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
  - Gradient Boosting Machines
  - Support Vector Machines
  - Neural Networks

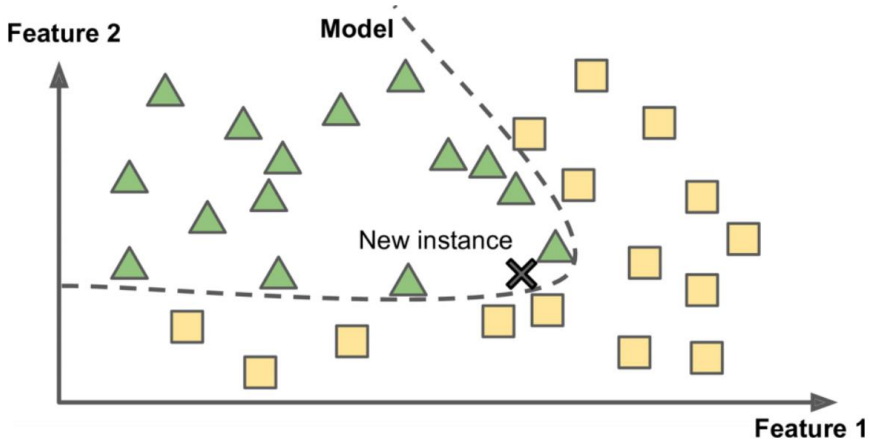
** Many algorithms have a classification and a regression variant, and we will describe both.*

** 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.*

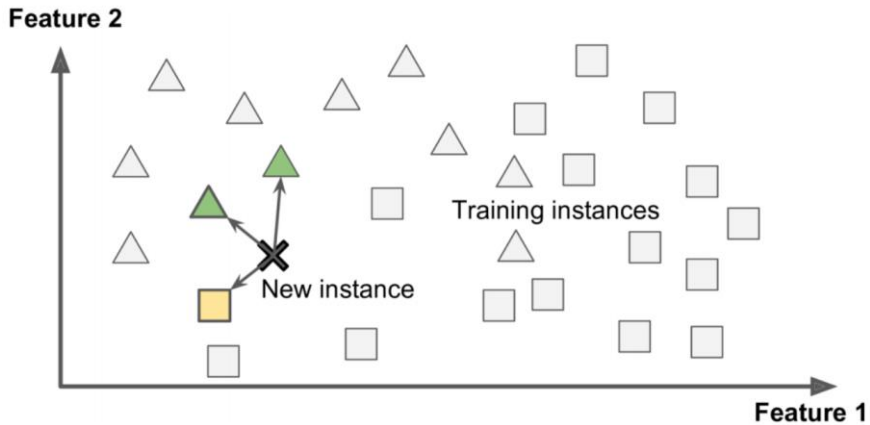
k-Nearest Neighbors

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.**

k-Nearest Neighbors

- 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.

k-Nearest Neighbors

- Given a (training) dataset $D = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_n, y_n)\}$ such that $\boldsymbol{x}_i = (x_{i1}, \dots, x_{id}) \in \mathbb{R}^d$ is the *i*-th input vector of *d* features and y_i is the corresponding target label.

- For a query data point $\boldsymbol{x}_{\text{new}}$
  1. Compute distance from $\boldsymbol{x}_{\text{new}}$ to each data point in D (distance metric)
  2. Identify *k* nearest neighbors of $\boldsymbol{x}_{\text{new}}$, $kNN(\boldsymbol{x}_{\text{new}}) = \{(\boldsymbol{x}_{(1)}, y_{(1)}), \dots, (\boldsymbol{x}_{(k)}, y_{(k)})\} \subset D$ (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?

k-Nearest Neighbors

- **For Classification,**

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

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

- **For Regression,**

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

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

$w(\boldsymbol{x}_{(i)}, \boldsymbol{x})$ is a weight function *(hyperparameter, not learned)*

e.g., inverse of Euclidean distance $\frac{1}{\|\boldsymbol{x}_{(i)} - \boldsymbol{x}\|_2}$

Hyperparameters

- **Distance metric**
  - Euclidean: $\left\|\boldsymbol{x}_{(i)} - \boldsymbol{x}\right\|_2$
  - Manhattan: $\left\|\boldsymbol{x}_{(i)} - \boldsymbol{x}\right\|_1$
  - Minkowski: $\left\|\boldsymbol{x}_{(i)} - \boldsymbol{x}\right\|_p$

  ** Distance Metrics available in scikit-learn*

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

- **The number of nearest neighbors *k***
  - Smaller *k* → capture local structure in data (but also noise)
  - Larger *k* → provide more smoothing, less noise, but may miss local structure

Hyperparameters

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

scikit-learn Practice: *KNeighborsClassifier*

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

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

Classifier implementing the k-nearest neighbors vote.

n_neighbors	*int, default=5* Number of neighbors to use by default for kneighbors queries.
weights	*{'uniform', 'distance'}, callable or None, 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. Refer to the example entitled Nearest Neighbors Classification showing the impact of the weights hyperparameter on the decision boundary.

scikit-learn Practice: *KNeighborsClassifier*

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

p	*float, default=2* Power hyperparameter for the Minkowski metric. When p = 1, this is equivalent to using manhattan_distance (l1), and euclidean_distance (l2) for p = 2. For arbitrary p, minkowski_distance (l_p) is used. This hyperparameter is expected to be positive.
metric	*str or callable, default='minkowski'* Metric to use for distance computation. Default is "minkowski", which results in the standard Euclidean distance when p = 2. See the documentation of scipy.spatial.distance and the metrics listed in distance_metrics for valid metric values. 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. If metric is a callable function, it takes two arrays representing 1D vectors as inputs and must return one value indicating the distance between those vectors. This works for Scipy's metrics, but is less efficient than passing the metric name as a string.
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.
predict(*X*)	Predict the class labels for the provided data X.
predict_proba(*X*)	Return probability estimates for the provided data X.

scikit-learn Practice: *KNeighborsClassifier*

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

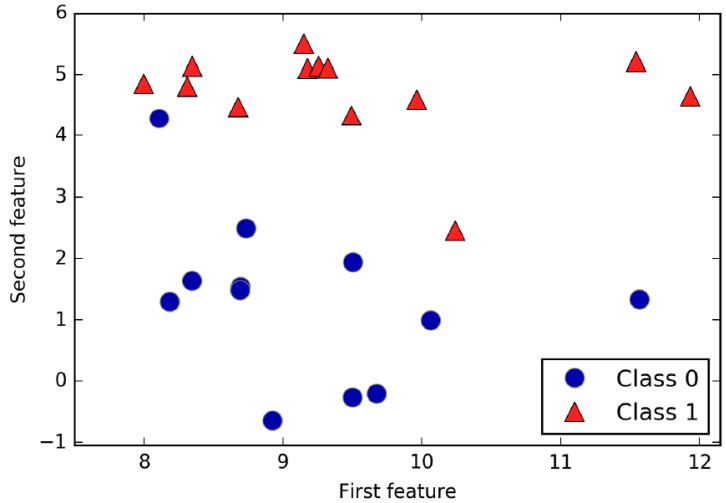
```
import mglearn
import matplotlib.pyplot as plt
```

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)
```



	X1	X2	Y
0	9.96347	4.59677	1
1	11.03295	-0.16817	0
2	11.54156	5.21116	1
3	8.69289	1.54322	0
4	8.10623	4.28696	0
5	8.30989	4.80624	1
6	11.93027	4.64866	1
7	9.67285	-0.20283	0
8	8.34810	5.13416	1
9	8.67495	4.47573	1
10	9.17748	5.09283	1
11	10.24029	2.45544	1
12	8.68937	1.48710	0
13	8.92230	-0.63993	0
14	9.49123	4.33225	1
15	9.25694	5.13285	1
16	7.99815	4.85251	1
17	8.18378	1.29564	0
18	8.73371	2.49162	0
19	9.32298	5.09841	1
20	10.06394	0.99078	0
21	9.50049	-0.26430	0
22	8.34469	1.63824	0
23	9.50169	1.93825	0
24	9.15072	5.49832	1
25	11.56396	1.33894	0

scikit-learn Practice: *KNeighborsClassifier*

- **Example (*forge* dataset): *k*=3**

[1]:
```
import mglearn
X, y = mglearn.datasets.make_forge()

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)
```

[2]:
```
from sklearn.neighbors import KNeighborsClassifier
clf = KNeighborsClassifier(n_neighbors=3)
clf.fit(X_train, y_train)
```

```
KNeighborsClassifier(n_neighbors=3)
```

[3]:
```
y_test_hat = clf.predict(X_test)
print(y_test)
print(y_test_hat)
```

```
[1 0 1 0 1 1 0]
[1 0 1 0 1 0 0]
```

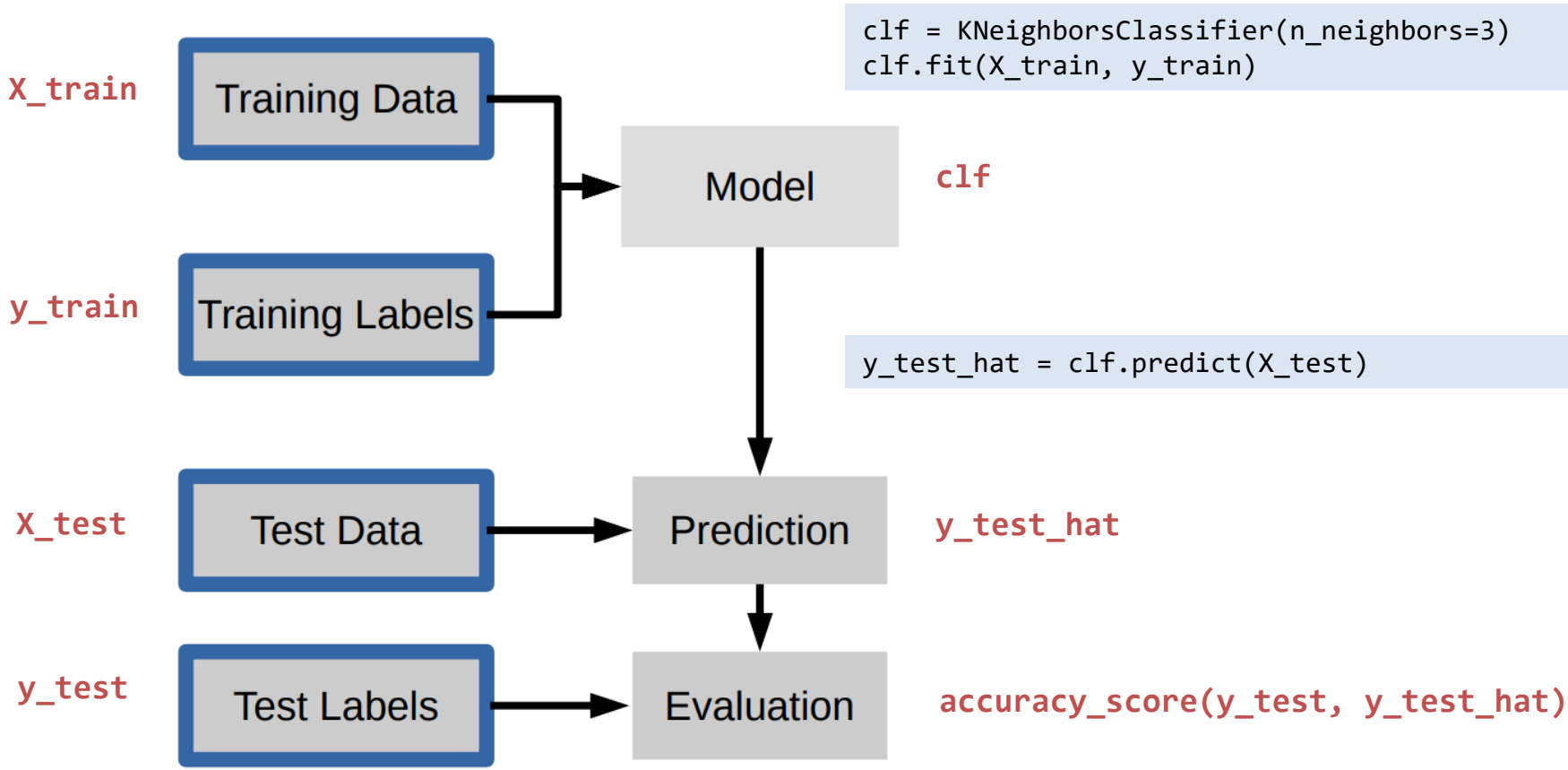
[4]:
```
from sklearn.metrics import accuracy_score
y_train_hat = clf.predict(X_train)
print('train accuracy: %.5f'%accuracy_score(y_train, y_train_hat))
y_test_hat = clf.predict(X_test)
print('test accuracy: %.5f'%accuracy_score(y_test, y_test_hat))
```

```
train accuracy: 0.94737
test accuracy: 0.85714
```

scikit-learn Practice: *KNeighborsClassifier*

- **Example (*forge* dataset): *k*=3**

```
X, y = mglearn.datasets.make_forge()
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.25, random_state=0)
```

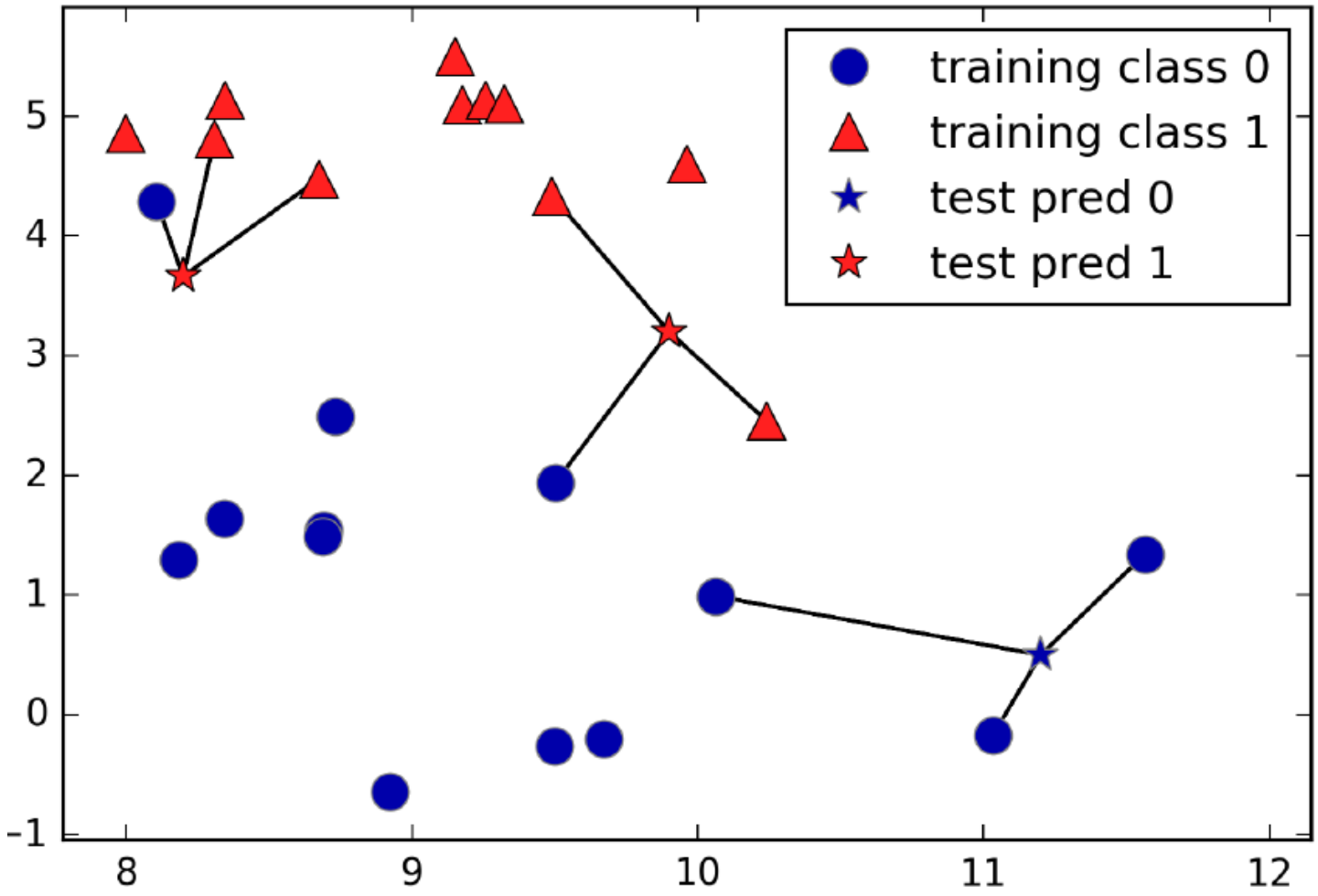



```
clf = KNeighborsClassifier(n_neighbors=3)
clf.fit(X_train, y_train)
```

```
y_test_hat = clf.predict(X_test)
```

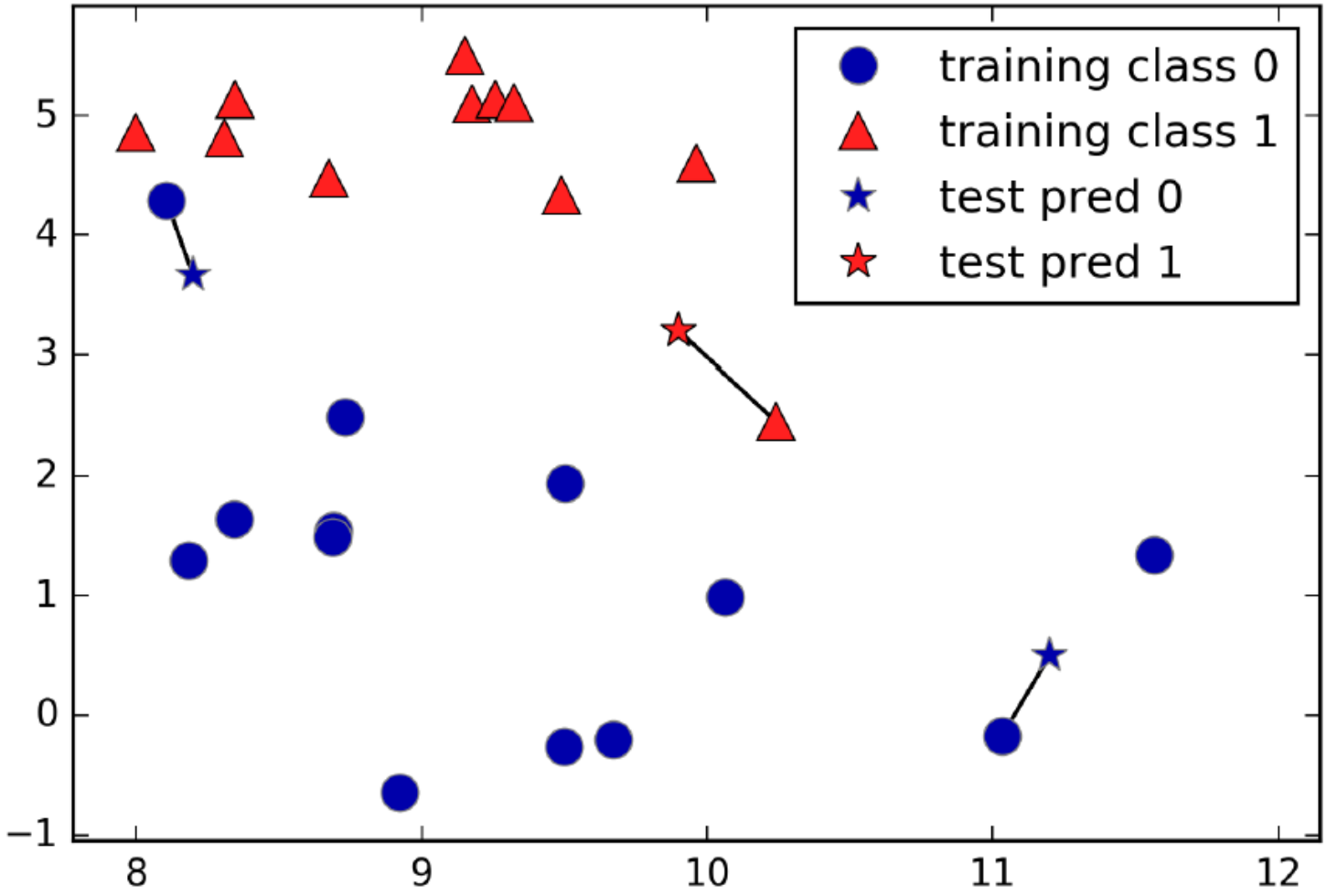
scikit-learn Practice: *KNeighborsClassifier*

- **Example (*forge* dataset): *k*=3**



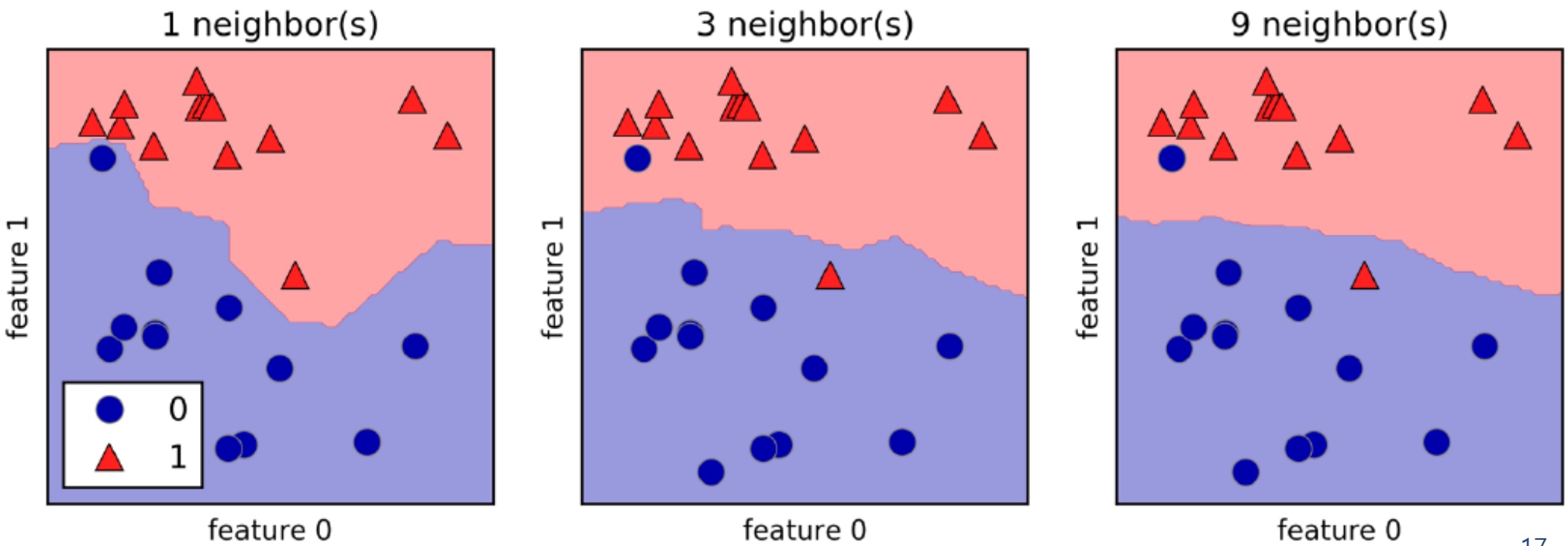
scikit-learn Practice: *KNeighborsClassifier*

- **Example (*forge* dataset): *k*=1**



scikit-learn Practice: *KNeighborsClassifier*

- **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)



scikit-learn Practice: *KNeighborsClassifier*

- **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.

scikit-learn Practice: *KNeighborsClassifier*

- **Example (*breast_cancer* dataset): varying the hyperparameter *k***

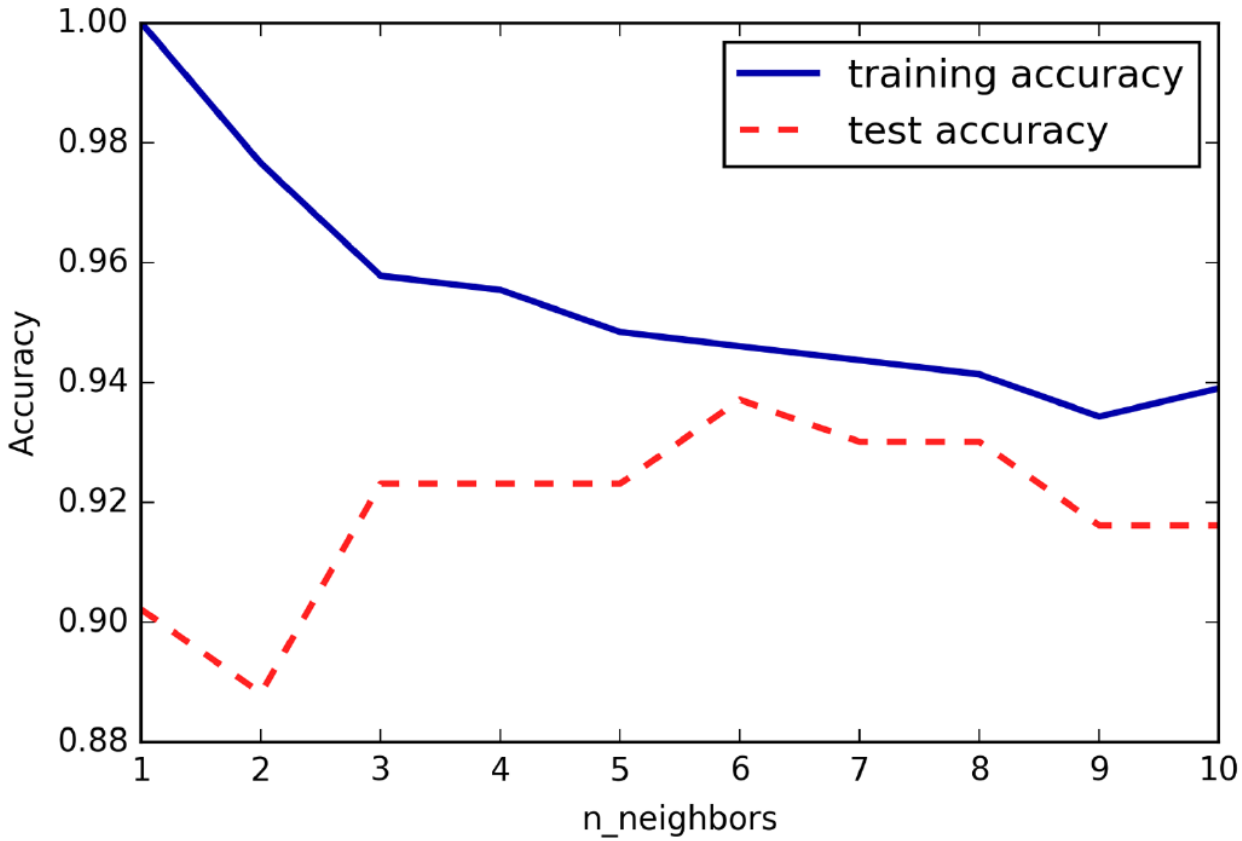
[1]:
```
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import accuracy_score

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)
```

[2]:
```
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

scikit-learn Practice: *KNeighborsClassifier*

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



scikit-learn Practice: *KNeighborsClassifier*

- **Example (*breast_cancer* dataset): varying the distance metric**

[1]:
```
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)
```

[2]:
```
training_accuracy = []
test_accuracy = []

p_settings = range(1, 6) # try n_neighbors from 1 to 10
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)

$$\left\|\boldsymbol{x}_{(i)} - \boldsymbol{x}\right\|_p$$

	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

scikit-learn Practice: *KNeighborsRegressor*

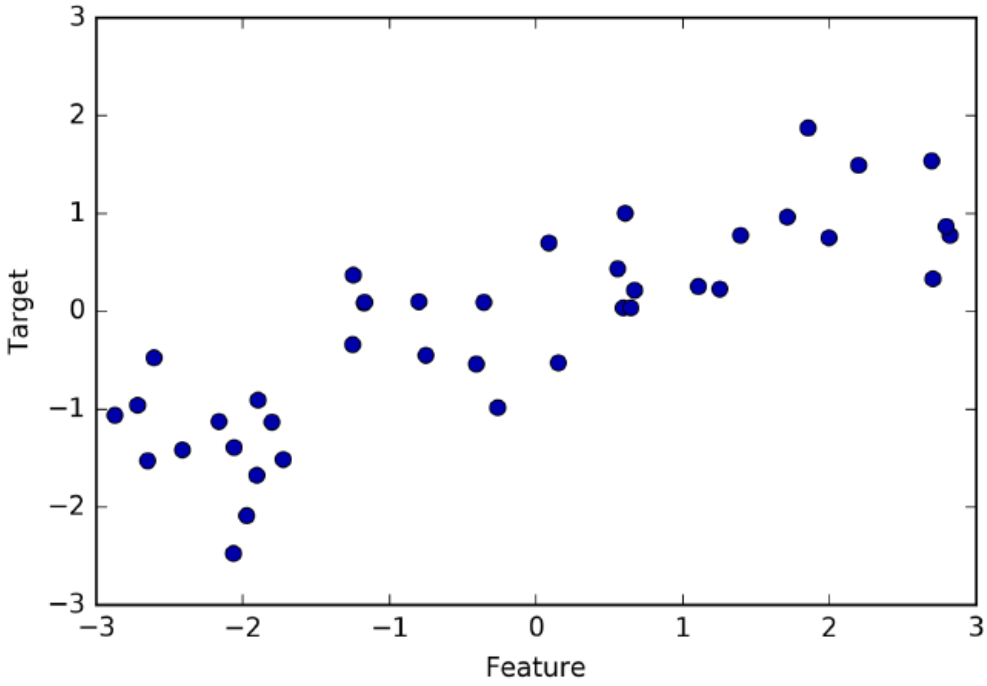
https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsRegressor.html

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

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.

scikit-learn Practice: *KNeighborsRegressor*

- **Example with the *wave* dataset**
  - The wave dataset is a synthetic dataset that has a single feature and a continuous target.



scikit-learn Practice: *KNeighborsRegressor*

- **Example (*wave* dataset): *k*=3**

[1]:
```
import mglearn
X, y = mglearn.datasets.make_wave(n_samples=40)

from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

[2]:
```
from sklearn.neighbors import KNeighborsRegressor
reg = KNeighborsRegressor(n_neighbors=3)
reg.fit(X_train, y_train)
```

```
KNeighborsRegressor(n_neighbors=3)
```

[3]:
```
y_test_hat = reg.predict(X_test)
print(y_test)
print(y_test_hat)
```

```
[ 0.37299 0.21778 0.96695 -1.38774 -1.0598 -0.90497 0.43656 0.77896 -0.54115 -0.95652]
[-0.05397 0.35686 1.13672 -1.89416 -1.13881 -1.63113 0.35686 0.91241 -0.4468 -1.13881]
```

[4]:
```
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
R_square: 0.83442
```

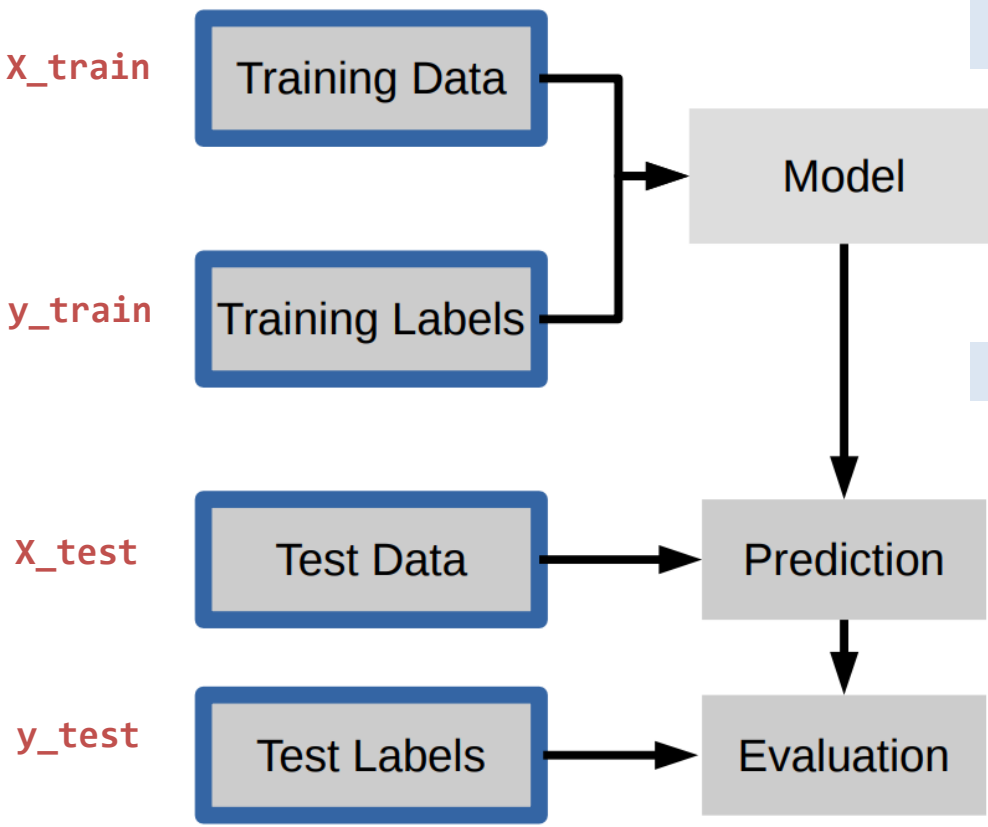
	X	Y
0	-0.75276	-0.44822
1	2.70429	0.33123
2	1.39196	0.77932
3	0.59195	0.03498
4	-2.06389	-1.38774
5	-2.06403	-2.47196
6	-2.65150	-1.52731
7	2.19706	1.49417
8	0.60669	1.00032
9	1.24844	0.22956
10	-2.87649	-1.05980
11	2.81946	0.77896
12	1.99466	0.75419
13	-1.72597	-1.51370
14	-1.90905	-1.67303
15	-1.89957	-0.90497
16	-1.17455	0.08449
17	0.14854	-0.52735
18	-0.40833	-0.54115
19	-1.25263	-0.34091
	⋮	⋮

scikit-learn Practice: *KNeighborsRegressor*

- **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)
```



reg

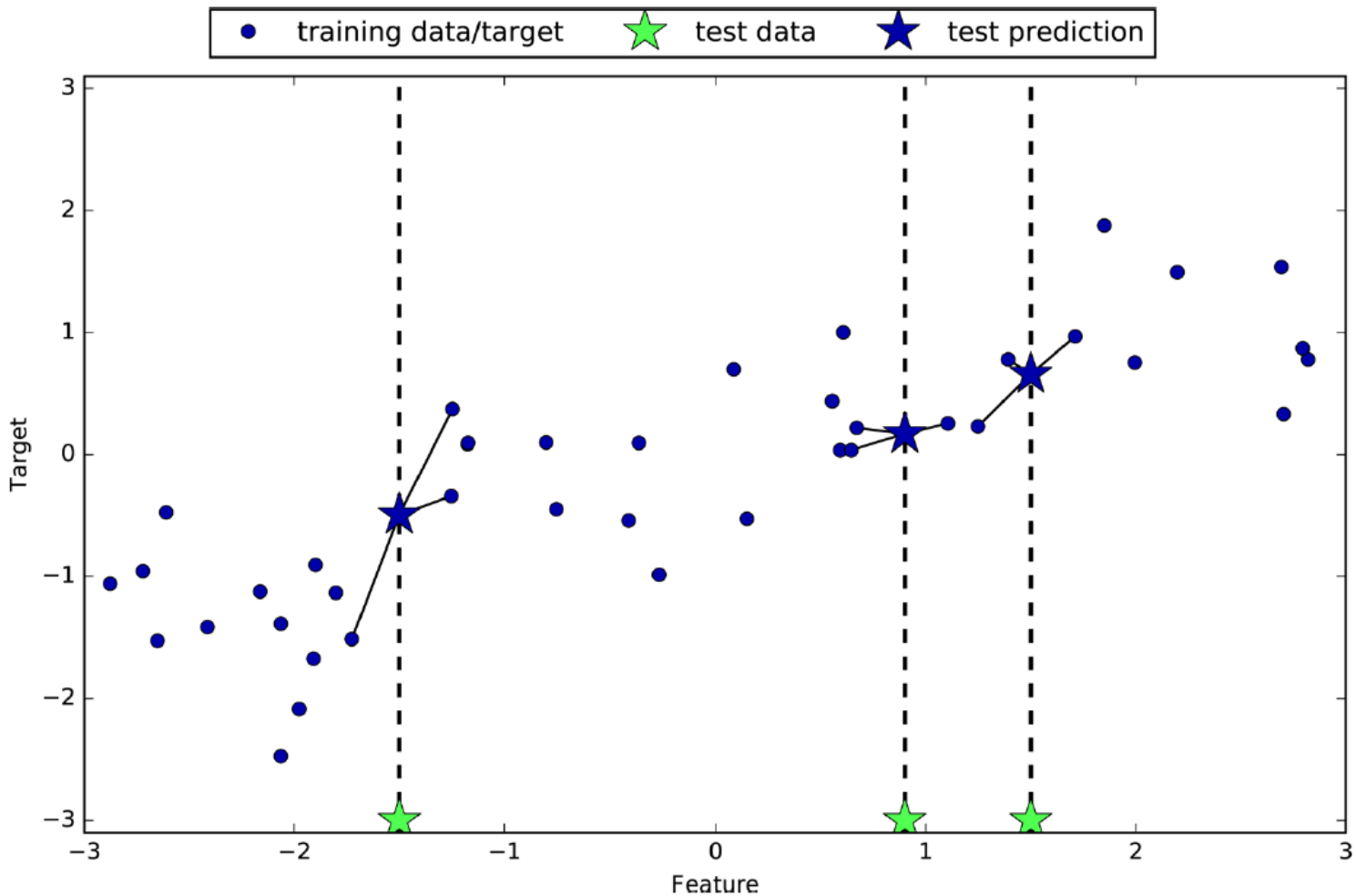
```
y_test_hat = reg.predict(X_test)
```

y_test_hat

```
mean_absolute_error(y_test,y_test_hat)
mean_squared_error(y_test,y_test_hat)**0.5
r2_score(y_test,y_test_hat)
```

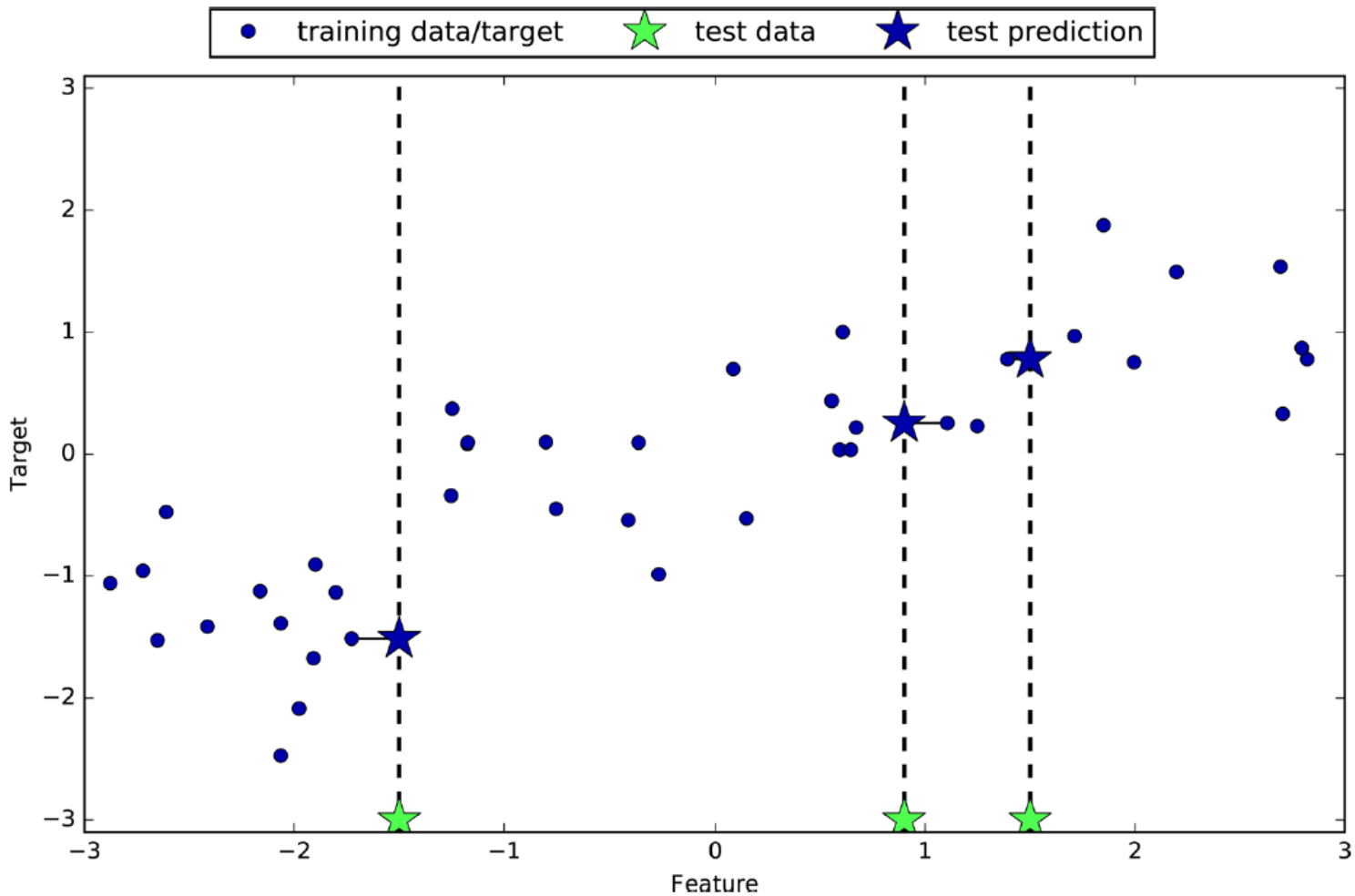
scikit-learn Practice: *KNeighborsRegressor*

- **Example (*wave* dataset): *k*=3**



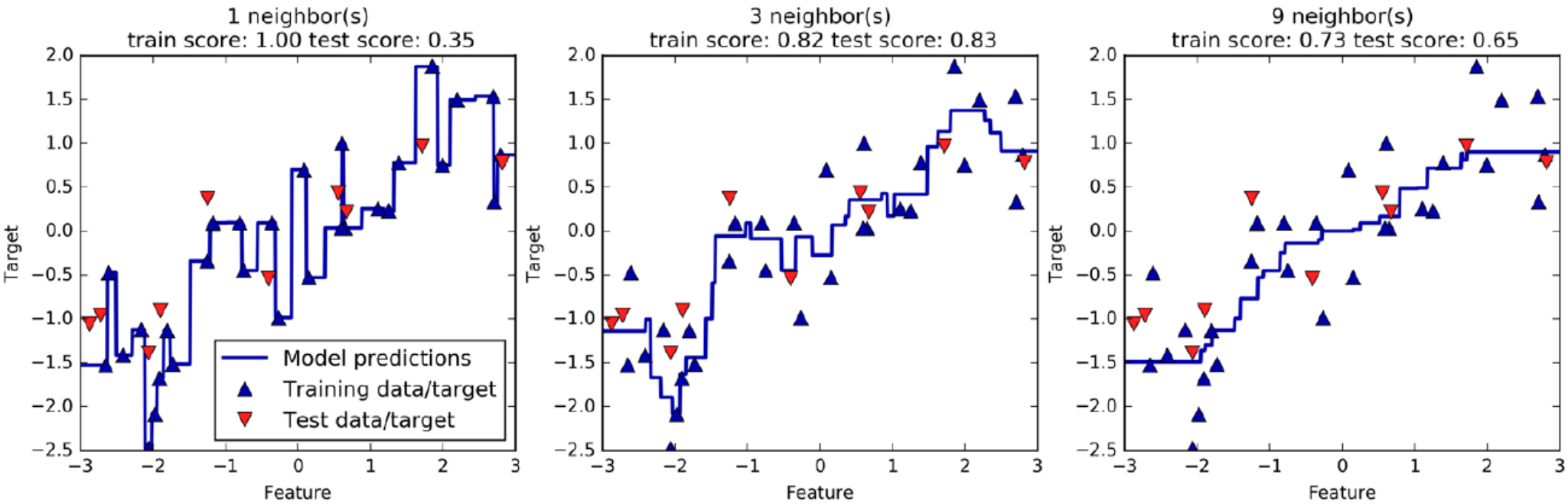
scikit-learn Practice: *KNeighborsRegressor*

- **Example (*wave* dataset): *k*=1**



scikit-learn Practice: *KNeighborsRegressor*

- **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 achieve the highest performance on validation data

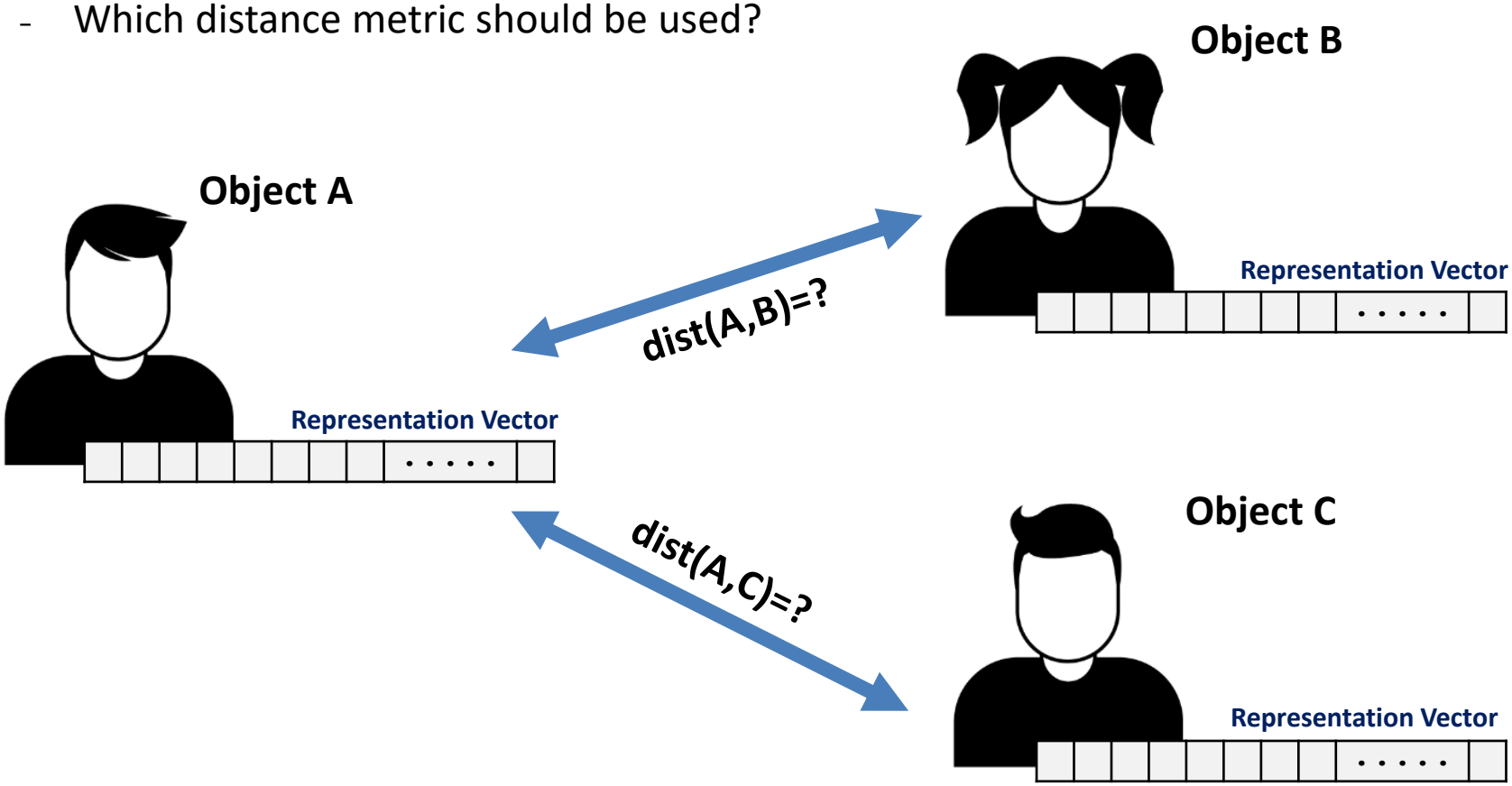
  * It's important to preprocess your data (including *data scaling* and *one-hot encoding*)

- **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)

Discussion

- **Determining distances between different objects**
  - Which features should be used?
  - How should the scale of each feature be determined?
  - Which distance metric should be used?



Discussion

- **How should the scale of each feature be determined?**
  - Certain features are more important than others in many applications.
  - It is often sensible to scale the features differently.

  - **Example: How feature scaling affects distance comparisons**

Original Dataset

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

$$\mathrm{dist}(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{10049} \simeq 100.2$$
$$\mathrm{dist}(\boldsymbol{a}, \boldsymbol{c}) = \sqrt{64} = 8$$

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

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

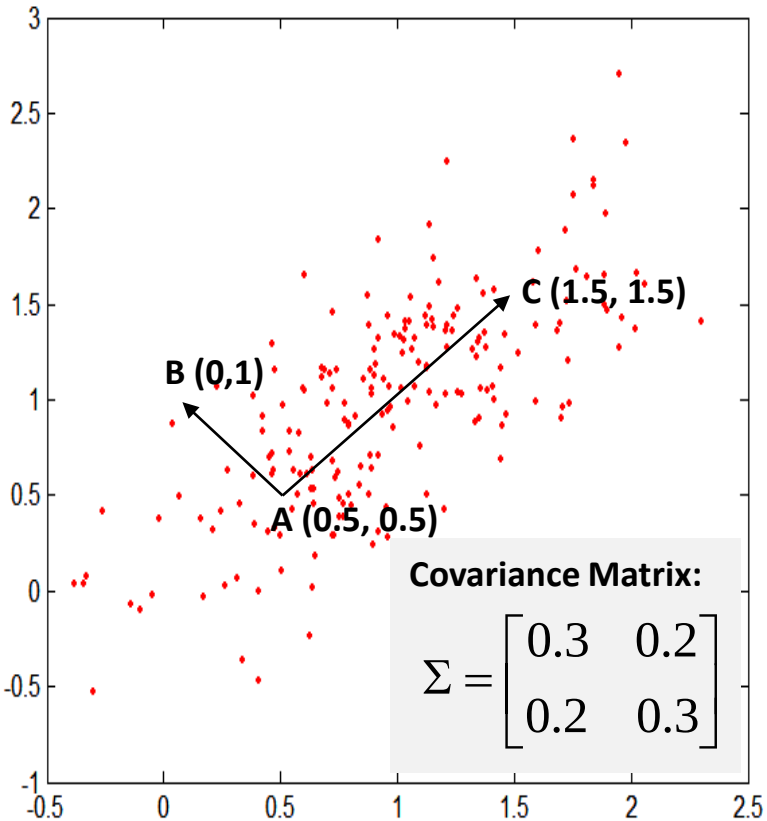
$$\mathrm{dist}(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{50} \simeq 7.1$$
$$\mathrm{dist}(\boldsymbol{a}, \boldsymbol{c}) = \sqrt{64} = 8$$

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

*** Assuming Euclidean distance as the distance metric**

Discussion

- **Which distance metric should be used?**



Euclidean Distance $d(\mathbf{x}, \mathbf{y}) = \|\mathbf{x} - \mathbf{y}\|_2 = \sqrt{(\mathbf{x} - \mathbf{y})^T (\mathbf{x} - \mathbf{y})}$

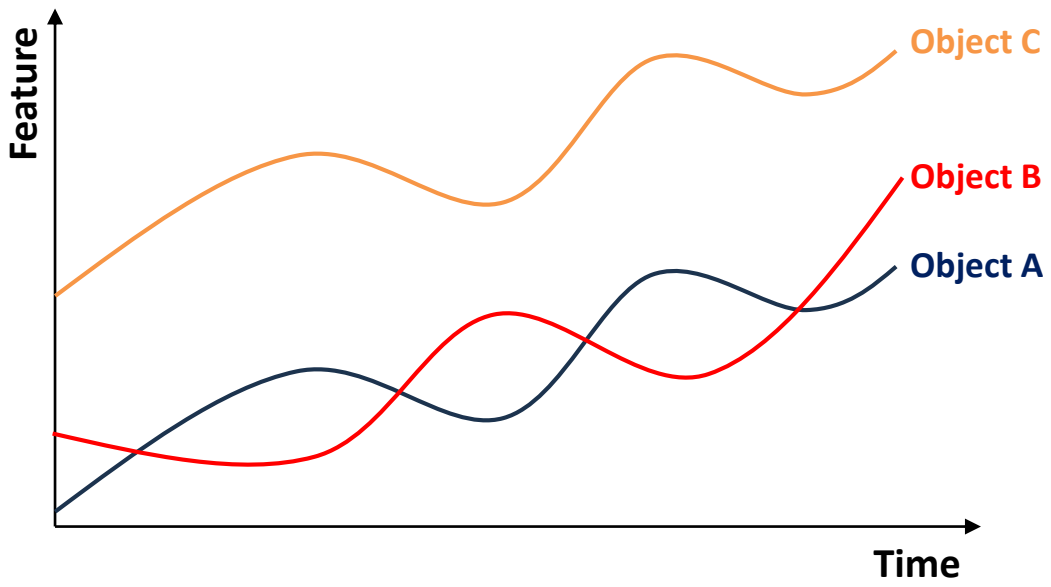
$d(\boldsymbol{A}, \boldsymbol{B}) = 0.707, \; d(\boldsymbol{A}, \boldsymbol{C}) = 1.414$

Mahalanobis Distance $d(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^T \Sigma^{-1} (\mathbf{x} - \mathbf{y})}$

$d(\boldsymbol{A}, \boldsymbol{B}) = 5, \; d(\boldsymbol{A}, \boldsymbol{C}) = 4$

Discussion

- **Subjectivity in determining distances**
  - The suitable distance metric may vary depending on the problem context.
  - It is important to choose or define distance metrics based on domain knowledge.
  - **Example: In the time-series data below, is object A more similar to B or C?**



Data Preprocessing and Scaling

Data Scaling

- **Some supervised learning algorithms, like *k*-nearest neighbors, support vector machines, and neural networks are very sensitive to the scaling of the data.**
  - It is important to adjust the features so that the data representation is more suitable for these algorithms.

- **Common practice: Putting all numeric features on the same scale**
  - It can be used when features with the largest scales would dominate and skew results.
  - It often improves the accuracy of supervised algorithms and leads to reduced memory and time consumption.

Data Scaling

- **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. This ensures that for each feature the mean is 0 and the variance is 1.

```
class sklearn.preprocessing.StandardScaler(*, copy=True, with_mean=True, with_std=True)
```

  - **MinMax Scaling:** Scale to [0,1] ([-1,1] recommended) by subtracting minimum and dividing by the range. This shifts and scales the data such that all features fall exactly within the specified range.

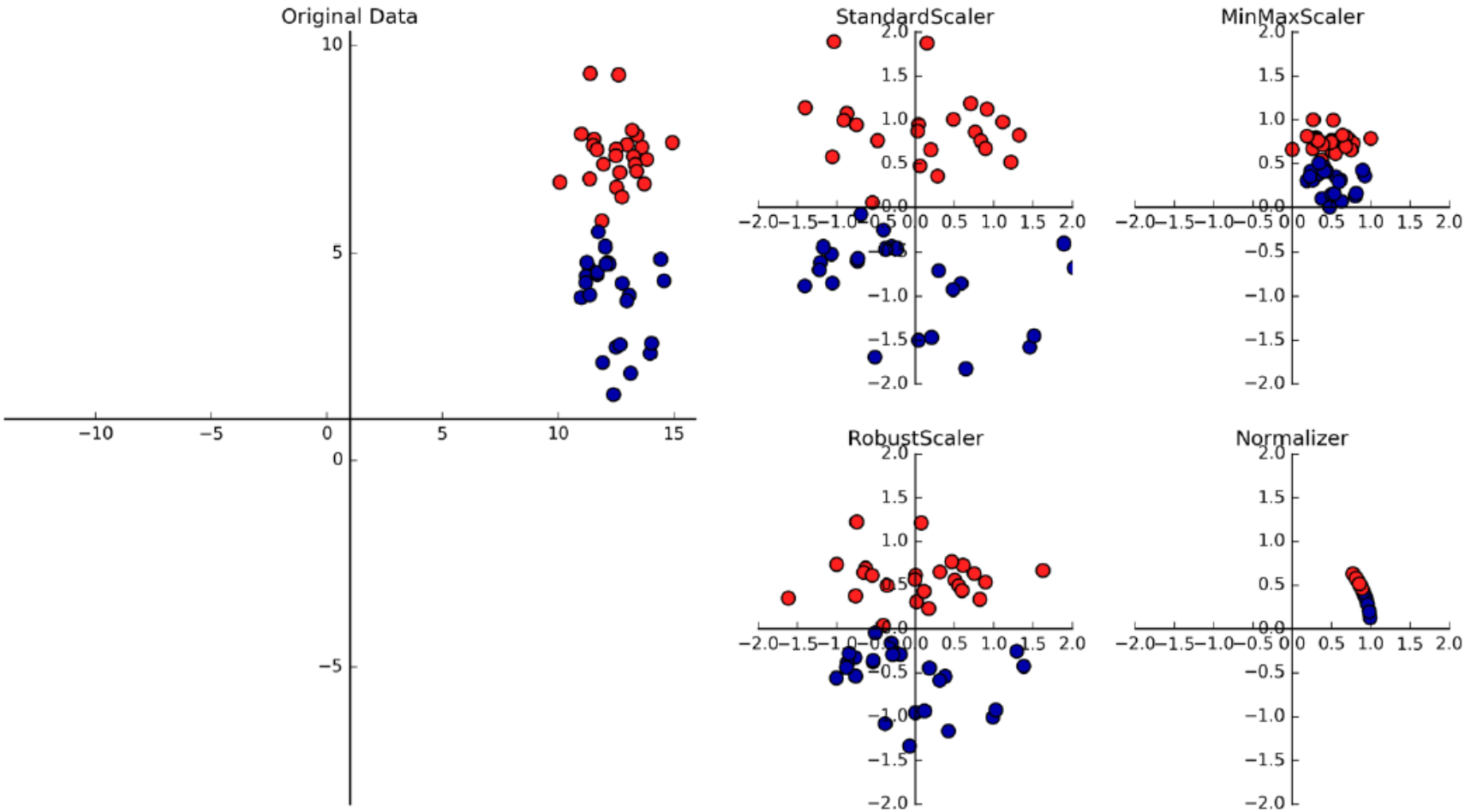
```
class sklearn.preprocessing.MinMaxScaler(feature_range=(0, 1), *, copy=True, clip=False)
```

  - **Robust Scaling**: Transform by subtracting the **median** (instead of mean) and then dividing by the **interquartile range** (instead of standard deviation). The median and interquartile range are used to ignore outliers.

```
class sklearn.preprocessing.RobustScaler(*, with_centering=True, with_scaling=True,
quantile_range=(25.0, 75.0), copy=True, unit_variance=False)
```

Data Scaling

- **Example: a synthetic two-class classification dataset with two features**



scikit-learn Practice: *StandardScaler*

https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html

```
class sklearn.preprocessing.StandardScaler(*, copy=True, with_mean=True, with_std=True)
```

Standardize features by removing the mean and scaling to unit variance.

The standard score of a sample x is calculated as:

z = (x - u) / s

where u is the mean of the training samples or zero if with_mean=False, and s is the standard deviation of the training samples or one if with_std=False.

Centering and scaling happen independently on each feature by computing the relevant statistics on the samples in the training set. Mean and standard deviation are then stored to be used on later data using transform.

Standardization of a dataset is a common requirement for many machine learning estimators: they might behave badly if the individual features do not more or less look like standard normally distributed data (e.g. Gaussian with 0 mean and unit variance).

For instance many elements used in the objective function of a learning algorithm (such as the RBF kernel of Support Vector Machines or the L1 and L2 regularizers of linear models) assume that all features are centered around 0 and have variance in the same order. If a feature has a variance that is orders of magnitude larger than others, it might dominate the objective function and make the estimator unable to learn from other features correctly as expected.

StandardScaler is sensitive to outliers, and the features may scale differently from each other in the presence of outliers. For an example visualization, refer to Compare StandardScaler with other scalers.

This scaler can also be applied to sparse CSR or CSC matrices by passing with_mean=False to avoid breaking the sparsity structure of the data.

scikit-learn Practice: *StandardScaler*

https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html

Methods	
fit(*X*, *y*=*None*, *sample_weight*=*None*)	Compute the mean and std to be used for later scaling.
fit_transform(*X*, *y*=*None*, ***fit_params*)	Fit to data, then transform it. Fits transformer to X and y with optional parameters fit_params and returns a transformed version of X.
inverse_transform(*X*, *copy*=*None*)	Scale back the data to the original representation.
transform(*X*, *copy*=*None*)	Perform standardization by centering and scaling.

scikit-learn Practice: *StandardScaler*

- **Example of Standard Scaling**

[1]:
```
import pandas as pd
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target, random_state=1)
```

[2]:
```
pd.DataFrame(X_train).head()
```

	0	1	2	3	4	5	6	7	8	9	...
0	15.22	30.62	103.40	716.9	0.10480	0.20870	0.25500	0.094290	0.2128	0.07152	...
1	14.96	19.10	97.03	687.3	0.08992	0.09823	0.05940	0.048190	0.1879	0.05852	...
2	14.68	20.13	94.74	684.5	0.09867	0.07200	0.07395	0.052590	0.1586	0.05922	...
3	10.32	16.35	65.31	324.9	0.09434	0.04994	0.01012	0.005495	0.1885	0.06201	...
4	11.85	17.46	75.54	432.7	0.08372	0.05642	0.02688	0.022800	0.1875	0.05715	...

[3]:
```
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
X_train_scaled = scaler.fit_transform(X_train)
```

[4]:
```
pd.DataFrame(X_train_scaled).head()
```

	0	1	2	3	4	5	6	7	8	9	...
0	0.305754	2.595219	0.462461	0.168272	0.604222	2.044178	2.093529	1.163667	1.181984	1.284296	...
1	0.233517	-0.053349	0.205731	0.086315	-0.474245	-0.124576	-0.366220	-0.016409	0.263950	-0.633174	...
2	0.155724	0.183459	0.113437	0.078562	0.159934	-0.639524	-0.183248	0.096223	-0.816308	-0.529925	...
3	-1.055627	-0.685603	-1.072681	-0.917106	-0.153894	-1.072608	-0.985935	-1.109322	0.286071	-0.118407	...
4	-0.630543	-0.430402	-0.660381	-0.618627	-0.923606	-0.945392	-0.775172	-0.666346	0.249202	-0.835245	...

scikit-learn Practice: *MinMaxScaler*

https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.MinMaxScaler.html

```
class sklearn.preprocessing.MinMaxScaler(feature_range=(0, 1), *, copy=True, clip=False)
```

Transform features by scaling each feature to a given range.

This estimator scales and translates each feature individually such that it is in the given range on the training set, e.g. between zero and one.

The transformation is given by:

```
X_std = (X - X.min(axis=0)) / (X.max(axis=0) - X.min(axis=0))
X_scaled = X_std * (max - min) + min
```

where min, max = feature_range.

This transformation is often used as an alternative to zero mean, unit variance scaling.

MinMaxScaler doesn't reduce the effect of outliers, but it linearly scales them down into a fixed range, where the largest occurring data point corresponds to the maximum value and the smallest one corresponds to the minimum value. For an example visualization, refer to Compare MinMaxScaler with other scalers.

feature_range	*tuple (min, max), default=(0, 1)* Desired range of transformed data.

scikit-learn Practice: *MinMaxScaler*

- **Example of MinMax Scaling**

[1]:
```
import pandas as pd
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target, random_state=1)
```

[2]:
```
pd.DataFrame(X_train).head()
```

	0	1	2	3	4	5	6	7	8	9	...
0	15.22	30.62	103.40	716.9	0.10480	0.20870	0.25500	0.094290	0.2128	0.07152	...
1	14.96	19.10	97.03	687.3	0.08992	0.09823	0.05940	0.048190	0.1879	0.05852	...
2	14.68	20.13	94.74	684.5	0.09867	0.07200	0.07395	0.052590	0.1586	0.05922	...
3	10.32	16.35	65.31	324.9	0.09434	0.04994	0.01012	0.005495	0.1885	0.06201	...
4	11.85	17.46	75.54	432.7	0.08372	0.05642	0.02688	0.022800	0.1875	0.05715	...

[3]:
```
from sklearn.preprocessing import MinMaxScaler
scaler = MinMaxScaler(feature_range=(-1,1))
X_train_scaled = scaler.fit_transform(X_train)
```

[4]:
```
pd.DataFrame(X_train_scaled).head()
```

	0	1	2	3	4	5	6	7	8	9	...
0	-0.220124	0.414271	-0.176145	-0.513552	-0.058048	0.416430	0.194939	-0.062724	0.078788	-0.064821	...
1	-0.244735	-0.364897	-0.264184	-0.538664	-0.326713	-0.410070	-0.721649	-0.520974	-0.172727	-0.636124	...
2	-0.271239	-0.295232	-0.295833	-0.541039	-0.168728	-0.606315	-0.653468	-0.477237	-0.468687	-0.605361	...
3	-0.683942	-0.550896	-0.702578	-0.846108	-0.246908	-0.771360	-0.952577	-0.945378	-0.166667	-0.482751	...
4	-0.539117	-0.475820	-0.561191	-0.754655	-0.438657	-0.722879	-0.874039	-0.773360	-0.176768	-0.696330	...

scikit-learn Practice: *RobustScaler*

https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.RobustScaler.html

```
class sklearn.preprocessing.RobustScaler(*, with_centering=True, with_scaling=True,
quantile_range=(25.0, 75.0), copy=True, unit_variance=False)
```

Scale features using statistics that are robust to outliers.

This Scaler removes the median and scales the data according to the quantile range (defaults to IQR: Interquartile Range). The IQR is the range between the 1st quartile (25th quantile) and the 3rd quartile (75th quantile).

Centering and scaling happen independently on each feature by computing the relevant statistics on the samples in the training set. Median and interquartile range are then stored to be used on later data using the transform method.

Standardization of a dataset is a common preprocessing for many machine learning estimators. Typically this is done by removing the mean and scaling to unit variance. However, outliers can often influence the sample mean / variance in a negative way. In such cases, using the median and the interquartile range often give better results. For an example visualization and comparison to other scalers, refer to Compare RobustScaler with other scalers.

quantile_range	*tuple (q_min, q_max), 0.0 < q_min < q_max < 100.0, default=(25.0, 75.0)* Quantile range used to calculate scale_. By default this is equal to the IQR, i.e., q_min is the first quantile and q_max is the third quantile.

Effect of Data Scaling on Supervised Learning

- **Example (*forge* dataset) with *StandardScaler***

[1]:
```
import mglearn
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import accuracy_score

X, y = mglearn.datasets.make_forge()
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.25, random_state=0)
```

[2]:
```
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

[3]:
```
clf = KNeighborsClassifier(n_neighbors=3)
clf.fit(X_train_scaled, y_train)
```

```
KNeighborsClassifier(n_neighbors=3)
```

[4]:
```
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))
```

```
train accuracy: 0.94737
test accuracy: 0.85714
```

	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
```

Effect of Data Scaling on Supervised Learning

- **Example (*forge* dataset) with *MinMaxScaler***

[1]:
```
import mglearn
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import accuracy_score

X, y = mglearn.datasets.make_forge()
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.25, random_state=0)
```

[2]:
```
scaler = MinMaxScaler(feature_range=(-1,1))
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

[3]:
```
clf = KNeighborsClassifier(n_neighbors=3)
clf.fit(X_train_scaled, y_train)
```

```
KNeighborsClassifier(n_neighbors=3)
```

[4]:
```
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))
```

```
train accuracy: 0.94737
test accuracy: 0.85714
```

	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
```

Effect of Data Scaling on Supervised Learning

- **Example (*breast_cancer* dataset) with *StandardScaler***

[1]:
```
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.svm import SVC
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, random_state=0)
```

[2]:
```
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

[3]:
```
clf = SVC()
clf.fit(X_train_scaled, y_train)
```

```
SVC()
```

[4]:
```
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))
```

```
train accuracy: 0.98592
test accuracy: 0.96503
```

Results without Scaling

```
train accuracy: 0.90376
test accuracy: 0.93706
```

Effect of Data Scaling on Supervised Learning

- **Example (*breast_cancer* dataset) with *MinMaxScaler***

[1]:
```
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler
from sklearn.svm import SVC
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, random_state=0)
```

[2]:
```
scaler = MinMaxScaler(feature_range=(-1,1))
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

[3]:
```
clf = SVC()
clf.fit(X_train_scaled, y_train)
```

```
SVC()
```

[4]:
```
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))
```

```
train accuracy: 0.98357
test accuracy: 0.97203
```

Results without Scaling

```
train accuracy: 0.90376
test accuracy: 0.93706
```

One-Hot Encoding

- **For most supervised learning algorithms, 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_output=True,
dtype=<class 'numpy.float64'>, handle_unknown='error', min_frequency=None, max_categories=None,
feature_name_combiner='concat')
```

- **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

One-hot encoding

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