K-Nearest Neighbor

K-Nearest Neighbors

K-Nearest neighbors for classification predicts the category using the K-closest observations

K-Nearest Neighbors

K-Nearest neighbors for classification predicts the class using the K-closest observations

K-Nearest Neighbors – Assumptions

- All Predictors (features) must be numeric
- Neighbors are rows in the dataset
- There is a distance between each pair of rows
- Distance between row p and row q is

$$\sqrt{(q_1-p_1)^2+(q_2-p_2)^2+\cdots+(q_n-p_n)^2}$$

where $(p_1, p_2,..., p_n)$ and $(q_1, q_2,..., q_n)$ are the values in the rows p and q

K-Nearest Neighbors – Assumptions

Distance =
$$\sqrt{(q_1-p_1)^2+(q_2-p_2)^2+\cdots+(q_n-p_n)^2}$$

- If distance is small, the rows are close to each other
- If distance is large, the rows are far from each other
- Each row has a closest neighbor
- Each row has K closest neighbors
- Each row has a category in column Y

K-Nearest Neighbors – Procedure

For each data point (row)

- Identify the K-nearest neighbors (rows)
- Count how many of them belong to each Y-category
- Identify the category with the largest count

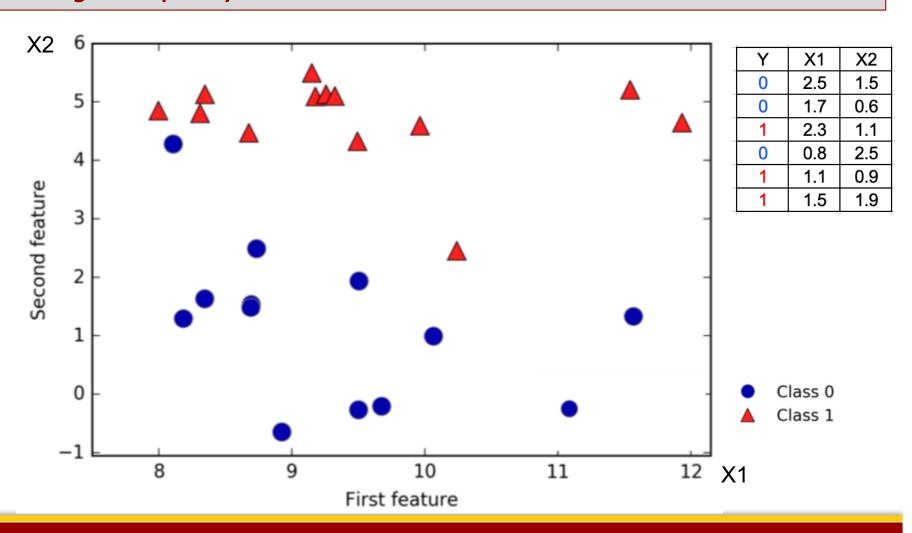
Classify the data point as member of that category

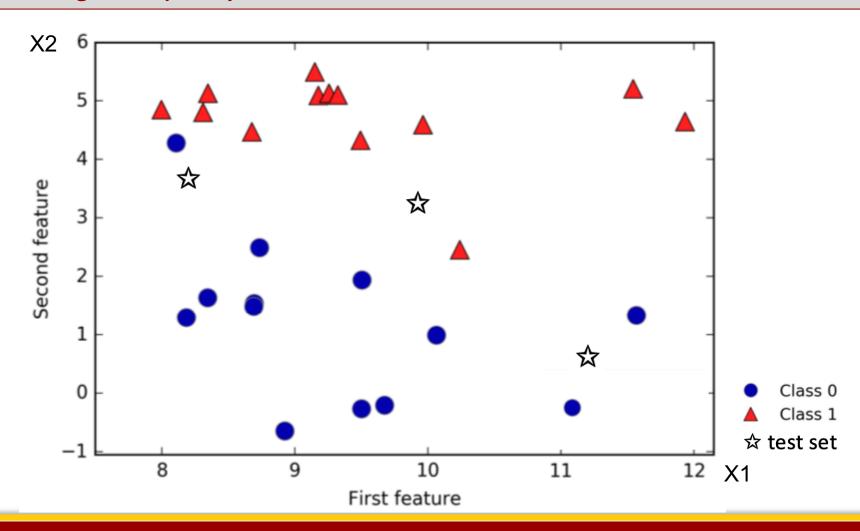
K-Nearest Neighbors - Notes

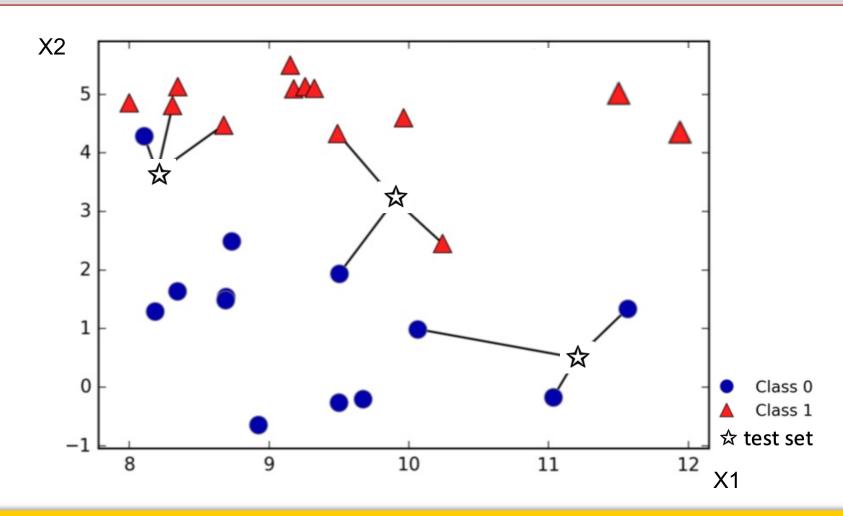
- KNN is a distance-based method
- Scaling of the data affects KNN performance
- K is a hyperparameter of the KNN Method
- Predictions depend on K
- Model performance is based on accuracy rate

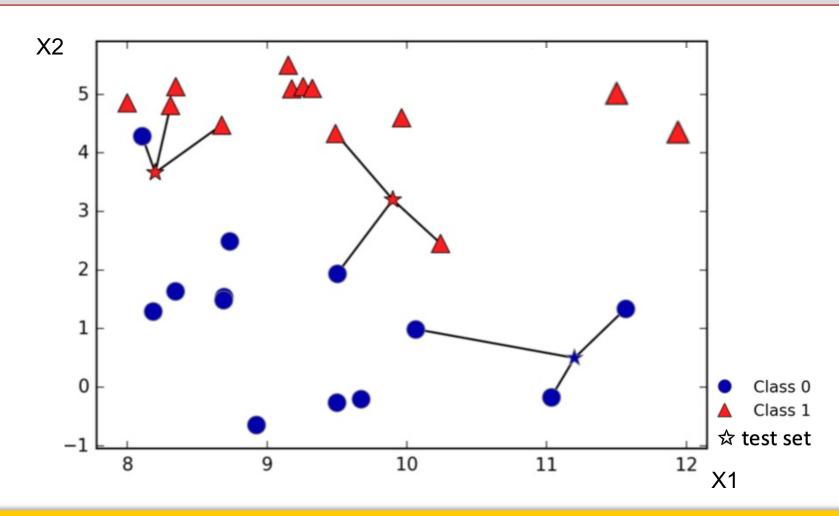
Predict the category (class) of new observations (rows) using the 3-closest neighbors

Υ	X1	X2
0	2.5	1.5
0	1.7	0.6
1	2.3	1.1
0	0.8	2.5
1	1.1	0.9
1	1.5	1.9









Predict the category (class) using the 3-closest observations

Υ	X1	X2	Yhat
	2.5	1.5	1
	1.7	0.6	0
	2.3	1.1	1
	8.0	2.5	0
	1.1	0.9	0
	1.5	1.9	1

Predict the category (class) using the 3-closest observations

Compare predictions with the actual categories

Υ	X1	X2	Yhat	error?
0	2.5	1.5	1	YES
0	1.7	0.6	0	NO
1	2.3	1.1	1	NO
0	8.0	2.5	0	NO
1	1.1	0.9	0	YES
1	1.5	1.9	1	NO

Error rate = 2/6



Hyperparameters

PARAMETERS vs HYPERPARAMETERS

Parameter

Coefficient in the model that is estimated from the data

Example: Coefficients from linear regression

PARAMETERS vs HYPERPARAMETERS

Hyperparameter

Model parameter that cannot be estimated from the data

Example: KNN (n. neighbors), RR (shrinkage parameter α)

Tree (depth), RF (n. trees), GB (learning rate)

PARAMETERS vs HYPERPARAMETERS

Hyperparameter

Model parameter that cannot be estimated from the data

Example: KNN (n. neighbors), RR (shrinkage parameter α)

Tree (depth), RF (n. trees), GB (learning rate)

- A hyperparameter is a parameter whose value is used to control the learning process
- Models may have one or many hyperparameters

MODELS WITH NO HYPERPARAMETERS

If no hyperparameters, the data should be split into 2 subsets

Train set (dataset to build the model)

Test set (dataset to test the model)

MODELS WITH HYPERPARAMETERS

Hyperparameter tuning

Needed to find optimal parameter values

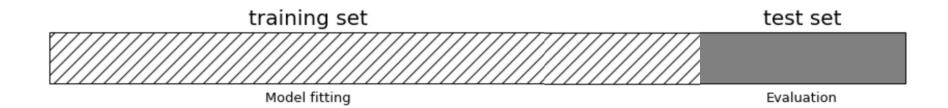
For Hyperparameter tuning the data should be split into 3 subsets

Train set (dataset to build the model)

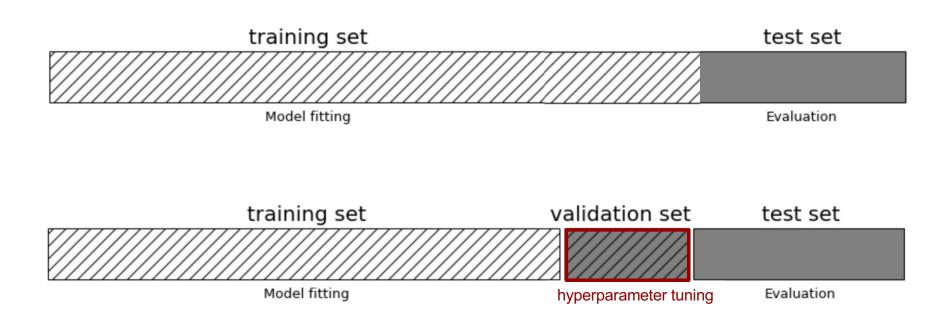
Validation set (dataset for tuning hyperparameters)

Test set (dataset to test the model)

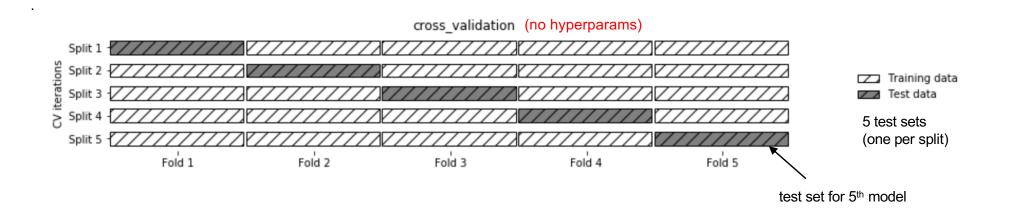
HOLDOUT CROSS VALIDATION – No hyperparameters

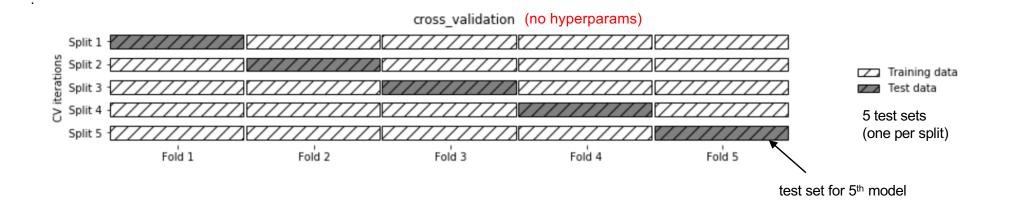


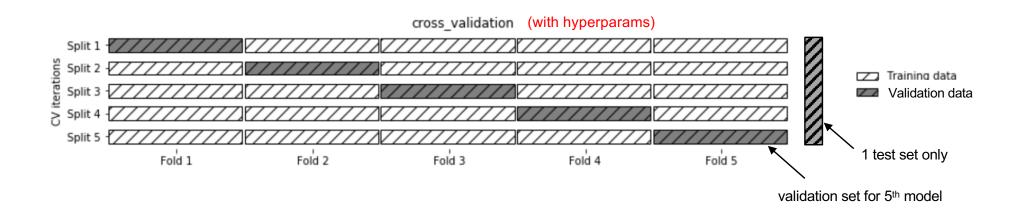
HOLDOUT CROSS VALIDATION - 3 SETS

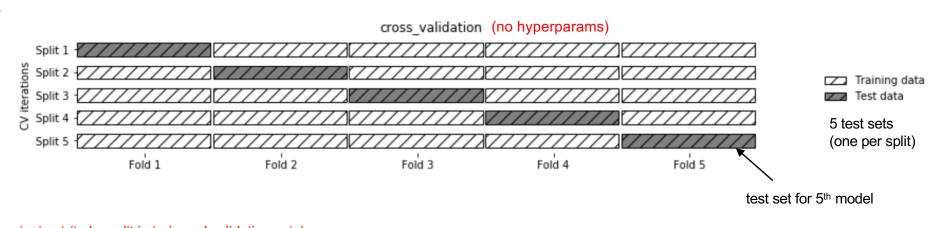


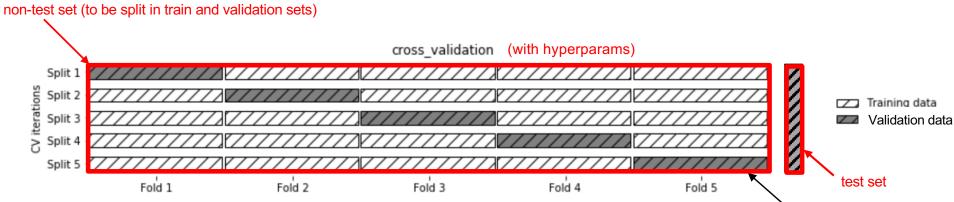
K-Fold CROSS VALIDATION – No hyperparameters



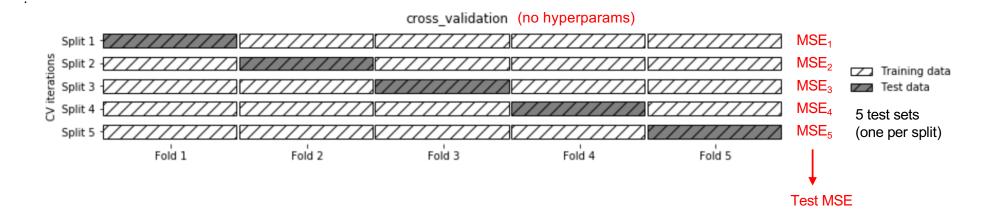


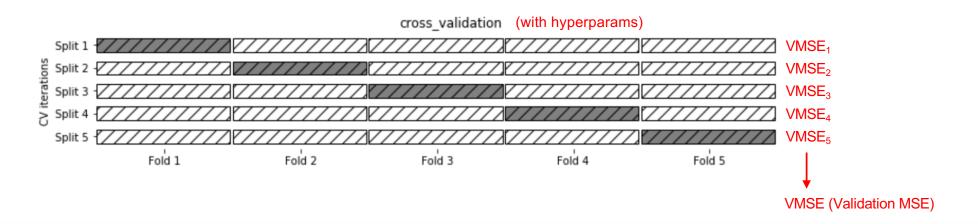


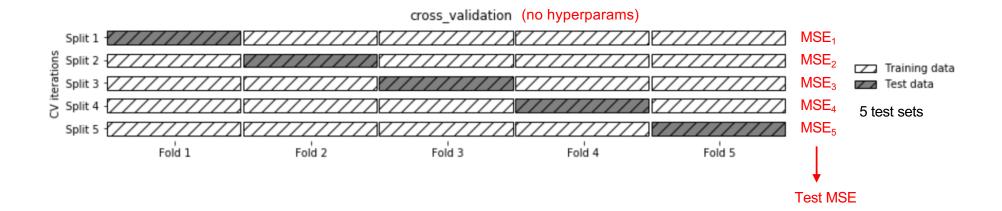


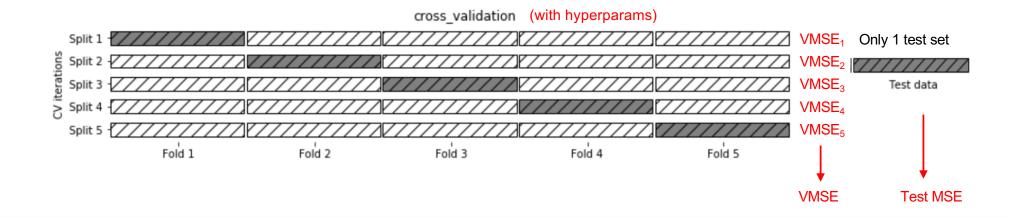


validation set for 5th model









Example – Cancer data

- The Cancer data from sklearn contains lab data of 569 patients
- It includes 30 patient lab measurements associated with breast cancer tumors. These measurements are the predictors.
- Some patients have cancer and others have a tumor but are healthy. The target data assigns a 0 or a 1 for the patients

- The Cancer data from sklearn contains lab data of 569 patients
- It includes 30 patient lab measurements associated with breast cancer tumors. These measurements are the predictors.
- Some patients have cancer and others have a tumor but are healthy. The target variable assigns a 0 or a 1 for the patients
- Build a KNN model (with K=3 nearest neighbors) to predict if the patient has cancer. Find the test accuracy rate.
- Compare Holdout Cross validation and K-fold Cross validation for hyperparameter tuning (the process of finding the number of neighbors K that maximizes the test accuracy rate)

Find the test accuracy rate with the following KNN models

- 1. Holdout CV model with fixed K on original data
- 2. Holdout CV loop to find best K on original data
- 3. Holdout CV loop to find best K on scaled data
- 4. k-Fold CV model with fixed K on original data
- 5. k-Fold CV loop to find best K on original data
- 6. k-Fold CV model with fixed K on scaled data
- 7. k-Fold CV loop to find best K on scaled data

```
← train_test_split

← train_test_split
(two times)

cross_val_score
cross_val_score,
pipeline
```

K-Nearest Neighbors - CANCER DATASET

	X																		
Y	<				average	values				>	<				worst	values			
out	radius	texture	perimeter	area	smoothness	compactness	concavity	concave p	symmetry	fractal_dir	radius	texture	perimeter	area	smoothness	compactness	concavity	concave p	ymmetry
M	17.99	10.38	122.8	1001	0.1184	0.2776	0.3001	0.1471	0.2419	0.07871	25.38	17.33	184.6	2019	0.1622	0.6656	0.7119	0.2654	0.4601
M	20.57	17.77	132.9	1326	0.08474	0.07864	0.0869	0.07017	0.1812	0.05667	24.99	23.41	158.8	1956	0.1238	0.1866	0.2416	0.186	0.275
M	19.69	21.25	130	1203	0.1096	0.1599	0.1974	0.1279	0.2069	0.05999	23.57	25.53	152.5	1709	0.1444	0.4245	0.4504	0.243	0.3613
M	11.42	20.38	77.58	386.1	0.1425	0.2839	0.2414	0.1052	0.2597	0.09744	14.91	26.5	98.87	567.7	0.2098	0.8663	0.6869	0.2575	0.6638
M	20.29	14.34	135.1	1297	0.1003	0.1328	0.198	0.1043	0.1809	0.05883	22.54	16.67	152.2	1575	0.1374	0.205	0.4	0.1625	0.2364
M	12.45	15.7	82.57	477.1	0.1278	0.17	0.1578	0.08089	0.2087	0.07613	15.47	23.75	103.4	741.6	0.1791	0.5249	0.5355	0.1741	0.3985
M	18.25	19.98	119.6	1040	0.09463	0.109	0.1127	0.074	0.1794	0.05742	22.88	27.66	153.2	1606	0.1442	0.2576	0.3784	0.1932	0.3063
M	13.71	20.83	90.2	577.9	0.1189	0.1645	0.09366	0.05985	0.2196	0.07451	17.06	28.14	110.6	897	0.1654	0.3682	0.2678	0.1556	0.3196
M	13	21.82	87.5	519.8	0.1273	0.1932	0.1859	0.09353	0.235	0.07389	15.49	30.73	106.2	739.3	0.1703	0.5401	0.539	0.206	0.4378
M	12.46	24.04	83.97	475.9	0.1186	0.2396	0.2273	0.08543	0.203	0.08243	15.09	40.68	97.65	711.4	0.1853	1.058	1.105	0.221	0.4366
M	16.02	23.24	102.7	797.8	0.08206	0.06669	0.03299	0.03323	0.1528	0.05697	19.19	33.88	123.8	1150	0.1181	0.1551	0.1459	0.09975	0.2948
M	15.78	17.89	103.6	781	0.0971	0.1292	0.09954	0.06606	0.1842	0.06082	20.42	27.28	136.5	1299	0.1396	0.5609	0.3965	0.181	0.3792
M	19.17	24.8	132.4	1123	0.0974	0.2458	0.2065	0.1118	0.2397	0.078	20.96	29.94	151.7	1332	0.1037	0.3903	0.3639	0.1767	0.3176
M	15.85	23.95	103.7	782.7	0.08401	0.1002	0.09938	0.05364	0.1847	0.05338	16.84	27.66	112	876.5	0.1131	0.1924	0.2322	0.1119	0.2809
M	13.73	22.61	93.6	578.3	0.1131	0.2293	0.2128	0.08025	0.2069	0.07682	15.03	32.01	108.8	697.7	0.1651	0.7725	0.6943	0.2208	0.3596
M	14.54	27.54	96.73	658.8	0.1139	0.1595	0.1639	0.07364	0.2303	0.07077	17.46	37.13	124.1	943.2	0.1678	0.6577	0.7026	0.1712	0.4218
M	14.68	20.13	94.74	684.5	0.09867		0.07395	0.05259		0.05922	19.07	30.88	123.4	1138	0.1464	0.1871	0.2914	0.1609	0.3029
M	16.13	20.68	108.1	798.8	0.117		0.1722	0.1028		0.07356	20.96	31.48	136.8	1315	0.1789	0.4233	0.4784	0.2073	0.3706
M	19.81	22.15	130	1260	0.09831	0.1027	0.1479	0.09498	0.1582	0.05395	27.32	30.88	186.8	2398	0.1512	0.315	0.5372	0.2388	0.2768
В	13.54	14.36	87.46		0.09779	0.08129	0.06664	0.04781	0.1885	0.05766	15.11	19.26	99.7	711.2	0.144	0.1773	0.239	0.1288	0.2977
В	13.08	15.71	85.63	520	0.1075		0.04568	0.0311	0.1967	0.06811	14.5	20.49	96.09		0.1312	0.2776	0.189	0.07283	0.3184
В	9.504	12.44			0.1024		0.02956	0.02076		0.06905	10.23	15.66	65.13		0.1324	0.1148	0.08867	0.06227	0.245
M	15.34	14.26	102.5	704.4	0.1073		0.2077	0.09756		0.07032	18.07	19.08	125.1		0.139	0.5954	0.6305	0.2393	0.4667
M	21.16	23.04	137.2	1404	0.09428	0.1022	0.1097	0.08632	0.1769	0.05278	29.17	35.59	188	2615	0.1401	0.26	0.3155	0.2009	0.2822

(569, 30)

Cesar Acosta Ph.D.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split
from sklearn.model_selection import KFold
from sklearn.model_selection import cross_val_score

from sklearn.datasets import load_breast_cancer
from sklearn.neighbors import KNeighborsClassifier

from sklearn.model_selection import StratifiedKFold
from sklearn.pipeline import Pipeline
```

from sklearn.datasets import load_breast_cancer

1. Hold out Cross validation -Fixed K, No Scaling-

K-Nearest Neighbors – holdout cross validation (hyperparameter known K=3)

```
y = cancer.target
X = cancer.data

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, random_state=66)

print('train_set:', X_train.shape, y_train.shape)
print('test_set:', X_test.shape, y_test.shape)

train_set: (426, 30) (426,)
test_set: (143, 30) (143,)

426/569

0.7486818980667839

train_size = 0.75
```

K-Nearest Neighbors – holdout cross validation (K=3)

Cesar Acosta Ph.D.

K-Nearest Neighbors – Test accuracy rate (K=3)

```
# Find test accuracy rate
model.score(X test, y test)
0.9230769230769231
# confusion matrix
yhat = model.predict(X test)
pd.crosstab(y test, yhat,
             rownames=['y test'],colnames=['predictions'])
predictions
          0 1
    y_test
        o 47 6
                    ← Six 'category 0' patients predicted as category 1
                    ← Five 'category 1' patients predicted as category 0
           5 85
(47+85)/143
                        accuracy rate
0.9230769230769231
```

Cesar Acosta Ph.D.

2. Hold out Cross validation -Search for K, No Scaling-

```
y0 = cancer.target
X0 = cancer.data
X0.shape
(569, 30)
```

Reserve test set until last step →

Split remaining data into train and validation sets →

```
print(X_train.shape, X_validation.shape)
(319, 30) (107, 30)
```

```
      val_acc

      1
      0.906542

      2
      0.915888

      3
      0.897196

      4
      0.906542

      5
      0.906542

      6
      0.915888

      7
      0.906542

      8
      0.925234

      9
      0.925234

      10
      0.925234

      11
      0.906542
```

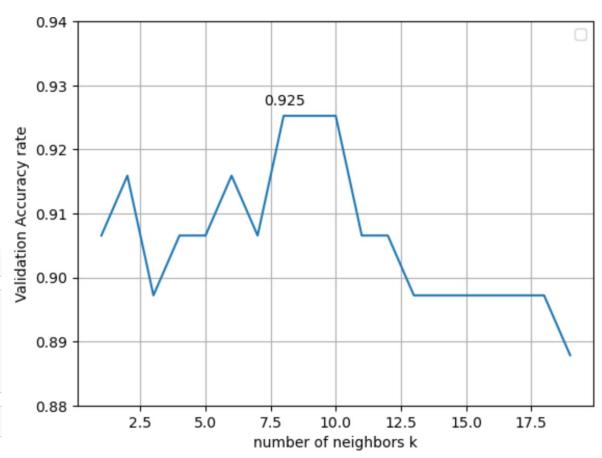
```
df.plot()
plt.ylabel("Validation Accuracy rate")
plt.xlabel("number of neighbors k")
plt.legend('')
plt.ylim(0.88,0.94)
plt.annotate('0.925',(7.25,0.927))
```

```
# test accuracy rate

# rebuild model on the
# combined (train+validation) set

model = KNeighborsClassifier(n_neighbors=8)
model.fit(X, y);

model.score(X_test,y_test)
0.9300699300699301
```



3. Hold out Cross validation -Search for K, Scaling the data-

K-Nearest Neighbors - Scaling the data

```
from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler()

# Find min/max of each feature in Train set
scaler.fit(X_train);

# then transform data into (0,1)
# by substracting the train set Min,
# and dividing by the train set range

X_train_scaled = scaler.transform(X_train)
X_validation_scaled = scaler.transform(X_validation)
```

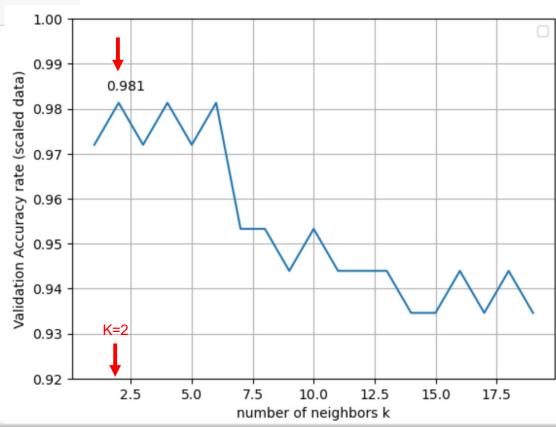
K-Nearest Neighbors - Holdout CrossValidation to find best K

```
validation_accuracy_scaled = []

for k in range(1,20):
    model = KNeighborsClassifier(n_neighbors=k)
    model.fit(X_train_scaled, y_train)
    score = model.score(X_validation_scaled,y_validation)
    validation_accuracy_scaled.append(score)
```

validation acc scaled

1	0.971963
2	0.981308
3	0.971963
4	0.981308
5	0.971963
6	0.981308
7	0.953271
8	0.953271
9	0.943925
10	0.953271
11	0.943925



K-Nearest Neighbors – Holdout CrossValidation to find best K

```
# Find test accuracy rate

scaler = MinMaxScaler()
scaler.fit(X);

X_scaled = scaler.transform(X)
X_test_scaled = scaler.transform(X_test)
```

```
# rebuild model on the
# combined (train+validation) set
model2 = KNeighborsClassifier(n_neighbors=2)
model2.fit(X_scaled, y);

model2.score(X_test_scaled,y_test)
0.9230769230769231
```

4. k-Fold Cross validation -Fixed K, No Scaling-

K-Nearest Neighbors – 5-fold Cross Validation (no scaling) with known K = 3

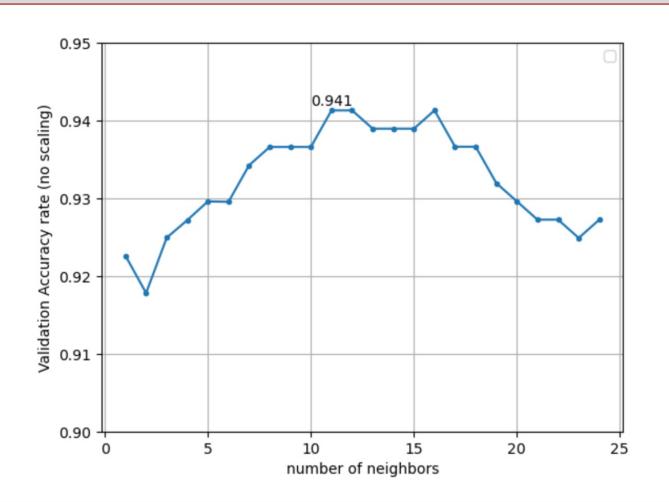
```
y = cancer.target
X = cancer.data
kfold = StratifiedKFold(n_splits = 5,shuffle = True,random_state=1)
model1 = KNeighborsClassifier(n_neighbors=3)
scores = cross val score(model1,X,y,cv=kfold)
# display all 5 test accuracy rates
scores
array([0.94736842, 0.89473684, 0.92982456, 0.94736842, 0.95575221])
# average test accuracy rate
scores.mean()
0.935010091600683
```

5. k-Fold Cross validation -Search for K, No Scaling-

K-Nearest Neighbors – 5-fold Cross Validation (no scaling) to select best K

```
y = cancer target
X = cancer.data
X_train,X_test,\
y train, y test = train test split(X,y,
                                   stratify=y,
                                    random_state=66)
val_acc_rate = []
for k in range(1,25):
    model1 = KNeighborsClassifier(n_neighbors=k)
    scores = cross_val_score(model1,X_train,y_train,cv=kfold)
    val_acc_rate.append(scores.mean())
df1 = pd.DataFrame(val_acc_rate,
                                                                to be split
                    columns=['val acc rate'])
                                                                into 5 folds
df1.index = range(1.25)
```

K-Nearest Neighbors - 5-fold Cross Validation (no scaling) to select best K



	average val_acc_rate
1	0.922599
2	0.917811
3	0.924925
4	0.927196
5	0.929603
6	0.929549
7	0.934254
8	0.936607
9	0.936607
10	0.936607
11	0.941313

K-Nearest Neighbors – 5-fold Cross Validation (no scaling) test accuracy rate

```
# Find test accuracy rate

# rebuild model on the
# combined (train+validation) set

model2 = KNeighborsClassifier(n_neighbors=11)
model2.fit(X_train, y_train);

model2.score(X_test,y_test)

0.916083916083916
```

	average val_acc_rate
1	0.922599
2	0.917811
3	0.924925
4	0.927196
5	0.929603
6	0.929549
7	0.934254
8	0.936607
9	0.936607
10	0.936607
11	0.941313

6. k-Fold Cross validation -Fixed K, Scaling the data-

K-Nearest Neighbors – 5-fold Cross Validation (K = 3)

```
y = cancer.target
X = cancer.data

kfold = StratifiedKFold(n_splits = 5,shuffle = True,random_state=1)

scaler = MinMaxScaler()
model1 = KNeighborsClassifier(n_neighbors=3)
pipel = Pipeline([('transformer1', scaler), ('estimator1', model1)])
```

K-Nearest Neighbors – 5-fold Cross Validation (K = 3)

```
y = cancer.target
X = cancer.data

kfold = StratifiedKFold(n_splits = 5,shuffle = True,random_state=1)

scaler = MinMaxScaler()
model1 = KNeighborsClassifier(n_neighbors=3)
pipe1 = Pipeline([('transformer1', scaler), ('estimator1', model1)])
```

K-Nearest Neighbors – 5-fold Cross Validation (hyperparameter known K = 3)

```
y = cancer target
X = cancer.data
kfold = StratifiedKFold(n_splits = 5,shuffle = True,random_state=1)
scaler = MinMaxScaler()
model1 = KNeighborsClassifier(n_neighbors=3)
pipe1 = Pipeline([('transformer1', scaler), ('estimator1', model1)])
scores = cross_val_score(pipe1,X,y,cv=kfold)
scores
array([0.95614035, 0.99122807, 0.98245614, 0.96491228, 0.96460177])
# test accuracy rate
scores.mean()
0.9718677224033534
```

7. k-Fold Cross validation -Search for K, Scaling the data-

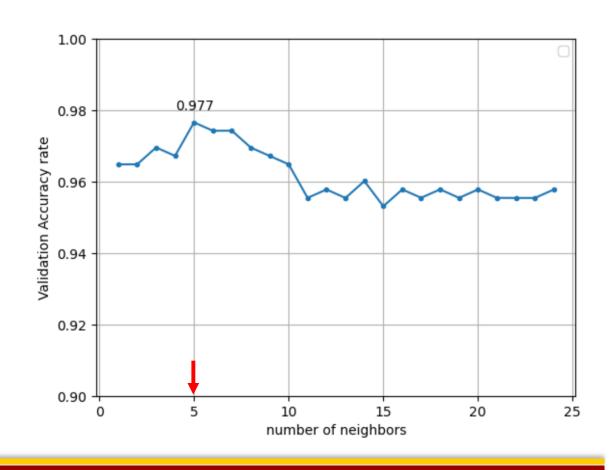
K-Nearest Neighbors – 5-fold Cross Validation to find best K

Reserve test set until last step →

```
y = cancer.target
X = cancer.data
X_train,X_test,\
y_train,y_test = train_test_split(X,y,stratify=y,
                                   random state=66)
val acc rate = []
for k in range(1,25):
    scaler = MinMaxScaler()
    model1 = KNeighborsClassifier(n neighbors=k)
    pipe1 = Pipeline([('transformer1', scaler),
                      ('estimator1', model1)])
    scores = cross_val_score(pipe1,X_train,y_train,cv=kfold)
    val_acc_rate.append(scores.mean())
df1 = pd.DataFrame(val_acc_rate,
                   columns=['val acc rate'])
```

K-Nearest Neighbors - 5-fold Cross Validation to find best K

val_acc_rate	
1	0.964843
2	0.964870
3	0.969576
4	0.967223
5	0.976607
6	0.974254
7	0.974282
8	0.969549
9	0.967196
10	0.964870
11	0.955458



K-Nearest Neighbors – 5-fold Cross Validation test accuracy rate

```
y = cancer.target
X = cancer.data

Reserve test set
until last step →

X_train, X_test, \
y_train, y_test = train_test_split(X, y, stratify=y, random_state=66)
```

Reserve test set

until last step →

K-Nearest Neighbors – 5-fold Cross Validation test accuracy rate

```
y = cancer.target
X = cancer.data
X train,X test,\
y_train,y_test = train_test_split(X,y,stratify=y,
                                   random state=66)
scaler = MinMaxScaler()
scaler.fit(X_train);
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
# rebuild model on the
# combined (train+validation) set
model2 = KNeighborsClassifier(n_neighbors=5)
model2.fit(X_train_scaled, y_train);
model2.score(X_test_scaled,y_test)
0.9440559440559441
```