## lab3-exercises

October 10, 2022

```
[]: # Lab 3 Exercises for COMP 6321 Machine Learning
```

In this lab you'll cluster and fit mixture models to data using the popular *scikit-learn* package. Lab3 requires a good understanding of Numpy and Matplotlib. Please complete Lab1 before attempting Lab3.

Run the code cell below to import the required packages.

```
[278]: import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
import sklearn
import sklearn.cluster  # For KMeans class
import sklearn.mixture  # For GaussianMixture class
import sklearn.preprocessing  # For scale function
import mpl_toolkits.mplot3d  # For enabling projection='3d' feature in

→Matplotlib
```

### 1 Introduction

This "introduction" group of code cells has no exercises. The goal is to provide you with examples. Run the code cells and learn from them.

Load the image *ladybug.png* as a Numpy array. The image should already have been unzipped into the same directory as this notebook.

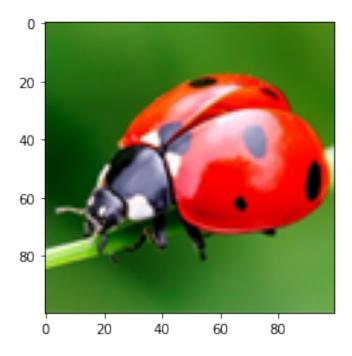
```
[279]: image = plt.imread('ladybug.png')
print(image.shape)
```

```
(100, 100, 3)
```

Notice the shape of the array. Entry image[y,x] in the array is a length-3 vector representing the RGB value of pixel at location (x,y) in the image.

Plot the image using Matplotlib's *imshow* function.

```
[280]: plt.imshow(image);
```



Reshape the image into a 2-dimensional matrix suitable for clustering the pixels by their RGB colour value. The data should be in array format

$$\begin{bmatrix} r_1 & g_1 & b_1 \\ r_2 & g_2 & b_2 \\ \vdots & \vdots & \vdots \\ r_N & g_N & b_N \end{bmatrix}$$

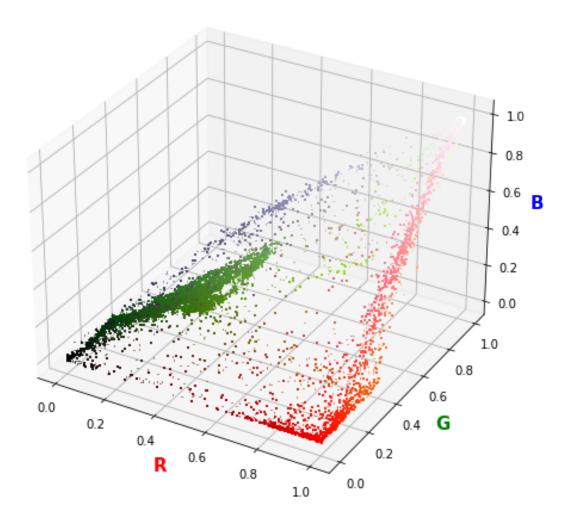
where N = 10000 and each  $\begin{bmatrix} r_i & g_i & b_i \end{bmatrix}$  is the colour of pixel with index i.

```
[281]: RGB = image.reshape(-1, 3)
       print(RGB.shape)
       print(RGB)
      (10000, 3)
      [[0.30588236 0.5568628
                               0.2
       [0.27058825 0.53333336 0.16470589]
       [0.27058825 0.53333336 0.16470589]
       [0.4509804
                               0.34901962]
                    0.6745098
       [0.4392157
                    0.6784314
                               0.34509805]
       [0.4666667 0.6901961
                               0.37254903]]
```

The top-left pixel (index i = 0) has colour [0.31 0.56 0.20], which is green-ish. Makes sense! Plot the pixel RGB values in 3-dimensional colour space.

```
[282]: | def plot_colour_space(RGB, title=None, hold=False, **kwargs):
           Plots Nx3 matrix RGB in 3 dimensions.
           The keyword arguments are passed to Matplotlib's scatter() function.
           If hold=True, the points will be added to the previous plot. Otherwise a_{\sqcup}
        \rightarrownew plot is generated.
           11 11 11
           if hold:
               ax = plt.gca()
           else:
               fig = plt.figure(figsize=(8,8))
               ax = fig.add_subplot(111, projection='3d')
           kwargs.setdefault('alpha', 1.0)
           ax.scatter(*RGB.T, **kwargs)
           ax.set_xlabel('R', color='r', fontweight='bold', fontsize=15)
           ax.set_ylabel('G', color='g', fontweight='bold', fontsize=15)
           ax.set_zlabel('B', color='b', fontweight='bold', fontsize=15)
           if title is not None:
               ax.set_title(title)
       plot_colour_space(RGB, c=RGB, s=0.5, marker='s', title="Pixels plotted in_
        ⇔colour space")
```

## Pixels plotted in colour space



Run the K-means clustering algorithm with K=5, using each RGB pixel colour vector as a data point.

```
[283]: def run_kmeans(data, k):

"""

Runs K-means on an NxD array using k clusters.

Returns a KxD matrix of centroids and a length-N vector of labels (cluster

→ assignments).

"""

kmeans = sklearn.cluster.KMeans(n_clusters=k, random_state=0).fit(data)

return kmeans.cluster_centers_, kmeans.labels_
```

```
centroids, labels = run_kmeans(RGB, k=5)
print(centroids)
print(labels, len(labels))
```

```
[[0.91830087 0.11951411 0.04882491]

[0.2199334 0.4692984 0.09348438]

[0.8889071 0.67274106 0.6811432 ]

[0.07332402 0.23711258 0.04663853]

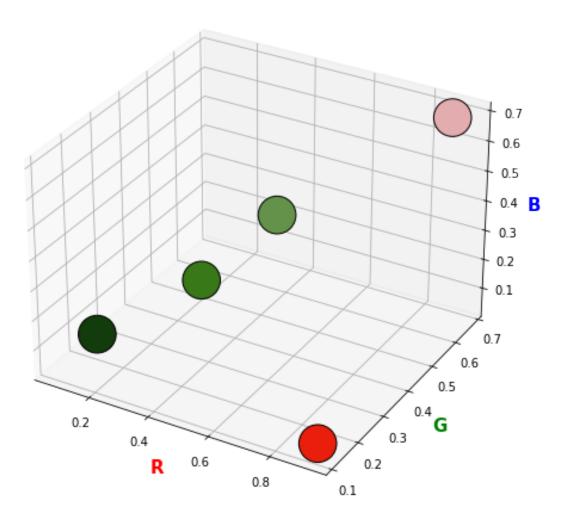
[0.39092913 0.5740281 0.2899987 ]]

[4 1 1 ... 4 4 4] 10000
```

The centroids array has shape (5,3) because there are K=5 centroids, a 3-dimensional vector. The labels are given as integer indices, as in the "alternate formulation for K-means" from Lecture 2.

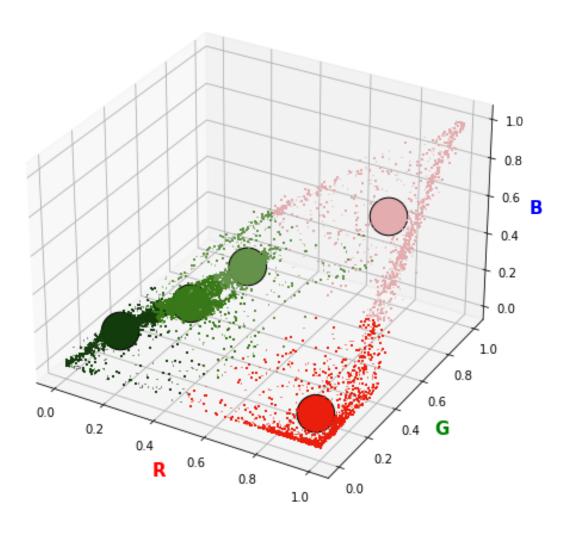
Plot the centroids in RGB colour space.

### Centroids only

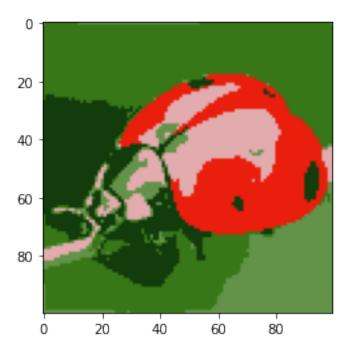


Plot the pixels in RGB space but with colour matching that of the centroid the pixel was assigned to. Include the centroids themselves in the same plot.

# Centroids and recoloured pixels



[286]: plt.imshow(RGB\_recoloured.reshape(image.shape));



Compare the above to Figure 9.3 (p.429) of the Bishop textbook.

# 2 1. Spatial clustering with K-means

Exercises 1.1–1.4 ask you to apply scikit-learn's **sklearn.cluster.KMeans** object to the pixels from the introduction, but on slightly different data.

It requires that you have already run the code cells from the introduction.

```
[287]: assert 'image' in globals(), "Did you run the code cells from introduction?" assert 'RGB' in globals(), "Did you run the code cells from introduction?"
```

#### 2.0.1 Exercise 1.1 — Add pixel location features

The introduction showed you how to cluster pixels by colour, like Figure 9.3 (p.429) of the Bishop book. The data that we clustered was an array of 3-dimensional features  $\begin{bmatrix} r_i & g_i & b_i \end{bmatrix}$ , stored in the array object referenced by variable RGB.

In exercises 1.2–1.4, you'll be asked to cluster the pixels by *colour* (rgb) and *location* (xy). To do this, you must first add pixel location features to the data.

Write a few lines of code to create a new array called RGBXY where each row is a 5-dimensional feature vector  $\begin{bmatrix} r_i & g_i & b_i & x_i & y_i \end{bmatrix}$ , with  $(x_i, y_i)$  being the location in the image where pixel i came from in the original image. Use the image variable to get the height and width of the original ladybug image. Then use the **np.arange** and **np.meshgrid** function to generate two arrays, each containing the individual  $x_i$  and  $y_i$  values respectively. Finally, use a matrix stacking function like

 $np.column\_stack$  to create the new array object RGBXY from the original RGB data and your new pixel location arrays.

If you have done everything correctly, your data with extra "pixel location features" should look like this:

```
>>> RGBXY
      [[ 0.30588236  0.55686277
                                                           0.
                                                                     ]
                                                                     1
       [ 0.27058825  0.533333336  0.16470589
                                              1.
                                                           0.
       [ 0.27058825  0.53333336  0.16470589
                                                                     1
                                                           0.
       . . .
       [ 0.4509804
                                                          99.
                                                                     ]
                      0.67450982
                                  0.34901962 97.
       [ 0.43921569  0.67843139
                                  0.34509805 98.
                                                          99.
                                                                     ]
                                                                     ]]
       [ 0.4666667
                      0.6901961
                                  0.37254903 99.
                                                          99.
[288]: x2d, y2d = np.meshgrid(np.arange(0, 100, dtype="float32"), np.arange(0, 100,

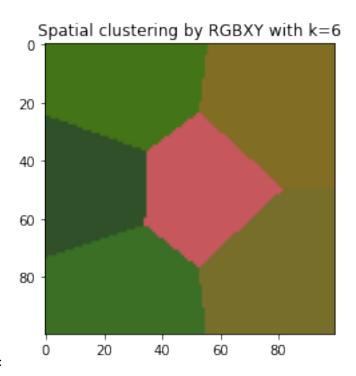
dtype="float32"))
       RGBXY = np.column_stack((RGB, x2d.ravel(), y2d.ravel()))
```

**Check your answer** by running the code cell below.

Correct!

#### 2.0.2 Exercise 1.2 — Cluster pixels spatially

Write a few lines of code to do the following: 1. Cluster the  $\begin{bmatrix} r_i & g_i & b_i & x_i & y_i \end{bmatrix}$  values that are currently stored in the RGBXY variable. Use K=6 clusters. You can use sklearn.cluster.KMeans directly or you can use the  $run\_kmeans$  function from the introduction. 2. Plot the re-coloured image, where each pixel's colour has been replaced by its corresponding centroid colour, as we did in the introduction.



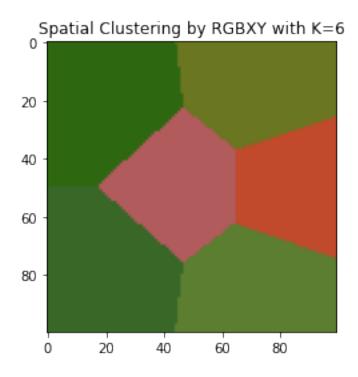
Your plot should look like this:

Hint: Your RGBXY array has shape (10000,5), but the imshow function expects an array of shape (height, width, 3). So you will need to slice out colour data and reshape it into a form that imshow expects.

```
[290]: from sklearn.cluster import KMeans

km = KMeans(n_clusters=6)
km.fit(RGBXY)
centroids, labels = km.cluster_centers_, km.labels_
plt.title("Spatial Clustering by RGBXY with K=6")
plt.imshow(centroids[labels][:,:3].reshape(image.shape))
```

[290]: <matplotlib.image.AxesImage at 0x7fc1cdfa0df0>



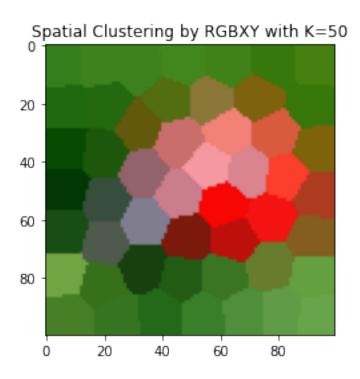
### 2.0.3 Exercise 1.3 — More clusters!

Repeat Exercise 1.2 but this time use K=50 clusters. It may take a few seconds. If you do not understand the result that you see, ask for insight from a TA or from someone else.

```
[291]: from sklearn.cluster import KMeans

km = KMeans(n_clusters=50)
km.fit(RGBXY)
centroids, labels = km.cluster_centers_, km.labels_
plt.title("Spatial Clustering by RGBXY with K=50")
plt.imshow(centroids[labels][:,:3].reshape(image.shape))
```

[291]: <matplotlib.image.AxesImage at 0x7fc1ce4a08b0>

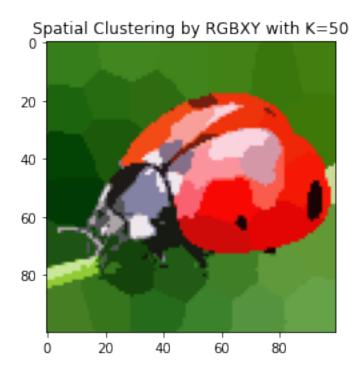


### 2.0.4 Exercise 1.4 — Feature scaling

Repeat Exercise 1.3 but this time scale the x and y features by a factor of 0.02 before clustering. Your answer should use Numpy's "broadcasting" mechanism to achieve the scaling in a single step.

Be sure to store the transformed values in a new array called  $RGBXY\_scaled$  rather than modifying the original RGBXY array. Otherwise you may end up having to re-run the code cell that generated the RGBXY variable.

[292]: <matplotlib.image.AxesImage at 0x7fc1ceaf1850>



The purpose of this exercise is to see that the clustering method is very sensitive to the scale of different features. If you were to scale the XY components all the way to zero, you would be back to clustering  $only\ by\ colour$ , as we did in the introduction.

Before continuing, try scaling (x, y) by different values, such as (0.05, 0.02) and see how that effects the pixel clusters.

# 3 2. Selecting K in K-means

Exercises 2.1-2.2 ask you to generate synthetic data and to apply the "elbow" heuristic for selecting optimal K in K-means.

Run the code cell below to define a function for sampling data from a mixture of Gaussians.

```
[293]: def sample_gmm(means, covs=None, weights=None, N=1):
    """
    Samples a K-component D-dimensional Gaussian mixture.

The means are KxD.
    The covariances are KxDxD. The default covariance is the DxD identity
    →matrix.

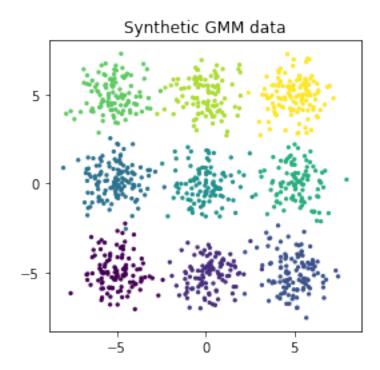
The weights are length K and must sum to 1. The default is uniform weights.

Returns (X, c) where X is an NxD array of samples and c is a length-N vector of component indices, i.e. X[i] was sampled from mixture component c[i].
```

```
nnn
   K, D = means.shape
   # Valudate inputs and set default values if needed
   if covs is None:
      covs = np.tile(np.eye(D), (K,1,1)) # Stack of K D-dimensional identity_
\rightarrow matricies
   if weights is None:
       weights = np.full(K, 1/K)
   assert covs.shape == (K,D,D)
   # Sample a vector of component choices in proportion to weights, one for
→each sample
   c = np.random.choice(K, N, p=weights) # choice() checks that weights has_
\rightarrow shape (K,1) and sums to 1
   \# Fill an array of N samples, one component at a time
  X = np.empty((N,D))
   for k in range(K):
      X[k==c] = np.random.multivariate_normal(means[k], covs[k], np.
return X, c
```

### 3.0.1 Exercise 2.1 — Generate synthetic GMM data

Write a few lines of code to generate 1000 samples from a 9-component Gaussian mixture, where the means are arranged in a 3x3 grid as shown below.



Use a single call to the *sample\_gmm* function to generate your data. That means you must build a *means* matrix with shape (9,2) containing the 9 means. You should know how to do this procedurally, either with for-loops or with a call to the *np.meshgrid* and *np.column\_stack* functions. (Do not write out all 9 of the mean vectors by hand.)

Create a variable called X that refers to your samples, and create a variable called c that refers to the mixture component indices (this value is directly returned by  $sample\_gmm$ , so just store the result).

The np.random.seed(0) ensures you always generate the same data each time you run the code cell.

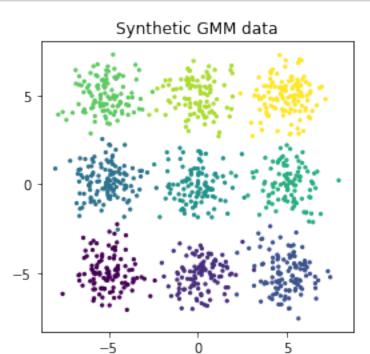
```
[294]: np.random.seed(0)

a, b = np.meshgrid([-5, 0, 5], [-5, 0, 5])
means = np.vstack((a.ravel(), b.ravel())).T
X, c = sample_gmm(means=means, N=1000)
```

Plot your data by running the code cell below.

```
plt.title("Synthetic GMM data")
plt.xticks([-5, 0, 5])
plt.yticks([-5, 0, 5])
plt.gca().set_aspect('equal') # It's important to see this data with equal

→scales on each axis
```



### 3.0.2 Exercise 2.2 — Choosing K with K-means

When applying K-means, it may be difficult to choose the best K for a particular data set. Recall the "elbow curve" method for selecting K as reviewed in Lecture 2. You are asked to apply this method to select a "good" K for the data set generated in Exercise 2.1.

Write a few lines of code to generate a plot of K (x-axis) versus the corresponding K-means objective value (y-axis) for each choice of  $K \in \{2, ... 15\}$ . Use the **sklearn.cluster.KMeans** object in your answer. Once you have called the *fit* method on a KMeans object you can recover the final objective value (at convergence) from the object's intertia attribute (as in kmeans\_object.inertia\_).

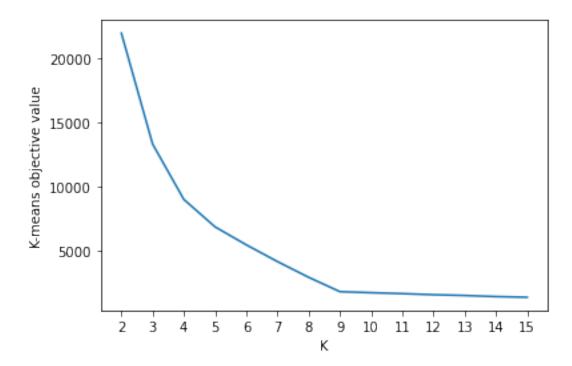
If you have done this correctly, you should see a 'kink' at K=9, which makes sense given that the data was indeed generated from 9 clusters.

```
[296]: from sklearn.cluster import KMeans

x_axis = np.arange(2, 16)
y_axis = [KMeans(n_clusters=x).fit(X).inertia_ for x in x_axis]
```

```
plt.xlabel("K")
plt.ylabel("K-means objective value")
plt.xticks(x_axis)
plt.plot(x_axis, y_axis)
```

[296]: [<matplotlib.lines.Line2D at 0x7fc1cfa9d580>]



# 4 3. Fitting a Gaussian Mixture Model (GMM)

Exercises 3.1–3.4 ask you fit 2D data with scikit-learn's **sklearn.mixture.GaussianMixture** object.

Run the code cell below to define a function that will help to visualize the placement and shape of GMM components.

```
[297]: def plot_gmm(gmm):
    """
    Plots the placement of components in a Gaussian Mixture.

    The gmm object should be of type sklean.mixture.GaussianMixture
    """
    ax = plt.gca()
    for weight, mean, cov in zip(gmm.weights_, gmm.means_, gmm.covariances_):
        v, w = np.linalg.eigh(cov)
        v = 2*np.sqrt(2*v)
```

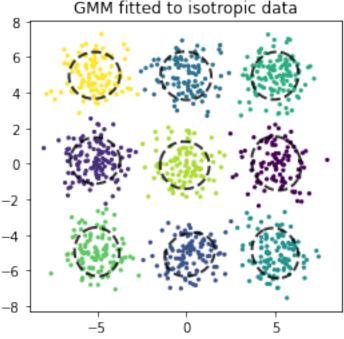
```
u = w[0] / np.linalg.norm(w[0])
angle = 180 * (1 + np.arctan(u[1]/u[0]) / np.pi) # Ellipse() function
→needs degrees
ell = mpl.patches.Ellipse(mean, v[0], v[1], angle, edgecolor='k',
facecolor='none', linestyle='--',
→linewidth=2, alpha=0.8)
ax.add_artist(ell)
```

#### 4.0.1 Exercise 3.1 — Fit a GMM to non-overlapping, isotropic data

Write fitting code to fit a sklearn.mixture.GaussianMixture object to the synthetic data from Exercise 2.1. Use 9 mixture components in your answer. You should use the argument  $random\_state=0$  to ensure reproducibility. Create a variable called gmm that refers to your new GaussianMixture object.

```
[298]: from sklearn.mixture import GaussianMixture
gmm = GaussianMixture(n_components=9, random_state=0, n_init=5).fit(X)
```

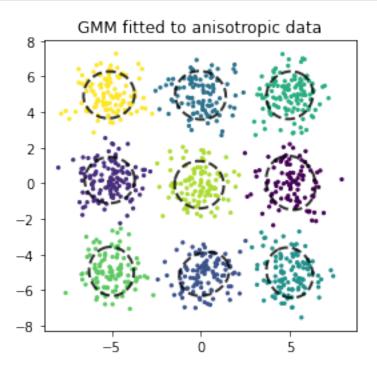
Write plotting code using the *plot\_gmm* function provided. Once you have the ellipses plotting correctly, use the **predict** method of the *GaussianMixture* object and use them to colour the points in the scatter plot. Your plot should look similar to:



If you find that the GMM components do not fit perfectly to the data, try adding  $n\_init=5$  to the arguments of your GaussianMixture object. This will run the EM algorithm multiple times from different randomized initializations, and may give a higher chance of getting the 'right' clustering.

```
[299]: plot_gmm(gmm)
    predicted = gmm.predict(X)

plt.scatter(*X.T, s=5, c=predicted)
    plt.title('GMM fitted to anisotropic data')
    plt.gca().set_aspect('equal')
```



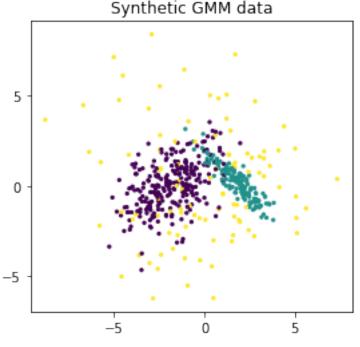
### 4.0.2 Exercise 3.2 — Generate overlapping, anisotropic synthetic GMM data

Write some code to generate 500 samples from 2-dimensional 3-component Gaussian mixture having the following parameters:

$$\begin{aligned} \pi_1 &= 0.5, \quad \boldsymbol{\mu}_1 = \begin{bmatrix} -2.0 & 0.0 \end{bmatrix}, \quad \boldsymbol{\Sigma}_1 = \begin{bmatrix} 2.0 & 1.0 \\ 1.0 & 2.0 \end{bmatrix} \\ \pi_2 &= 0.3, \quad \boldsymbol{\mu}_2 = \begin{bmatrix} 2.0 & 0.0 \end{bmatrix}, \quad \boldsymbol{\Sigma}_2 = \begin{bmatrix} 1.0 & -0.9 \\ -0.9 & 1.0 \end{bmatrix} \\ \pi_3 &= 0.2, \quad \boldsymbol{\mu}_3 = \begin{bmatrix} 0.0 & 0.0 \end{bmatrix}, \quad \boldsymbol{\Sigma}_3 = \begin{bmatrix} 10.0 & 0.0 \\ 0.0 & 10.0 \end{bmatrix} \end{aligned}$$

Use the  $sample\_gmm$  function from part 2. Create a variable called X that refers to your samples, and create a variable called c that refers to the mixture component indices (this value is directly returned by  $sample\_gmm$ , so just store the result).

Plot your data by running the code cell below. The plot should look like this:



```
[301]: assert 'X' in globals(), "You must create a variable called 'X' that refers to → your samples!"

assert 'c' in globals(), "You must create a variable called 'c' that refers to → your component indices!"

assert X.shape == (500,2), "X should have shape (500, 2)!"

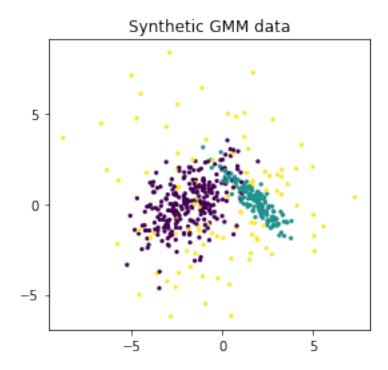
assert c.shape == (500,), "c should have shape (500,)!"

plt.scatter(*X.T, c=c, s=5) # Plot each point (X[i,0], X[i,1]) using colour → index c[i] and point size 5

plt.title("Synthetic GMM data")
```

```
plt.xticks([-5, 0, 5])
plt.yticks([-5, 0, 5])
plt.gca().set_aspect('equal') # It's important to see this data with equal

⇒scales on each axis
```

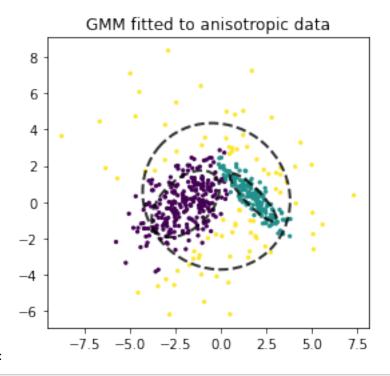


### 4.0.3 Exercise 3.3 — Fit a GMM to the anisotropic, overlapping data

Write fitting code to fit a sklearn.mixture.GaussianMixture object to the synthetic data you generated in Exercise 3.2. Use 3 mixture components in your answer. You should use the argument  $random\_state=0$  to ensure reproducibility. Create a variable called gmm that refers to your new GaussianMixture object.

```
[302]: from sklearn.mixture import GaussianMixture
gmm = GaussianMixture(n_components=3, random_state=0).fit(X)
```

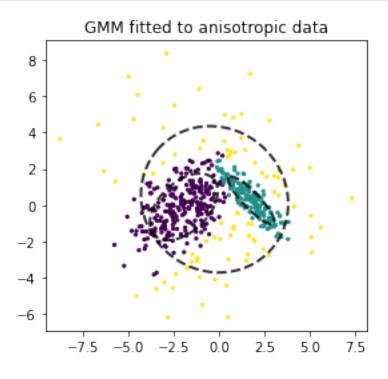
Write plotting code (like Exercise 3.1) using the predict method. Your plot should look like



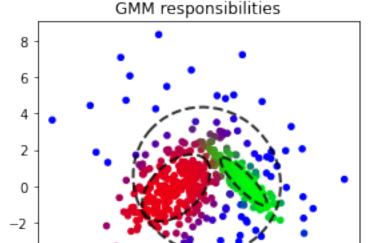
this (colours may differ):

```
[303]: predicted = gmm.predict(X)
plot_gmm(gmm)

plt.scatter(*X.T, s=5, c=predicted)
plt.title('GMM fitted to anisotropic data')
plt.gca().set_aspect('equal')
```



Write plotting code to visualize the probability  $p(z_{ik} \mid \mathbf{x}_i)$  that component k generated data point  $\mathbf{x}_i$ . Use the **predict\_proba** method of the GaussianMixture object to get the probabilities. Because there are K = 3 components, you can visualize these probabilities by using  $[p(z_{i1} \mid \mathbf{x}_i) \quad p(z_{i2} \mid \mathbf{x}_i) \quad p(z_{i3} \mid \mathbf{x}_i)]$  as the values colour  $[r_i \quad g_i \quad b_i]$  for data point i. Your plot



0.0

2.5

5.0

7.5

should look like this:

-6

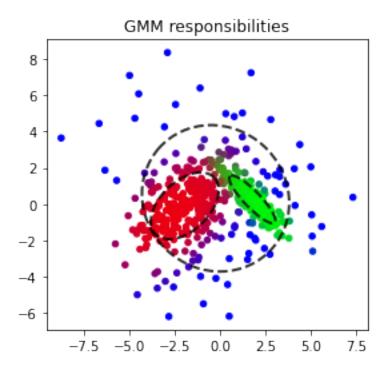
-7.5

```
[304]: plot_gmm(gmm)
    predicted = gmm.predict_proba(X)

plt.scatter(*X.T, s=20, c=predicted)
    plt.title('GMM responsibilities')
    plt.gca().set_aspect('equal')
```

-2.5

-5.0



### 4.0.4 Exercise 3.4 — Sample from spatially clustered pixels using a GMM

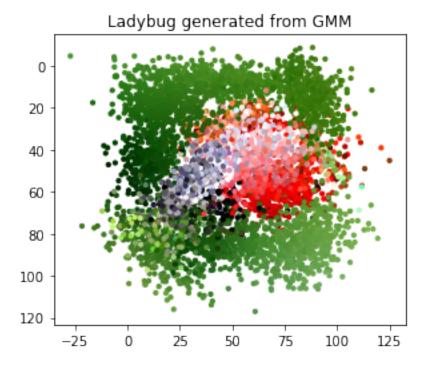
Write fitting code to fit a sklearn.mixture.GaussianMixture object to the RGBXY data (the ladybug) that you generated in Exercise 1.2. Use 15 mixture components in your answer. You should use the argument random\_state=0 to ensure reproducibility. Create a variable called gmm that refers to your new GaussianMixture object.

```
[305]: from sklearn.mixture import GaussianMixture
gmm = GaussianMixture(n_components=15, random_state=0).fit(RGBXY)
```

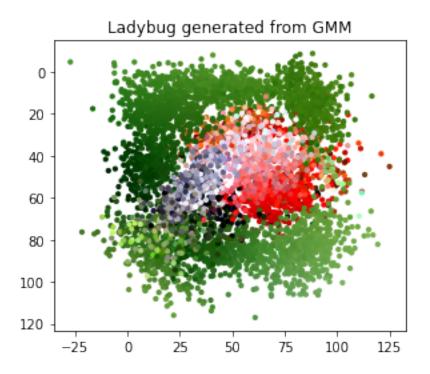
Generate 5000 samples from your fitted mixture model by using the sample method of the GaussianMixture object. The resulting sample matrix should have shape (5000,5) where each row is a vector  $\begin{bmatrix} r & g & b & x & y \end{bmatrix}$ . Create a variable X to refer to your new samples. Note that the sample function also returns a component membership vector, but you can ignore it.

```
[306]: X, _ = gmm.sample(n_samples=5000)
```

Plot the samples as if they were pixels at location (x, y) with colour (r, g, b). Use a single call to Matplotlib's scatter function. Your ladybug should look something like this:



*Hint:* The *scatter* function will fail if you use any colour values outside range [0.0, 1.0], yet there's no guarantee that a Gaussian will produce values within this range. Use the **np.clip** function to clamp the (r, g, b) values to this range.



This final exercise was designed to show: \* how to train a GMM on 5-dimensional data (RGBXY); \* how to visualize 5 dimensional samples in a 2D plot, by using a combination of colour and space; \* that sampling from a generative model, such as a GMM, is a good way to see whether the samples it generates are "realistic" or whether they're missing important aspects of the real data; and \* that a Gaussian or a GMM, when used as a generative model, can produce samples that have values outside the range of the original training data (for example, negative XY coordinates).