Machine Learning Tutorial

Week2

Introduction to Supervised Learning

Supervised Learning

$$(x_i, y_i) \propto p(x, y) \text{ i.i.d.}$$

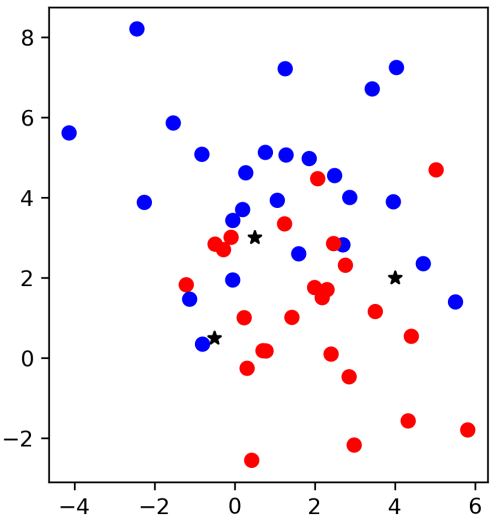
$$x_i \in \mathbb{R}^p$$

$$y_i \in \mathbb{R}$$

$$f(x_i) \approx y_i$$

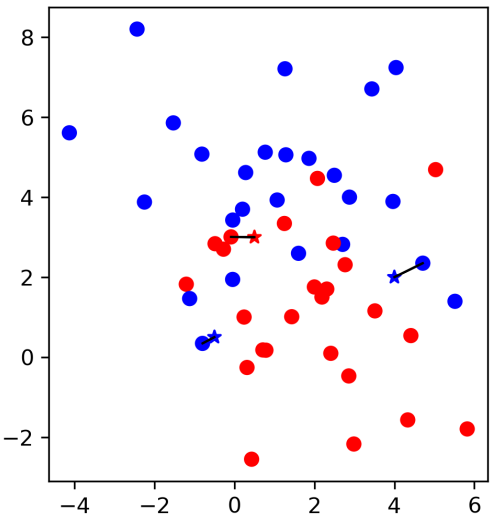
$$f(x) \approx y$$

Nearest Neighbors



$$f(x) = y_i, i = \text{argmin}_j ||x_j - x||$$

Nearest Neighbors



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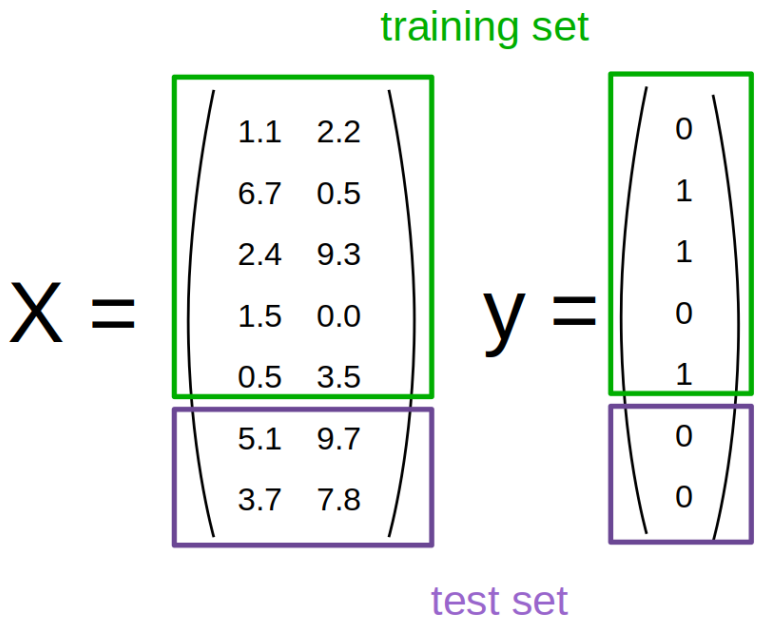
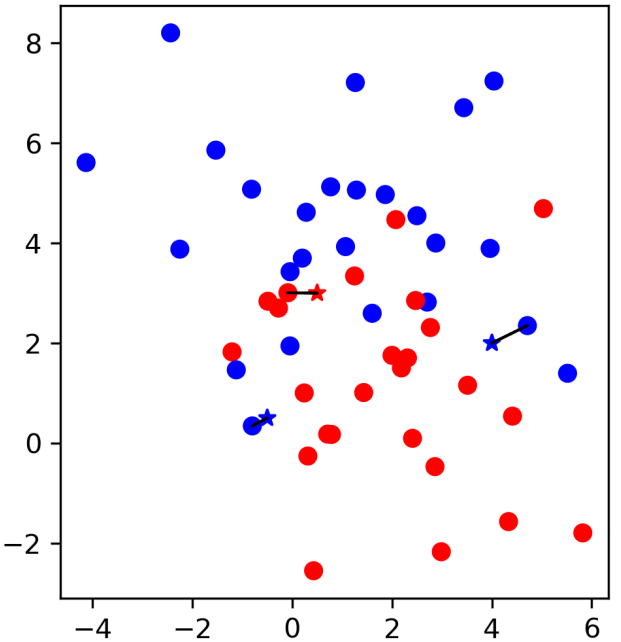

training set
X =
1.1 2.2
6.7 0.5
2.4 9.3
1.5 0.0
0.5 3.5
5.1 9.7
3.7 7.8
y =
0
1
1
0
1
0
0
test set

KNN with scikit-learn

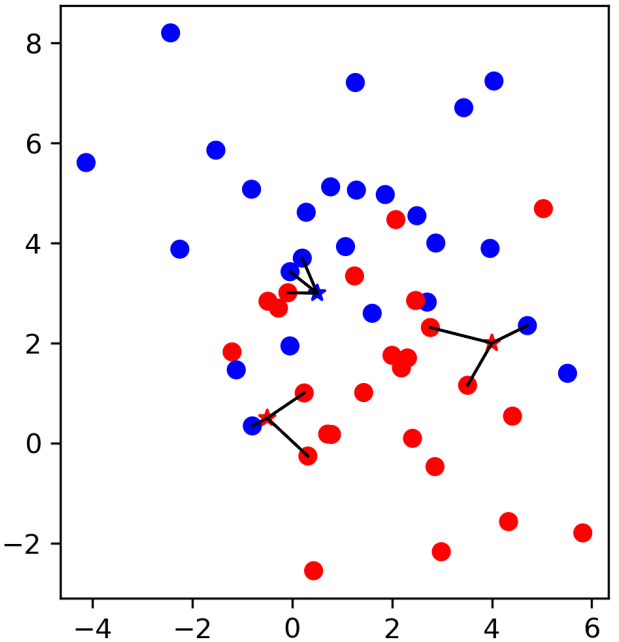
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y)

from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=1)
knn.fit(X_train, y_train)
print("accuracy: {:.2f}".format(knn.score(X_test, y_test)))
y_pred = knn.predict(X_test)
```

accuracy: 0.77

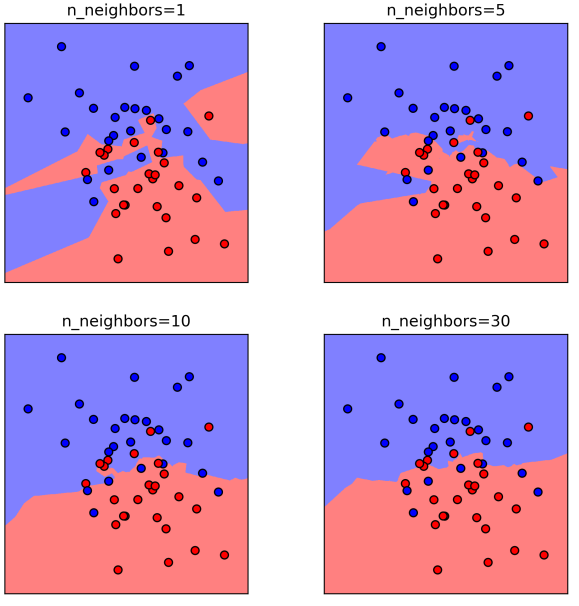
More neighbors



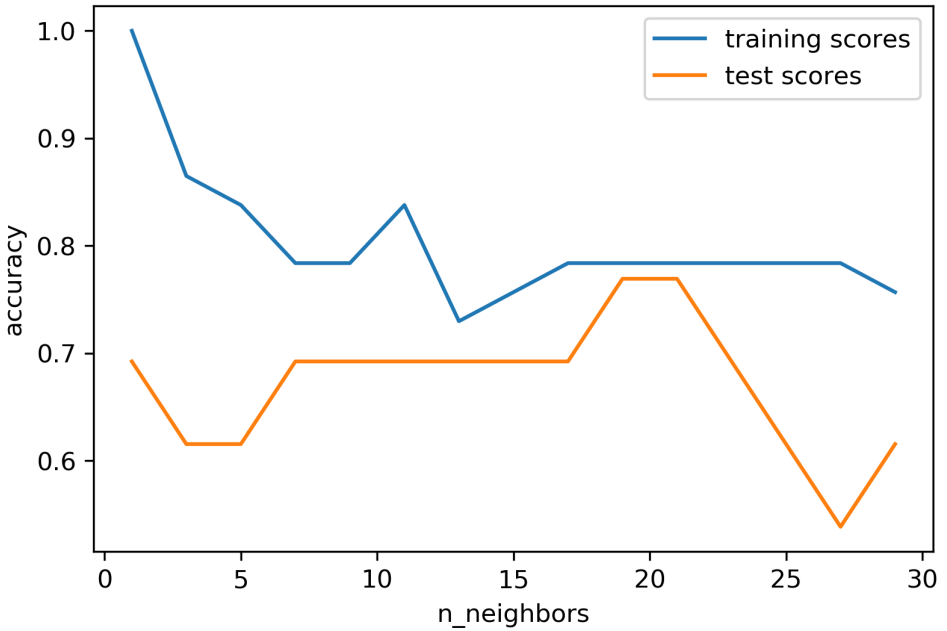
More neighbors



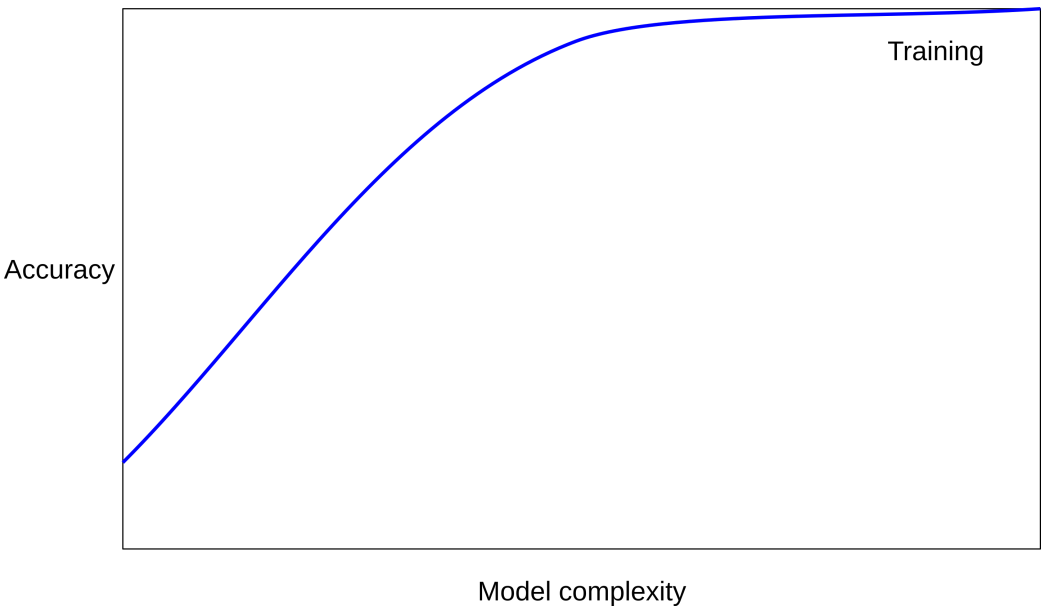
Influence of n_neighbors



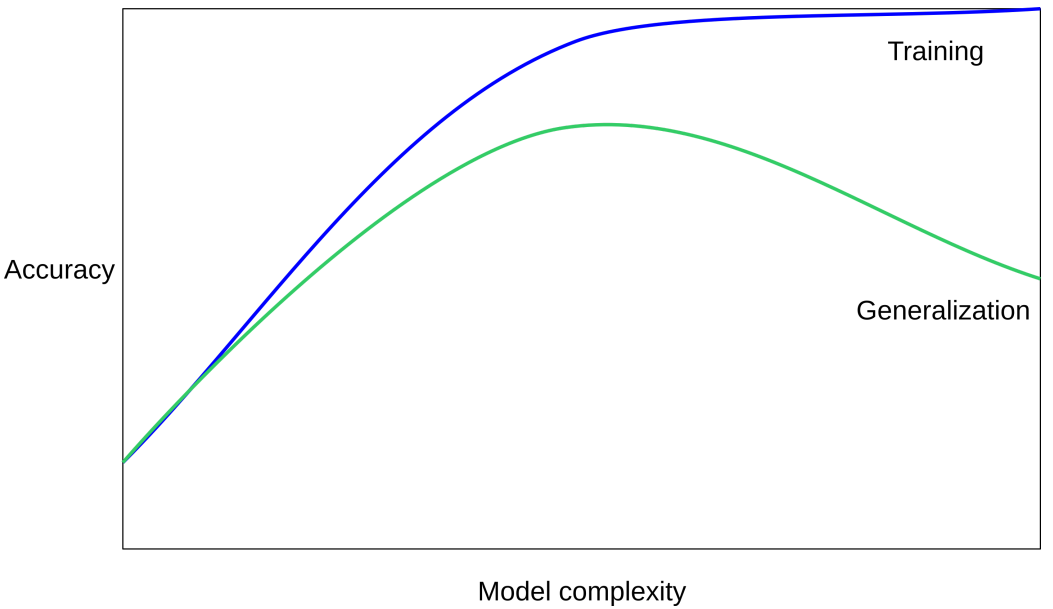
Model complexity



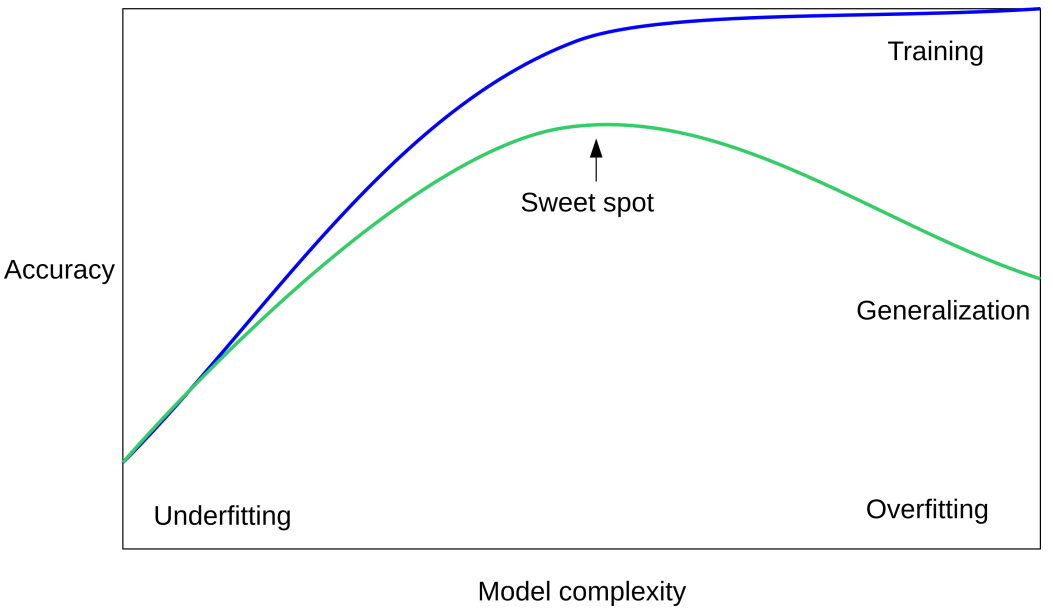
Overfitting and Underfitting



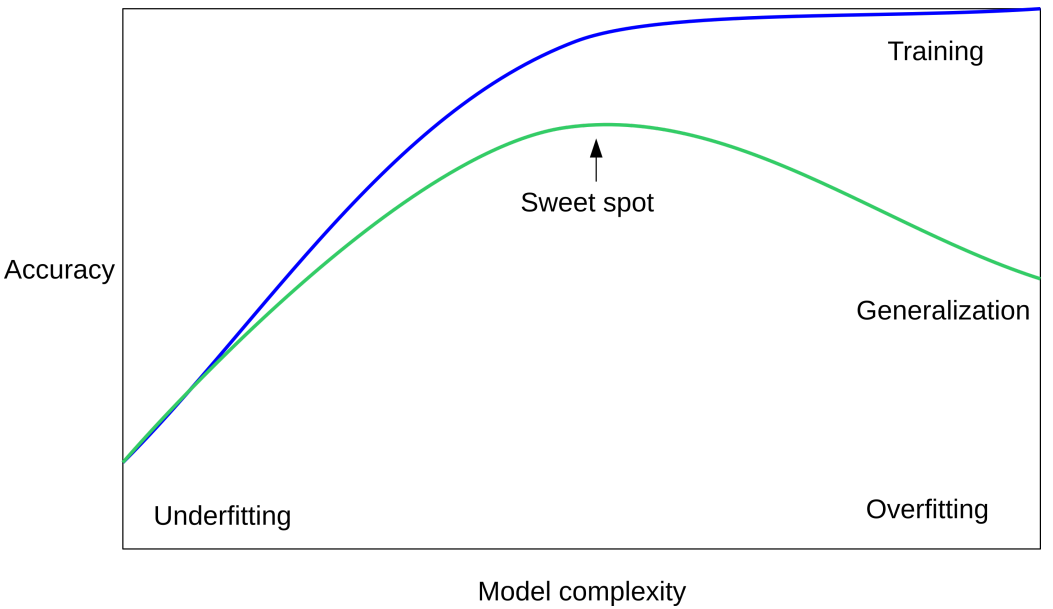
Overfitting and Underfitting

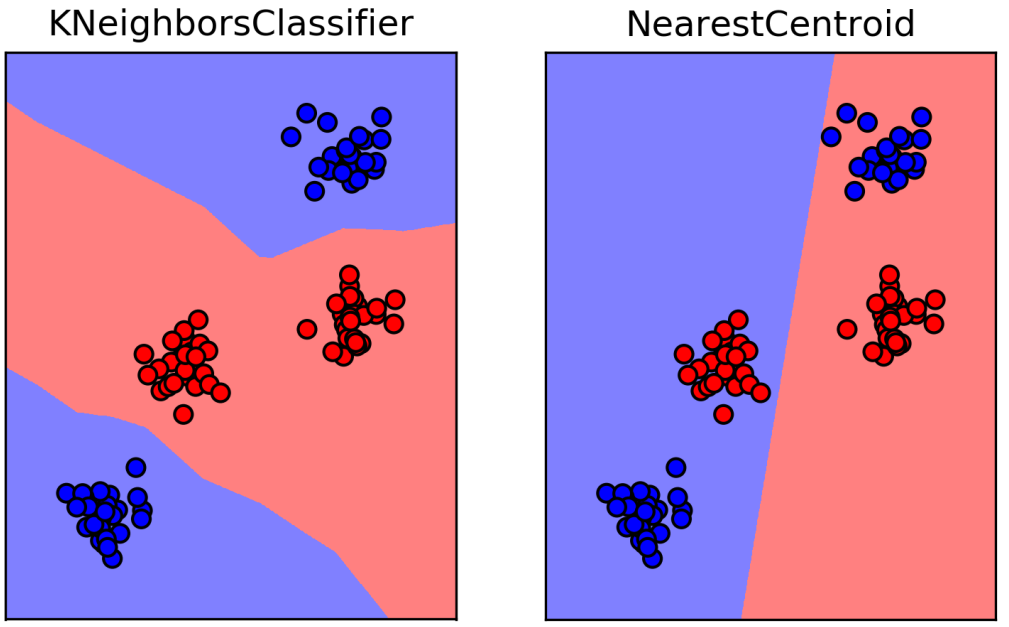


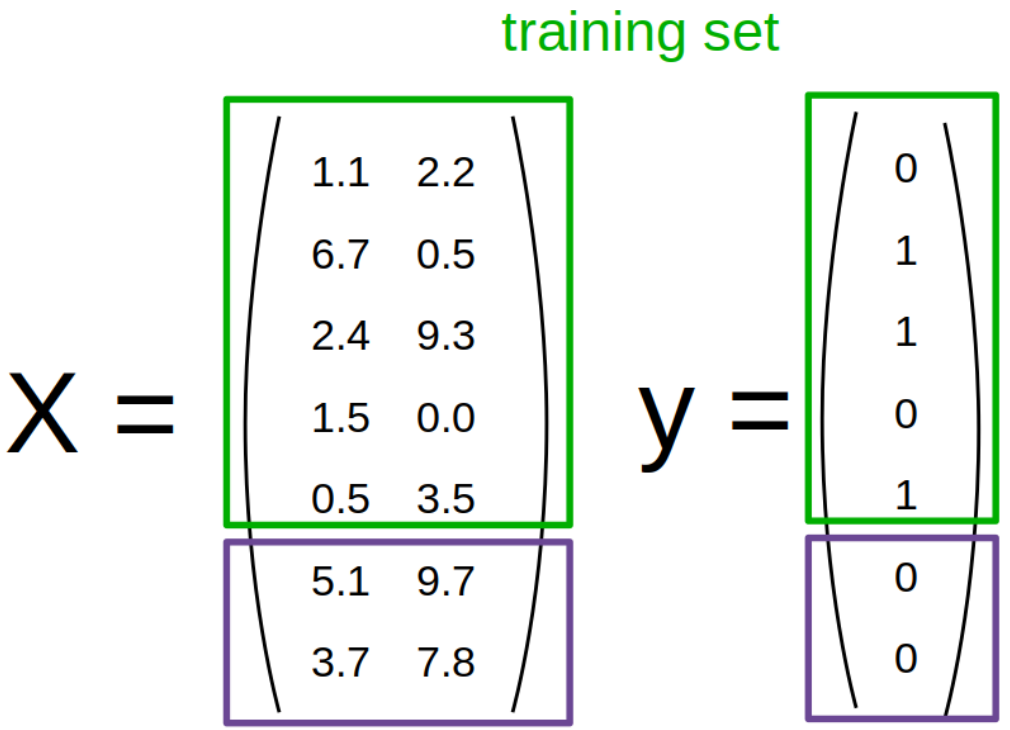
Overfitting and Underfitting



Overfitting and Underfitting




KNeighborsClassifier
NearestCentroid


training set
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1.5 0.0
0.5 3.5
5.1 9.7
3.7 7.8
y =
0
1
1
0
1
0
0

Overfitting the validation set

```
from sklearn.datasets import load_breast_cancer
from sklearn.preprocessing import scale

data = load_breast_cancer()
X, y = data.data, data.target
X = scale(X)

X_trainval, X_test, y_trainval, y_test = train_test_split(X, y)
X_train, X_val, y_train, y_val = train_test_split(
    X_trainval, y_trainval)

knn = KNeighborsClassifier(n_neighbors=5).fit(X_train, y_train)

print("Validation: {:.3f}".format(knn.score(X_val, y_val)))
print("Test: {:.3f}".format(knn.score(X_test, y_test)))
```

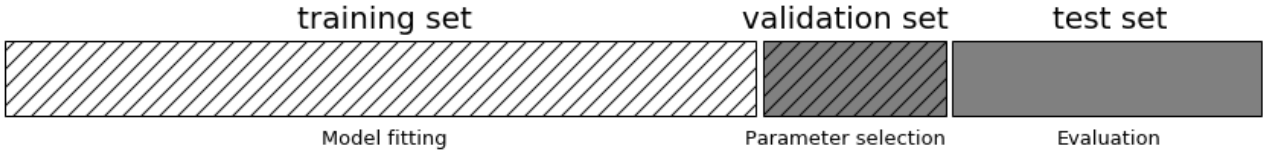
```
Validation: 0.972
Test: 0.965
```

Overfitting the validation set

```
val = []
test = []

for i in range(1000):
    rng = np.random.RandomState(i)
    noise = rng.normal(scale=.1, size=X_train.shape)
    knn = KNeighborsClassifier(n_neighbors=5)
    knn.fit(X_train + noise, y_train)
    val.append(knn.score(X_val, y_val))
    test.append(knn.score(X_test, y_test))

print("Validation: {:.3f}".format(np.max(val)))
print("Test: {:.3f}".format(test[np.argmax(val)]))
```

```
Validation: 1.000
Test: 0.958
```

Threefold split

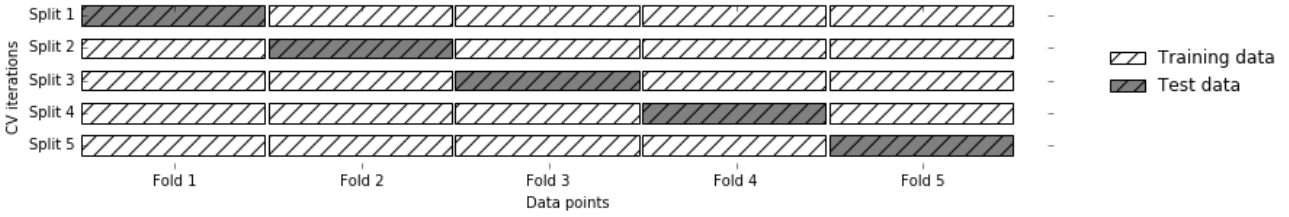


Implementing threefold split

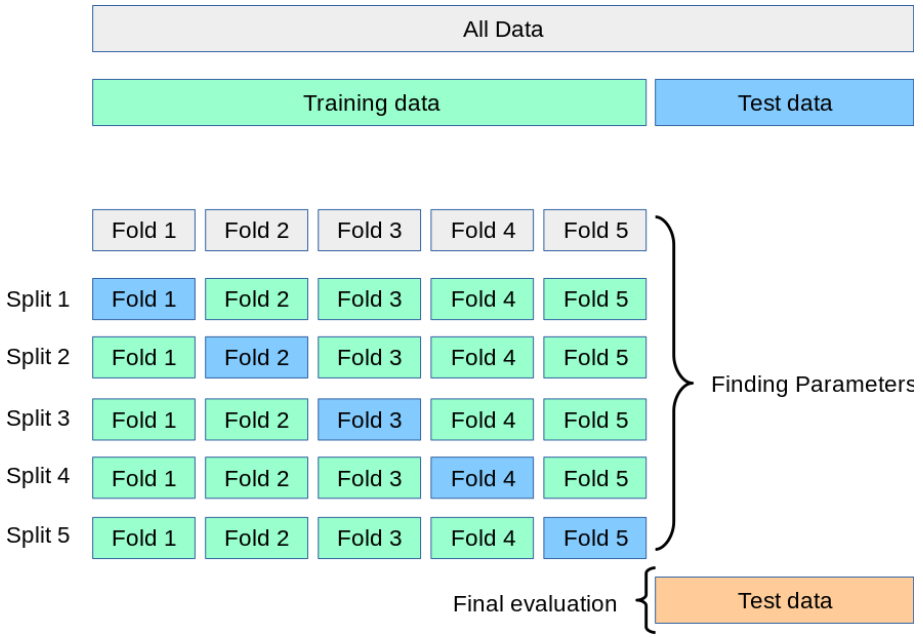
```
X_trainval, X_test, y_trainval, y_test = train_test_split(X, y)
X_train, X_val, y_train, y_val = train_test_split(X_trainval, y_trainval)

val_scores = []
neighbors = np.arange(1, 15, 2)
for i in neighbors:
    knn = KNeighborsClassifier(n_neighbors=i)
    knn.fit(X_train, y_train)
    val_scores.append(knn.score(X_val, y_val))
print("best validation score: {:.3f}".format(np.max(val_scores)))
best_n_neighbors = neighbors[np.argmax(val_scores)]
print("best n_neighbors: {}".format(best_n_neighbors))

knn = KNeighborsClassifier(n_neighbors=best_n_neighbors)
knn.fit(X_trainval, y_trainval)
print("test-set score: {:.3f}".format(knn.score(X_test, y_test)))
```

```
best validation score: 0.991
best n_neighbors: 11
test-set score: 0.951
```

Cross-validation



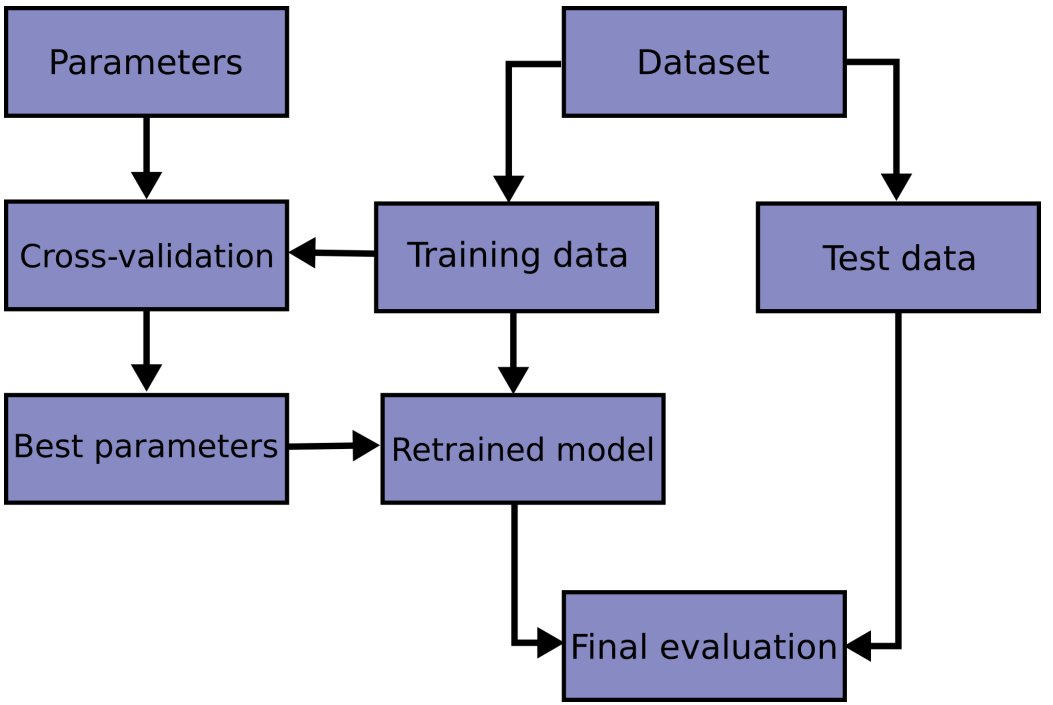
Cross-validation + test set



Grid-Search with Cross-Validation

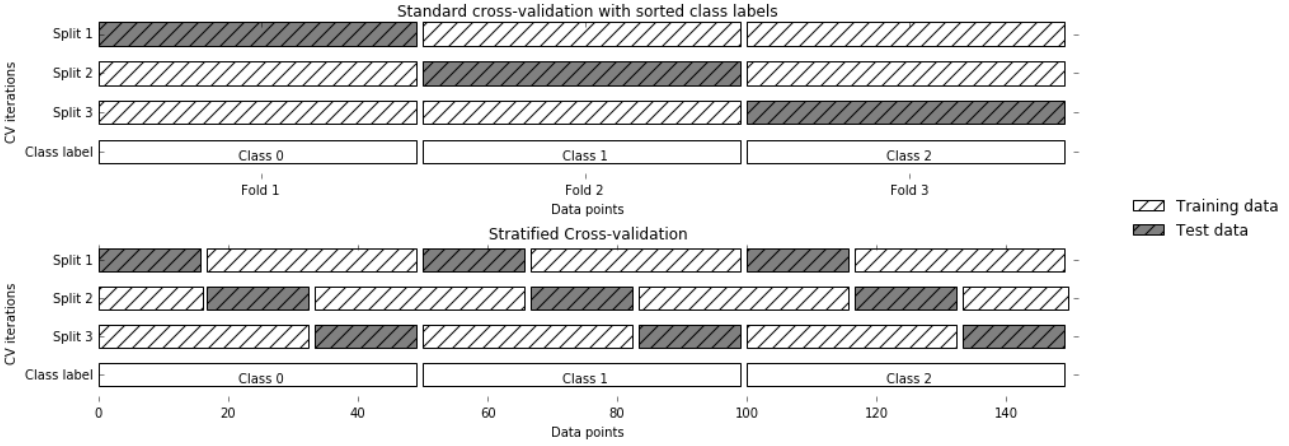
```
from sklearn.model_selection import cross_val_score

X_train, X_test, y_train, y_test = train_test_split(X, y)
cross_val_scores = []

for i in neighbors:
    knn = KNeighborsClassifier(n_neighbors=i)
    scores = cross_val_score(knn, X_train, y_train, cv=10)
    cross_val_scores.append(np.mean(scores))

print("best cross-validation score: {:.3f}".format(np.max(cross_val_scores)))
best_n_neighbors = neighbors[np.argmax(cross_val_scores)]
print("best n_neighbors: {}".format(best_n_neighbors))

knn = KNeighborsClassifier(n_neighbors=best_n_neighbors)
knn.fit(X_train, y_train)
print("test-set score: {:.3f}".format(knn.score(X_test, y_test)))
```

```
best cross-validation score: 0.967
best n_neighbors: 9
test-set score: 0.965
```


Parameters
Dataset
Cross-validation
Training data
Test data
Best parameters
Retrained model
Final evaluation

Cross-Validation Strategies

StratifiedKFold

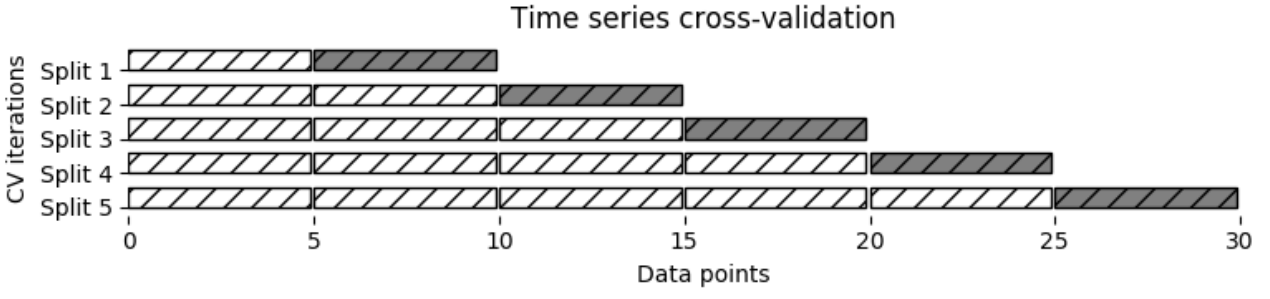


Stratified: Ensure relative class frequencies in each fold reflect relative class frequencies on the whole dataset.

Repeated KFold and LeaveOneOut

- LeaveOneOut : KFold(n_folds=n_samples) High variance, takes a long time
- Better: RepeatedKFold. Apply KFold or StratifiedKFold multiple times with shuffled data. Reduces variance!

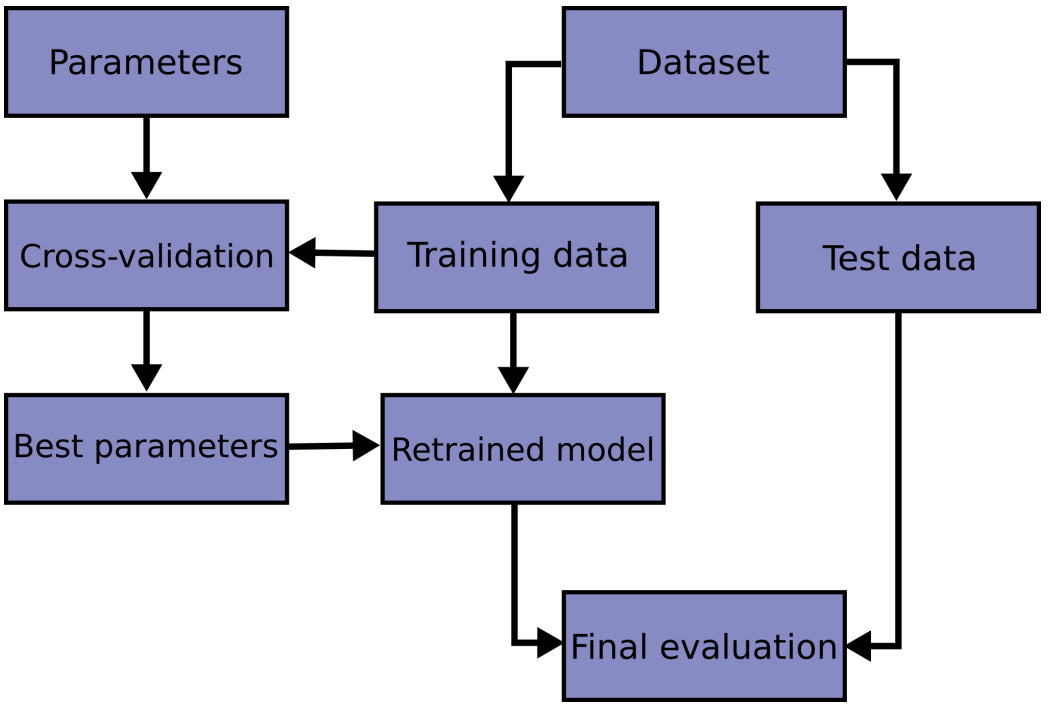
TimeSeriesSplit



Using Cross-Validation Generators

```
from sklearn.model_selection import KFold, StratifiedKFold
kfold = KFold(n_splits=5)
skfold = StratifiedKFold(n_splits=5, shuffle=True)

print("KFold:\n{}".format(
      cross_val_score(KNeighborsClassifier(), X, y, cv=kfold)))

print("StratifiedKFold:\n{}".format(
      cross_val_score(KNeighborsClassifier(), X, y, cv=skfold)))
```

```
KFold:
[ 0.93  0.96  0.96  0.98  0.96]
StratifiedKFold:
[ 0.97  0.95  0.98  0.96  0.96]
```


Parameters
Dataset
Cross-validation
Training data
Test data
Best parameters
Retrained model
Final evaluation

GridSearchCV

```
from sklearn.model_selection import GridSearchCV

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y)


param_grid = {'n_neighbors':  np.arange(1, 15, 2)}

grid = GridSearchCV(KNeighborsClassifier(), param_grid=param_grid, cv=10)
grid.fit(X_train, y_train)

print("best mean cross-validation score: {:.3f}".format(grid.best_score_))
print("best parameters: {}".format(grid.best_params_))

print("test-set score: {:.3f}".format(grid.score(X_test, y_test)))
```

```
best mean cross-validation score: 0.967
best parameters: {'n_neighbors': 9}
test-set score: 0.993
```

GridSearchCV Results

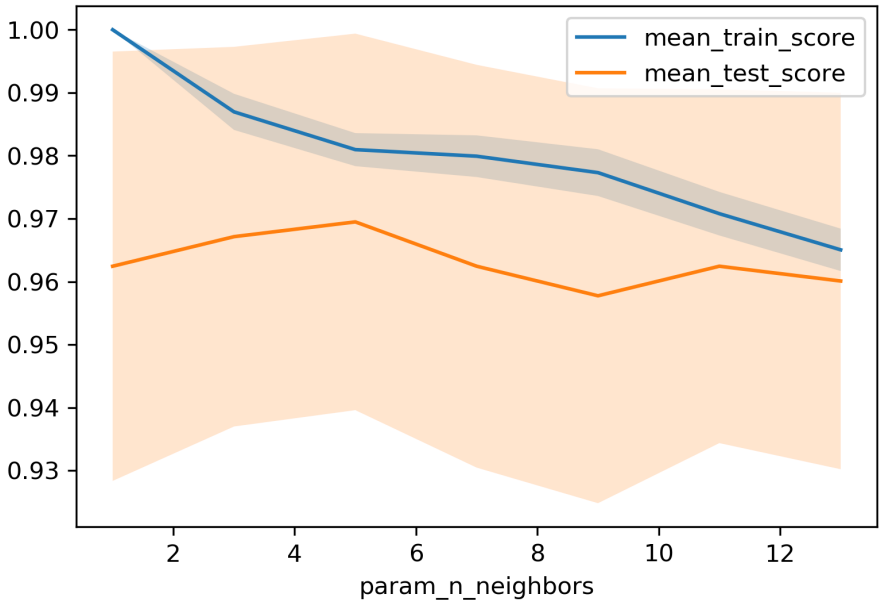
```
import pandas as pd
results = pd.DataFrame(grid.cv_results_)
results.columns
```

```
Index(['mean_fit_time', 'mean_score_time', 'mean_test_score',
       'mean_train_score', 'param_n_neighbors', 'params', 'rank_test_score',
       'split0_test_score', 'split0_train_score', 'split1_test_score',
       'split1_train_score', 'split2_test_score', 'split2_train_score',
       'split3_test_score', 'split3_train_score', 'split4_test_score',
       'split4_train_score', 'split5_test_score', 'split5_train_score',
       'split6_test_score', 'split6_train_score', 'split7_test_score',
       'split7_train_score', 'split8_test_score', 'split8_train_score',
       'split9_test_score', 'split9_train_score', 'std_fit_time',
       'std_score_time', 'std_test_score', 'std_train_score'],
      dtype='object')
```

```
results.params
```

```
0     {'n_neighbors': 1}
1     {'n_neighbors': 3}
2     {'n_neighbors': 5}
3     {'n_neighbors': 7}
4     {'n_neighbors': 9}
5    {'n_neighbors': 11}
6    {'n_neighbors': 13}
Name: params, dtype: object
```

n_neighbors Search Results



Questions ?