W4995 Applied Machine Learning

Introduction to Supervised Learning

02/03/20

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Supervised Learning

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

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

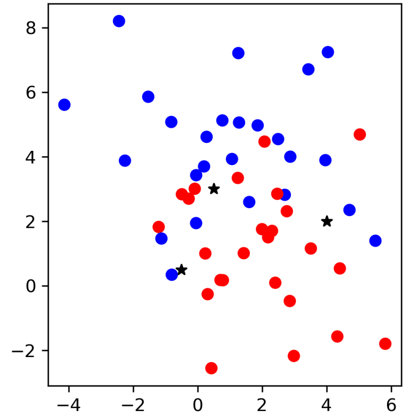
$$y_i \in \mathbb{R}$$

$$\text{learn } f(x_i) \approx y_i$$

such that

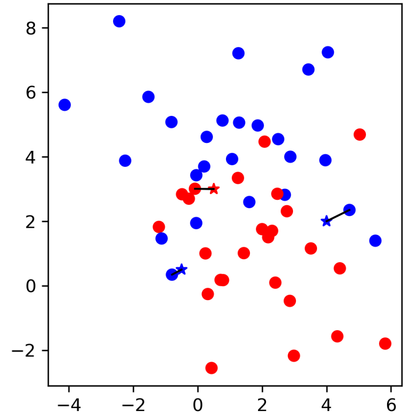
$$f(x) \approx y$$

Nearest Neighbors



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

Nearest Neighbors



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

training set

$$X = \begin{pmatrix} 1.1 & 2.2 \\ 6.7 & 0.5 \\ 2.4 & 9.3 \\ 1.5 & 0.0 \\ 0.5 & 3.5 \\ 5.1 & 9.7 \\ 3.7 & 7.8 \end{pmatrix} \quad y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

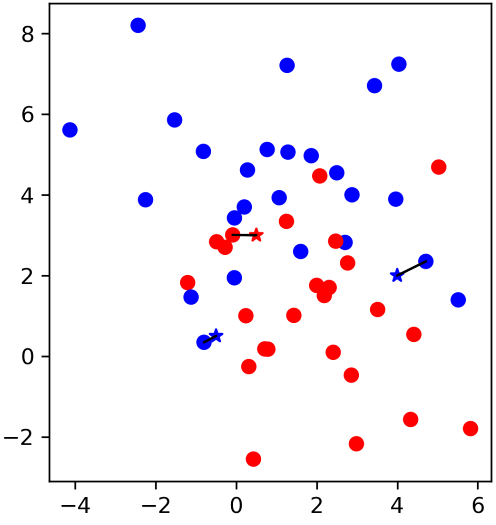
test set

KNN with scikit-learn

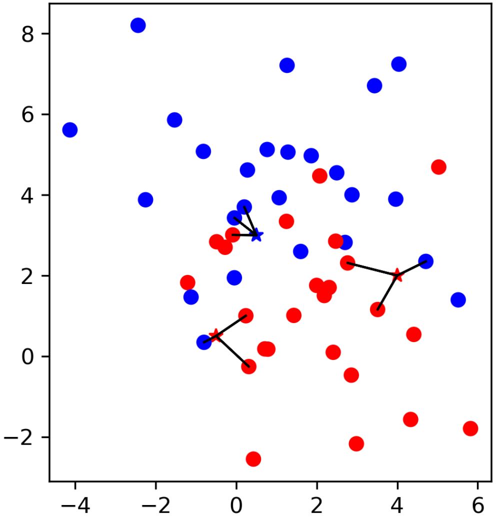
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y)

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

accuracy: 0.77

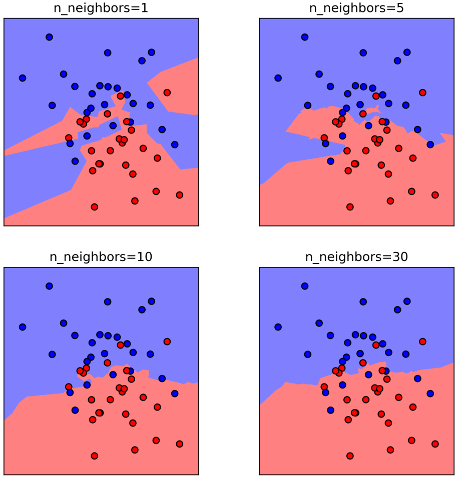
Influence of Number of Neighbors



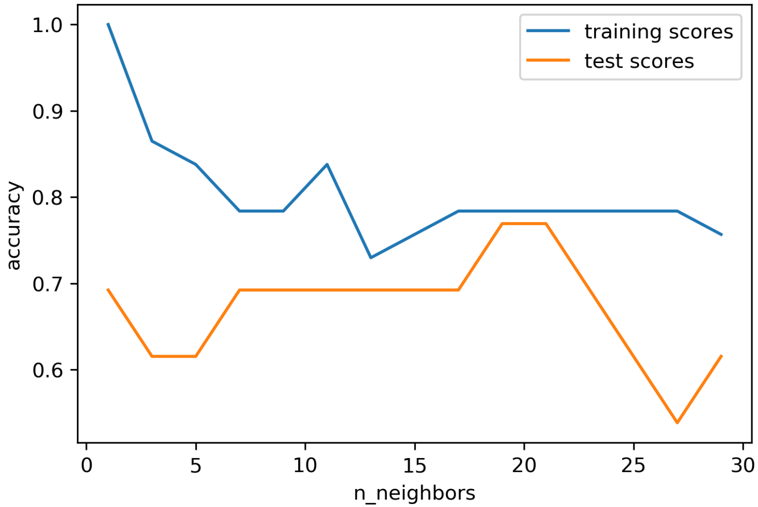
Influence of Number of Neighbors



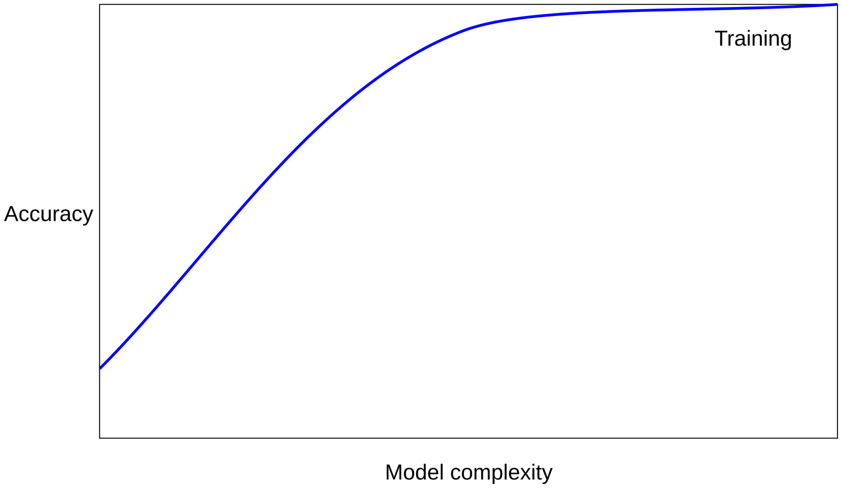
Influence of n_neighbors



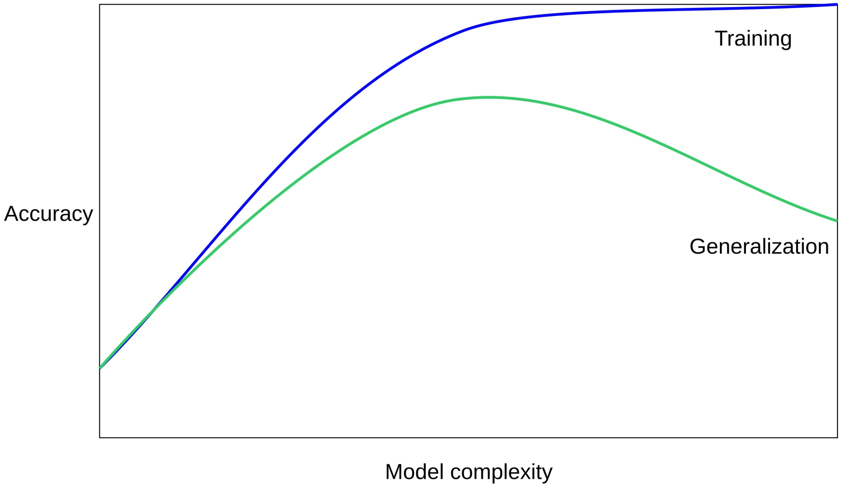
Model complexity



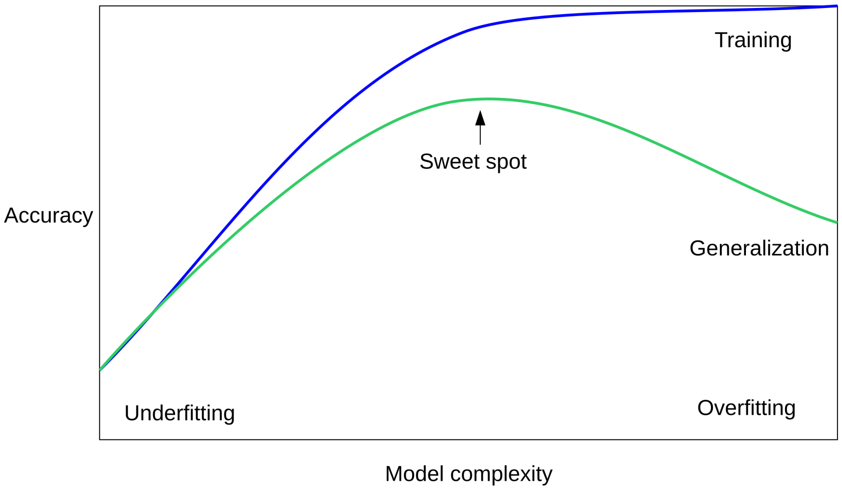
Overfitting and Underfitting



Overfitting and Underfitting



Overfitting and Underfitting



Computational Properties

Naive

- fit: no time
- memory: O(n * p)
- predict: O(n * p)

n=n_samples p=n_features

Computational Properties

Naive

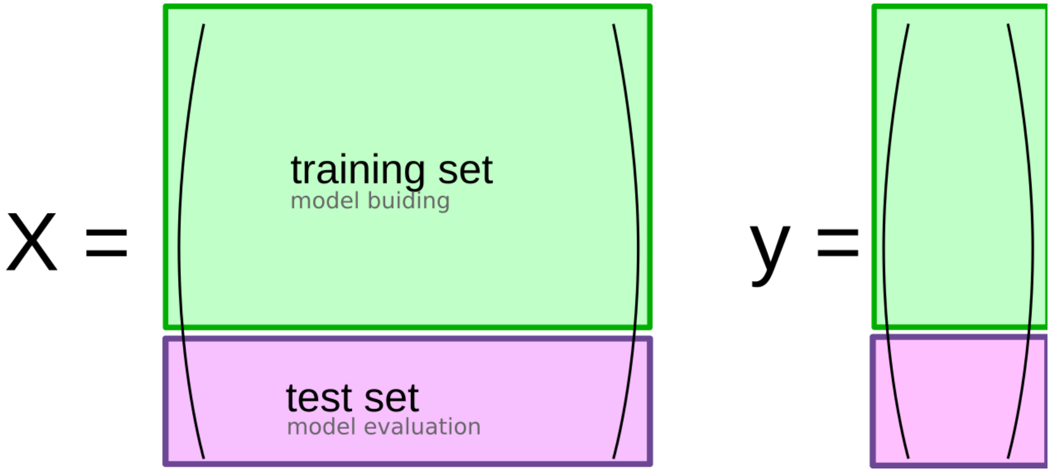
- fit: no time
- memory: O(n * p)
- predict: O(n * p)

Kd-tree

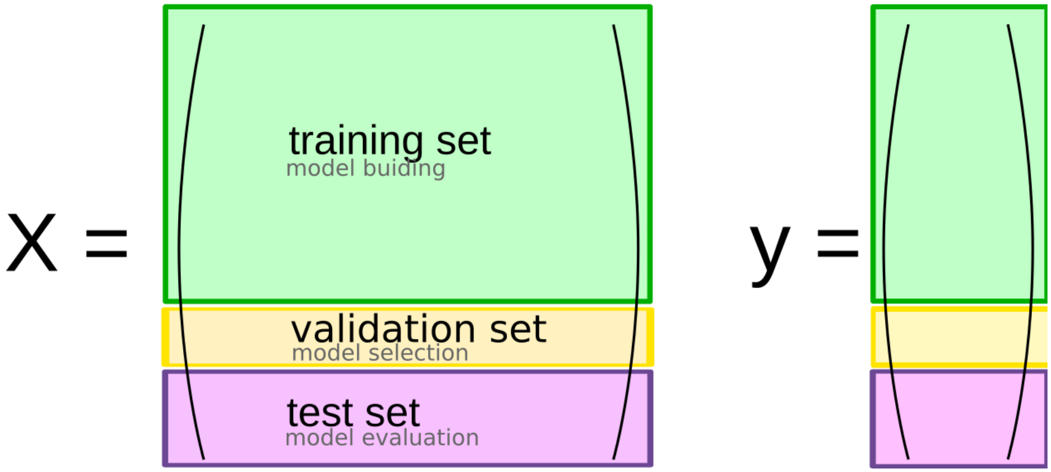
- fit: O(p * n log n)
- memory: O(n * p)
- predict:
- O(k * log(n))
  FOR FIXED p!

n=n_samples p=n_features

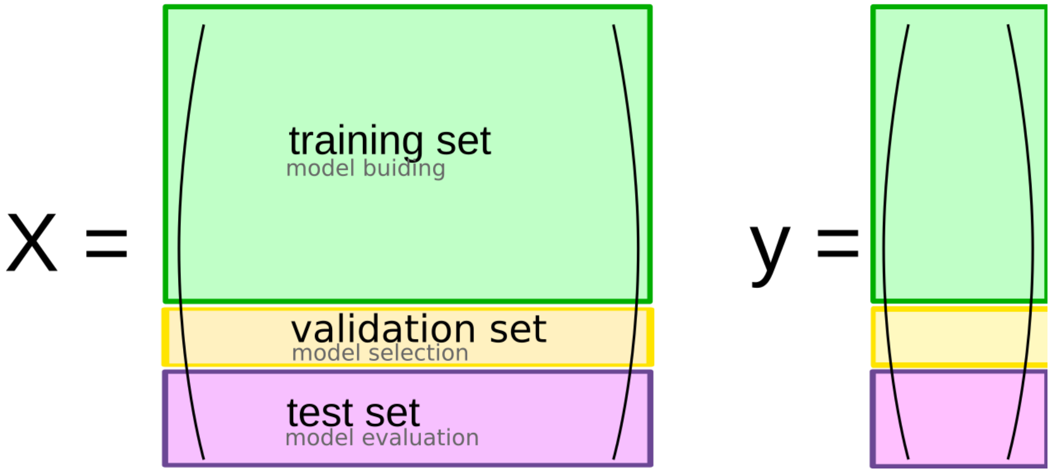
So far: Train-test-split



Threefold split

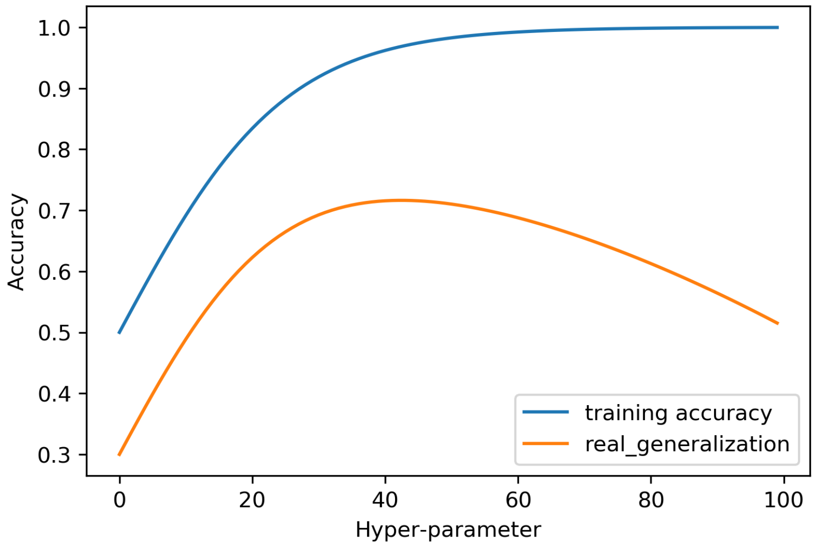


Threefold split

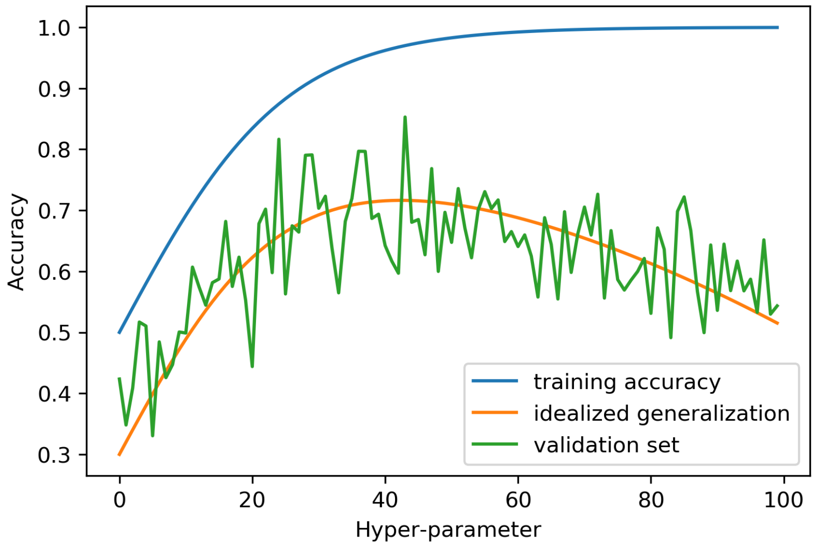


Interesting related read on overfitting in cross-validation [Preventing Overfitting in cross-validation - Ng 1997]

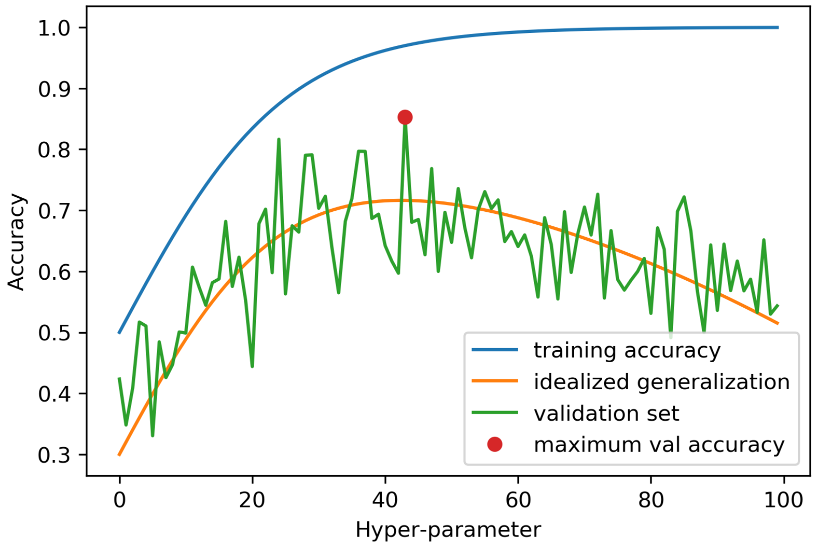
Overfitting the validation set



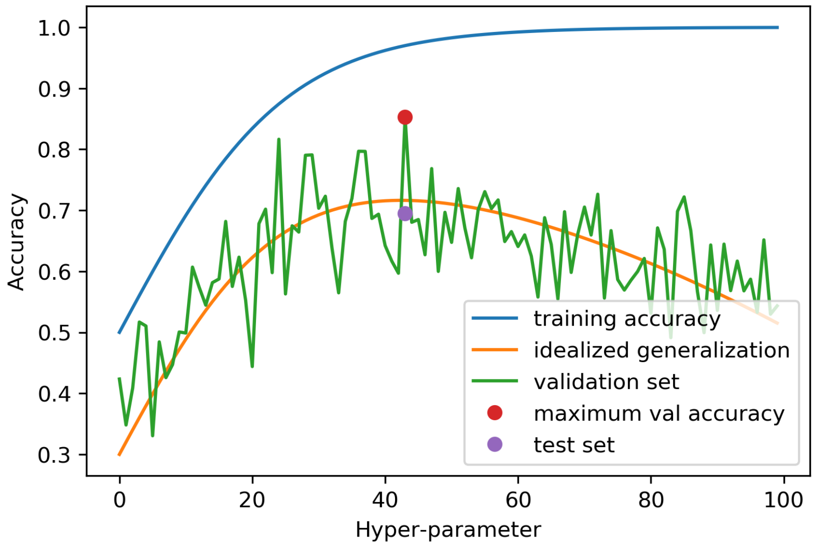
Overfitting the validation set



Overfitting the validation set



Overfitting the validation set

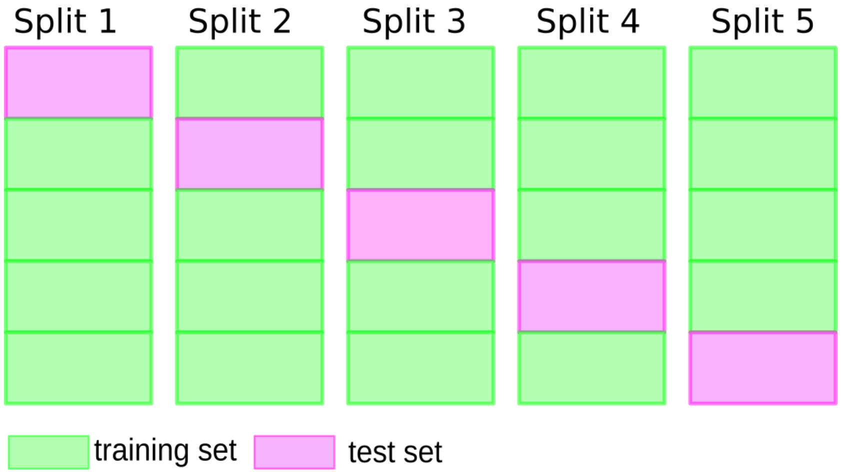


Threefold Split for Hyper-Parameters

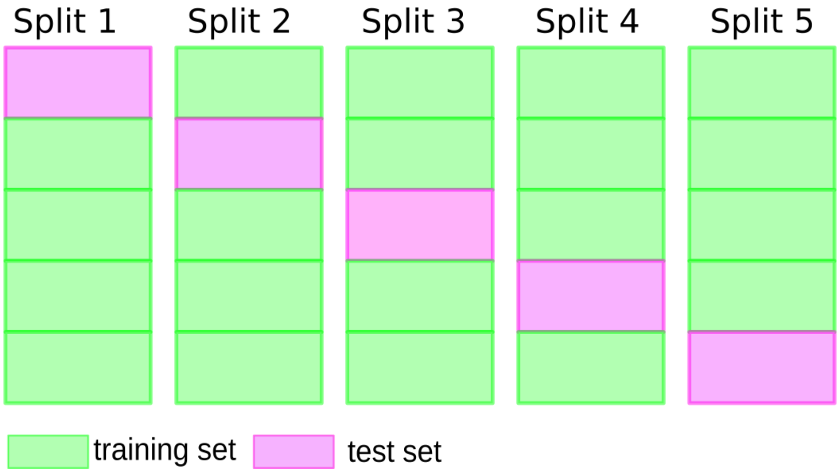
```
X_trainval, X_test, y_trainval, y_test = train_test_split(X, y)
X_train, X_val, y_train, y_val = train_test_split(X_trainval, y_trainval)

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(f"best validation score: {np.max(val_scores):.3}")
best_n_neighbors = neighbors[np.argmax(val_scores)]
print("best n_neighbors:", best_n_neighbors)

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

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

Cross-validation



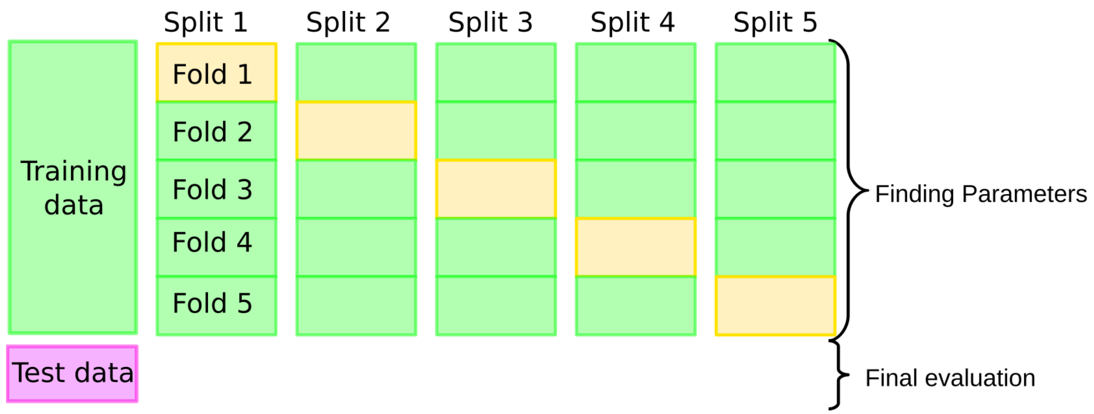
Cross-validation



pro: more stable, more data

con: slower

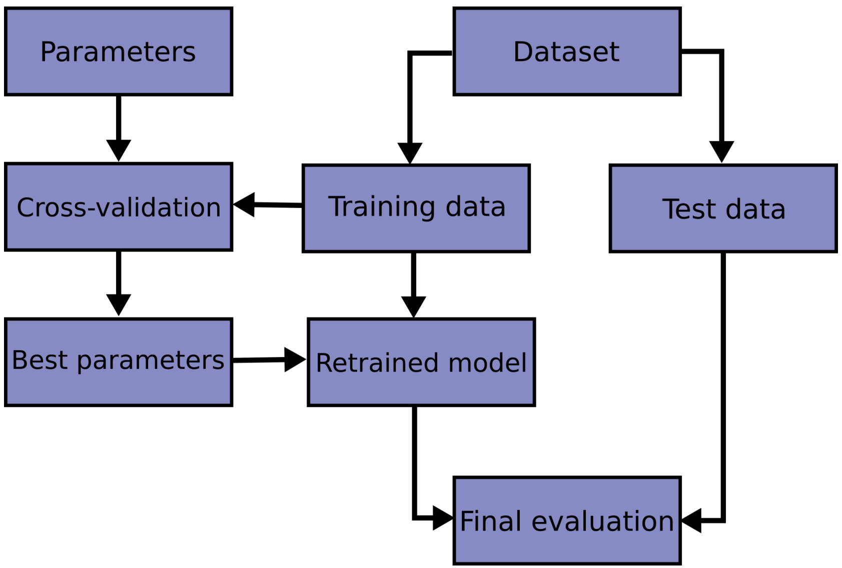
Cross-validation + test set



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

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

```
best cross-validation score: 0.967
best n_neighbors: 9
```


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, 30, 2)}
grid = GridSearchCV(KNeighborsClassifier(), param_grid=param_grid, cv=10,
                   return_train_score=True)
grid.fit(X_train, y_train)
print(f"best mean cross-validation score: {grid.best_score_}")
print(f"best parameters: {grid.best_params_}")
print(f"test-set score: {grid.score(X_test, y_test):.3f}")
```

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

GridSearchCV Results

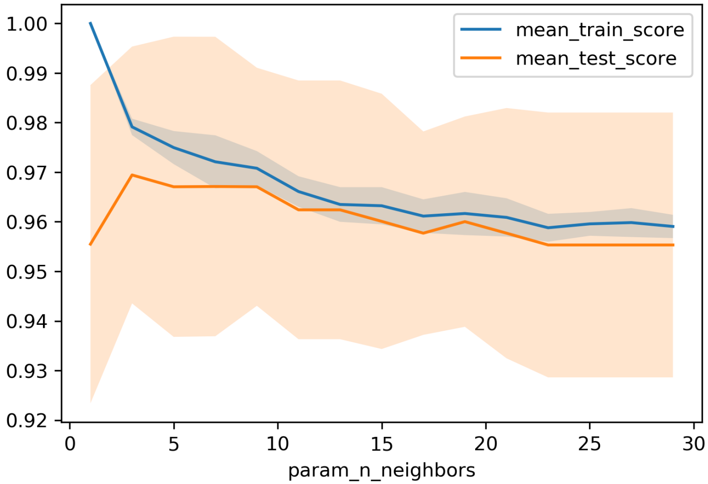
```python
import pandas as pd
results = pd.DataFrame(grid.cv_results_)
results.columns
```

```
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')
```

```python
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
```

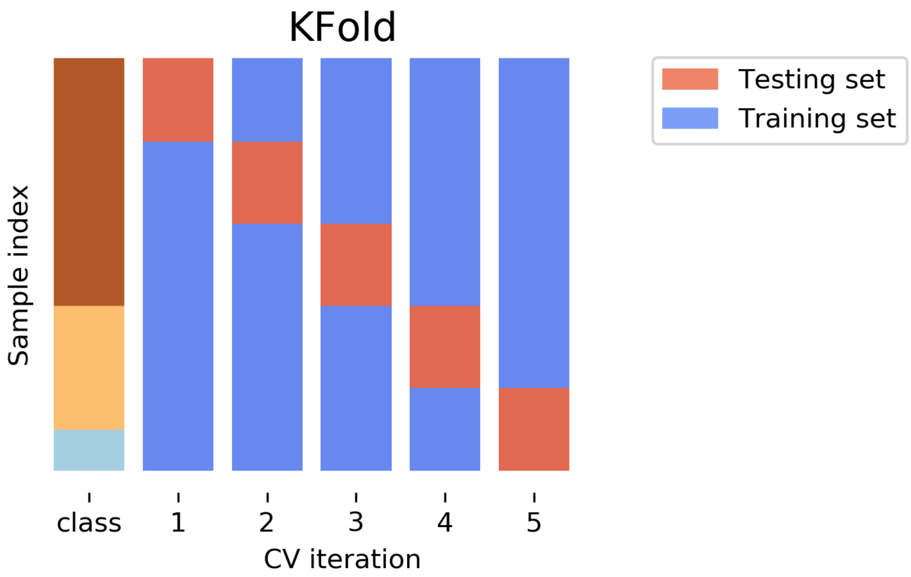
n_neighbors Search Results

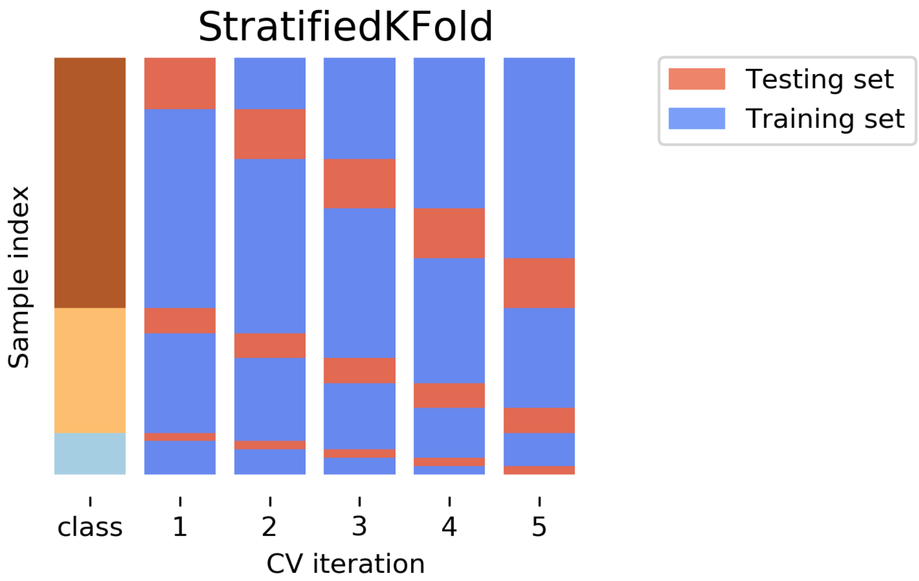


Nested Cross-Validation

- Replace outer split by CV loop
- Doesn't yield single model (inner loop might have different best parameter settings)
- Takes a long time, not that useful in practice

Cross-Validation Strategies


KFold
Testing set
Training set
Sample index
class
1
2
3
4
5
CV iteration



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

Importance of Stratification

```
y.value_counts()
```

```
0    60
1    40
```

```
from sklearn.model_selection import cross_val_score, KFold, StratifiedKFold
from sklearn.dummy import DummyClassifier

dc = DummyClassifier('most_frequent')
skf = StratifiedKFold(n_splits=5, shuffle=True)
res = cross_val_score(dc, X, y, cv=skf)
np.mean(res), res.std()
```

```
(0.6, 0.0)
```

```
kf = KFold(n_splits=5, shuffle=True)
res = cross_val_score(dc, X, y, cv=kf)
np.mean(res), res.std()
```

```
(0.6, 0.063)
```

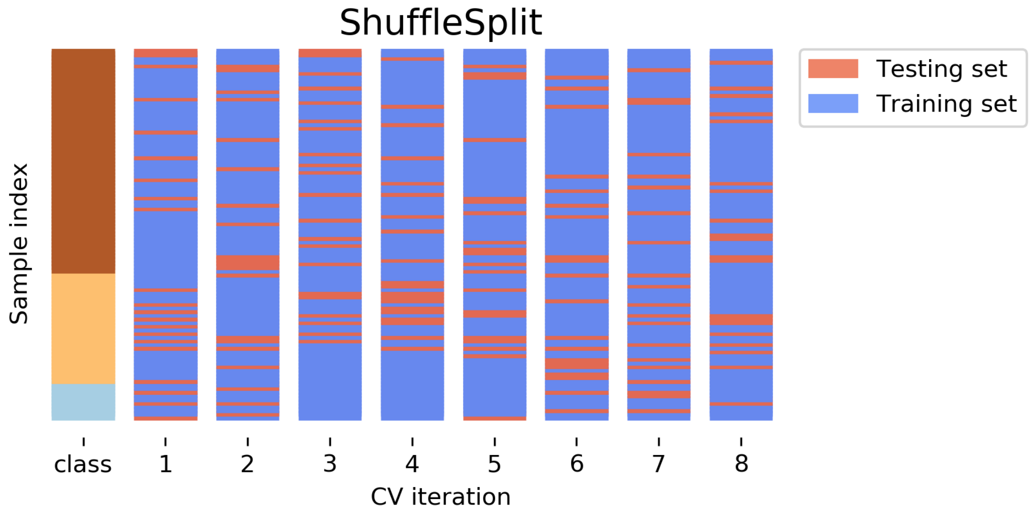
Repeated KFold and LeaveOneOut

- LeaveOneOut : KFold(n_folds=n_samples)
  High variance, takes a long time

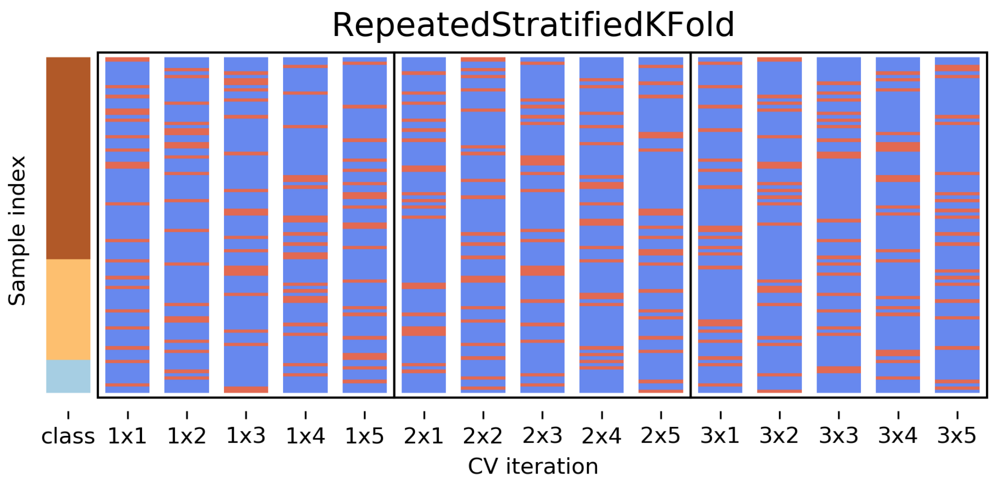
  (see Raschka for a review and Varoquaux for empirical evaluation)

- Better: ShuffleSplit (aka Monte Carlo)
  Repeatedly sample a test set with replacement

- Even Better: RepeatedKFold.
  Apply KFold or StratifiedKFold multiple times with shuffled data.



Number of iterations and test set size independent



Potentially less variance than StratifiedShuffleSplit.
Five times five fold or at most ten times ten fold is sufficient.

Defaults in scikit-learn

- 5-fold in 0.22 (used to be 3 fold)
- For classification cross-validation is stratified
- train_test_split has stratify option: train_test_split(X, y, stratify=y)
- No shuffle by default!

Cross-Validation with non-iid data

Grouped Data

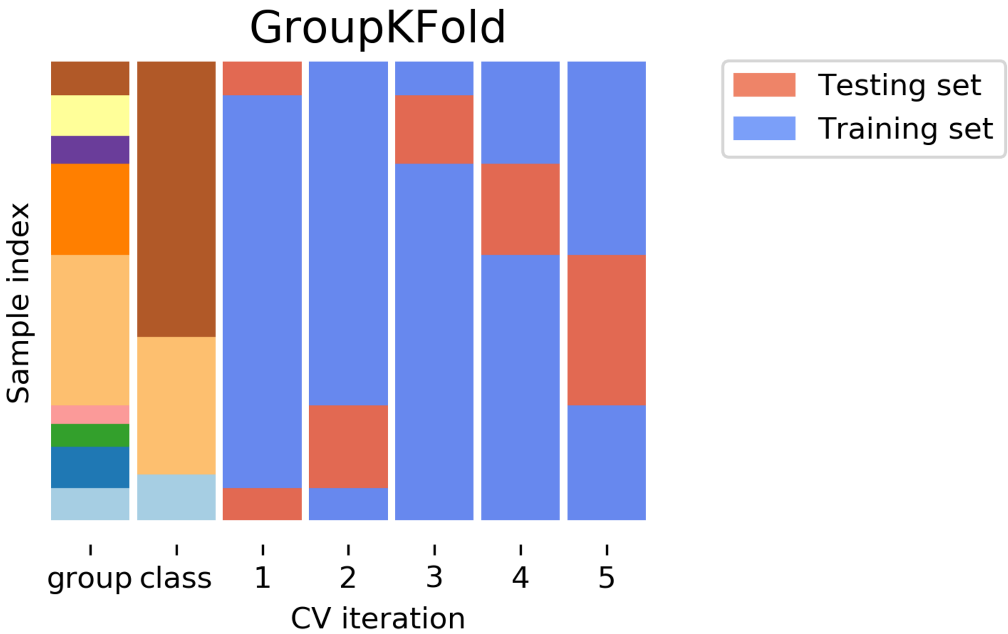
Assume have data (medical, product, user...) from 5 cities

- New York, San Francisco, Los Angeles, Chicago, Houston.

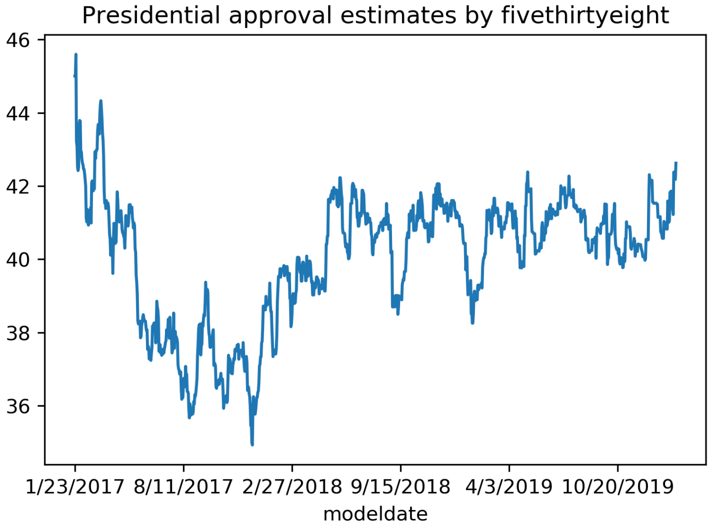
We can assume data within a city is more correlated then between cities.

Usage Scenarios

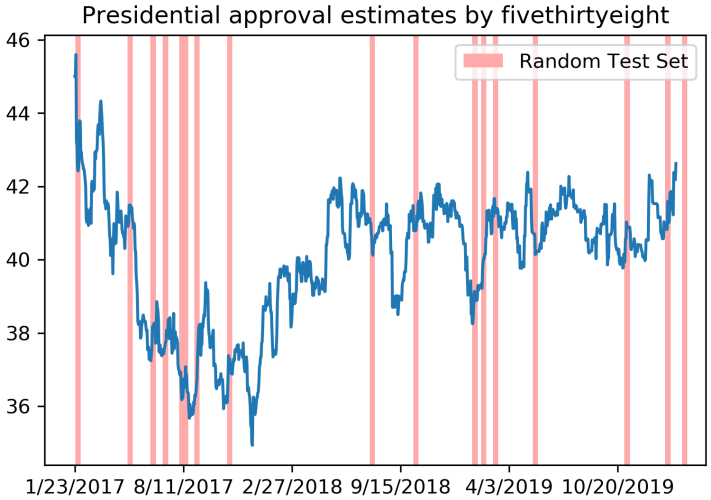
- Assume all future users will be in one of these cities: i.i.d.
- Assume we want to generalize to predict for a new city: not i.i.d.


GroupKFold
Sample index
group
class
1
2
3
4
5
CV iteration
Testing set
Training set

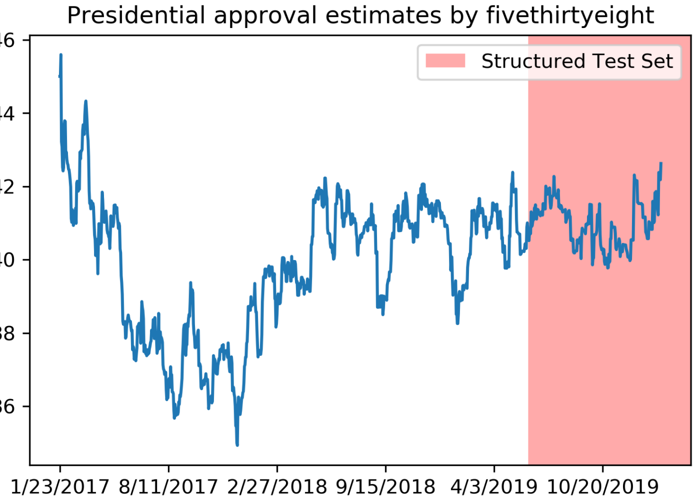
Correlations in time (and/or space)

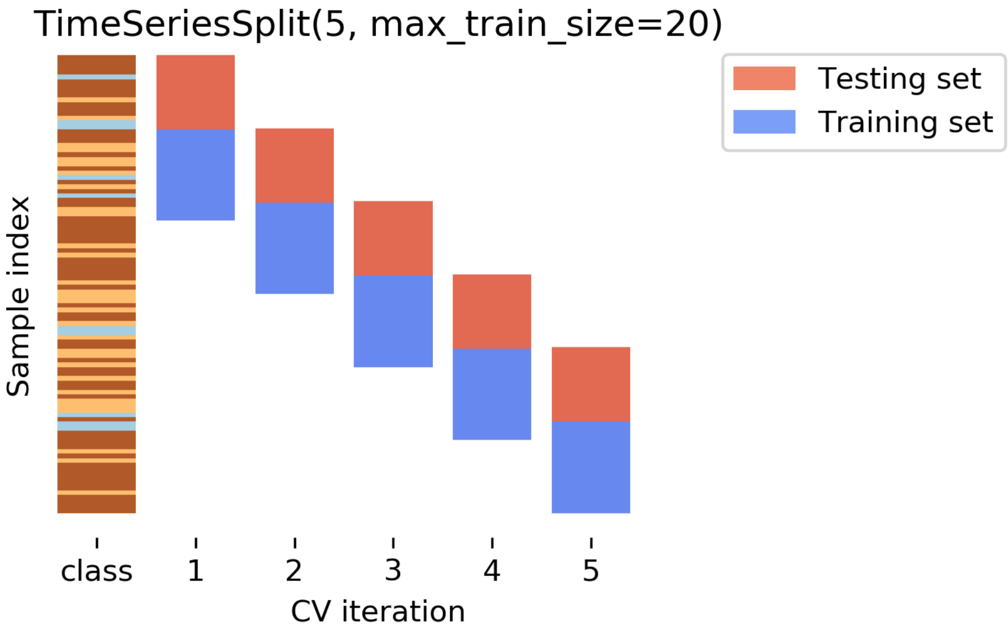


Correlations in time (and/or space)



Correlations in time (and/or space)




TimeSeriesSplit(5, max_train_size=20)
Testing set
Training set
Sample index
class
1
2
3
4
5
CV iteration


TimeSeriesSplit
Testing set
Training set
Sample index
class
1
2
3
4
5
CV iteration

Using Cross-Validation Generators

```
from sklearn.model_selection import KFold, StratifiedKFold, ShuffleSplit, RepeatedStratifiedKFold
kfold = KFold(n_splits=5)
skfold = StratifiedKFold(n_splits=5, shuffle=True)
ss = ShuffleSplit(n_splits=20, train_size=.4, test_size=.3)
rs = RepeatedStratifiedKFold(n_splits=5, n_repeats=10)

print("KFold:")
print(cross_val_score(KNeighborsClassifier(), X, y, cv=kfold))

print("StratifiedKFold:")
print(cross_val_score(KNeighborsClassifier(), X, y, cv=skfold))

print("ShuffleSplit:")
print(cross_val_score(KNeighborsClassifier(), X, y, cv=ss))

print("RepeatedStratifiedKFold:")
print(cross_val_score(KNeighborsClassifier(), X, y, cv=rs))
```

```
KFold:
[0.93 0.96 0.96 0.98 0.96]
StratifiedKFold:
[0.98 0.96 0.96 0.97 0.96]
ShuffleSplit:
[0.98 0.96 0.96 0.98 0.94 0.96 0.95 0.98 0.97 0.92 0.94 0.97 0.95 0.92
 0.98 0.98 0.97 0.94 0.97 0.95]
RepeatedStratifiedKFold:
[0.99 0.96 0.97 0.97 0.95 0.98 0.97 0.98 0.97 0.96 0.97 0.99 0.94 0.96
 0.96 0.98 0.97 0.96 0.96 0.97 0.97 0.96 0.96 0.96 0.98 0.96 0.97 0.97
 0.97 0.96 0.96 0.95 0.96 0.99 0.98 0.93 0.96 0.98 0.98 0.96 0.96 0.95
 0.97 0.97 0.96 0.97 0.97 0.97 0.96 0.96]
```

cross_validate function

```
from sklearn.model_selection import cross_validate
res = cross_validate(KNeighborsClassifier(), X, y, return_train_score=True,
                     scoring=["accuracy", "roc_auc"])
res_df = pd.DataFrame(res)
```

fit_time	score_time	test_accuracy	test_roc_auc	train_accuracy	train_roc_auc
0.000839	0.010204	0.965217	0.996609	0.980176	0.997654
0.000870	0.014424	0.956522	0.983689	0.975771	0.998650
0.000603	0.009298	0.982301	0.999329	0.971491	0.996977
0.000698	0.006670	0.955752	0.984071	0.978070	0.997820
0.000611	0.006559	0.964602	0.994634	0.978070	0.998026

Questions ?