Artificial Intelligent and Its Application

Laboratory 3: Scikit-learn

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Outline

- A brief introduction to Scikit-learn (sklearn)
- Data Pre-processing
- Training
- Evaluation
- Dataset Generation
- Unsupervised learning



What is Scikit-learn?

- A power library for machine learning
- User-friendly APIs
- Based on NumPy and SciPy, run fast





Why Scikit-learn?

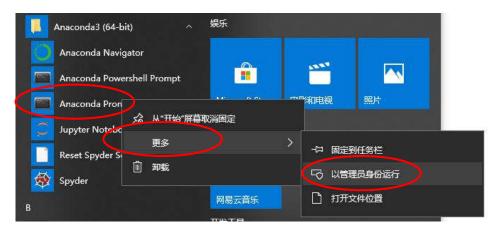
- Contains a lot of ML algorithms
 - □ Decision tree, SVM, k-NN, MLP, etc
- Consistent APIs
 - □ Same standard interface for all algorithms
- Data processing
 - ☐ For example: scaling, sampling
- Integrate open source datasets
 - ☐ For example: mnist, iris



Install Scikit-learn

- Use Anaconda to install Scikit-learn
 - □conda install -c anaconda scikitlearn

Right click



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Install Scikit-learn

- Use Anaconda to install Scikit-learn
 - □conda install -c anaconda scikitlearn



scikit-learn will be downloaded and installed



Install Scikit-learn

- Check if scikit-learn is installed
 - ☐ Try to import **sklearn**

```
import sklearn
sklearn

<module 'sklearn' from 'C:\\Users\\xhote-packages\\sklearn\\_init_.py'>
```

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Simple Example

```
Data Preparation

Data Prepara
```



Type of Functions

- 1. Dataset Preparation
- 2. Data Preprocessing
- 3. Classifier
- 4. Training/Prediction
- 5. Evaluation
- 6. Plotting
- 7. Unsupervised Learning

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DATASET PREPARATION



Dataset Format

- Dataset used in Scikit-learn should be in numpy array format
- Depend on the file type, different functions in libraries can be used to load the dataset into the memory
- Data stored in other format should be converted to numpy



Dataset Preparation

Load Data from a file

Example:

Dataset in npy (numpy format)

dataset = numpy.load(filename)

Dataset in csv (pandas should be used)

- df = pandas.read csv(filename)



Load build-in Data

Scikit-learn contains some well-known datasets in a library called datasets

■ from sklearn import datasets

E.g. mnist dataset

- datasets.load digits()
 - ☐ Both data and labels are **numpy array**



Dataset Preparation

Load build-in Data

Other well-known datasets

- datasets.load iris()
- datasets.load boston()
- datasets.load_wine()
- datasets.load breast cancer()
- datasets.load_diabetes()

Reference:

https://scikit-learn.org/stable/datasets/index.html



Generation

Generate data randomly

- make_classification([samNum, featNum, claNum])
 - ☐ samNum: sample #
 - ☐ featNum: **feature** #
 - □ claNum: class #
 - □ return: numpy arrays: data and labels

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.datasets.make_classification.html#sklearn.datasets.make_classification

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Dataset Preparation

Generation

Generate data followed Normal distribution

- - □ mean: array, mean of each dimenion
 - □ cov: matrix, the covariance matrix
 - ☐ samNum: sample #
 - ☐ featNum: **feature** #
 - □ claNum: class #
 - □ return: numpy arrays: data and labels



Dataset Preparation

Generation

More functions for generating data

- make_biclusters(shape, clusterNum)
- make circles([samNum])

Reference:

https://scikit-learn.org/stable/modules/classes.html #samples-generator

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DATA PREPROCESSING



Scaling

Value Scaling

- from sklearn.preprocessing import MinMaxScaler
- Transform the value and the label





Data Preprocessing

Scaling

- MinMaxScaler([FectRange, copy])
 - □ Normalize the features values into a range
 - ☐ FectRange: tuple, normalized range
 - □ copy: bool, True: the old data will be copied
- StandardScalar()
 - $\Box x = (x u) / s$, where u, s are mean and standard deviation
- Normalizer()
 - □ Normalize samples individually to unit norm



Scaling

An example



Data Preprocessing

Scaling

Label Encoding

- LabelEncoder()
 - □ Encode labels with value between 0 and c-1,c is the class number

Reference:

https://scikit-learn.org/stable/modules/classes.html# module-sklearn.preprocessing



Training and Test Set

Split dataset into training and test set

- train_test_split(data, label[,
 test size])
 - □data: numpy array, all data
 - □label: all corresponding labels
 - ☐ test size: float, proportion of the test set
 - return: numpy arrays: training set, test set, training labels and test labels

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Data Preprocessing

Training and Test Set

Example



Feature Selection

- VarianceThreshold([threshold])
 - □ Remove feature with low variance
 - □ threshold: float, remove the features with variance not larger than threshold

2 features' variance are both 0, will be removed

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Data Preprocessing

Feature Selection

Select k features with highest scores

- selectKBest([score func, k]):
 - □ score func: a function, to calculate the scores

Select % features with highest scores

- selectPercentile([score_func,
 percentile])
 - □ score func: a function, to calculate the scores
- Reference:

https://scikit-learn.org/stable/modules/feature selection.html



- Given a dataset with 4 samples
 - [[1, 2, 5, 6, 3], [1, 3, 8, 5, 5], [2, 5, 2, 6, 4], [1, 6, 1, 5, 4]]
 - □ Remove the features whose variance is <= 0.3
 - □ Select the best 2 feature by Chi-squared stats



Data Preprocessing

Resampling

Resampling for imbalance problem

- conda install -c conda-forge imbalanced-learn
 - ☐ Same as installing sklearn



Oversampling

- from imblearn.over_sampling import RandomOverSampler
- RandomOverSampler([sam_strategy, random state])
 - ☐ sam strategy: specify how to resample the dataset
 - ☐ random state: control randomization of algorithm

Reference:

https://imbalanced-learn.readthedocs.io/en/stable/generated/imblearn.over_sampling.RandomOverSampler.html

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Data Preprocessing

Oversampling

```
from collections import Counter
X, y = make_classification(n_samples=5000, n_features=2, n_informative=2,
                          n redundant=0, n repeated=0, n classes=3,
                           n_clusters_per_class=1,
                          weights=[0.01, 0.05, 0.94],
                           class_sep=0.8, random_state=0)
sorted(Counter(y).items())
                                        Before sampling:
                                        Class0
                                                       64 samples
[(0, 64), (1, 262), (2, 4674)]
                                        Class1
                                                       262 samples
                                        Class2
                                                       4674 samples
from imblearn.over_sampling import RandomOverSampler
ros = RandomOverSampler(random_state=0)
X_resampled, y_resampled = ros.fit_resample(X, y)
sorted(Counter(y_resampled).items())
                                        After sampling:
[(0, 4674), (1, 4674), (2, 4674)]
                                        Each class
                                                     4674 samples
```



Undersampling

- from imblearn.under_sampling import RandomUnderSampler
- RandomUnderSampler([sam_strategy, random state])
 - □ sam strategy: specify how to resample the dataset
 - ☐ random state: control randomization of algorithm

Reference:

https://imbalanced-learn.readthedocs.io/en/stable/generated/imblearn.under_sampling.RandomUnderSampler.html

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Data Preprocessing

Undersampling

```
from collections import Counter
X, y = make_classification(n_samples=5000, n_features=2, n_informative=2,
                           n redundant=0, n repeated=0, n classes=3,
                           n clusters per class=1,
                           weights=[0.01, 0.05, 0.94],
                           class_sep=0.8, random_state=0)
sorted(Counter(v).items())
                                      Before sampling:
                                      Class0
                                                      64 samples
[(0, 64), (1, 262), (2, 4674)]
                                      Class1
                                                      262 samples
                                                      4674 samples
                                      Class2
from imblearn.under_sampling import RandomUnderSampler
rus = RandomUnderSampler(random_state=0)
X resampled, y resampled = rus.fit resample(X, y)
sorted(Counter(y_resampled).items())
                                     After sampling:
[(0, 64), (1, 64), (2, 64)]
                                     Each class
                                                       64 samples
```



Resampling

Other resampling technique

- Over sampling
 - □ SMOTE ()
 - □ ADASYN ()
 - □ Reference:
 https://imbalanced-learn.org/en/stable/over_sampling.html
- Under sampling
 - ☐ ClusterCentroids()
 - ☐ EditedNearestNeighbours()
 - □ Reference:
 https://imbalanced-learn.org/en/stable/under_sampling.html

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CLASSIFIER DEFINITION

Classifier

- Bayes Classifier
- Decision tree
- SVM
- K-NN
- MLP
- Random forest
- Ensemble



Classifier

Bayes Classifier

- from sklearn import GaussianNB
- cls = GaussianNB([priors, var smoothing])
 - □ priors: Prior probabilities of the classes. If specified the priors are not adjusted according to the data.
 - □ var_smoothing: Portion of the largest variance of all features that is added to variances for calculation stability
- Reference:

https://scikit-learn.org/stable/modules/classes.html# module-sklearn.naive_bayes



Decision Tree

- from sklearn import tree
- cls = tree.DecisionTreeClassifier
 ([max depth])
 - □ max_depth: maximum depth of the tree, no limitation by default
 - ☐ Supports multi-label classification

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html



Classifier

SVM

- from sklearn.svm import SVC
- cls = SVC([kernel, gamma])
 - □ kernel: str, specify the kernel type
 - □ gamma: kernel coefficient for "rbf", "poly" and "sigmoid"
 - ☐ Supports multi-label classification

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.svm.SVC.html



Classifier

K-NN

- from sklearn.neighbors import KNeighborsClassifier
- cls = KNeighborsClassifier
 ([n neighbors])
 - □ n_neighbors: Number of neighbors to use for kneighbors queries, 5 by default

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html



Classifier

MLP

- from sklearn.neural_network import
 MLPClassifier
- cls = MLPClassifier([activation, ..])
 - □ activation: str, activation function for the hidden layer, "relu" by default
 - □ hidden_layer_sizes: tuple, the ith number represents the number of neurons in the ith hidden layer
 - □ batch_size: int, decide how many samples are used for one update, min(200, n_samples) by default



MLP

- □ solver: str, the solver for weight optimization, "adam" by default
- □ alpha: float, L2 penalty (regularization term) parameter, 0.0001 by default
- □ learning_rate_init: float, initial learning rate, 0.001 by default, only used when solver="sgd"
- learning_rate: str, learning rate schedule, "constant"
 by default, only used when solver="sgd"
- □ max_iter: int, maximum number of iterations, 200 by default



Classifier

MLP

- □ shuffle: bool, set True to shuffle samples in each iteration, True by default
- momentum: float, between 0 to 1, momentum for gradient update, 0.9 by default, only used when solver="sgd"

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.neural_network.MLPClassifier.html



Ensemble: Random Forest

- from sklearn.ensemble import RandomForestClassifier
- cls = RandomForestClassifier
 ([n estimators])
 - ☐ n estimators: int, n decision trees, 10 by default
 - ☐ Supports multi-label classification

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

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Classifier

Ensemble: Voting

- from sklearn.ensemble import
 VotingClassifier
- voting = VotingClassifier
 (estimators[, voting])
 - ☐ estimators: list, contains tuples as (str, estimator)
 - □ voting: 'hard', majority voting; if 'soft', argmax of the sums of the predicted probabilities

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.ensemble. VotingClassifier.html#sklearn.ensemble.VotingClassifier



Ensemble: Bagging

- from sklearn.ensemble import
 BaggingClassifier
- bagging = BaggingClassifier
 ([base_estimator, n_estimators,
 max samples, max features])
 - □ base_estimator: the base estimator to fit on random subset of the dataset, decision tree by default
 - □ n_estimators: int, n estimators in the ensemble, 10 by default
 - max_samples: int or float, specify how many samples are drawn from the whole dataset



Classifier

Ensemble: Bagging

- max_features: int or float, specify how many features are drawn from all features
- Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html



Ensemble: Boosting

- from sklearn.ensemble import GradientBoostingClassifier
- boosting= GradientBoostingClassifier
 ([n estimators])
 - □ n_estimators: int, the number of boosting stages to perform, 10 by default
 - ☐ Supports multi-label classification

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html



Classifier

Load/Save Classifier

Load a trained classifier by pickle

- import pickle as pkl
- f = open(filepath, "rb")
- classifier = pkl.load(f)
- f.close()
 - A trained classifier will be loaded from disk according to the given filepath



Load/Save Classifier

Save a trained classifier by pickle

- import pickle as pkl
- f = open(filepath, "wb")
- pkl.dump(classifier, f)
- f.close()
 - ☐ The trained classifier will be saved to the given filepath





Classifier

■ Reference:

https://scikit-learn.org/stable/supervised_learning.html #supervised-learning



- Given dataset in "lab2_Trylt.csv"
 - □ Train a Bayes classifier on the dataset, calculate the test accuracy (Split the dataset into training set and test set)
 - □ Evaluate its performance in terms of F1score, average precision, ROC-curve and AUC

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Try It

- Given dataset in "lab2_Trylt.csv"
 - □ Train a decision tree classifier on the dataset, calculate the test accuracy
 - ☐ Change the depth of the decision tree, calculate the test accuracy



- Given dataset in "lab2_Trylt.csv"
 - □ Train a SVM classifier on the dataset, calculate the test accuracy
 - ☐ Use different kernels for the SVM, and compare the test accuracies

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Try It!

- Given dataset in "lab2_Trylt.csv"
 - ☐ Train **k-NN** classifiers on the dataset where k from 1 to 5
 - ☐ Find out the corresponding value of k when the test accuracy is the highest



- Given dataset in "lab2_Trylt.csv"
 - ☐ Train a MLP with the following structures on the dataset and calculate test accuracy
 - 2 hidden layers (3 neurons in each hidden layer)
 - 2 hidden layers (6 neurons in each hidden layer)
 - □ Try other parameters in MLP to see if better performance can be achieved





Try It!

- Given dataset in "lab2_Trylt.csv"
 - □ Train random forest classifiers on the dataset where the number of trees from 1 to 10
 - ☐ Find out the corresponding value of n when the test accuracy is the highest



- Given dataset in "lab2_Trylt.csv"
 - Use n SVMs as a base classifier for Bagging on the dataset and calculate test accuracy, n = 2, 4, ...,10
 - □ Try other classifiers (DT, knn)

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CLASSIFIER TRAINING/PREDICTION



Training

- After the classifier is defined, the training can start
- classifier.fit(data, label)
 - □ data and label must be numpy array or list
 - □ classifier will be updated and returned by calling fit()
- train_set and train_label are numpy
 arrays in this example



Training/Prediction

Prediction

Label Prediction

- classifier.predict(data)
 - data: numpy array or list, contains data of each samples
 - return: 1-D numpy array: labels of each sample

Probability Prediction

- classifier.predict proba(data)
 - data: numpy array or list, contains data of each samples
 - □ return: 2-D numpy array: element[i, j] is the probability of sample i belonging to class j



Training/Prediction

Prediction

```
pred = cls.predict(test_set)
        pred
        array([0, 1, 1, 1, 0, 1, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1,
               1, 1, 1, 1, 1, 1, 1, 1, 0, 1, 0, 0, 1, 1, 1, 1, 1, 1, 0, 1, 0,
               0, 1, 0, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 1, 1, 0, 1, 0, 0, 1, 1, 1,
               1, 0, 1, 1, 1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1,
               0, 0, 1, 1, 1, 1, 0, 1, 0, 1, 0, 1, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1,
               1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 0, 0,
               0, 1, 0, 1, 1, 1, 1, 0, 0, 0, 1, 1, 0, 1, 0, 1, 0, 1, 1, 1],
              dtype=int64)
        pred_proba = cls.predict_proba(test_set)
        pred_proba
        array([0.58395574, 0.41604426]
                [0. 08836755, 0. 91163245]
                0.94146387,
                            0.05853613]
Probability of
                                           Probability of
being class 0
                                          being class 1
               [0. 27435561,
                            0.72564439]
                0. 23595516,
                            0.76404484]
                            0.89747868]
                0. 10252132,
```

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EVALUATION



Evaluation

- Accuracy
- F1-score
- Average precision
- ROC
- AUC
- Confusion matrix



Evaluation

Accuracy

- from sklearn.metrics import accuracy_score
- accuracy_score(true_labels,
 predicted labels)

F1-score

- from sklearn.metrics import f1_score
- f1_score(true_labels,
 predicted labels)

Evaluation

Precision

- from sklearn.metrics import average precision score
- average_precision_score(true_labels, predicted labels)

Confusion matrix

- from sklearn.metrics import confusion matrix
- confusion_matrix(true_labels, predicted_labels)

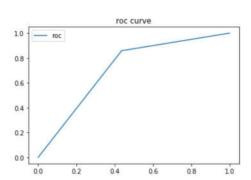


Evaluation

ROC curve

thresholds: [2 1 0]

- from sklearn.metrics import roc_curve
- roc_curve(true_labels,
 predicted labels)



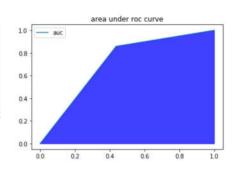


Evaluation

AUC

- from sklearn.metrics import roc auc score
- roc_auc_score(true_labels,
 predicted labels)

```
from sklearn.metrics import roc_auc_score
auc = roc_auc_score(test_label, pred)
auc
0.71111111111111111
```



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Evaluation

■ Reference:

https://scikitlearn.org/stable/modules/classes.html#modulesklearn.metrics



PLOTTING

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Plot Decision Boundary

- How to plot a figure?
 - 1. Construct dense grid that fills the entire space
 - 2. Predict labels for all points in the grid
 - Use different colors to represent points with different labels



Example

Bayes classifier decision boundary

1. Construct the grid

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Decision Boundary Plotting

Example

Bayes classifier decision boundary

2. Predict all values in the grid

```
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5

h = 0.01
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))

Z = bayes.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

plt.contourf(xx, yy, Z)
plt.scatter(X[:, 0], X[:, 1], c=y, cmap=plt.cm.Spectral)
plt.show()
```



Example

Bayes classifier decision boundary

3. Colour and plot the grid

```
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
h = 0.01
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = bayes.predict(np.c_[xx.ravel(), yy.ravel()])
Z = Z.reshape(xx.shape)

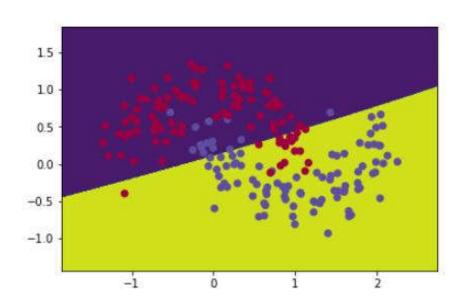
plt.contourf(xx, yy, Z)
plt.scatter(X[:, 0], X[:, 1], c=y, cmap=plt.cm.Spectral)
plt.show()
```

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Decision Boundary Plotting

Example





Return values within a range with an interval

- np.range([start,]stop[, step])
 - □ start and stop decide the interval [start, stop)
 - □ step: spacing between values. If start is given, step must be given
- **e.g.** np.range(1,2,0.25) = [1,1.25,1.5,1.75]

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Decision Boundary Plotting

Return matrices from coordinate vectors

- np.meshgrid([x_1 , x_2 , .., x_n])
 - $\square \ x_i$: is 1-D array representing the coordinates of a grid, where i=1..n, n is the dimensionality of the coordinate
 - □ the returned matrices for n coordinate vectors are n-D matrices

```
e.g.
np.meshgrid(
    array([1,2]),
    array([1,2])
)
4 points:
(1,2), (2,2)
(1,1), (2,1)
```



Flatten arrays

- np.ravel(array[, order])
 array.ravel([order])
 - □ array will be flattened into 1-D array
 - order: decide how to index, default is to index the elements in row-major
- e.g.
 - □ np.ravel(array([[1,2], [3,4]]))
 array([1,2,3,4])

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Decision Boundary Plotting

Generate a coordinator of a sample

- \blacksquare np.c_(x1, x2)
 - $\square \times 1$ and $\times 2$ are the feature 1 and 2d
- e.g.

```
np.c_(array([1,2]), array([3,4]))
array([ [1,3], [2,4] ])

5
2 points:
(1,3), (2,4)
```



Plot contours

- plt.contourf([x, y,]z[, colors, cmap])
 - $\square \times$ and y are the coordinates of the values in z
 - □ z: the height values over which the contour is drawn
 - □ colors: the colors of the levels, i.e. the lines for contour and the areas for contour
 - □ cmap: a Colormap instance or registered colormap name, maps the level values to colors

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Decision Boundary Plotting

Plot points

- plt.scatter(x, y[, c, cmap])
 - $\square \times$ and y are the coordinates of the points
 - □ c: one color for all points or specify colors for each points
 - □ cmap: a Colormap instance or registered colormap
 name, only used if c is an array of floats



UNSUPERVISED LEARNING

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Sklearn: Unsupervised learning

- K-means
- PCA



Unsupervised Learning

Clustering: K-means

- from sklearn.cluster import KMeans
- max iter])
 Means([n_clusters,
 max iter])
 - ☐ n clusters: int, n clusters, 8 by default
 - max_iter: maximum number of iterations, 300 by
 default
- Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.cluster.KMeans.html

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Try It!

- Given dataset in "lab2_Try_data.csv", assume the data is unlabeled
 - ☐ Use **k-means** to split the data in to n clusters, where n from 2 to 5
 - ☐ Use different colors to plot different clusters, then observe how the value of n effects the results



Unsupervised Learning

Clustering: Others

- SpectralClustering()
- DBSCAN()
- MeanShift()

Reference:

https://scikit-learn.org/stable/modules/classes.html #module-sklearn.cluster

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Unsupervised Learning

PCA

- from sklearn.decomposition import PCA
- pca = PCA([n_components])
 - □ n_components: int, float, string or None, keep n components

Reference:

https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html



- Given dataset in "lab2_Trylt.csv"
 - □ Apply **k-means** to split the samples in to 2 clusters
 - □ Use different colors to plot different labeled samples
 - □ Do this exercise again in the first principle component of PCA