Pattern Recognition
and Applications Lab

Data Sampling, Visualization, Learning and Classification

Machine Learning – Laboratory

Battista Biggio

Department of Electrical and Electronic Engineering
University of Cagliari, Italy

Exercise 1

- Consider the function `make_gaussian_dataset` defined in the previous lab session

- Extend it to handle:
  1. more than two dimensions
  2. more than two classes
  3. non-isotropic Gaussians
     - covariance matrix is a positive-definite matrix, not necessarily proportional to the identity matrix (namely, features are correlated!)

Exercise 1 – This is the starting point…

```python
import numpy as np

def make_gaussian_dataset(n0, n1, mu0, mu1):
    """ Creates a 2-class 2-dimensional Gaussian dataset. """
   d = 2  # hard-coded for convenience, we will improve this later on

   x0 = np.random.randn(n0, d) + mu0  # uses broadcasting...
   x1 = np.random.randn(n1, d) + mu1

   # sample labels
   y0 = np.zeros(n0)
   y1 = np.ones(n1)

   # concatenate data and labels
   x = np.vstack((x0, x1))
   y = np.hstack((y0, y1))

   return x, y


# generate data with 10 samples/class, and means [-1,-1], [1, 1]
xn, yn = make_gaussian_dataset(10, 10, [-1, -1], [+1, +1])
print('xn: ', xn)
print('yn: ', yn)
```

Exercise 1: Solution

```python
def make_gaussian_dataset(n, mu):
    """
    Creates a k-class d-dimensional Gaussian dataset.
    :param n: vector containing the number of samples for each class
    :param mu: matrix containing the mean vector for each class
    :return: x,y, the gaussian dataset
    """

    n = np.array(n)  # convert to np.array if list is passed as input
    mu = np.array(mu)
    n_classes = mu.shape[0]  # number of classes
    n_features = mu.shape[1]  # number of features
    n_samples = n.sum()  # total number of samples

    x = np.zeros(shape=(n_samples, n_features))
    y = np.zeros(shape=(n_samples,))

    start_index = 0
    for i in xrange(n_classes):
        x_tmp = np.random.randn(n[i], n_features) + mu[i, :]  # broadcasting...
        x[start_index:start_index + n[i], :] = x_tmp
        y[start_index:start_index + n[i]] = i
        start_index += n[i]
    return x, y
```

Exercise 1: Solution

- This is still not considering different covariance matrices per class

```
import numpy as np

def make_gaussian_dataset(n, mu):
    [...]

# generate data
xn, yn = make_gaussian_dataset([10, 5, 2], [[-1, -1],
                                             [+1, -1],
                                             [-1, +1]])
```

- How to extend it to use a different covariance matrix per class?
  make_gaussian_dataset(n, mu, ***cov***)?

Exercise 2

Define a function that plots a dataset using a different color for each class:

```
plot_dataset (x, y, feat_1=0, feat_2=1)
```

Hints:

```
import matplotlib.pyplot as plt
plt.scatter(x1, x2, color='r')
```

plots the point (x1, x2) as a red point

Colors are: `['k','b','r','g','c','m','y']`

```
bool_class0=(y==0)  # select samples belonging to class 0
```

Other useful functions:

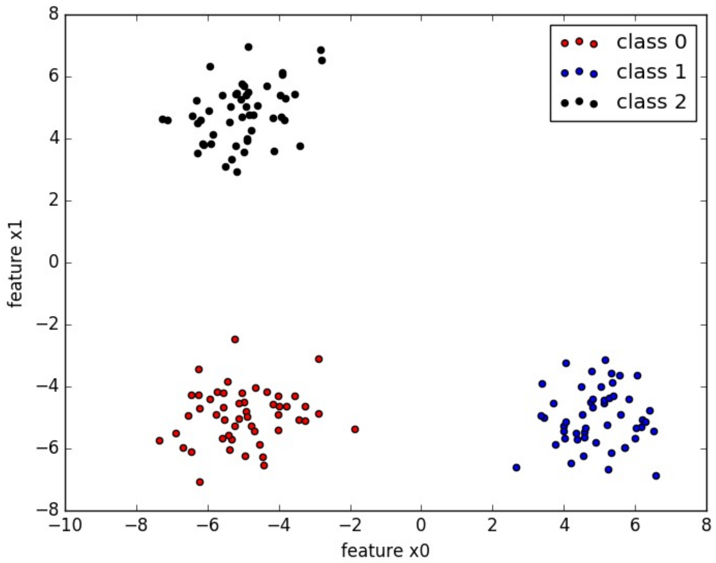
```
plt.xlabel(), plt.ylabel(), plt.legend(), plt.show()
```

Exercise 2: Solution

```python
import matplotlib.pyplot as plt


def plot_dataset(x, y, feat_1=0, feat_2=1):
    n_classes = len(np.unique(y))
    colors = ['r', 'b', 'k', 'g', 'c', 'm', 'y']

    for y0 in xrange(n_classes):
        x0 = x[y == y0, feat_1]  # y0 is the current class in the loop
        x1 = x[y == y0, feat_2]
        plt.scatter(x0, x1, c=colors[y0], label='class ' + str(y0))

    plt.legend()
    plt.xlabel('feature x' + str(feat_1))
    plt.ylabel('feature x' + str(feat_2))

    return
```

Exercise 2: Solution

```
# generate data
xn, yn = make_gaussian_dataset([50, 50, 50], [[-5, -5],[+5, -5],[-5, +5]])
plot_dataset(xn, yn, 0, 1)
```



Learning and Classification

What's next? Learning and Classification

- Now we can sample data and visualize it in two dimensions
- The goal of the next exercises is to implement a simple classifier
  - The Nearest Mean Classifier (NMC)
- We will implement its learning and classification procedures

Ex. 3: NMC – Learning & Classification

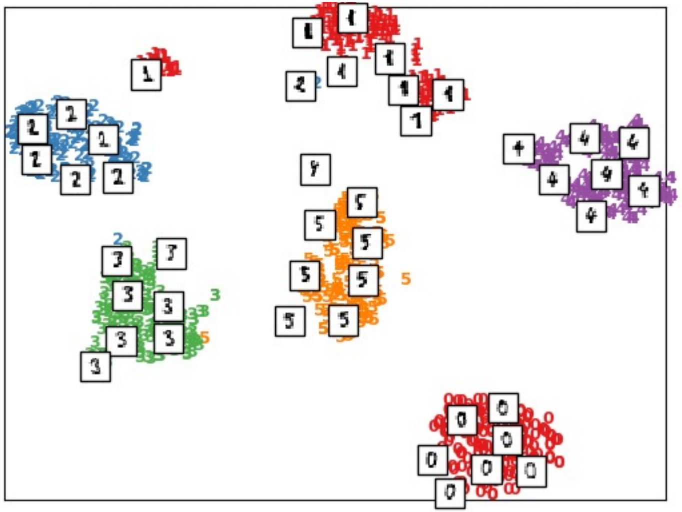
- During the learning phase, NMC is given a training set consisting of pairs (x, y) of samples along with their labels
- For each class y0 in y
  - NMC estimates the mean of the samples in class y0
  - stores the mean vector (centroid)

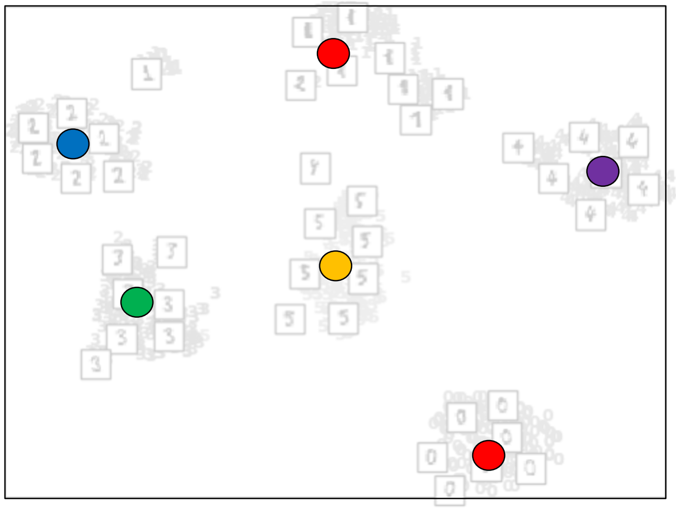
- During classification, NMC assigns the current test sample x to the class whose mean vector (centroid) is the closest one to x

- Implement the functions
  - `centroids = fit(x,y)`, corresponding to the learning phase, and
  - `y_pred, distances = predict(x, centroids)`, corresponding to the classification phase, where `y_pred` is the label of the predicted class, and `distances` are the distance values w.r.t the centroids

NMC Classifier: «*fit*»

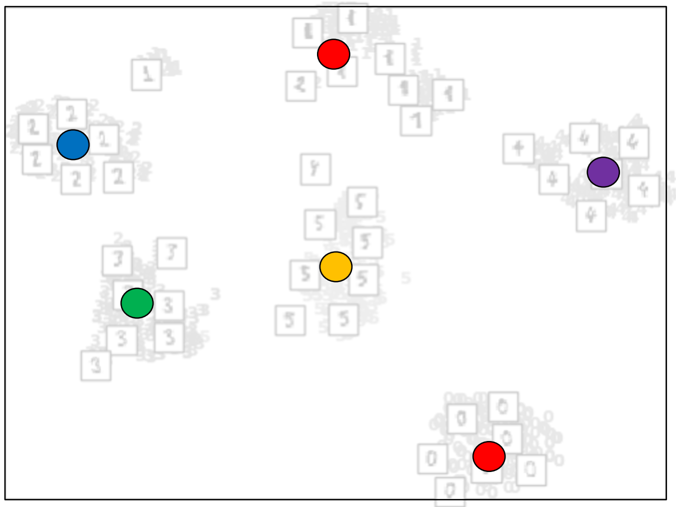
- Each sample is represented as a point in the feature space (e.g., for images, each dimension may correspond to the value of each pixel)
  - we can plot different classes with different colors / markers
  - *fit* estimates the average (centroid) for each class

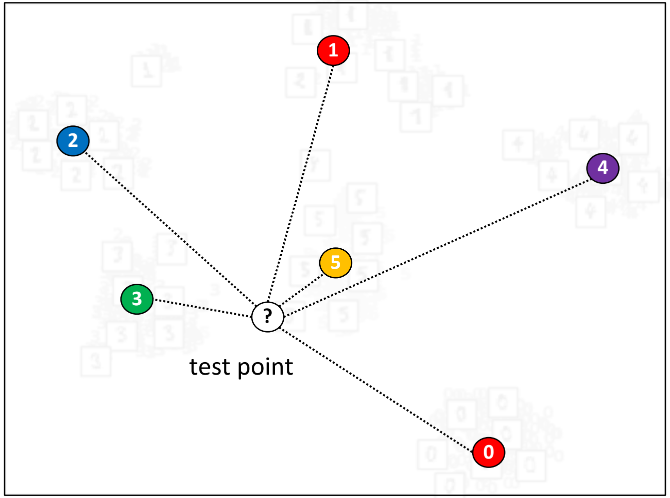




NMC Classifier: *«predict»*

- *Predict* computes the Euclidean distance of a given test point against all centroids, and assigns it to the class of the closest centroid
  - The test point ('?') below is classified as a '5', as it is closer to the centroid of class '5'
  - The length of each dashed line is the distance between the test point and the given centroid





Exercise 3: Solution

```python
import numpy as np


def fit(x, y):
    n_classes = np.unique(y).size
    n_features = x.shape[1]

    centroids = np.zeros(shape=(n_classes, n_features))
    for k in xrange(n_classes):
        centroids[k] = x[y == k, :].mean(axis=0)
    return centroids

def predict(x, centroids):
    n_samples = x.shape[0]
    n_classes = centroids.shape[0]
    distances = np.zeros(shape=(n_samples, n_classes))

    for k in xrange(n_classes):
        distances[:,k] = np.linalg.norm(x-centroids[k, :], axis=1)
    y_pred = np.argmin(distances, axis=1)

    return y_pred, distances
```

Let's create a *class*

```
class CNearestMeanClassifier(object):
    """Class implementing a nearest mean classifier"""

    def __init__(self):
        self._centroids = None
        return

    def fit(self, x, y):
        n_classes = np.unique(y).size
        n_features = x.shape[1]
        centroids = np.zeros(shape=(n_classes, n_features))
        for k in xrange(n_classes):
            centroids[k] = x[y == k, :].mean(axis=0)
        self._centroids = centroids
        return

    def predict(self, x):
        n_samples = x.shape[0]
        n_classes = self._centroids.shape[0]
        distances = np.zeros(shape=(n_samples, n_classes))
        for k in xrange(n_classes):
            distances[:, k] = np.linalg.norm(x - self._centroids[k, :], axis=1)
        y_pred = np.argmin(distances, axis=1)
        return y_pred, distances
```

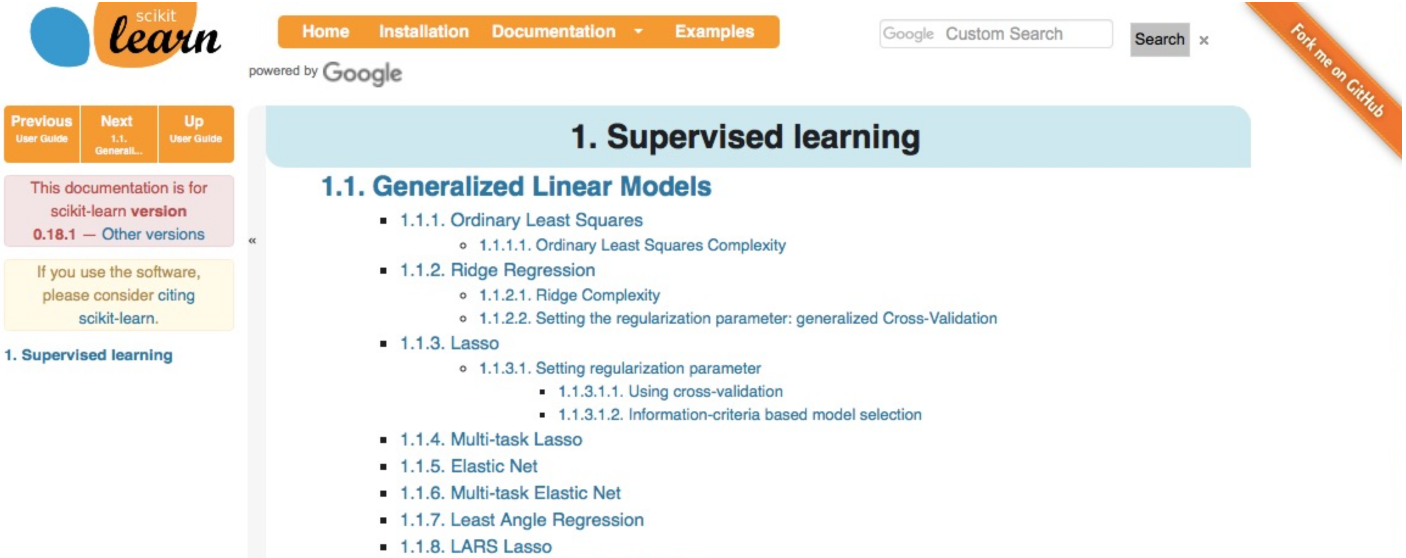
Class Properties

- Python decorator to access class private members
  - See also 'setters'

```
class CNearestMeanClassifier(object):
    """Class implementing a nearest mean classifier"""

    def __init__(self):
        self._centroids = None
        return

    @property
    def centroids(self):
        return self._centroids

    [...]
```

Scikit-learn Classifiers

- Check http://scikit-learn.org/stable/supervised_learning.html
- NearestCentroid implements our CNearestMeanClassifier
  - http://scikit-learn.org/stable/modules/neighbors.html#nearest-centroid-classifier

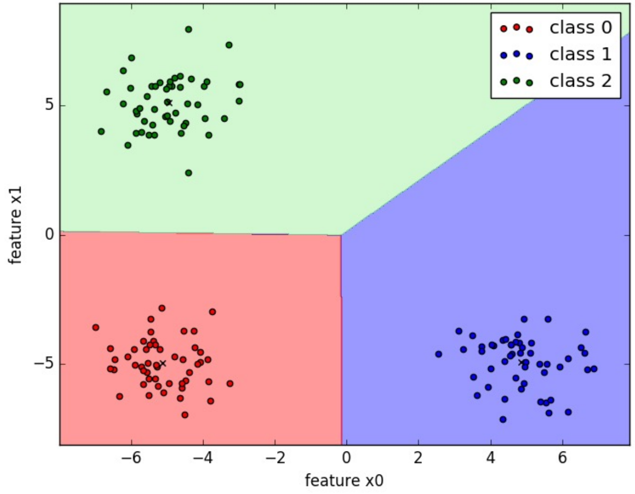


Ex. 4: Visualizing the decision regions

```python
def plot_decision_regions(x, y, classifier, resolution=0.02):
    # setup marker generator and color map
    colors = ('red', 'blue', 'lightgreen', 'black', 'gray', 'cyan')
    cmap = ListedColormap(colors[:len(np.unique(y))])

    # plot the decision surface
    x1_min, x1_max = x[:, 0].min() - 1, x[:, 0].max() + 1
    x2_min, x2_max = x[:, 1].min() - 1, x[:, 1].max() + 1
    xx1, xx2 = np.meshgrid(np.arange(x1_min, x1_max, resolution),
                           np.arange(x2_min, x2_max, resolution))
    Z, score = classifier.predict(np.array([xx1.ravel(), xx2.ravel()]).T)
    Z = Z.reshape(xx1.shape)
    plt.contourf(xx1, xx2, Z, alpha=0.4, cmap=cmap)
    plt.xlim(xx1.min(), xx1.max())
    plt.ylim(xx2.min(), xx2.max())

    # plot class samples
    plot_dataset(x,y)
    return
```

Exercise 4: Solution

```
from src.prlib import CNearestMeanClassifier, \
    make_gaussian_dataset, plot_decision_regions
import matplotlib.pyplot as plt

x, y = make_gaussian_dataset([50, 50, 50], [[-5, -5],
                                            [+5, -5],
                                            [-5, +5]])

classifier = CNearestMeanClassifier()
classifier.fit(x, y)

plot_decision_regions(x, y, classifier)

# plot centroids
plt.scatter(classifier.centroids[:, 0],
            classifier.centroids[:, 1],
            marker='x', color='k')
plt.show()
```



Ex. 5: Testing performance on unseen data

- To assess classifier performance, one should estimate the classification error on never-before-seen data
  - The training data should not be used to this end, as it provides an optimistic estimate of the real performance!
- Therefore, the correct procedure amounts to:
  1. Sampling a training and a testing set (from the same underlying distribution), e.g., with `make_gaussian_data(n, mu)`
  2. Fitting the classifier on training data
  3. Predicting the class labels of testing data
  4. Evaluating the fraction of wrong labels

```
x_tr, y_tr = make_gaussian_dataset(n, mu)
x_ts, y_ts = make_gaussian_dataset(n, mu)
clf = CNeareastMeanClassifier()
clf.fit(x_tr,y_tr)
y_pred, dist = clf.predict(x_ts)
error = (y_pred != y_ts).mean()
```

What happens if one changes means and/or covariances of the Gaussian classes?
How does the error vary?

Lessons learned

- Visualize data and decision regions
- Implementation of a simple classifier (using a Python class)
- Create packages and dedicated function libraries
- Basic estimation of classifier performance on unseen data

Student challenges:

1. Extend make_gaussian_dataset to handle covariance matrices
2. Implement a k-Nearest Neighbor (kNN) classifier
3. Visualize decision regions of scikit-learn classifiers using
   - Nearest Centroid, and kNN (you may try other algorithms as well!)
4. Estimate performance of each classifier on unseen data

Please e-mail us if you are able to solve any of them!