DNN wine iris QNJL

DNN (Wine, Iris)¶

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Abstract¶

- Datasets: Wine and Iris (UC Irvine Machine Learning Repository)
- Machine learning methods: Decision Trees, naïve Bayes, k-nearest neighbors and SVM (linear and RBF), DNN
- Objective: Compare the performance (confusion matrix and accuracy) of different methods for the classification task by using two different data sets: Wine and Iris.

In [291]:

```
import numpy as np
import pandas as pd
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.datasets import load_wine, load_iris
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix, precision_score, accuracy_score
from sklearn.neural_network import BernoulliRBM
from sklearn.model_selection import ParameterGrid
import time
import matplotlib.pyplot as plt
import seaborn as sns
#visulize tree
from io import StringIO
import pydotplus
import matplotlib.image as mpimg
from sklearn import tree
```

```
Iris dataset¶
In [292]:
iris = load_iris()
In [293]:
X_iris = iris.data
y_iris = iris.target
a) 80% training and 20% testing In [294]:
X_train_50_iris, X_test_50_iris, y_train_50_iris, y_test_50_iris = train_test_split(X_iris,
b) 50% training and 50% testing¶
In [295]:
X_train_80_iris, X_test_80_iris, y_train_80_iris, y_test_80_iris = train_test_split(X_iris,
Wine dataset¶
In [296]:
wine = load_wine()
In [297]:
# Split datasets into features (X) and labels (y)
X_{wine} = wine.data
y_wine = wine.target
a ) 80% training and 20% testing¶ In [298]:
X_train_50_wine, X_test_50_wine, y_train_50_wine, y_test_50_wine = train_test_split(X_wine,
b) 50% training and 50% testing¶
In [299]:
X_train_80_wine, X_test_80_wine, y_train_80_wine, y_test_80_wine = train_test_split(X_wine,
function to train and evaluate a classifier¶
In [300]:
def train_and_evaluate(classifier, X_train, X_test, y_train, y_test):
    # train
    classifier.fit(X_train, y_train)
```

import matplotlib.pyplot as plt

```
# predict
y_pred = classifier.predict(X_test)

# accuracy
acc = accuracy_score(y_test, y_pred)
# confusion matriz
cm = confusion_matrix(y_test, y_pred)
return acc, cm
```

Decision trees ID3¶

Entropy: The amount of information disorder or amount of randomness in the nodes (amount of impurity).

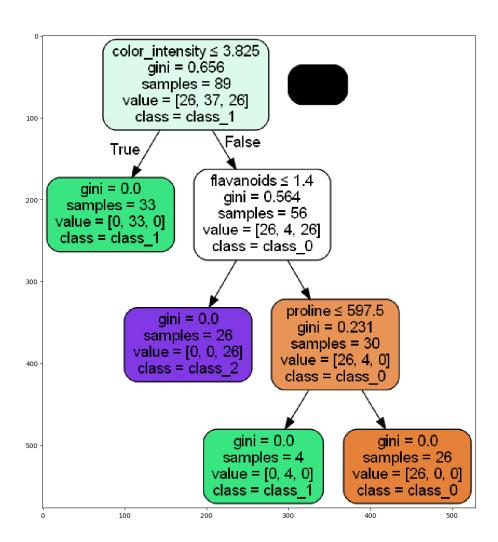
The formula for the entropy of any given attribute, \$A_k\$, is given as:

```
\ H(C|A_k) = \sum_{j=1}^{M_k} p(a_k,j) \cdot [-\sum_{i=1}^{N} p(c_i|a_k,j) \cdot p(c_i|a_k,j)
```

 $H(C|A_k) =$ \$ entropy of the classification property of attribute A_k \$ $p(a_k, j) =$ \$ probability of attribute k\$ being at value j\$ $p(c_i|a_k, j) =$ \$ probability that the class value is c_i \$ when attribute k\$ is at its jth value $M_k =$ \$ total number of values for atribute $A_k =$ 1, $1, 2, ..., M_k$ \$ 1, 2, ..., M\$ 1, 2, ..., M\$ total number of attributes; 1, 2, ..., M\$ 1, 2, ..., M\$

wine 50% train¶

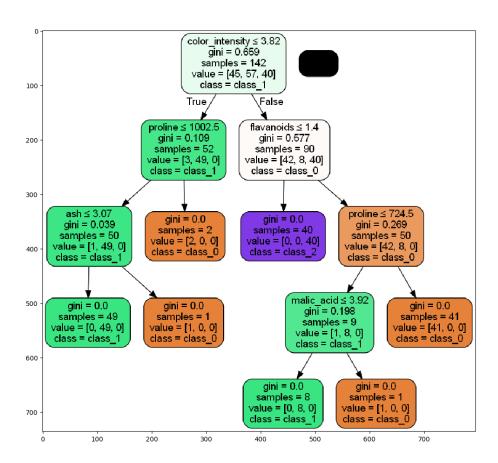
[0 1 21]]



wine 80% train¶

```
In [305]:
tree_classifier_wine = DecisionTreeClassifier()
In [306]:
tree_acc_80_wine, tree_cm_80_wine = train_and_evaluate(tree_classifier_wine, X_train_80_wine)
In [307]:
print("Results for Wine with 80% of training and testing data:")
print("Decision tree - Accuracy:", tree_acc_80_wine)
print("Decision tree - Confusion matrix:")
print(tree_cm_80_wine)
```

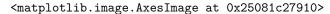
```
Results for Wine with 80\% of training and testing data:
Decision tree - Confusion matrix:
[[13 1 0]
[ 0 14 0]
[ 0 1 7]]
In [308]:
dot_data = StringIO()
filename = "tree.png"
out = tree.export_graphviz(tree_classifier_wine, out_file=dot_data,
                    filled=True, rounded=True, special_characters=True,
                    feature_names=wine.feature_names,
                    class_names=[str(target) for target in wine.target_names])
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png(filename)
img = mpimg.imread(filename)
plt.figure(figsize=(12,15))
plt.imshow(img,interpolation='nearest')
Out[308]:
<matplotlib.image.AxesImage at 0x25087916410>
```

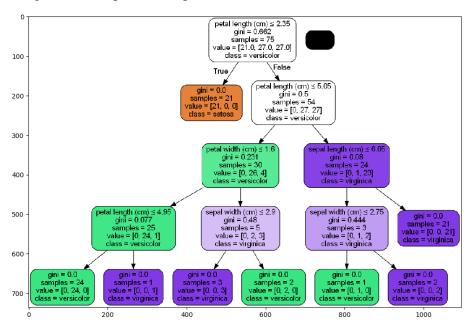


iris 50%¶

In [309]:

```
tree_classifier_iris = DecisionTreeClassifier()
In [310]:
tree_acc_50_iris, tree_cm_50_iris = train_and_evaluate(tree_classifier_iris, X_train_50_iris)
In [311]:
print("Results for Iris with 50% of training and testing data:")
print("Decision tree - Accuracy:", tree_acc_50_iris)
print("Decision tree - Confusion matrix:")
print(tree_cm_50_iris)
Results for Iris with 50% of training and testing data:
Decision tree - Accuracy: 0.9466666666666667
Decision tree - Confusion matrix:
[[29 0 0]
```



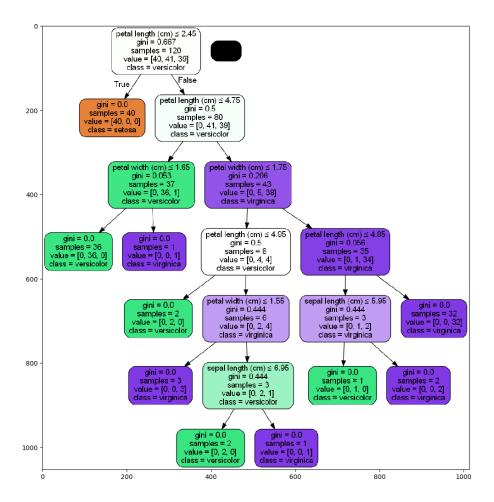


iris $80\%\P$

In [313]:

tree_classifier_iris = DecisionTreeClassifier()

```
In [314]:
tree_acc_80_iris, tree_cm_80_iris = train_and_evaluate(tree_classifier_iris, X_train_80_iris
In [315]:
print("Results for Iris with 80% of training and testing data:")
print("Decision tree - Accuracy:", tree_acc_80_iris)
print("Decision tree - Confusion matrix:")
print(tree_cm_80_iris)
Results for Iris with 80% of training and testing data:
Decision tree - Accuracy: 1.0
Decision tree - Confusion matrix:
[[10 0 0]
[0 9 0]
[ 0 0 11]]
In [316]:
dot_data = StringIO()
filename = "tree.png"
out = tree.export_graphviz(tree_classifier_iris, out_file=dot_data,
                      filled=True, rounded=True, special_characters=True,
                      feature_names=iris.feature_names,
                      class_names=[str(target) for target in iris.target_names])
graph = pydotplus.graph_from_dot_data(dot_data.getvalue())
graph.write_png(filename)
img = mpimg.imread(filename)
plt.figure(figsize=(12,15))
plt.imshow(img,interpolation='nearest')
Out[316]:
<matplotlib.image.AxesImage at 0x250863c4e90>
```



naïve Bayes¶

The assumption of the naive classifier is that the attributes are independent of each other with respect to the concept are independent of each other with respect to the target concept and, therefore, they are independent of the target concept:

$$P(a_i,a_2,...,a_n|v_j) = \prod_{i} P(a_i|v_j)$$

The naive Bayesian classifier approach is:

$$\ v_nb = \arg \max_{v_j \in V} P(v_j) \pmod_{i} P(a_i|v_j) \$$

The probabilities $P(a_i|v_j)$ are much easier to estimate than $P(a_i,a_2,...a_n)$

wine 50%¶

In [317]:

```
naive_bayes_classifier_wine = GaussianNB()
In [318]:
nb_acc_50_wine, nb_cm_50_wine = train_and_evaluate(naive_bayes_classifier_wine, X_train_50_t
In [319]:
print("Results for Wine with 50% of training and testing data:")
print("Naive Bayes - Accuracy:", nb_acc_50_wine)
print("Naive Bayes- Confusion matrix:")
print(nb_cm_50_wine)
Results for Wine with 50% of training and testing data:
Naive Bayes - Accuracy: 0.9887640449438202
Naive Bayes- Confusion matrix:
[[32 1 0]
 [ 0 34 0]
 [ 0 0 22]]
wine 80\%¶
In [320]:
naive_bayes_classifier_wine = GaussianNB()
In [321]:
nb_acc_80_wine, nb_cm_80_wine = train_and_evaluate(naive_bayes_classifier_wine, X_train_80_t
print("Results for Wine with 80% of training and testing data:")
print("Naive Bayes - Accuracy:", nb_acc_80_wine)
print("Naive Bayes- Confusion matrix:")
print(nb_cm_80_wine)
Results for Wine with 80% of training and testing data:
Naive Bayes - Accuracy: 1.0
Naive Bayes- Confusion matrix:
[[14 0 0]
[ 0 14 0]
 [[8 0 0]
Iris 50%¶
In [323]:
naive_bayes_classifier_iris = GaussianNB()
In [324]:
nb_acc_50_iris, nb_cm_50_iris = train_and_evaluate(naive_bayes_classifier_iris, X_train_50_:
```

```
In [325]:
print("Results for Iris with 50% of training and testing data:")
print("Naive Bayes - Accuracy:", nb_acc_50_iris)
print("Naive Bayes- Confusion matrix:")
print(nb_cm_50_iris)
Results for Iris with 50% of training and testing data:
Naive Bayes - Accuracy: 0.986666666666667
Naive Bayes- Confusion matrix:
[[29 0 0]
 [ 0 23 0]
 [ 0 1 22]]
Iris 80%¶
In [326]:
naive_bayes_classifier_wine = GaussianNB()
In [327]:
nb_acc_80_iris, nb_cm_80_iris = train_and_evaluate(naive_bayes_classifier_wine, X_train_80_:
In [328]:
print("Results for Iris with 80% of training and testing data:")
print("Naive Bayes - Accuracy:", nb_acc_80_iris)
print("Naive Bayes- Confusion matrix:")
print(nb_cm_80_iris)
Results for Iris with 80% of training and testing data:
Naive Bayes - Accuracy: 1.0
Naive Bayes- Confusion matrix:
[[10 0 0]
 [ 0 9 0]
 [ 0 0 11]]
```

k-Nearest neighbors¶

- Non-parametric, meaning that it does not make explicit assumptions about the functional form of the data, avoiding mis-modeling the underlying distribution of the data.
- It memorizes the training instances that are later used as "knowledge" for the prediction phase.
- The minimal training phase of KNN is performed at both a memory cost, since we must store a potentially huge dataset, and a computational cost during test time, since the classification of a given observation requires an exhaustion of the entire dataset.

Find nearest similar points¶

The distance between points is found, using one of the distance measures:

• Euclidean distance:

```
\ \sqrt{\sum_{i=1}^{k} (\mathbb{x}_i} - \mathbb{y}^2} $$
```

- Manhattan distance: $\ \sum_{i=1}^{k} |\mathcal{x}_i| \mathcal{y}_i|$
- 1. Calculate the distance
- 2. Find its nearest neighbors
- 3. Vote for the labels

Define the value of K

- The number of neighbors (K) is a hyperparameter to be chosen at the time of model construction.
- The number of neighbors (K) is a hyperparameter to be chosen at the time of model construction.
- There is no optimal number of neighbors that fits all types of datasets, each dataset has its own requirements.
- A small number of neighbors will have a low skewness but a high variance, and a large number of neighbors will have a lower variance but a higher skewness.

funtion select the best parameter to ${\bf k}$

```
In [329]:
```

```
from sklearn.model_selection import GridSearchCV
def find_best_parameter_k_neighbors (classifier, X_train, X_test, y_train, y_test):
    param_grid = {'n_neighbors': [3, 5, 7, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20]}
    grid_search = GridSearchCV(classifier, param_grid, cv=5)
    grid_search.fit(X_train, y_train)
    best_k = grid_search.best_params_['n_neighbors']
    best_knn = KNeighborsClassifier(n_neighbors=best_k, metric= 'minkowski', p=2)
    best_knn.fit(X_train, y_train)
    y_pred = best_knn.predict(X_test)
    acc = accuracy_score(y_test, y_pred)
```

```
cm = confusion_matrix(y_test, y_pred)
   return acc, cm, best_k
wine 50\%¶
In [330]:
knn = KNeighborsClassifier()
knn_acc_50_wine, knn_cm_50_wine, knn_best_k_wine_50 = find_best_parameter_k_neighbors(knn, X
In [332]:
print("Results for wine with 50% of training and testing data:")
print("Best k:", knn_best_k_wine_50)
print("Knn - Accuracy:", knn_acc_50_wine)
print("Knn - Confusion matrix:")
print(knn_cm_50_wine)
Results for wine with 50% of training and testing data:
Best k: 14
Knn - Accuracy: 0.6629213483146067
Knn - Confusion matrix:
[[27 0 6]
[ 1 20 13]
[ 0 10 12]]
wine 80\%¶
In [333]:
knn = KNeighborsClassifier()
In [334]:
knn_acc_80_wine, knn_cm_80_wine, knn_best_k_wine_80 = find_best_parameter_k_neighbors(knn, Z
In [335]:
print("Results for wine with 80% of training and testing data:")
print("Best k:", knn_best_k_wine_80)
print("Knn - Accuracy:", knn_acc_80_wine)
print("Knn - Confusion matrix:")
print(knn_cm_80_wine)
Results for wine with 80% of training and testing data:
Best k: 17
Knn - Accuracy: 0.7777777777778
```

```
Knn - Confusion matrix:
[[14 0 0]
[ 0 9 5]
 [1 2 5]]
Iris 50\%\P
In [336]:
knn = KNeighborsClassifier()
knn_acc_50_iris, knn_cm_50_iris, knn_best_k_iris_50 = find_best_parameter_k_neighbors(knn, X
In [338]:
print("Results for Iris with 50% of training and testing data:")
print("Best k:", knn_best_k_iris_50)
print("Knn - Accuracy:", knn_acc_50_iris)
print("Knn - Confusion matrix:")
print(knn_cm_50_iris)
Results for Iris with 50% of training and testing data:
Best k: 17
Knn - Accuracy: 0.96
Knn - Confusion matrix:
[[29 0 0]
[ 0 23 0]
[ 0 3 20]]
iris 80%¶
In [339]:
knn = KNeighborsClassifier()
In [340]:
knn_acc_80_iris, knn_cm_80_iris, knn_best_k_iris_80 = find_best_parameter_k_neighbors(knn, Z
In [341]:
print("Results for Iris with 80% of training and testing data:")
print("Best k:", knn_best_k_iris_80)
print("Knn - Accuracy:", knn_acc_80_iris)
print("Knn - Confusion matrix:")
print(knn_cm_80_iris)
Results for Iris with 80% of training and testing data:
Best k: 3
Knn - Accuracy: 1.0
```

```
Knn - Confusion matrix:
[[10  0  0]
  [ 0  9  0]
  [ 0  0  11]]
```

Support Vector Machines (SVM)¶

- Algoritmh based on supervised learning (labeling data)
- This algoritmh is cable to perform regression and classification linear and non-linear
- Works very well for small to medium sized complex datasets
- It can be applied in different ways depending on the data set:
 - Linearly separeble datasets:
 - * Hard Margin Classification
 - * Soft Margin Classification
 - Non-linearly separable datasets:
 - * kernels

Disadvantages:

- only works with linearly separable dataset
- is very sensitive to anomalous data

```
In [342]:
```

```
from sklearn.pipeline import Pipeline
from sklearn.svm import SVC
from sklearn.preprocessing import StandardScaler, RobustScaler
```

Gasussian Kernel¶ In [343]:

```
y_pred = rbf_kernel_svm_clf.predict(X_test)
                                  acc = accuracy_score(y_test, y_pred)
                                  if acc > best_acc:
                                             best_acc = acc
                                             best_params = (gamma_, C_)
                                             best_cm = confusion_matrix(y_test, y_pred)
           return (best_acc, best_cm, best_params[0], best_params[1])
Wine 50\%¶
In [344]:
svm_acc_50_wine, svm_cm_50_wine, svm_gamma_50_wine, svm_C_50_wine = find_best_parameter_gamma_50_wine, svm_cm_50_wine = find_best_parameter_gamma_50_wine, svm_cm_50_wine, svm
In [345]:
print("Results for wine with 50% of training and testing data:")
print("Best gamma:", svm_gamma_50_wine )
print("Best C_ ", svm_C_50_wine)
print("svm - Accuracy:", svm_acc_50_wine)
print("svm - Confusion matrix:")
print(svm_cm_50_wine)
Results for wine with 50% of training and testing data:
Best gamma: 0.1
Best C_ 1.0
svm - Accuracy: 0.9775280898876404
svm - Confusion matrix:
[[26 0 0]
  [ 0 36 1]
  [ 0 1 25]]
Wine 80\%¶
In [346]:
svm_acc_80_wine, svm_cm_80_wine, svm_gamma_80_wine, svm_C_80_wine = find_best_parameter_gam
In [347]:
print("Results for wine with 80% of training and testing data:")
print("Best gamma:", svm_gamma_80_wine )
print("Best C_ ", svm_C_80_wine)
print("svm - Accuracy:", svm_acc_80_wine)
```

rbf_kernel_svm_clf.fit(X_train, y_train)

```
print("svm - Confusion matrix:")
print(svm_cm_80_wine)
Results for wine with 80% of training and testing data:
Best gamma: 0.1
Best C_ 1.0
svm - Accuracy: 0.9647887323943662
svm - Confusion matrix:
[[43 2 0]
  [ 1 55 1]
  [ 0 1 39]]
Iris 50%¶
In [348]:
svm_acc_50_iris, svm_cm_50_iris, svm_gamma_50_iris, svm_C_50_iris = find_best_parameter_gamma_50_iris
In [349]:
print("Results for iris with 50% of training and testing data:")
print("Best gamma:", svm_gamma_50_iris )
print("Best C_ ", svm_C_50_iris)
print("svm - Accuracy:", svm_acc_50_iris)
print("svm - Confusion matrix:")
print(svm_cm_50_iris)
Results for iris with 50% of training and testing data:
Best gamma: 0.1
Best C_ 10.0
svm - Accuracy: 0.96
svm - Confusion matrix:
[[21 0 0]
 [ 0 24 3]
  [ 0 0 27]]
Iris 80%¶
In [350]:
svm_acc_80_iris, svm_cm_80_iris, svm_gamma_80_iris, svm_C_80_iris = find_best_parameter_gamma_80_iris, svm_cm_80_iris, svm_cm_
In [351]:
print("Results for iris with 80% of training and testing data:")
print("Best gamma:", svm_gamma_80_iris )
print("Best C_ ", svm_C_80_iris)
print("svm - Accuracy:", svm_acc_80_iris)
print("svm - Confusion matrix:")
print(svm_cm_80_iris)
```

```
Results for iris with 80% of training and testing data:
Best gamma: 0.001
Best C_ 100000.0
svm - Accuracy: 0.966666666666667
svm - Confusion matrix:
[[40 0 0]
[ 0 39 2]
[ 0 2 37]]
DNN\P
In [352]:
def reconstruct_from_hidden(hidden, rbm):
    #Reconstruct visible layer from hidden activations
   p = 1.0 / (1 + np.exp(-np.dot(hidden, rbm.components_) - rbm.intercept_visible_))
   return (p > 0.5).astype(int)
# Define hyperparameter grid for grid search
param_grid = {
    'n_components': [4],
    'learning_rate': [0.1],
    'batch_size': [3],
    'n_iter': [100]
}
def train_and_evaluate_dnn(TrainData):
   results = []
   start_time_total = time.time()
    # Perform grid search
    for params in ParameterGrid(param_grid):
        start_time = time.time()
        rbm = BernoulliRBM(**params, verbose=0)
        rbm.fit(TrainData)
        hidden_data = rbm.transform(TrainData)
        reconstructed_data = reconstruct_from_hidden(hidden_data, rbm)
        accuracy = np.mean(reconstructed_data == TrainData)
        end_time = time.time()
        execution_time = end_time - start_time
```

Wine 50%¶

In [353]:

dnn_results_wine_50= train_and_evaluate_dnn(X_train_50_wine)

dnn_results_wine_50

Out[353]:

	$n_components$	$learning_rate$	$batch_size$	n_iter	accuracy	$execution_time$
0	4	0.1	3	100	0.001729	0.189876

Wine 80%¶

In [354]:

dnn_results_wine_80= train_and_evaluate_dnn(X_train_80_wine)

dnn_results_wine_80

Out[354]:

	$n_components$	$learning_rate$	$batch_size$	n_iter	accuracy	execution_time
0	4	0.1	3	100	0.001083	0.268337

Iris $50\%\P$

In [355]:

```
dnn_results_iris_50= train_and_evaluate_dnn(X_train_50_iris)
dnn_results_iris_50
Out[355]:
```

	n_components	learning_rate	$batch_size$	n_iter	accuracy	execution_time
0	4	0.1	3	100	0.01	0.391826

Iris $80\%\P$

In [356]:

dnn_results_iris_80= train_and_evaluate_dnn(X_train_80_iris)

dnn_results_iris_80

Out[356]:

Out[358]:

	n_components	learning_rate	batch_size	n_iter	accuracy	execution_time
0	4	0.1	3	100	0.016667	0.619345

Dataset: Wine Training: 50% Testing: 50%¶

```
In [358]:
acc = [tree_acc_50_wine, nb_acc_50_wine, knn_acc_50_wine, svm_acc_50_wine]
models = ['Decision tree', 'Naive Bayes', 'K-NN', 'SVM']
best_ks = ['', '', knn_best_k_wine_50, f'gamma: {svm_gamma_50_wine} C: {svm_C_50_wine}']
data = {
    'Classifier': models,
    'best parameters': best_ks,
    'Accuracy': acc
}
table_df1 = pd.DataFrame(data)
table_df1
```

	Classifier	best parameters	Accuracy
0	Decision tree		0.910112
1	Naive Bayes		0.988764
2	K-NN	14	0.662921

	Classifier	best parameters	Accuracy
3	SVM	gamma: 0.1 C: 1.0	0.977528

Dataset: Wine Training: 80% Testing: 20%¶

```
In []:
acc = [tree_acc_80_wine, nb_acc_80_wine, knn_acc_80_wine, svm_acc_80_wine]
models = ['Decision tree', 'Naive Bayes', 'K-NN', 'SVM']
best_ks = ['', '', knn_best_k_wine_80, f'gamma: {svm_gamma_80_wine} C: {svm_C_80_wine}']
data = {
    'Classifier': models,
    'best parameters': best_ks,
    'Accuracy': acc
}
table_df2 = pd.DataFrame(data)
table_df2
Out[]:
```

	Classifier	best parameters	Accuracy
0	Decision tree		0.944444
1	Naive Bayes		1.000000
2	K-NN	17	0.777778
3	SVM	gamma: 0.1 C: 1.0	0.964789

Dataset: Iris Training: 50% Testing: 50%¶

```
In [359]:
acc = [tree_acc_50_iris, nb_acc_50_iris, knn_acc_50_iris, svm_acc_50_iris]
models = ['Decision tree', 'Naive Bayes', 'K-NN', 'SVM']
best_ks = ['', '', knn_best_k_iris_50, f'gamma: {svm_gamma_50_iris} C: {svm_C_50_iris}']
data = {
    'Classifier': models,
    'best parameters': best_ks,
    'Accuracy': acc
}
table_df3 = pd.DataFrame(data)
```

Out[359]:

	Classifier	best parameters	Accuracy
0	Decision tree		0.946667
1	Naive Bayes		0.986667
2	K-NN	17	0.960000
3	SVM	gamma: 0.1 C: 10.0	0.960000

Dataset: Iris Training: 80% Testing: 20%¶

```
In []:
acc = [tree_acc_80_iris, nb_acc_80_iris, knn_acc_80_iris, svm_acc_80_iris]
models = ['Decision tree', 'Naive Bayes', 'K-NN', 'SVM']
best_ks = ['', '', knn_best_k_iris_80, f'gamma: {svm_gamma_80_iris} C: {svm_C_80_iris}']
data = {
    'Classifier': models,
    'best parameters': best_ks,
    'Accuracy': acc
}
table_df4 = pd.DataFrame(data)
table_df4
Out[]:
```

	Classifier	best parameters	Accuracy
0	Decision tree		1.000000
1	Naive Bayes		1.000000
2	K-NN	3	1.000000
3	SVM	gamma: 0.001 C: 100000.0	0.966667

Conclusions

In the case of the Wine data set (50% and 50%), the best classifier is Naive Bayes with 98% accuracy; for (80% and 20%), Naive Bayes is also the best with 1 accuracy.

While for Iris (50% and 50%), the best is Naive Bayes with 98%, and for (80% and 20%) there is a tie with the three classifiers with 100%.

References¶

 - Fisher, R. A.. (1988). Iris. UCI Machine Learning Repository. https://doi.org/10.24432/C56C76.

- Aeberhard, Stefan and Forina, M.. (1991). Wine. UCI Machine Learning Repository. https://doi.org/10.24432/C5PC7J.
- Scikit-learn: Machine Learning in Python, Pedregosa et al., JMLR 12, pp. 2825-2830, 2011. http://jmlr.org/papers/v12/pedregosa11a.html