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Exercise 1: Python Tutorial, Probability Density, GMM, EM

due on 2023-11-04

Important information regarding the exercises:

- Use the Moodle system to submit your solution. You will also find your corrections there.
- Due to the large number of participants, we require you to submit your solution to Moodle in groups of 3 students. You can use Moodle to form groups.
- Upload your pen & paper solutions as PDF. If your solutions are handwritten, ensure that your handwriting is legible, and that the pictures are not blurred and are taken under appropriate lighting conditions. All non-readable submissions will be discarded immediately.

Question	Points	Bonus	Score
Python Tutorial	0	0	
Warming up!	4	0	
Maximum Likelihood	6	0	
Expectation Maximization (EM) Algorithm	10	4	
Σ Points	20	4	

• Upload your implementation as '.zip' or '.tar.gz' file.

- (a) Install Python from https://www.python.org/downloads/ Set the Python environment and run Python using the command python in your shell (see https: //docs.python.org/3/tutorial/interpreter.html).
- (b) Go through chapters 3, 4, and 5 in https://docs.python.org/3/tutorial/.
- (c) Install NumPy and Matplotlib by running pip install numpy matplotlib in your shell.
- (d) Walk through the basic NumPy tutorial (https://numpy.org/doc/stable/user/ quickstart.html).

Note: We suggest you to use Visual Studio Code (https://code.visualstudio. com/) together with the Python extension, or the PyCharm IDE (https://www.jetbrains. com/pycharm/) for writing Python code.

- - (a) What is the probability of selecting an apple?

(b) If we observe that the selected fruit is in fact an orange, what is the probability that (2 pts) it came from the green box?

Question 3: Maximum Likelihood $(\Sigma = 6)$ Consider the following probability density function

$$p(x|\theta) = \frac{1}{\sqrt{2\pi\theta}} \exp\left(-\frac{(x-3)^2}{2\theta}\right).$$

Given N measurements $x_1, ..., x_n > 0$ of x, what is the maximum likelihood estimate $\hat{\theta}$?

Notes:

- For your reference, the equations for the *D*-dimensional GMMs can be found in the book of C. M. Bishop "Pattern Recognition and Machine Learning" (Chapter 9).
- You will need to install the following dependencies: pip install scikit-learn numpy matplotlib imageio
- You can use the provided 'apply.py' script to test your implementation. Comment out the unrelated parts to test the individual subexercises.
- (a) Implement the function getLogLikelihood that computes the log-likelihood

(2 pts)

$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$

of a mixture of Gaussian distributions with the signature

```
1 def getLogLikelihood(means, weights, covariances, X):
2
      # Log Likelihood estimation
      #
3
      # INPUT:
4
      # means
                       : Mean for each Gaussian KxD
5
      # weights
                      : Weight vector 1xK for K Gaussians
6
                      : Covariance matrices for each gaussian DxDxK
      # covariances
7
      # X
                        : Input data NxD
8
      # where N is number of data points
9
      # D is the dimension of the data points
10
      # K is number of gaussians
11
12
      # OUTPUT:
13
      # logLikelihood : log-likelihood
14
      return logLikelihood
15
```

(b) Implement the function EStep that performs the expectation step of the EM algorithm, (2 pts) i.e. computes the responsibilities $\gamma_i(\mathbf{x}_n)$:

```
1 def EStep(means, covariances, weights, X):
2  # Expectation step of the EM Algorithm
3  #
```

```
# INPUT:
4
      # means
                       : Mean for each Gaussian KxD
\mathbf{5}
      # weights : Weight vector 1xK for K Gaussians
6
      # covariances : Covariance matrices for each gaussian DxDxK
7
      # X
                        : Input data NxD
8
9
      #
      # N is number of data points
10
      # D is the dimension of the data points
11
      # K is number of gaussians
12
13
      # OUTPUT:
14
      # logLikelihood : Log-likelihood (a scalar).
15
                       : NxK matrix of responsibilities for N
16
      # gamma
         datapoints and K gaussians.
      return [logLikelihood, gamma]
17
```

(c) Implement the function MStep that performs the maximization step of the EM algorithm. i.e. $\hat{\pi}_{j}^{new}, \hat{\mu}_{j}^{new}, \hat{\Sigma}_{j}^{new}$: (2 pts)

```
1 def MStep(gamma, X):
      # Maximization step of the EM Algorithm
2
3
      #
      # INPUT:
4
               : NxK matrix of responsibilities for N
5
      # gamma
        datapoints and K gaussians.
                      : Input data (NxD matrix for N datapoints of
      # X
6
        dimension D).
      #
7
      # N is number of data points
8
      # D is the dimension of the data points
Q
     # K is number of gaussians
10
11
      #
      # OUTPUT:
12
      # logLikelihood : Log-likelihood (a scalar).
13
     # means : Mean for each gaussian (KxD).
14
      # weights
                     : Vector of weights of each gaussian (1xK).
15
      # covariances : Covariance matrices for each component(
16
         DxDxK).
     return [weights, means, covariances, logLikelihood]
17
```

(d) As mentioned in the lecture, it is often necessary to introduce a regularization for (1 pt) EM to work robustly. One possibility is to add a small value to the diagonal entries of all covariance matrices: $\Sigma_{\text{reg}} = \Sigma + \varepsilon \mathbf{I}$. This ensures that the covariance matrix has a low condition number, which makes the computation of the inverse more stable. Implement the function

```
1 def regularize_cov(covariance, epsilon):
     # regularize a covariance matrix, by enforcing a minimum
2
      # value on its singular values. Explanation see exercise sheet
3
      #
4
     # INPUT:
5
     # covariance
                      : matrix
6
     # epsilon
                       : minimum value for singular values
7
     #
8
    # OUTPUT:
9
```

10 # regularized_cov: reconstructed matrix 11 return regularized_cov

that regularizes a covariance matrix as described above.

(e) Implement the function estGaussMixEM for performing EM for estimating Gaussian (1 pt) Mixture Models of D-dimensional data.

```
1 def estGaussMixEM(data, K, n_iters, epsilon):
      # EM algorithm for estimation gaussian mixture mode
2
      #
3
      # INPUT:
4
                         : input data, N observations, D dimensional
\mathbf{5}
      # data
      # K
                         : number of mixture components (modes)
6
      #
7
      # OUTPUT:
8
      # weights
                        : mixture weights - P(j) from lecture
9
10
      # means
                         : means of gaussians
      # covariances
                       : covariancesariance matrices of gaussians
11
      return [weights, means, covariances]
12
```

Use the functions from the previous subquestions for the implementation of this function. Initialize the weights uniformly

weights = numpy.ones(K) / K

and the means and the covariances using the K-Means algorithm:

```
kmeans = KMeans(n_clusters = K, n_init = 10).fit(data)
1
      cluster_idx = kmeans.labels_
2
      means = kmeans.cluster_centers_
3
4
      # Create initial covariance matrices
5
      for j in range(K):
6
          data_cluster = data[cluster_idx == j]
7
          min_dist = np.inf
8
          for i in range(K):
9
               # compute sum of distances in cluster
10
               dist = np.mean(euclidean_distances(data_cluster, [
11
                  means[i]], squared=True))
               if dist < min dist:</pre>
12
                   min_dist = dist
13
          covariances[:, :, j] = np.eye(n_dim) * min_dist
14
```

(f) Test your EM implementation on the provided synthetic data data1, data2, data3 (2 pts) and visualize your fitted model. Submit screen-shots of the visualizations. They should look similar to this:

Now, repeat the experiment for different number of mixture models (e.g. $K = 4, 5, 6, \ldots$ etc). Examine how the likelihood of the computed model changes with K. Are these likelihoods comparable? Which is the best K and why?

(g) Use the provided datasets of RGB pixel values for skin (sdata) and non-skin (ndata) (2 bonus) regions for a skin detection experiment. First, train a Gaussian Mixture Model for each dataset using your implementation from previous part. Based on these two Mixture Models, classify the pixels in the provided image faces.png according to the Likeli-



Figure 1: This figure shows the visualisation for the fitted models.

hood Ratio:

$$\frac{p(\text{color}|\text{skin})}{p(\text{color}|\text{non-skin})} > \theta$$

Implement this in the function skinDetection. Use different θ and compare your results to the groundtruth faces_groundtruth.png. Which parameters θ , κ , etc. work well? Give possible explanations.

(h) Try your algorithm on some images. Can you find examples where it works or does (2 bonus) not work? Give some possible explanations.