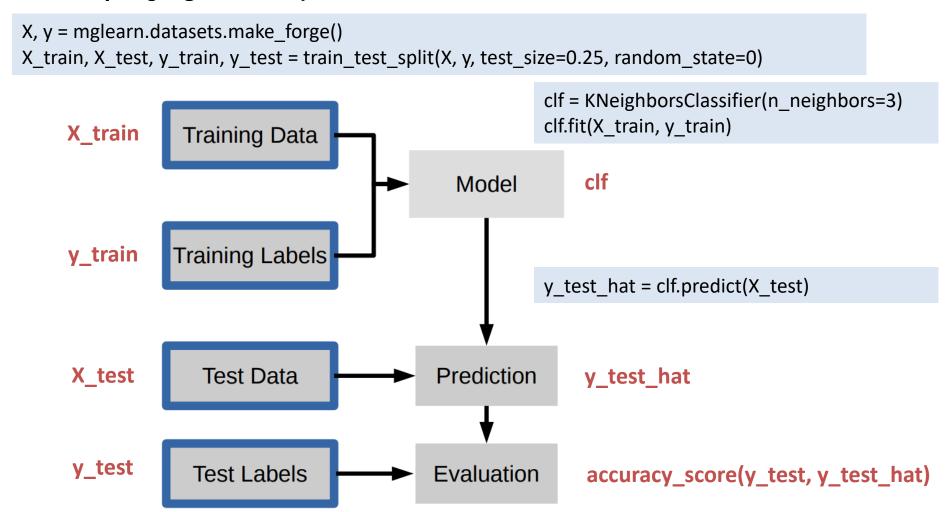
X1 X2 Y 9.96347 4.59677 1 11.03295 -0.16817 2 11.54156 5.21116 8.69289 1.54322 0 8.10623 4.28696 8.30989 4.80624 6 11.93027 4.64866 9.67285 -0.20283 0 8.34810 5.13416 8.67495 4.47573 1 9.17748 5.09283 11 10.24029 2.45544 1 8.68937 1.48710 0 8.92230 -0.63993 0 9.49123 4.33225 9.25694 5.13285 7.99815 4.85251 1.29564 0 2.49162 0 9.32298 5.09841 10.06394 0.99078 9.50049 -0.26430 0 8.34469 1.63824 0 1.93825 0 9.15072 5.49832 1 **25** 11.56396 1.33894 0

• Example (forge dataset): k=3

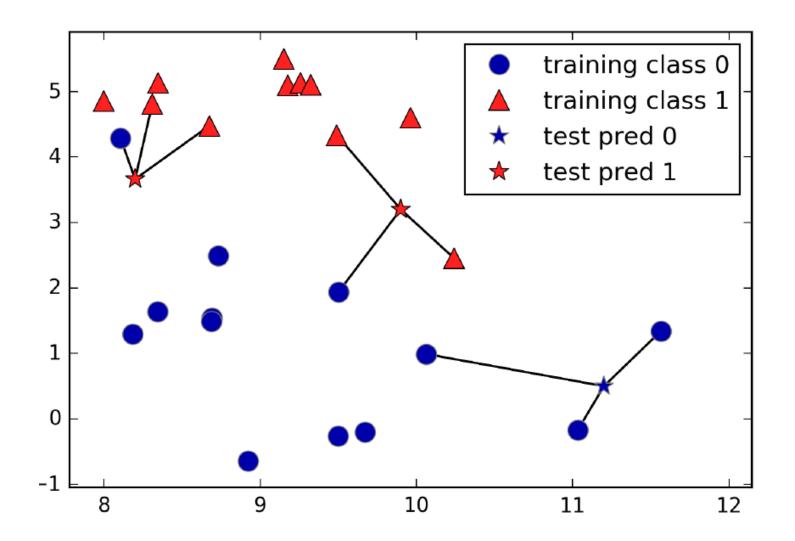
test accuracy: 0.85714

```
In [2]: import malearn
        X, y = mglearn.datasets.make_forge()
In [3]: from sklearn.model_selection import train_test_split
        X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random_state=0)
In [4]: from sklearn.neighbors import KNeighborsClassifier
        clf = KNeighborsClassifier(n neighbors=3)
        clf.fit(X train, y train)
Out[4]:
                 KNeighborsClassifier
         KNeighborsClassifier(n neighbors=3)
In [5]: y_test_hat = clf.predict(X_test)
        print(y test)
        print(y_test_hat)
        [1010110]
        [1010100]
In [6]: from sklearn.metrics import accuracy_score
        y_train_hat = clf.predict(X_train)
        print('train accuracy: %.5f'%accuracy_score(y_train, y_train_hat))
        y_test_hat = clf.predict(X test)
        print('test accuracy: %.5f'%accuracy_score(y_test, y_test_hat))
        train accuracy: 0.94737
```

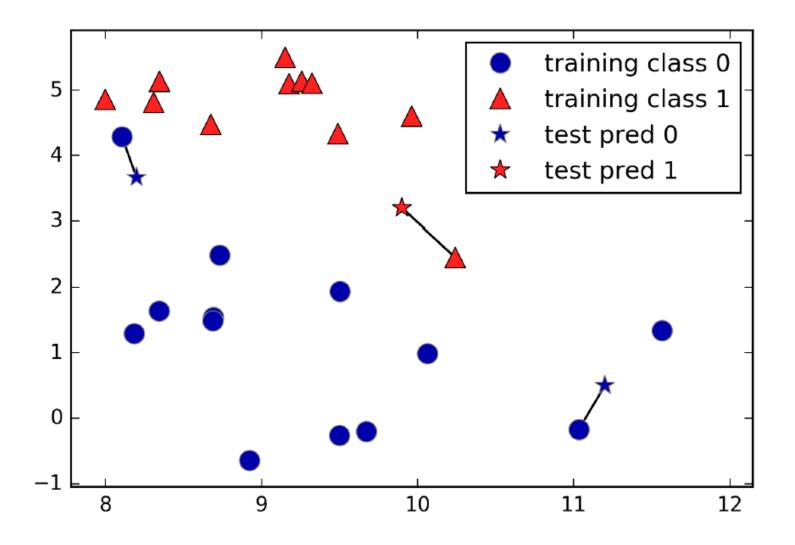
Example (forge dataset): k=3



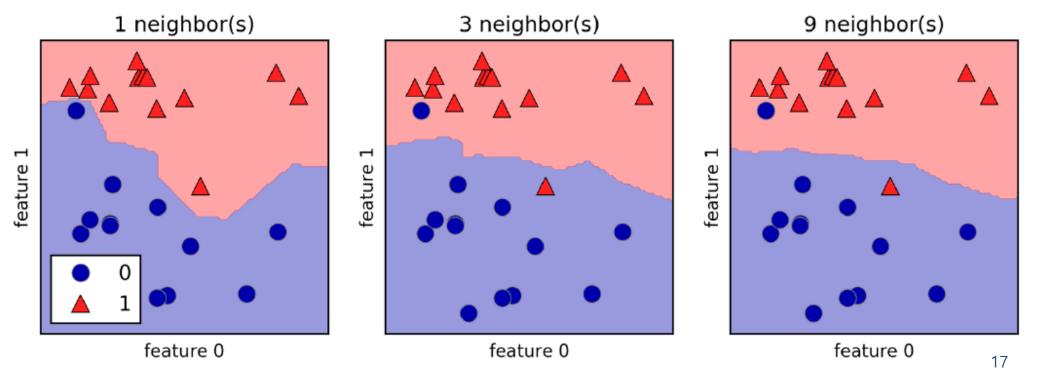
• Example (forge dataset): k=3



Example (forge dataset): k=1



- The effect of the hyperparameter k (n_neighbors)
 - Decision boundaries created by k-NN
 - Using a single neighbor (k=1) results in a decision boundary that follows the training data closely. (corresponds to high model complexity)
 - Considering more neighbors leads to a smoother decision boundary. (corresponds to low model complexity)



Example with the breast_cancer dataset

- The dataset consists of 569 data points with 30 features
- Each data point (tumor) is labeled as "benign" (for harmless tumors) or "malignant" (for cancerous tumors) binary classification
- Of these 569 data points, 212 are labeled as malignant and 357 as benign.
- The classification task is to learn to predict whether a tumor is malignant based on the measurements of the tissue.

In [7]: from sklearn.datasets import load_breast_cancer

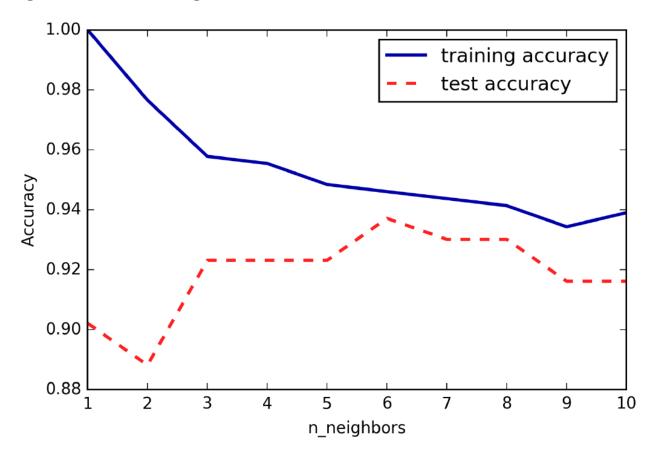
from sklearn.model_selection import train_test_split

Example (breast_cancer dataset): varying the hyperparameter k

```
from sklearn, neighbors import KNeighborsClassifier
        from sklearn.metrics import accuracy_score
        cancer = load_breast_cancer()
        X train, X test, y train, y test = train test split(
            cancer.data, cancer.target, stratify=cancer.target, random state=66)
In [8]: training accuracy = []
        test accuracy = []
        k_settings = range(1, 11) # try n_neighbors from 1 to 10
        for k in k settings:
            # build the model
            clf = KNeighborsClassifier(n_neighbors=k
            clf.fit(X_train, y_train)
            # accuracy on the training set
            y_train_hat = clf.predict(X_train)
            training_accuracy.append(accuracy_score(y_train, y_train_hat))
            # accuracy on the test set (generalization)
            y_test_hat = clf.predict(X test)
            test accuracy.append(accuracy score(y test, y test hat))
```

	k	training accuracy	test accuracy
0	1	1.00000	0.90210
1	2	0.97653	0.88811
2	3	0.95775	0.92308
3	4	0.95540	0.92308
4	5	0.94836	0.92308
5	6	0.94601	0.93706
6	7	0.94366	0.93007
7	8	0.94131	0.93007
8	9	0.93427	0.91608
9	10	0.93897	0.91608

- Example (breast_cancer dataset): varying the hyperparameter k
 - Comparison of training and test accuracy as a function of k (n_neighbors)
 - Smaller $k \rightarrow$ overfitting
 - Larger k → underfitting



Example (breast_cancer dataset): varying the distance metric

```
In [10]: from sklearn.datasets import load breast cancer
         from sklearn, model selection import train test split
         from sklearn, neighbors import KNeighborsClassifier
         from sklearn.metrics import accuracy_score
         cancer = load breast cancer()
         |X train, X test, y train, y test = train test split(
             cancer.data, cancer.target, stratify=cancer.target, random_state=66)
In [11]: training_accuracy = []
         test_accuracy = []
         p_settings = range(1, 6) # try minkowski p from 1 to 5
         for p in p settings:
             # build the model
             clf = KNeighborsClassifier(n_neighbors=5, metric='minkowski', p=p)
             clf.fit(X train, y train)
             # accuracy on the training set
             y_train_hat = clf.predict(X_train)
             training accuracy.append(accuracy score(y train, y train hat))
             # accuracy on the test set (generalization)
             y_test_hat = clf.predict(X_test)
             test accuracy.append(accuracy score(y test, y test hat))
```

Minkowski Distance (p) $\|x_{(i)} - x\|_p$

	p	training accuracy	test accuracy
0	1	0.96479	0.93706
1	2	0.94836	0.92308
2	3	0.94366	0.93007
3	4	0.94366	0.92308
4	5	0.94366	0.92308

https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsRegressor.html

sklearn.neighbors.KNeighborsRegressor¶

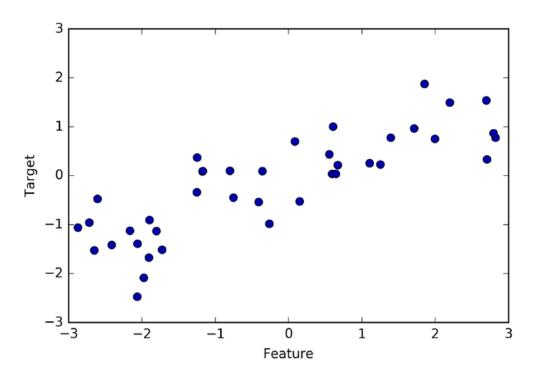
 $class \ \, sklearn.neighbors. \ \, KNeighborsRegressor (n_neighbors=5, \ ^*, weights='uniform', algorithm='auto', leaf_size=30, p=2, \\ metric='minkowski', metric_params=None, n_jobs=None, \ ^*kwargs) \\ [source]$

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.

Example with the wave dataset

- The wave dataset is a synthetic dataset that has a single feature and a continuous target.



Example (wave dataset): k=3

R square: 0.83442

In [13]: import mglearn

```
X, y = mglearn.datasets.make_wave(n_samples=40)
In [14]: from sklearn.model_selection import train_test_split
         X_train, X_test, y_train, y_test = train_test_split(X, y, random state=0)
In [15]: from sklearn.neighbors import KNeighborsRegressor
         reg = KNeighborsRegressor(n_neighbors=3)
         reg.fit(X_train, y_train)
Out[15]:
                  KNeighborsRegressor
          KNeighborsRegressor(n neighbors=3)
In [16]: y_test_hat = reg.predict(X_test)
         print(v test)
         print(y_test_hat)
         [ 0.37299  0.21778  0.96695 -1.38774 -1.0598 -0.90497  0.43656  0.77896
          -0.54115 -0.956521
         [-0.05397 0.35686 1.13672 -1.89416 -1.13881 -1.63113 0.35686 0.91241
          -0.4468 -1.13881]
In [17]: from sklearn.metrics import mean absolute error, mean squared error, r2 score
         print('MAE: %.5f'%mean absolute error(y test,y test hat))
         print('RMSE: %.5f'%mean_squared_error(y_test,y_test_hat)**0.5)
         print('R_square: %.5f'%r2_score(y_test,y_test_hat))
         MAE: 0.25372
         RMSE: 0.32966
```

24

Х

0 -0.75276 -0.44822

2 1.39196 0.77932

5 -2.06403 -2.47196

6 -2.65150 -1.52731 **7** 2.19706 1.49417

8 0.60669 1.00032

11 2.81946 0.77896

12 1.99466 0.75419

13 -1.72597 -1.51370

14 -1.90905 -1.67303

15 -1.89957 -0.90497

16 -1.17455 0.08449

18 -0.40833 -0.54115

19 -1.25263 -0.34091

0.14854 -0.52735

9 1.24844 0.22956 **10** -2.87649 -1.05980

3 0.59195 0.03498 **4** -2.06389 -1.38774

1 2.70429

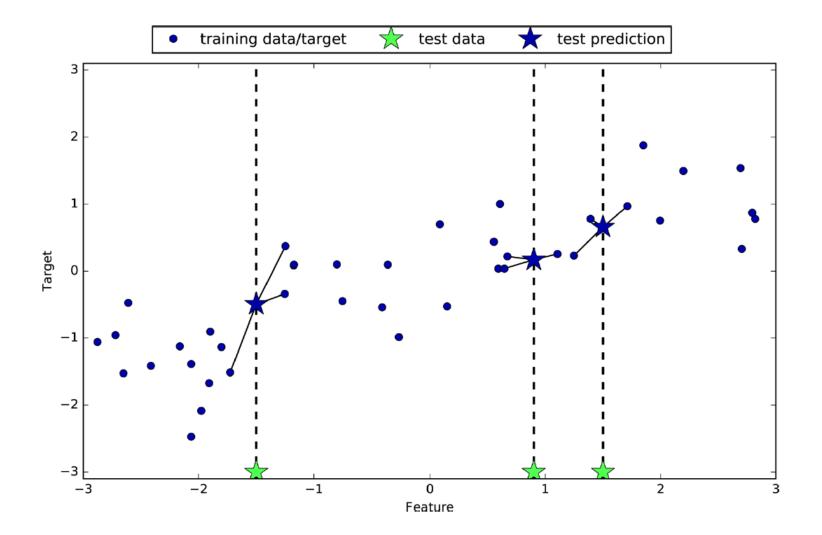
Υ

0.33123

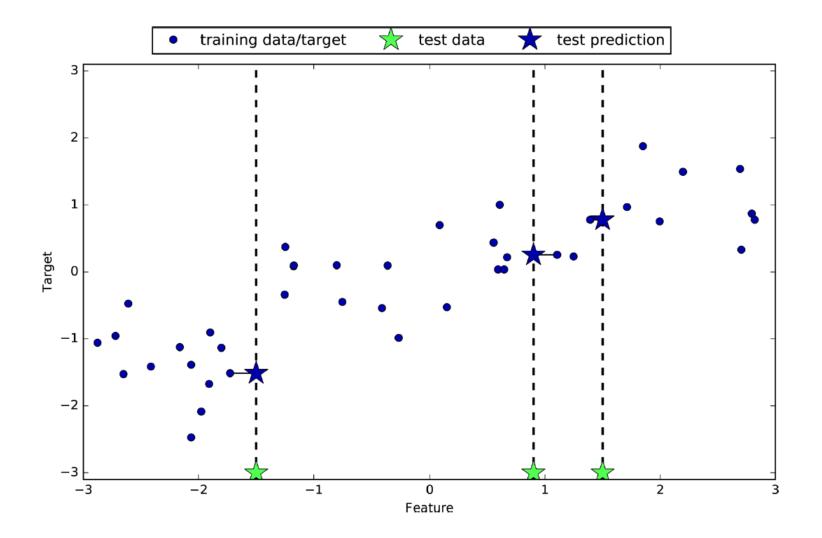
Example (wave dataset): k=3

```
X, y = mglearn.datasets.make_wave(n_samples=40)
X train, X test, y train, y test = train test split(X, y, random_state=0)
                                                          reg = KNeighborsRegressor(n neighbors=3)
                                                          reg.fit(X train, y train)
    X train
                 Training Data
                                              Model
                                                             reg
               Training Labels
    y_train
                                                          y_test_hat = reg.predict(X_test)
    X_test
                   Test Data
                                            Prediction
                                                             y test hat
                                                             mean_absolute_error(y_test,y_test_hat)
    y test
                  Test Labels
                                            Evaluation
                                                             mean_squared_error(y_test,y_test_hat)**0.5
                                                             r2 score(y test, y test hat)
```

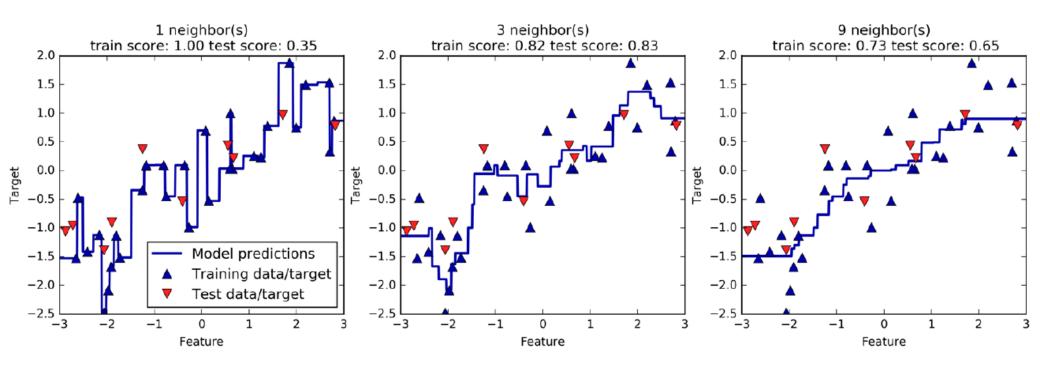
Example (wave dataset): k=3



Example (wave dataset): k=1



- The effect of the hyperparameter k (n_neighbors)
 - Comparing predictions made by k-NN
 - By using a single neighbor (k=1), each point in the training set has an obvious influence on the predictions. (high model complexity)
 - Considering more neighbors leads to smoother predictions. (low model complexity)



Discussion

The main hyperparameters to the k-NN algorithm

- n_neighbor (the number of neighbors k)
- metric (distance metric)
- weights (weighting scheme)
- * Typically chosen to have the highest performance in validation data
- * It's important to preprocess your data (including data scaling and one-hot encoding)

Strengths

- The algorithm is very easy to understand
- The algorithm often gives reasonable performance without a lot of adjustments (good baseline method to try)

Weaknesses

- Prediction can be slow when your training set is very large (either in number of features or in number of data points)
- The algorithm often does not perform well on datasets with many features (hundreds or more)

Feature Scaling for Distance Metric

- Certain features are more important than others in many applications.
- It is often sensible to scale the features differently.

Original Dataset

	x_1	x_2
data point a	3	200
data point b	10	100
data point c	11	200

$$dist(\mathbf{a}, \mathbf{b}) = \sqrt{10049} \approx 100.2$$

 $dist(\mathbf{a}, \mathbf{c}) = \sqrt{64} = 8$

$$dist(\boldsymbol{a}, \boldsymbol{b}) > dist(\boldsymbol{a}, \boldsymbol{c})$$

Same Dataset (but different feature scales)

	x_1	$x_2/100$
data point a	3	2
data point b	10	1
data point c	11	2

$$\operatorname{dist}(\boldsymbol{a},\boldsymbol{b}) = \sqrt{50} \simeq 7.1$$

$$dist(a, c) = \sqrt{64} = 8$$

$$dist(\boldsymbol{a}, \boldsymbol{b}) < dist(\boldsymbol{a}, \boldsymbol{c})$$

- Feature Scaling: Puts all numeric features on same scale
 - It must be used when features with the largest scales would dominate and skew results
- Scaling functions
 - **Standard Scaling:** Transform to have a mean of 0 and a standard deviation of 1 by subtracting mean and dividing by standard deviation

```
class skilearn.preprocessing.StandardScaler(*, copy=True, with_mean=True, with_std=True) [source]
```

- MinMax Scaling: Scale to 0-1 by subtracting minimum and dividing by the range

```
class skilearn.preprocessing.MinMaxScaler(feature_range=(0, 1), *, copy=True, clip=False) [source]
```

Robust Scaling: Transform by subtracting the median and then dividing by the interquartile range

```
class \  \, \text{sklearn.preprocessing.} \\ \textbf{RobustScaler}(*, with\_centering=True, with\_scaling=True, quantile\_range=(25.0, 75.0), copy=True, \\ unit\_variance=False) \\ [\text{source}]
```

Example (forge dataset) with StandardScaler

```
In [19]: import mglearn
         X, y = mglearn.datasets.make forge()
In [20]: from sklearn.model_selection import train_test_split
         X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
In [21]: from sklearn, preprocessing import StandardScaler
         scaler = StandardScaler()
         scaler.fit(X_train)
         X_train_scaled = scaler.transform(X_train)
         X test scaled = scaler.transform(X test)
In [22]: from sklearn.neighbors import KNeighborsClassifier
         clf = KNeighborsClassifier(n neighbors=3)
         clf.fit(X train scaled, y train)
Out[22]:
                  KNeighborsClassifier
         |KNeighborsClassifier(n_neighbors=3)
In [23]: from sklearn.metrics import accuracy_score
         y train hat = clf.predict(X train scaled)
         print('train accuracy: %.5f'%accuracy_score(y_train, y_train_hat))
         y_test_hat = clf.predict(X_test_scaled)
         print('test accuracy: %.5f'%accuracy score(y test, y test hat))
```

	X1_train	X2_train	X1_train_scaled	X2_train_scaled
0	8.92230	-0.63993	-0.43383	-1.66209
1	8.73371	2.49162	-0.61218	-0.21838
2	9.32298	5.09841	-0.05489	0.98339
3	7.99815	4.85251	-1.30782	0.87003
4	11.03295	-0.16817	1.56227	-1.44460
5	9.17748	5.09283	-0.19250	0.98082
6	11.56396	1.33894	2.06445	-0.74979
7	9.15072	5.49832	-0.21780	1.16776
8	8.34810	5.13416	-0.97686	0.99988
9	11.93027	4.64866	2.41088	0.77605
		:		:

Results without Scaling

train accuracy: 0.94737 test accuracy: 0.85714

• Example (forge dataset) with MinMaxScaler

```
In [25]: import mglearn
         X, y = mglearn.datasets.make_forge()
In [26]: from sklearn.model selection import train test split
         X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
In [27]: from sklearn.preprocessing import MinMaxScaler
         scaler = MinMaxScaler()
         scaler.fit(X train)
         X train scaled = scaler.transform(X train)
         X_test_scaled = scaler.transform(X_test)
In [28]: from sklearn.neighbors import KNeighborsClassifier
         clf = KNeighborsClassifier(n neighbors=3)
         clf.fit(X train scaled, y train)
Out[28]:
                  KNeighborsClassifier
         KNeighborsClassifier(n_neighbors=3)
In [29]: from sklearn.metrics import accuracy_score
         y train hat = clf.predict(X train scaled)
         print('train accuracy: %.5f'%accuracy score(y train, y train hat))
         y_test_hat = clf.predict(X_test_scaled)
         print('test accuracy: %.5f'%accuracy_score(y_test, y_test_hat))
```

	X1_train	X2_train	X1_train_scaled	X2_train_scaled
0	8.92230	-0.63993	0.23502	0.00000
1	8.73371	2.49162	0.18706	0.51017
2	9.32298	5.09841	0.33693	0.93485
3	7.99815	4.85251	0.00000	0.89479
4	11.03295	-0.16817	0.77180	0.07686
5	9.17748	5.09283	0.29992	0.93394
6	11.56396	1.33894	0.90684	0.32238
7	9.15072	5.49832	0.29312	1.00000
8	8.34810	5.13416	0.08900	0.94067
9	11.93027	4.64866	1.00000	0.86158
		•		:

Results without Scaling

train accuracy: 0.94737 test accuracy: 0.85714

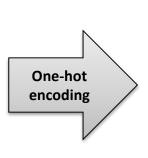
One-Hot Encoding

- Categorical features must be transformed into numeric features
- One-Hot Encoding: replace a categorical feature with multiple new features that can have the values 0 and 1 (one new feature per category)

class sklearn.preprocessing.OneHotEncoder(*, categories='auto', drop=None, sparse=True, dtype=<class 'numpy.float64'>, handle_unknown='error')

Example: Color Categories {Red, Green, Blue}

ID	Color	
1	Red	
2	Green	
3	Green	
4	Blue	
5	Green	
6	Red	
7	Red	
8	Red	
9	Green	
10	Blue	



ID	Color_Red	Color_Green	Color_Blue
1	1	0	0
2	0	1	0
3	0	1	0
4	0	0	1
5	0	1	0
6	1	0	0
7	1	0	0
8	1	0	0
9	0	1	0
10	0	0	1



