

## Section 2.1

Exercise 2.1.1 (Jupyter Notebook) Let

$$X = \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} \quad Y = [1 \quad 2 \quad 3] \quad Z = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 7 \end{bmatrix}$$

Perform the following numpy operations:

- Define each of X, Y and Z as a 2d numpy arrays
- Concatenate X and Y in the row direction (X on top of Y)
- Reshape Z into a 2 row and 3 column 2d numpy array
- Compute  $X + 3*Y + \text{reshapedZ}$
- Compute  $X*Y$  (componentwise multiplication with broadcasting)

Hint: look at UnsupervisedML/Examples/Section02/NumpyBasic.ipynb

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.1.1.ipynb

Exercise 2.1.2 (Jupyter Notebook) Let

$$X = \begin{bmatrix} 1 & 2 & 3 & -1 & -3 & -4 \\ 4 & 5 & 7 & -6 & -5 & -7 \\ 7 & 8 & 9 & 2 & 4 & 6 \end{bmatrix} \quad \text{and } a = [0 \quad 1 \quad 1 \quad 0 \quad 1 \quad 1]$$

Perform the following numpy operations:

- Use np.where to find the indices where  $a = 0$
- Create a 2d array from X by indexing into its columns where  $a=0$  - call it Y
- Compute the mean of Y in the column direction (use np.mean with the appropriate axis option and keepdims=True)
- Use np.where to find the indices where  $a = 1$
- Create a 2d array from X by indexing into columns 0 and 3 – call it Z
- Compute the mean of Z in the column direction

Note: we will be using this approach for the K Means clustering algorithm

Hint: see UnsupervisedML/Examples/Section02/NumpyBasic.ipynb

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.1.2.ipynb

## Section 2.2

Exercise 2.2.1 (Jupyter Notebook) Let

$$W = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \quad X = \begin{bmatrix} 1 & 2 & 4 \\ -2 & -5 & -8 \end{bmatrix} \quad Y = [1 \quad 2 \quad 3] \quad Z = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 7 \end{bmatrix}$$

Compute the following (all multiplications here are matrix multiplications)

- (a)  $X + Y$
- (b)  $WX$
- (c)  $Z + Y^T$
- (d)  $XZW^{-1}$
- (e)  $X + Z^T$
- (f)  $ZX$
- (g)  $X^T Z^T$

Hint: see UnsupervisedML/Exercises/Section02/NumpyMatrixOperations.ipynb

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.2.1.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 2.3

Exercise 2.3.1 (Jupyter Notebook) Using numpy and matplotlib functionality plot the following functions for x between -5 and 5.

(a)  $f(x) = \frac{1}{1+e^{-x}}$  - Hint: use numpy exp function

(b)  $f(x) = \log(1 + e^x)$  Hint: use numpy log and exp functions

(c) Create an object oriented subplot with 1 row and 2 columns and add the plots in (a) and (b).

Note: you need not specify the column index in the ax object since there is only 1 row. Use ax[0] and ax[1] to refer to the individual subplots in the figure.

Hint: see UnsupervisedML/Examples/Section02/NumpyBasic.ipynb and

UnsupervisedML/Examples/Section02/MatplotlibBasic.ipynb

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.3.1.ipynb

## Section 2.4

### Exercise 2.4.1 (Jupyter Notebook)

(a) Consider the following matrix:

$$X = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

Plot using pcolormesh. What digit is it? (You will need to use flipud)

(b) Create the matrices for digits 3 and 6 and plot using pcolormesh.

Hint: see UnsupervisedML/Examples/Section02/MatplotlibAdvanced.ipynb

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.4.1.ipynb

### Exercise 2.4.2 (Jupyter Notebook)

The goal of this problem is to create an animation that combines the 2 animations in the demo in UnsupervisedML/Examples/Section02/MatplotlibAdvanced.ipynb.

(1) Change colors for a fixed set of 50 randomly chosen data points in 2 dimensions:

(2) Change the locations of 5 randomly chosen data points in 2 dimensions:

Hint: create a single figure and create separate scatter objects to hold (1) and (2). Update both scatter objects in the update function. This approach will be used for animation for the K Means algorithm.

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.4.2.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

## Section 2.5

Exercise 2.5.1 (Jupyter Notebook) Repeat the first part of Unsupervised/ML/Examples/Section02/PandasDemo.ipynb.

Read data from mydf1.csv and

- (a) Output a Y numpy array that has the square of the entries in the “label” column of the file
- (b) Output a X numpy array whose first column has the square root of the entries in the “feature 1” column and whose second column has the exponential of the entries in the “feature 2” column.

Solution: see UnsupervisedML/Exercises/Section02/Exercise\_02.5.1.ipynb

### Section 3.1

Exercise 3.1.1 (Jupyter Notebook) Consider the messages:

“A bird in the hand is worth two in the bush”, “The early bird gets the worm”, “Time is money”  
“Honesty is the best policy”

- (a) Repeat the countvectorizer example in UnsupervisedML/Examples/Section03/SklearnText.ipynb for this new dataset including creation of the word cloud.
- (b) Repeat (a) using stop words (“the”, “is”, “in”). Stop words are typically common words that should not have an impact to sentiment or topic. Hint: create an instance of the CountVectorizer with the format: CountVectorizer(stop\_words=[“the”, “is”, “in”]). Notice that the stop words are not in the word cloud.

Solution: See UnsupervisedML/Exercises/Section03/Exercise\_03.1.1.ipynb

Exercise 3.1.1 (Jupyter Notebook) Let’s go back to the example from the demo with documents:

“Call me soon”, “CALL to win”, “Pick me up soon”

The goal of this exercise is to generate the Tfidf matrix from the Countvectorizer matrix.

- (a) The document frequency  $df(i)$  is the number of documents in which word  $i$  appears. For example, “call” appears in 2 documents (once we convert to lowercase) and “soon” appears in 2 documents. Starting with the Countvectorizer matrix, create a column vector (# of word rows and 1 column) representing the document frequency.
- (b) Create the inverse document frequency vector  $idf(i)$  defined by following formula, where  $n$  is number of documents:

$$idf(i) = \log\left(\frac{1+n}{1+df(i)}\right) + 1$$

- (c) Compute the unscaled tfidf matrix defined by:

$$U_{ij} = \text{Count}(i, j) * idf(i)$$

Here  $U_{ij}$  is entry of unscaled tfidf matrix for word  $i$  and document  $j$  and  $\text{Count}(i, j)$  is the result of the countvectorizer for word  $i$  and document  $j$ .

- (d) Compute the scaled tfidf matrix  $T$ , where entries are obtained by scaling the unscaled matrix  $U$  using the following formula ( $W$  is number of words) and compare with tfidf matrix obtained directly from sklearn Tfidf vectorizer

$$T_{ij} = \frac{U_{ij}}{[\sum_{i=0}^{W-1} U_{ij}^2]^{1/2}}$$

Hint: see demo UnsupervisedML/Examples/Section03/SklearnText.ipynb

Solution: see UnsupervisedML/Exercises/Section03/Exercise\_03.1.2.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 3.2

Exercise 3.2.1 (Theory and Jupyter Notebook) Consider matrix/matrix multiplication  $A \cdot A$  where  $A$  is an  $M \times M$  matrix.

- (a) What is the computational complexity (number of operations) for this calculation as  $M \rightarrow \infty$  - work this out on paper.
- (b) Confirm the computational complexity in (a) by computing time to perform  $A \cdot A$  for matrices of various dimensions. Hint: see UnsupervisedML/Examples/Section03/Complexity.ipynb

Solution: see next page and also UnsupervisedML/Exercises/Section03/Exercise\_03.2.1.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

Solution: Exercise 3.2.1(a)

Consider matrix multiplication  $B = A * A$ , where  $A$  is  $M \times M$ .  $B$  is of dimension  $M \times M$ , so it has  $M^2$  entries. It can be shown that  $B_{ij}$  is dot product of row  $i$  of  $A$  and column  $j$  of  $A$ . Each dot product requires  $O(M)$  operations as  $M \rightarrow \infty$ . Hence, the total number of operations for computing all entries of  $B$  is  $O(M^3)$  as  $M \rightarrow \infty$ .

Solution: Exercise 3.2.1(b) see Unsupervised/Exercises/Section03/Exercise\_03.2.1.ipynb



### Section 3.3

Exercise 3.3.1 (Jupyter Notebook) Consider the following datasets/clusters:

$$X = \begin{bmatrix} 1 & 5 & 9 \\ 2 & 6 & 10 \\ 3 & 7 & 11 \\ 4 & 8 & 12 \end{bmatrix} \quad Y = \begin{bmatrix} 11 & 15 & -9 \\ 2 & -6 & 1 \\ 13 & 7 & -11 \\ 4 & 18 & 12 \end{bmatrix}$$

- (a) Compute the mean of each dataset. (Hint: express X and Y as 2d arrays in numpy and use np.mean() function to compute the mean. Make sure that you take the mean in the appropriate direction with the axis setting and make sure you use the appropriate keepdims setting.) The output for the mean should be a 2d array column vector of dimension 3x1.
- (b) Compute the distances between the 2 clusters defined as distance between cluster means.

Exercise 3.3.2 (Jupyter Notebook) In the demo for this section we looked at 2 different functions (looping version and vectorized version) for computing distance between a vector Y and a dataset X. Confirm that the computational complexity of this calculation is  $O(M)$  operations as  $M \rightarrow \infty$  for both approaches, where M is the number of data points in the dataset.

Hint: follow the approach for determining the computational complexity power shown in UnsupervisedML/Examples/Section03/Complexity.ipynb

Solution: UnsupervisedML/Exercises/Section03/Exercise\_03.3.1.ipynb

### Section 3.4

Exercise 3.4.1 (Jupyter Notebook) Consider the following matrix:

$$X = \begin{bmatrix} 11 & 15 & -9 \\ 2 & -6 & 1 \\ 13 & 7 & -11 \\ 4 & 18 & 12 \end{bmatrix}$$

- (a) Compute the compact SVD and confirm that  $X = U\Sigma V^T$
- (b) Confirm that each column of U has L2 length = 1 and that the columns are pairwise orthogonal.  
(For example confirm that  $U_0^T U_1 = 0$  and similar for other pairs of columns.)
- (c) Repeat (b) for the columns of V

Hint: see UnsupervisedML/Examples/Section03/SVD.ipynb

Solution: see UnsupervisedML/Exercises/Section03/Exercise\_03.4.1.ipynb

Exercise 3.4.2 (Jupyter Notebook) Consider an  $M \times M$  matrix A. Confirm that the computational complexity for the SVD calculation is  $O(M^3)$  as  $M \rightarrow \infty$ .

Hint: follow the approach in UnsupervisedML/Examples/Section03/Complexity.ipynb

Solution: see UnsupervisedML/Exercises/Section03/Exercise\_03.4.2.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 3.5

Exercise 3.5.1 (Jupyter Notebook) Consider the following dataset:

$$X = \begin{bmatrix} 1 & -2 & 3 & -4 & 5 \\ 6 & 7 & -10 & 11 & 3 \\ 8 & 9 & 12 & -13 & 2 \end{bmatrix}$$

- (a) Compute the mean of the dataset
- (b) Compute the covariance matrix for the dataset

Hint: see UnsupervisedML/Examples/Section03/MeanCovariance.ipynb

Solution: see UnsupervisedML/Exercises/Section03/Exercise\_03.5.1.ipynb

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 4.1

Exercise 4.1.1 (Theory) Suppose that a dataset has  $M$  data points. Provide an explanation for the complexity estimate of  $O(M^3)$  as  $M \rightarrow \infty$  to determine the clusters at all levels for hierarchical clustering algorithm.

Solution: see next page

Solution 4.1.1: Suppose that there are  $M$  points in the dataset. Initially, there are  $M$  clusters. Now suppose that we are at the level where there are  $m$  clusters. To determine clusters at the next level, one must compute all pairwise distances between clusters and combine the clusters that are closest to each other. If there are  $m$  clusters, then there are  $m(m-1)/2$  pairwise distances to compute. Hence there are  $O(m^2)$  pairwise distances to compute as  $m \rightarrow \infty$ . The amount of work to compute each pairwise distance between clusters is  $O(d)$  as  $d \rightarrow \infty$  (assuming we measure distance between clusters as distance between cluster centres and we store the cluster centres). Summing over  $m$ , we have:

$$\sum_{m=1}^M m(m-1)/2 = O(M^3) \quad \text{as } M \rightarrow \infty$$

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 4.3

Exercise 4.3.1 (Testing) Experiment with the `driver_hierarchical.py` code and try the other cases: `blobs`, `varied_blobs2`, `aniso`, `noisy_moons`, and `noisy_circles`. For the latter 2 cases, set the `nlevel=2` when plotting results.

Exercise 4.3.2 (Programming) Suppose that a dataset has  $M$  data points. For the Hierarchical Clustering Algorithm, confirm that the number of operations is  $O(M^3)$  as  $M \rightarrow \infty$  by measuring time for completing the algorithm for various values of  $M$ .

Hint: use one of the sklearn datasets for this Exercise and run the hierarchical clustering algorithm code for various values of  $M$ . I suggest going up to  $M = 200$  or else the clustering code may take too long to run. See `UnsupervisedML/Exercises/Section02/Complexity.ipynb` notebook for an example of how to determine the power in the complexity estimate.

Solution: see `UnsupervisedML/Exercises/Section04/Exercise_04.3.2.py`. Run this program in folder `UnsupervisedML/Code/Programs`

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

## Section 5.1

Exercise 5.1.1 (Theory) Suppose that a dataset has  $M$  data points. Can you provide an explanation as to why the worst case complexity for number of operations for the DBSCAN algorithm is  $O(M^2)$  as  $M \rightarrow \infty$ .

Solution: see next page

Exercise 5.1.2 (Programming) Create a program to generate the nearest neighbour plots as seen in the lecture. Use the varied\_blob1 dataset with  $M = 200$  and  $1500$  data points and set minpts = 4.

Solution: see file UnsupervisedML/Exercises/Section05/Exercise\_05.1.2.py. Run this program in the UnsupervisedML/Code/Programs folder

Exercise 5.1.3 (Theory) Suppose that DBSCAN is performed with minpts = 4 and  $\varepsilon = 0.3$ . It found that a new cluster is created with exactly 2 points. How is this possible?

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

Solution 5.1.1: The amount of work to determine the number of points in the  $\varepsilon$  neighbourhood for a single data point is  $O(M)$  as  $M \rightarrow \infty$ , since one must compute the distances to all other data points before determining the number within a distance  $\varepsilon$ . In the case of all noise points, we must do this distance calculation for all data points. Since there are  $M$  data points, then total work is  $O(M^2)$  as  $M \rightarrow \infty$ . There may be more efficient ways to determine points in the  $\varepsilon$  neighbourhood. These are mentioned in the Wikipedia page on DBSCAN (see section on Complexity):

<https://en.wikipedia.org/wiki/DBSCAN>

Solution 5.1.3: For DBSCAN with  $\text{minpts} = 4$  and  $\varepsilon = 0.3$  a cluster is created if there is a core point (with at least 4 points within  $\varepsilon = 0.3$ , including the core point itself.) If 2 of the neighbours are border points that belong to other clusters and they have been assigned to that other cluster first, then one is left with a cluster with 2 points.



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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 5.3

Exercise 5.3.1 (Testing) Experiment with the driver\_kmeans.py code and try the other cases: blobs, varied\_blobs2, aniso, noisy\_moons, and noisy\_circles. Experiment with the minpts and epsilon and the number of samples as well.

Exercise 5.3.2 (Programming) Suppose that a dataset has  $M$  data points. Confirm that the number of operations is  $O(M^2)$  as  $M \rightarrow \infty$  for the DBSCAN algorithm by measuring time for completing the algorithm for various values of  $M$ .

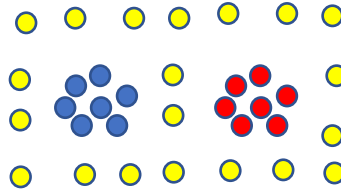
Hint: use one of the sklearn datasets for this Exercise and run the DBSCAN algorithm code for various values of  $M$ .

Solution: see UnsupervisedML/Exercises/Section05/Exercise\_05.3.2.py. Run this program in the UnsupervisedML/Code/Programs folder.

### Section 6.1

Exercise 6.1.1 (Theory) Suppose that a dataset has  $M$  data points. Can you provide an explanation as to why the complexity for number of operations for the K Means algorithm is  $O(M)$  as  $M \rightarrow \infty$ .

Exercise 6.1.2 (Theory) Explain why the following final cluster assignment cannot be generated by the K Means algorithm. (Blue dots belong to cluster 0, Red dots belong to cluster 1, Yellow dots belong to cluster 2.)



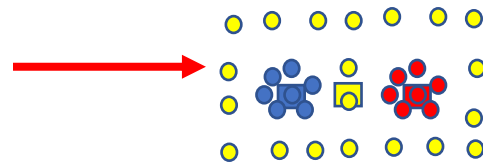
Solution 6.1.1: At each iteration of the algorithm one must perform the following steps:

- (1) Compute distance between each data point and each of cluster means
- (2) Compute the closest cluster mean for each data point
- (3) Compute the updated cluster mean values

Each of these steps requires  $O(M)$  operations as  $M \rightarrow \infty$ . If we assume a fixed number of iterations for convergence as  $M$  increases, the total work is  $O(M)$  operations as  $M \rightarrow \infty$ .

Solution 6.1.2: See figure below to the final cluster assignment with the cluster means in the square symbols. Remember that a data point belongs to the cluster corresponding to the nearest cluster mean, so the yellow point on the left should be in the blue cluster and not the yellow cluster. Same logic applies to other yellow data points on left and right.

This point is closer to blue mean than yellow mean, so it should belong to blue cluster



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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 6.3

Exercise 6.3.1 (Testing) Experiment with the driver\_kmeans.py code and try the other cases: blobs, varied\_blobs2, aniso, noisy\_moons, and noisy\_circles. Experiment with the number of clusters and initialization and number of samples.

Exercise 6.3.2 (Programming) Write a program to create the elbow plot for the varied\_blobs1 dataset with 200 points. Use the K Means with “random” initialization.

Solution: see UnsupervisedML/Exercises/Section06/Exercise\_06.3.2.py. Run this program in folder UnsupervisedML/Code/Programs.

Exercise 6.3.3 (Programming) Suppose that a dataset has  $M$  data points. Confirm that the number operations is  $O(M)$  as  $M \rightarrow \infty$  for the K Means algorithm by measuring time for completing the algorithm for various values of  $M$ .

Hint: use one of the sklearn datasets for this Exercise and run the K Means algorithm code for various values of  $M$ .

Solution: see UnsupervisedML/Exercises/Section06/Exercise\_06.3.3.py. Run this program in folder UnsupervisedML/Code/Programs

## Section 7.1

### Exercise 7.1.1 (Jupyter Notebook)

Let  $\phi=1$  and define:

$$\mu = \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad \Sigma = \begin{bmatrix} 2 & 0.5 \\ 0.5 & 3 \end{bmatrix}$$

Plot the contours for the 2d normal distribution pdf

$$N(X, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{1}{2}(X-\mu)^T \Sigma^{-1} (X-\mu)} = c$$

for  $c = 0.04, 0.06$  and  $d=2$  using the Matplotlib Ellipse approach shown in the demo. What happens when  $c$  is large? Why?

Hint: see UnsupervisedML/Examples/Section07/Normal.ipynb

Solution: see next page and UnsupervisedML/Exercises/Section07/Exercise\_07.1.1.ipynb

### Exercise 7.1.2 (Jupyter Notebook)

The goal of this problem is to help you create a vectorized version of the function to compute the multi-dimensional normal probability density function.

- (a) We start off with a vectorized version of the dot product. Define the following  $d$ -dimensional column vectors:  $X_0, \dots, X_{M-1}$  and  $Y_0, \dots, Y_{M-1}$ . Define  $X$  and  $Y$  to be the  $dxM$  dimensional matrices:

$$X = [X_0 \ X_1 \ \dots \ X_{M-1}] \quad Y = [Y_0 \ Y_1 \ \dots \ Y_{M-1}]$$

Create a function using numpy functionality that takes in  $X$  and  $Y$  and computes the dot products  $X_0^T Y_0, X_1^T Y_1, \dots, X_{M-1}^T Y_{M-1}$  **without explicit looping**. The output should be a 2d numpy array with dimension  $1 \times M$ . Hint: use component-wise multiplication and numpy sum.

- (b) Using the approach from (a) create a function that takes in  $X = [X_0 \ X_1 \ \dots \ X_{M-1}]$  ( $dxM$ ), mean  $\mu$  ( $dx1$ ), and covariance  $\Sigma$  ( $dxd$ ) and computes the normal pdf  $N(X, \mu, \Sigma)$  for each of the vectors in  $X$ . The output should be a 2d numpy array ( $1 \times M$ ). There should not be any explicit looping. Hint: one can compute  $\Sigma^{-1}(X - \mu)$  using appropriate numpy functions and then compute  $(X - \mu)^T \Sigma^{-1} (X - \mu)$  using the approach in (a).
- (c) Consider the normal pdf calculation for dataset  $X$  for  $d=2$  dimensions and  $M=100000$  samples for the mean and covariance from 7.1.1. Compare time for computing the normal pdf for columns of  $X$  for the non-vectorized version (from demo) and the vectorized version (from (b)).

Solution: see UnsupervisedML/Exercises/Section07/Exercise\_07.1.2.ipynb

Exercise 7.1.2: Solution: Consider the equation:

$$N(X, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{1}{2}(X-\mu)^T \Sigma^{-1} (X-\mu)} = c$$

If  $c$  is sufficiently large, then there are no real value solutions  $X$  for this equation. From the document UnsupervisedML\_GMM.pdf, the width (long dimension) of the elliptical contour is:

$$width = 2\sqrt{-2\log [c2\pi\sqrt{|\Sigma|}]\sqrt{\sigma_0}}$$

If  $c$  is too large, then the term in the first square root will be negative, so you will get an error when trying to compute width. Same issue occurs for the height.

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

## Section 7.2

Exercise 7.2.1 (Theory) Suppose that a dataset has  $M$  data points. Can you provide an explanation as to why the complexity for number of operations for the Gaussian Mixture Model algorithm is  $O(M)$  as  $M \rightarrow \infty$ .

Solution: see next page

Solution 7.2.1: At each iteration of the algorithm one performs:

(1) Expectation Step:

Compute the conditional probabilities  $\gamma_{ki}$  for clusters  $k=0,\dots,K-1$  and data points  $i=0,\dots,M-1$ .

(2) Maximization Step:

Compute the means  $\{\mu_k\}$ , covariances  $\{\Sigma_k\}$ , weights  $\{\phi_k\}$  for clusters  $k = 0,\dots,K-1$ .

In (1), there  $K*M$  probabilities to compute, where  $K$  is the number of clusters and  $M$  is the number of data points. Each of these probabilities involves a computation of the normal distribution pdf given by the formula:

$$N(X, \mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^d |\Sigma|}} e^{-\frac{1}{2}(X-\mu)^T \Sigma^{-1} (X-\mu)}$$

This computation is done  $K*M$  times for the  $K$  clusters and the  $M$  data points  $X_0, X_1, X_2, \dots, X_{M-1}$ .

In (2), one must compute  $K$  mean, covariances, and  $K$  weight. Each of these calculations involves summing from 0 to  $M-1$ . For example, for the means we have:

$$\mu_k = \frac{1}{M_k} \sum_{i=0}^{M-1} \gamma_{ki} X_i$$

Hence, the amount of work for each of the mean, covariance, and weight calculations is  $O(M)$  operations as  $M \rightarrow \infty$  as the sum is over the  $M$  data points.

Looking at each of these calculations carefully, it can be shown that the total amount of work  $O(M)$  operations as  $M \rightarrow \infty$ . Note that the amount of will depend on the number of clusters, the dimension, and the number of iterations. The  $O(M)$  estimate assumes that the number of iterations is bounded (has a maximum independent of the number of data points  $M$ ).



## Section 7.4

Exercise 7.4.1 (Testing) Experiment with the `driver_gaussianmm.py` code and try the other cases: `blobs`, `varied_blobs2`, `aniso`, `noisy_moons`, and `noisy_circles`. Experiment with the number of clusters and number of samples.

Exercise 7.4.2 (Programming) For the `varied_blobs1` dataset, write a program to determine the number of clusters for the Gaussian Mixture Model using the elbow method. (Plot final log likelihood value as a function of number of clusters for various number of clusters for the `varied_blobs1` dataset with 200 points.)

Solution: see `UnsupervisedML/Exercises/Section07/Exercise_7.3.2.py`. Run this program in folder `UnsupervisedML/Code/Programs`.

Exercise 7.4.3 (Programming) Suppose that a dataset has  $M$  data points. Confirm that the number of operations is  $O(M)$  as  $M \rightarrow \infty$  for the GaussianMM algorithm by measuring time for completing the algorithm for various values of  $M$ .

Hint: use one of the sklearn datasets for this Exercise and run the GaussianMM algorithm code for various values of  $M$ .

Solution: see `UnsupervisedML/Exercises/Section07/Exercise_7.3.3.py`. Run this program in folder `UnsupervisedML/Code/Programs`

Exercise 7.4.4 (Programming) Write a code to perform the Expectation Maximization algorithm in the case of the “spherical” approach. In this approach each covariance matrix is diagonal with the same variance value in each entry. The algorithm for this case is described in the `UnsupervisedML_GMM.pdf` file.

Hints: You can implement the algorithm using any approach that you like. Here are suggestions:

- (1) Create a function to compute the multi-dimensional normal pdf in case of constant variance (instead of a full covariance matrix).
- (2) Create a derived class `gaussianmm_spherical` with parent `gaussianmm`
- (3) Use a variable to track the variance for each component of the mixture at each iteration
- (4) Keep `self.Covsave` variable and update it after each maximization step with the constant diagonal covariance matrix for each component at each iteration. This will allow you to use the `plot_cluster` and `plot_cluster_animation` methods without any changes.

Use the spherical approach to perform clustering for the `varied_blobs1` dataset.

Solution: see `UnsupervisedML/Exercises/Section07/gaussianmm_spherical.py` and `Exercise_7.4.4.py` and run these files in folder `UnsupervisedML/Code/Programs`. I have created a separate class. It is probably better coding practice to implement both the original case and spherical case in the same class.

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### Section 8.1

Exercise 8.1.1 (Programming) Confirm that the number of operations for the Davies-Bouldin calculation is  $O(M)$  as  $M \rightarrow \infty$ . Confirm that the number of operations for the Silhouette is  $O(M^2)$  as  $M \rightarrow \infty$ .

Hint: perform clustering with K Means for one of the sklearn datasets and measure time to compute Davies-Bouldin and Silhouette as a function of M.

Solution: see next page and UnsupervisedML/Exercises/Section08/Exercise\_08.1.1.py

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

Solution 8.1.1: For Davies-Bouldin, I am finding a complexity power of 0.87 instead of 1. For Silhouette, I am finding a complexity power of around 1.5 instead of 2. The Silhouette power seems to be on the low side. For Silhouette I am using M up to around 25000. This suggests one should increase the value of M to get a result that is closer to the power of 2.

## Section 9.1

Exercise 9.1.1 (Jupyter Notebook) Consider the following dataset:

$$X = \begin{bmatrix} 1 & -2 & 7 & -8 \\ -3 & 4 & -9 & 10 \\ 5 & 6 & -11 & 12 \end{bmatrix}$$

- Compute the compact SVD of  $X$  using `numpy.linalg.svd` function and confirm that  $X = U\Sigma V^T$ .
- Determine the new dataset  $R$  using only the first 2 principal components.
- Determine the reconstructed  $X$  using the first 2 principal components.
- What proportion of the variance is captured by the first 2 principal components?

Solution: See UnsupervisedML/Exercises/Section09/Exercise\_09.1.1.ipynb

Exercise 9.1.2 (Jupyter Notebook) Consider the following dataset:

$$X = \begin{bmatrix} 1 & 3 \\ 5 & 7 \\ 2 & 4 \\ 6 & 8 \end{bmatrix} \quad X_0 = \begin{bmatrix} 1 \\ 5 \\ 2 \\ 6 \end{bmatrix} \quad X_1 = \begin{bmatrix} 3 \\ 7 \\ 4 \\ 8 \end{bmatrix}$$

This is an example of a dataset with 2 data points and 4 dimensions. We can represent  $X$  in 2 dimensions and still retain all the “information”.

- Compute the compact SVD of  $X$  using the `numpy.linalg.svd` function.
- Compute the representation  $R$  using 2 dimensions.
- Determine the length (L2 Euclidean) of the individual data points  $X_0$  and  $X_1$  and the L2 distance between these points.
- Determine the length (L2 Euclidean) of the individual data points  $R_0$  and  $R_1$  and the L2 distance between these points. The lengths and distance should be the same as in (c), so no “information” is lost.

Solution: see UnsupervisedML/Exercises/Section09/Exercise\_09.1.2.ipynb

### Section 9.3

Exercise 9.3.1 (Testing) Consider the matrix:

$$X = \begin{bmatrix} 1 & 2 & 11 & -12 & 2 \\ 3 & 4 & 13 & 1 & -7 \\ -1 & -2 & -1 & -2 & -3 \\ -7 & -1 & -4 & -5 & -6 \end{bmatrix}$$

Use the code in `pca.py` to answer the following questions:

- (a) Compute the compact version of the singular value decomposition and plot the cumulative variance proportion.
- (b) Compute the reduced dimension version of  $X-X\text{mean}$  capturing 0.99 proportion of the variance.
- (c) Compute the reconstructed version of  $X$  capturing 0.99 proportion of the variance.

Solution: see `UnsupervisedML/Exercises/Section09/Exercise_09.3.1.py` and run this file in `UnsupervisedML/Code/Programs`

Exercise 9.3.2 (Testing) Consider a 50x1000 random dataset (50 dimensions and 1000 samples). Use the `pca` code to estimate number of principal components needed to capture 0.85 proportion of the variance.

Solution: see next page and `UnsupervisedML/Exercises/Section09/Exercise_09.3.2.py` and run this file in `UnsupervisedML/Code/Programs`

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

Exercise 9.3.2 Solution: in my example 40 principal components are required to capture 0.85 proportion of the variance.

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### **Section 9.4**

Exercise 9.4.1 (Testing) Run the driver\_pca\_mnist.py (with 60000 samples and the train dataset) to answer the following questions

- (a) What is minimum number of dimensions to capture 50%, 90%, and 99% of the variance?
- (b) What is the minimum number of dimensions for you to be able distinguish the digits?

If 60000 samples is too many for your computer, change to 10000 samples (or fewer) with the valid dataset.

Solution: see next page

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

Exercise 9.4.1 Solution: run the driver\_pca\_mnist.py in UnsupervisedML/Code/Programs and vary the variance\_capture setting.

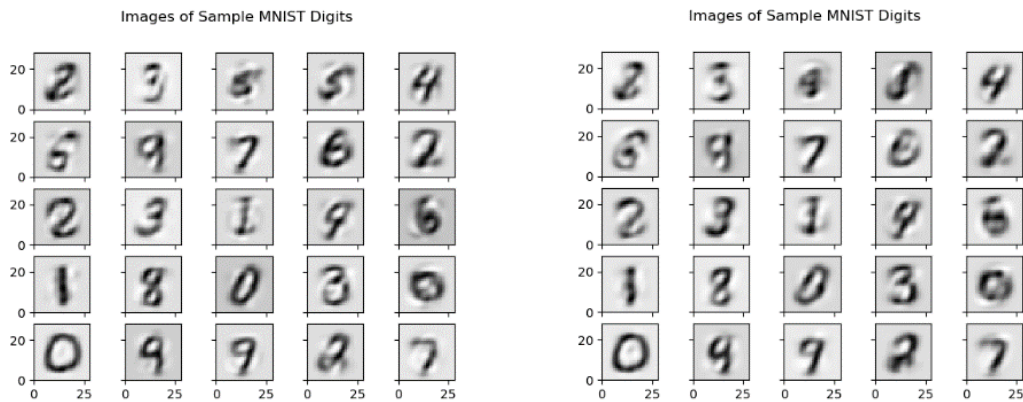
For 0.50 variance capture: 11 dimensions

For 0.95 variance capture: 154 dimensions

For 0.99 variance capture: 331 dimensions

Exercise 9.4.2 Solution:

The plot on the left is based on 20 dimensions (capturing 0.644 proportion of the variance). The plot on the right is based on 15 dimensions (capturing 0.529 proportion of the variance). With the figure on the right, the digits are a bit fuzzy and starting to be difficult to identify.





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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

## **Section 10.2**

Exercise 10.2.1 (Programming) Perform clustering for the Iris Flower dataset using the DBSCAN, K Means, and Gaussian Mixture Model methods after using PCA to reduce the number of dimensions to 2.

Solution: See files

UnsupervisedML/Exercises/Exercise\_10.2.1\_DBSCAN.py

UnsupervisedML/Exercises/Exercise\_10.2.1\_KMeans.py

UnsupervisedML/Exercises/Exercise\_10.2.1\_GMM.py

Run these files in the UnsupervisedML/Code/Programs folder.

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### **Section 10.3**

**Exercise 10.3.1 (Testing)** The idea with this Exercise is to determine the lowest proportion of variance capture that still yields reasonable results for MNIST Digits Dataset clustering. I will let you define “reasonable” for yourself. Experiment with the `casestudy_mnist.py` code and examine results as a function of the PCA variance capture amount. (Use the K Means algorithm for clustering)

**Exercise 10.3.2 (Testing)** In Section 07, we talked about the “spherical” approach for the Gaussian Mixture Model. This approach appears to be more stable and runs faster than the full covariance matrix approach that is implemented in the file `gaussianmm.py`. Do the same thing as Exercise 10.3.1 with this spherical approach.

**Solution:** use the code in `UnsupervisedML/Exercises/Section07/gaussianmm_spherical.py` with driver in `UnsupervisedML/Exercises/Section10/Exercise_10.3.2.py`. Run these files in the folder `UnsupervisedML/Code/Programs`.

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Solution files located at Github site: <https://github.com/satishchandrareddy/UnsupervisedML>

### **Section 10.4**

Exercise 10.4.1 (Testing) The idea with this Exercise is to determine the lowest proportion of variance capture that still yields reasonable results for BBC Text clustering. I will let you define “reasonable” for yourself. Experiment with the `casestudy_bbctext.py` code and examine results as a function of the PCA variance capture amount.