ML23

Lecture notes for Fall 2023 at Arkansas Tech University

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Preface

This is the lecture notes for STAT 4803/5803 Machine Learning Fall 2023 at ATU. If you have any comments/suggetions/concers about the notes please contact us at xxiao@atu.edu.

References

1 Introduction

In this Chapter we will discuss

- What is Machine Learning?
- What do typical Machine Learning problems look like?
- What is the basic structure of Machine Learning models?
- What is the basic work flow to use Machine Learning to solve problems?
- Some supplementary materials, such as Linear Algebra and Python.

```
import sys

print(sys.executable)

!mamba list
```

```
C:\Users\Xinli\mambaforge\python.exe
# packages in environment at C:\Users\Xinli\mambaforge\envs\base23:
#
# Name                    Version                   Build  Channel
anyio                     3.5.0           py310haa95532_0
appdirs                   1.4.4              pyhd3eb1b0_0
argon2-cffi               21.3.0             pyhd3eb1b0_0
argon2-cffi-bindings      21.2.0          py310h2bbff1b_0
asttokens                 2.0.5              pyhd3eb1b0_0
attrs                     22.1.0          py310haa95532_0
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```

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icc_rt                    2022.1.0             h6049295_2
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```

```
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libpng                    1.6.39               h8cc25b3_0
libsodium                 1.0.18               h62dcd97_0
libsqlite                 3.42.0               hcfcfb64_0    conda-forge
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python                    3.10.11         h4de0772_0_cpython    conda-forge
python-dateutil           2.8.2              pyhd3eb1b0_0
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vs2015_runtime            14.34.31931          hed1258a_16    conda-forge
wcwidth                   0.2.5               pyhd3eb1b0_0
```

```
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win_inet_pton             1.1.0           py310haa95532_0
winpty                    0.4.3                         4
xz                        5.4.2                h8cc25b3_0
yaml                      0.2.5                he774522_0
zeromq                    4.3.4                hd77b12b_0
zipp                      3.11.0          py310haa95532_0
zlib                      1.2.13               hcfcfb64_5    conda-forge
zstd                      1.5.5                hd43e919_0
```

2 k-Nearest Neighbors algorithm (k-NN)

This algorithm is different from other algorithms covered in this course, that it doesn't really extract features from the data. However, since its idea is easy to understand, we use it as our first step towards machine learning world.

Similar to other algorithms, we will only cover the beginning part of the algorithm. All later upgrades of the algorithms are left for yourselves to learn.

References: {cite:p}`Har2012`.

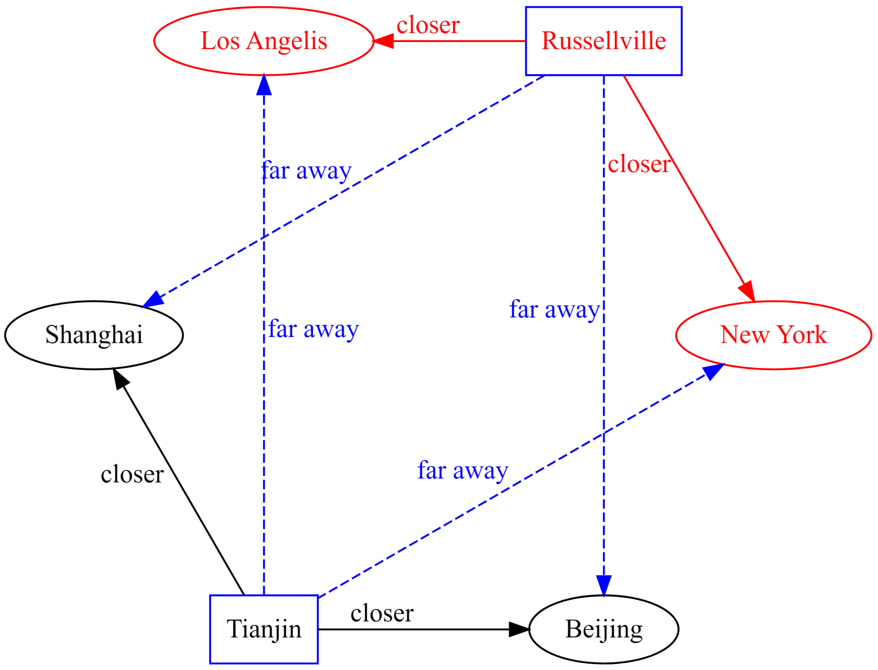
2.1 k-Nearest Neighbors Algorithm (k-NN)

2.1.1 Ideas

Assume that we have a set of labeled data $\{(X_i, y_i)\}$ where y_i denotes the label. Given a new data X, how do we determine the label of it?

k-NN algorithm starts from a very straightforward idea. We use the distances from the new data point X to the known data points to identify the label. If X is closer to y_i points, then we will label X as y_i.

Let us take cities and countries as an example. New York and Los Angeles are U.S cities, and Beijing and Shanghai are Chinese cities. Now we would like to consider Tianjin and Russellville. Do they belong to China or U.S? We calculate the distances from Tianjin (resp. Russellville) to all four known cities. Since Tianjin is closer to Beijing and Shanghai comparing to New York and Los Angeles, we classify Tianjin as a Chinese city. Similarly, since Russellville is closer to New York and Los Angeles comparing to Beijing and Shanghai, we classify it as a U.S. city.



This naive example explains the idea of k-NN. Here is a more detailed description of the algorithm.

2.1.2 The Algorithm

k-NN Classifier **Inputs** Given the training data set $\{(X_i, y_i)\}$ where $X_i = (x_i^1, x_i^2, \ldots, x_i^n)$ represents n features and y_i represents labels. Given a new data point $\tilde{X} = (\tilde{x}^1, \tilde{x}^2, \ldots, \tilde{x}^n)$.

Outputs Want to find the best label for $\tilde{X}$.

1. Compute the distance from $\tilde{X}$ to each X_i.
2. Sort all these distances from the nearest to the furthest.
3. Find the nearest k data points.
4. Determine the labels for each of these k nearest points, and compute the frenqucy of each labels.
5. The most frequent label is considered to be the label of $\tilde{X}$.

2.1.3 Details

- The distance between two data points are defined by the Euclidean distance:

$$dist\left((x_i^j)_{j=1}^n, (\tilde{x}^j)_{j=1}^n\right) = \sqrt{\sum_{j=1}^n (x_i^j - \tilde{x}^j)^2}.$$

- Using linear algebra notations:

$$dist(X_i, \tilde{X}) = \sqrt{(X_i - \tilde{X}) \cdot (X_i - \tilde{X})}.$$

- All the distances are stored in a 1-dim numpy array, and we will combine it together with another 1-dim array that store the labels of each point.

2.1.4 The codes

- `argsort`
- `get`
- `sorted`

```python
def classify_kNN(inX, X, y, k):
    # create a new 2-d numpy array by copying inX for each row.
    Xmat = np.tile(np.array([inX]), (X.shape[0], 1))
    # compute the distance between each row of X and Xmat
    Dmat = np.sqrt(np.sum((Xmat - X)**2, axis=1))
    # sort by distance
    sortedlist = Dmat.argsort()
    # count the freq. of the first k items
    k = min(k, len(sortedlist))
    classCount = dict()
    for i in sortedlist[:k]:
        classCount[y[i]] = classCount.get(y[i], 0) + 1
    # find out the most freqent one
    sortedCount = sorted(classCount.items(), key=lambda x:x[1],
                         reverse=True)
    return sortedCount[0][0]
```

2.1.5 `sklearn` packages

You may also directly use the kNN function `KNeighborsClassifier` packaged in `sklearn.neighbors`. You may check the description of the function online from here.

There are many ways to modify the kNN algorithm. What we just mentioned is the simplest idea. It is correspondent to the argument `weights='uniform'`, `algorithm='brute` and metric='euclidean'. However due to the implementation details, the results we got from sklearn are still a little bit different from the results produced by our naive codes.

```
from sklearn.neighbors import KNeighborsClassifier
clf = KNeighborsClassifier(n_neighbors=10, weights='uniform', algorithm='brute',
                             metric='euclidean')
clf.fit(X_train, y_train)
y_pred = ckf.predict(X_test)
```

2.1.6 Normalization

Different features may have different scales. It might be unfair for those features that have small scales. Therefore usually it is better to rescale all the features to make them have similar scales. After examining all the data, we find the minimal value minVal and the range ranges for each column. The normalization formula is:

$$X_{norm} = \frac{X_{original} - minVal}{ranges}.$$

We could also convert the normalized number back to the original value by

$$X_{original} = X_{norm} \times ranges + minVal.$$

The sample codes are listed below.

```
def encodeNorm(X, parameters=None):
    # parameters contains minVals and ranges
    if parameters is None:
        minVals = np.min(X, axis=0)
        maxVals = np.max(X, axis=0)
        ranges = np.maximum(maxVals - minVals, np.ones(minVals.size))
        parameters = {'ranges': ranges, 'minVals': minVals}
    else:
        minVals = parameters['minVals']
        ranges = parameters['ranges']
    Nmat = np.tile(minVals, (X.shape[0], 1))
    Xnorm = (X - Nmat)/ranges
    return (Xnorm, parameters)


def decodeNorm(X, parameters):
    # parameters contains minVals and ranges
    ranges = parameters['ranges']
    minVals = parameters['minVals']
    Nmat = np.tile(minVals, (X.shape[0], 1))
    Xoriginal = X * ranges + Nmat
    return Xoriginal
```

2.2 k-NN Project 1: `iris` Classification

This data is from `sklearn.datasets`. This dataset consists of 3 different types of irises' petal / sepal length / width, stored in a 150×4 `numpy.ndarray`. We already explored the dataset briefly in the previous chapter. This time we will try to use the feature provided to predict the type of the irises. For the purpose of plotting, we will only use the first two features: `sepal length` and `sepal width`.

2.2.1 Explore the dataset

We first load the dataset.

```
from sklearn import datasets
iris = datasets.load_iris()
X = iris.data[:, :2]
y = iris.target
```

Then we would like to split the dataset into trainning data and test data. Here we are going to use `sklearn.model_selection.train_test_split` function. Besides the dataset, we should also provide the propotion of the test set comparing to the whole dataset. We will choose `test_size=0.1` here, which means that the size of the test set is 0.1 times the size of the whole dataset. `stratify=y` means that when split the dataset we want to split respects the distribution of labels in `y`.

The split will be randomly. You may set the argument `random_state` to be a certain number to control the random process. If you set a `random_state`, the result of the random process will stay the same. This is for reproducible output across multiple function calls.

After we get the training set, we should also normalize it. All our normalization should be based on the training set. When we want to use our model on some new data points, we will use the same normalization parameters to normalize the data points in interests right before we apply the model. Here since we mainly care about the test set, we could normalize the test set at this stage.

Note that in the following code, I import functions `encodeNorm` from `assests.codes.knn`. You need to modify this part based on your file structure. See here for more details.

```
from sklearn.model_selection import train_test_split
from assests.codes.knn import encodeNorm
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.1, random_state=1, s

X_train_norm, parameters = encodeNorm(X_train)
X_test_norm, _ = encodeNorm(X_test, parameters=parameters)
```

Before we start to play with k-NN, let us look at the data first. Since we only choose two features, it is able to plot these data points on a 2D plane, with different colors representing different classes.

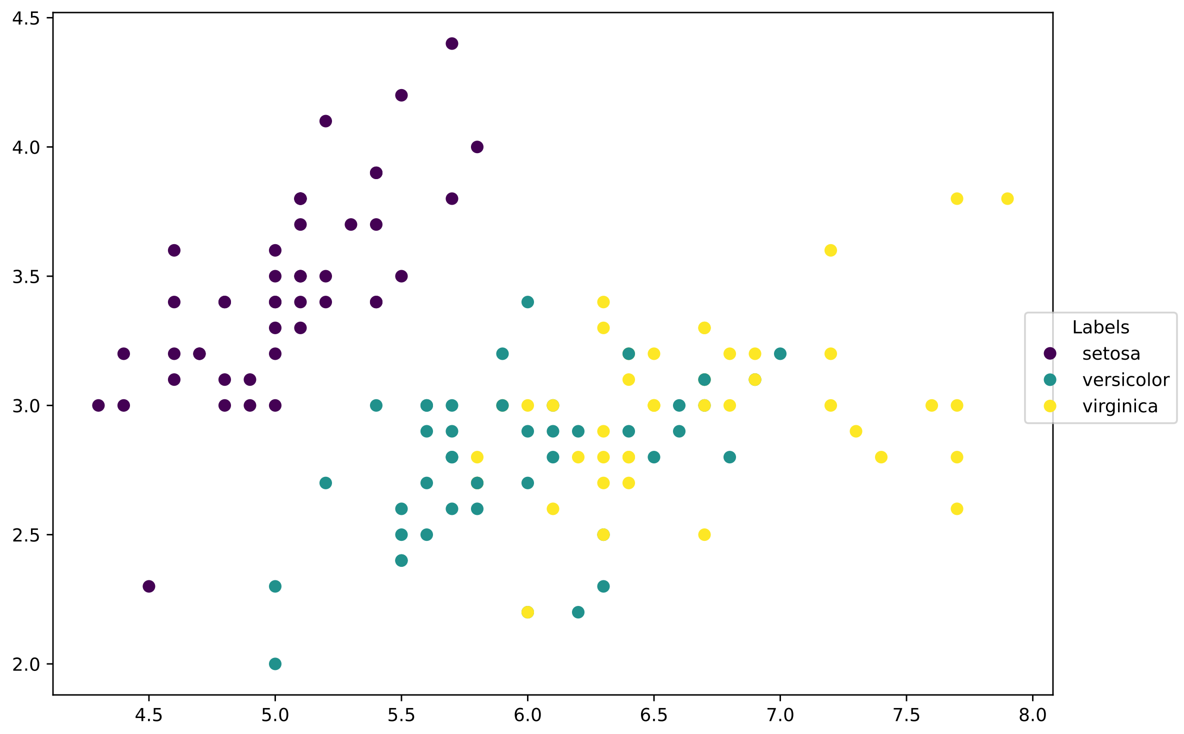
```
import matplotlib.pyplot as plt
import numpy as np

# Plot the scatter plot.
fig = plt.figure(figsize=(10,7))
ax = fig.add_subplot(111)
scatter = ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train)

# Generate legends.
labels = ['setosa', 'versicolor', 'virginica']
fig.legend(handles=scatter.legend_elements()[0], labels=labels,
           loc="right", title="Labels")

# plt.show()
```

```
<matplotlib.legend.Legend at 0x2df4c55f790>
```



(section:applyourknn)= ### Apply our k-NN model

Now let us apply k-NN to this dataset. We first use our codes. Here I use `from assests.codes.knn` to import our functions since I put all our functions in `./assests/codes/knn.py`. Then the poential code is

```
y_pred = classify_kNN(X_test, X_train, y_train, k=10)
```

Note that the above code is actually wrong. The issue ist that our function `classify_kNN` can only classify one row of data. To classify many rows, we need to use a `for` loop.

```
from assests.codes.knn import classify_kNN

n_neighbors = 10
y_pred = list()
for row in X_test_norm:
    row_pred = classify_kNN(row, X_train_norm, y_train, k=n_neighbors)
    y_pred.append(row_pred)
y_pred = np.array(y_pred)
```

We could use list comprehension to simply the above codes.

```python
from assests.codes.knn import classify_kNN

n_neighbors = 10
y_pred = np.array([classify_kNN(row, X_train_norm, y_train, k=n_neighbors)
                   for row in X_test_norm])
```

This `y_pred` is the result we got for the test set. We may compare it with the real answer `y_test`, and calcuate the accuracy.

```python
acc = np.mean(y_pred == y_test)
print(acc)
```

```
0.7333333333333333
```

2.2.2 Apply k-NN model from `sklearn`

Now we would like to use `sklearn` to reproduce this result. Since our data is prepared, what we need to do is directly call the functions.

```python
from sklearn.neighbors import KNeighborsClassifier
n_neighbors = 10
clf = KNeighborsClassifier(n_neighbors, weights="uniform", metric="euclidean",
                           algorithm='brute')
clf.fit(X_train_norm, y_train)
y_pred_sk = clf.predict(X_test_norm)

acc = np.mean(y_pred_sk == y_test)
print(acc)
```

```
0.7333333333333333
```

2.2.3 Using data pipeline

We may organize the above process in a neater way. After we get a data, the usual process is to apply several transforms to the data before we really get to the model part. Using terminolgies from `sklearn`, the former are called *transforms*, and the latter is called an *estimator*. In this example, we have exactly one tranform which is the normalization. The estimator here we use is the k-NN classifier.

sklearn provides a standard way to write these codes, which is called pipeline. We may chain the transforms and estimators in a sequence and let the data go through the pipeline. In this example, the pipeline contains two steps: 1. The normalization transform sklearn.preprocessing.MinMaxScaler. When we directly apply it the parameters ranges and minVals and will be recorded automatically, and we don't need to worry about it when we want to use the same parameters to normalize other data. 2. The k-NN classifier sklearn.neighbors.KNeighborsClassifier. This is the same one as we use previously.

The code is as follows. It is a straightforward code. Note that the () after the class in each step of steps is very important. The codes cannot run if you miss it.

After we setup the pipeline, we may use it as other estimators since it is an estimator. Here we may also use the accuracy function provided by sklearn to perform the computation. It is essentially the same as our acc computation.

```python
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import MinMaxScaler
from sklearn.metrics import accuracy_score

steps = [('scaler', MinMaxScaler()),
         ('knn', KNeighborsClassifier(n_neighbors, weights="uniform",
                                      metric="euclidean", algorithm='brute'))]
pipe = Pipeline(steps=steps)
pipe.fit(X_train, y_train)
y_pipe = pipe.predict(X_test)
print(accuracy_score(y_pipe, y_test))
```

```
0.7333333333333333
```

2.2.4 Visualize the Decision boundary

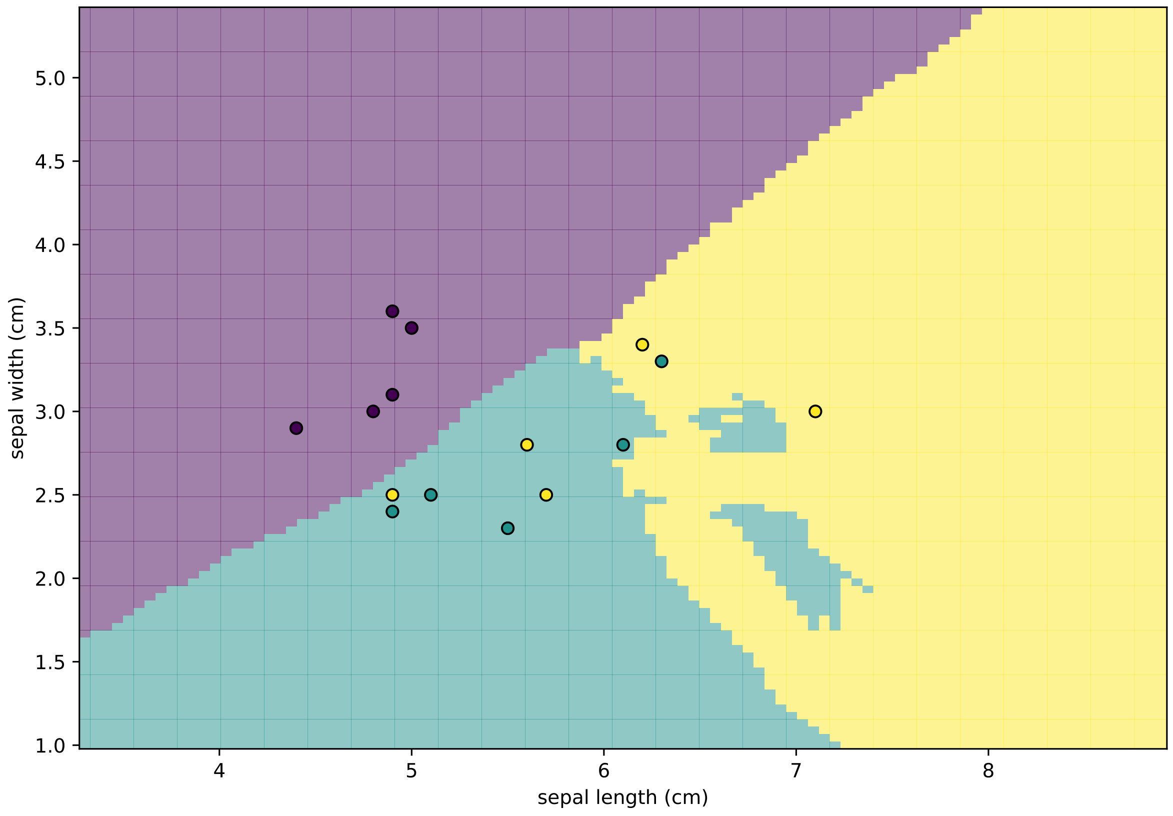
Using the classifier we get above, we are able to classify every points on the plane. This enables us to draw the following plot, which is called the Decision boundary. It helps us to visualize the relations between features and the classes.

We use DecisionBoundaryDisplay from sklearn.inspection to plot the decision boundary. The function requires us to have a fitted classifier. We may use the classifier pipe we got above. Note that this classifier should have some build-in structures that our classify_kNN function doesn't have. We may rewrite our codes to make it work, but this goes out of the scope of this section. This is supposed to be Python programming exercise. We will talk about it in the future if we have enough time.

We first plot the dicision boundary using `DecisionBoundaryDisplay.from_estimator`. Then we plot the points from `X_test`. From the plot it is very clear which points are misclassified.

```python
from sklearn.inspection import DecisionBoundaryDisplay

disp = DecisionBoundaryDisplay.from_estimator(
            pipe,
            X_train,
            response_method="predict",
            plot_method="pcolormesh",
            xlabel=iris.feature_names[0],
            ylabel=iris.feature_names[1],
            alpha=0.5)
disp.ax_.scatter(X_test[:, 0], X_test[:, 1], c=y_test, edgecolor="k")
disp.figure_.set_size_inches((10,7))
```



(section-cross-validation)= ### k-Fold Cross-Validation

Previously we perform a random split and test our model in this case. What would happen if we fit our model on another split? We might get a different accuracy score. So in order to evaluate the performance of our model, it is natual to consider several different split and compute the accuracy socre for each case, and combine all these socres together to generate an index to indicate whehter our model is good or bad. This naive idea is called *k-Fold Cross-Validation*.

The algorithm is described as follows. We first randomly split the dataset into `k` groups. We use one of them as the test set, and the rest together forming the training set, and use this setting to get an accuracy score. We did this for each group to be chosen as the test set. Then the final score is the mean.

`sklearn` provides a function `sklearn.model_selection.cross_val_score` to perform the above computation. The usage is straightforward, as follows.

```python
from sklearn.model_selection import cross_val_score
cv_scores = cross_val_score(pipe, X, y, cv=5)
print(cv_scores)
print(np.mean(cv_scores))
```

```
[0.66666667 0.8        0.63333333 0.8        0.7       ]
0.7200000000000001
```

2.2.5 Choosing a `k` value

In the previous example we choose `k` to be `10` as an example. To choose a `k` value we usually run some test by trying different `k` and choose the one with the best performance. In this case, best performance means the highest cross-validation score.

`sklearn.model_selection.GridSearchCV` provides a way to do this directly. We only need to setup the esitimator, the metric (which is the cross-validation score in this case), and the hyperparameters to be searched through, and `GridSearchCV` will run the search automatically.

We let `k` go from `1` to `100`. The code is as follows.

Note that `parameters` is where we set the search space. It is a dictionary. The key is the name of the estimator plus double `_` and then plus the name of the parameter.

```python
from sklearn.model_selection import GridSearchCV
n_list = list(range(1, 101))
parameters = dict(knn__n_neighbors=n_list)
clf = GridSearchCV(pipe, parameters)
```

```
clf.fit(X, y)
print(clf.best_estimator_.get_params()["knn__n_neighbors"])
```

```
35
```

After we fit the data, the `best_estimator_.get_params()` can be printed. It tells us that it is best to use `31` neibhours for our model. We can directly use the best estimator by calling `clf.best_estimator_`.

```
cv_scores = cross_val_score(clf.best_estimator_, X, y, cv=5)
print(np.mean(cv_scores))
```

```
0.82
```

The cross-validation score using `k=31` is calculated. This serves as a benchmark score and we may come back to dataset using other methods and compare the scores.

2.3 k-NN Project 2: Dating Classification

The data can be downloaded from {Download}`here<./assests/datasets/datingTestSet2.txt>`.

2.3.1 Background

Helen dated several people and rated them using a three-point scale: 3 is best and 1 is worst. She also collected data from all her dates and recorded them in the file attached. These data contains 3 features:

- Number of frequent flyer miles earned per year
- Percentage of time spent playing video games
- Liters of ice cream consumed per week

We would like to predict her ratings of new dates when we are given the three features.

The data contains four columns, while the first column refers to `Mileage`, the second `Gamingtime`, the third `Icecream` and the fourth `Rating`.

2.3.2 Look at Data

We first load the data and store it into a DataFrame.

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

df = pd.read_csv('./assests/datasets/datingTestSet2.txt', sep='\t', header=None)
df.head()
```

```
C:\Users\Xinli\AppData\Roaming\Python\Python310\site-packages\IPython\core\formatters.py:343
  return method()
```

	0	1	2	3
0	40920	8.326976	0.953952	3
1	14488	7.153469	1.673904	2
2	26052	1.441871	0.805124	1
3	75136	13.147394	0.428964	1
4	38344	1.669788	0.134296	1

To make it easier to read, we would like to change the name of the columns.

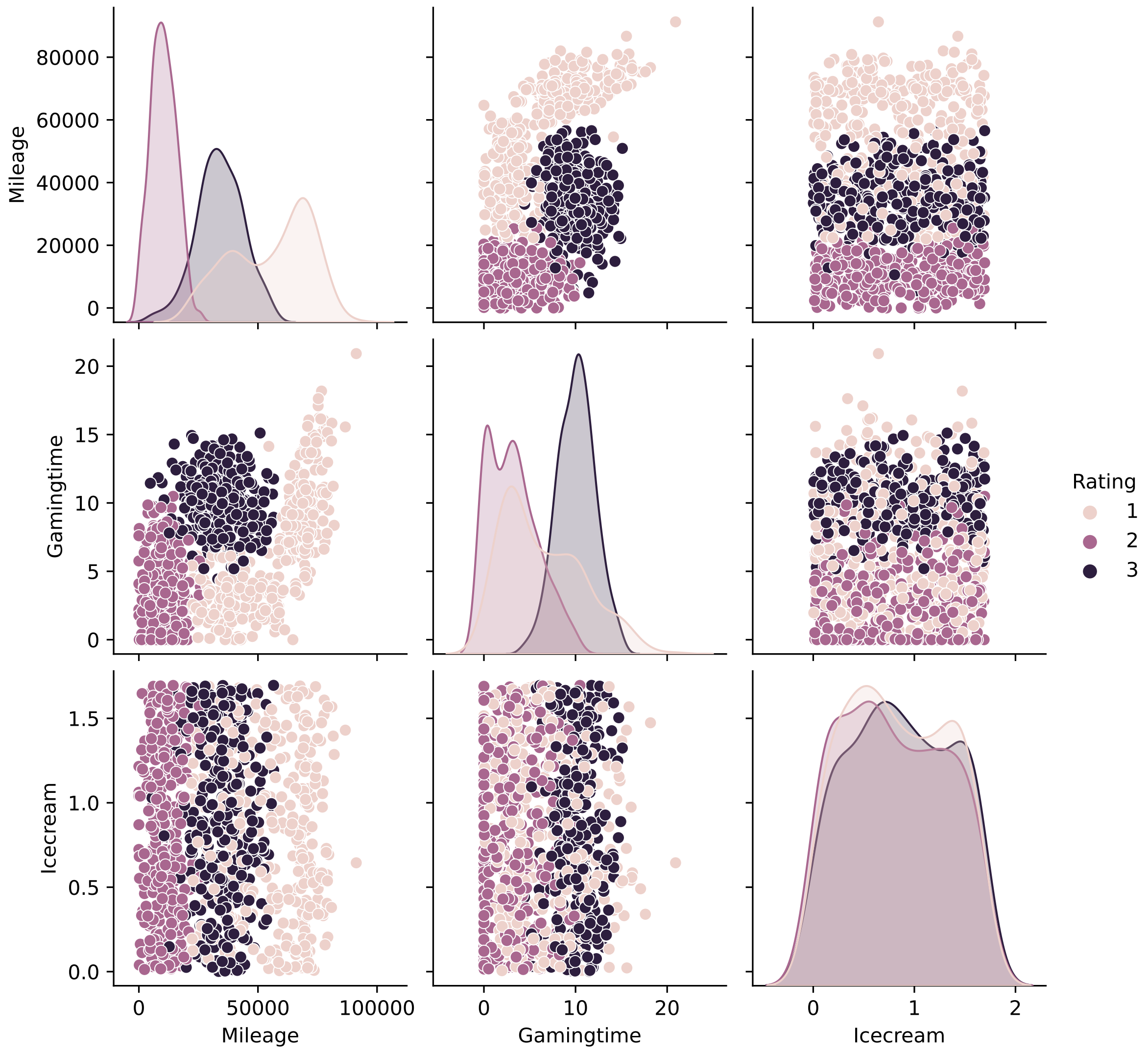
```python
df = df.rename(columns={0: "Mileage", 1: "Gamingtime", 2: 'Icecream', 3: 'Rating'})
df.head()
```

```
C:\Users\Xinli\AppData\Roaming\Python\Python310\site-packages\IPython\core\formatters.py:343
  return method()
```

	Mileage	Gamingtime	Icecream	Rating
0	40920	8.326976	0.953952	3
1	14488	7.153469	1.673904	2
2	26052	1.441871	0.805124	1
3	75136	13.147394	0.428964	1
4	38344	1.669788	0.134296	1

Since now we have more than 2 features, it is not suitable to directly draw scatter plots. We use `seaborn.pairplot` to look at the pairplot. From the below plots, before we apply any tricks, it seems that `Milegae` and `Gamingtime` are better than `Icecream` to classify the data points.

```python
import seaborn as sns
sns.pairplot(data=df, hue='Rating')
```



2.3.3 Applying kNN

Similar to the previous example, we will apply both methods for comparisons.

```
from sklearn.model_selection import train_test_split
from assests.codes.knn import encodeNorm
X = np.array(df[['Mileage', 'Gamingtime', 'Icecream']])
y = np.array(df['Rating'])

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.1, random_state=40,
```

```python
X_train_norm, parameters = encodeNorm(X_train)
X_test_norm, _ = encodeNorm(X_test, parameters=parameters)
```

```python
# Using our codes.
from assests.codes.knn import classify_kNN

n_neighbors = 10
y_pred = np.array([classify_kNN(row, X_train_norm, y_train, k=n_neighbors)
                   for row in X_test_norm])

acc = np.mean(y_pred == y_test)
print(acc)
```

```
0.93
```

```python
# Using sklearn.
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import MinMaxScaler
from sklearn.neighbors import KNeighborsClassifier
from sklearn.metrics import accuracy_score

steps = [('scaler', MinMaxScaler()),
         ('knn', KNeighborsClassifier(n_neighbors, weights="uniform",
                                      metric="euclidean", algorithm='brute'))]
pipe = Pipeline(steps=steps)
pipe.fit(X_train, y_train)
y_pipe = pipe.predict(X_test)
print(accuracy_score(y_pipe, y_test))
```

```
0.93
```

2.3.4 Choosing `k` Value

Similar to the previous section, we can run tests on `k` value to choose one to be used in our model using `GridSearchCV`.

```python
from sklearn.model_selection import GridSearchCV, cross_val_score
n_list = list(range(1, 101))
parameters = dict(knn__n_neighbors=n_list)
```

```
clf = GridSearchCV(pipe, parameters)
clf.fit(X, y)
print(clf.best_estimator_.get_params()["knn__n_neighbors"])
```

```
4
```

From this result, in this case the best `k` is `4`. The corresponding cross-validation score is computed below.

```
cv_scores = cross_val_score(clf.best_estimator_, X, y, cv=5)
print(np.mean(cv_scores))
```

```
0.952
```

2.4 Exercises and Projects

““wsfzkikzpl Handwritten example :label: ex2handwritten Consider the 1-dimensional data set shown below.

“‘yyrlrjxeotts Dataset :header-rows: 1

- - x
  - 1.5
  - 2.5
  - 3.5
  - 4.5
  - 5.0
  - 5.5
  - 5.75
  - 6.5
  - 7.5
  - 10.5
- - y
  - $+$
  - $+$
  - $-$
  - $-$
  - $-$
  - $+$

$-$ $+$
$-$ $-$
$-$ $+$
$-$ $+$

```
Please use the data to compute the class of $x=5.5$ according to $k=1$, $3$, $6$ and $9$
```

```
lvrxwaawfx ex2handwritten :class: dropdown Not yet done!
```

```
:label: ex2titanic
Please download the titanic dataset from {Download}`here<./assests/datasets/titanic.csv>`.

Please analyze the dataset and build a k-NN model to predict whether someone is survived o
```

““lvrxwaawfx ex2titanic :class: dropdown

Not yet done! ““