Homework 4: Clustering

Due: 23:59 on Mon 21 November

You have 3 weeks so no extensions.

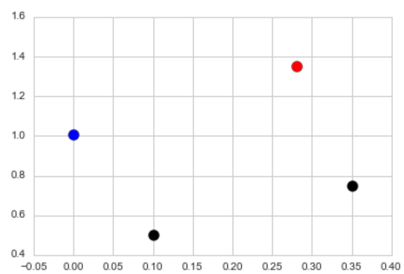
You will do this assignment individually and submit your answers via the Blackboard course website.

Problem 1 (The Curse of Dimensionality, 9pts)

In d dimensions, consider a hypersphere of unit radius, centered at zero, which is inscribed in a hypercube, also centered at zero, with edges of length two. What fraction of the hypercube's volume is contained within the hypersphere? Write this as a function of d. What happens when d becomes large?

Problem 2 (Norms, Distances, and Hierarchical Clustering, 10 pts)

Consider the following four data points, belonging to three clusters: the black cluster $((x_1, y_1) = (0.1, 0.5)$ and $(x_2, y_2) = (0.35, 0.75))$, the red cluster $(x_3, y_3) = (0.28, 1.35)$ cluster, and the blue cluster $(x_4, y_4) = (0, 1.01)$.



At each step of hierarchical clustering, the two most similar (or least dissimilar) clusters are merged together. This step is repeated until there is one single group. Different distances can be used to measure group dissimilarity. Recall the definition of the l_1, l_2, and l_∞ norm:

- For $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$
- For $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$
- For $\mathbf{x} \in \mathbb{R}^n$, $\|\mathbf{x}\|_\infty = \max_{i=1}^n |x_i|$

Also recall the definition of single-link distance, complete-link distance, and average-link distance between two clusters:

- Single-link clustering: for clusters G and H, $d_S(G, H) = \min_{i \in G, j \in H} d(i, j)$
- Complete-link clustering: for clusters G and H, $d_C(G, H) = \max_{i \in G, j \in H} d(i, j)$
- Average-link clustering: for clusters G and H, $d_A(G, H) = \frac{1}{|G||H|} \sum_{i \in G} \sum_{j \in H} d(i, j)$

Warm up question. Draw the 2D unit sphere for each norm, defined as $\mathcal{S} = \{x \in \mathbb{R}^2 : \|x\| = 1\}$. Feel free to do it by hand, take a picture and include it in your pdf.

Main question. For each norm (l_1, l_2, l_∞) and each clustering method (single, complete, or average link clustering), specify which 2 clusters would be the first to merge.

K-Means [30 pts]

Implement K-Means clustering from scratch.[1]. You have been provided with the MNIST dataset. The MNIST task is widely used in supervised learning, and modern algorithms with neural networks do very well on this task. We can also use MNIST for interesting unsupervised tasks. You are given representations of 6000 MNIST images, each of which are 28×28 handwritten digits. In this problem, you will implement K-means clustering on MNIST, to show how this relatively simple algorithm can cluster similar-looking images together quite well.

Problem 3 (K-means, 30pts)

The given code loads the images into your environment as a 6000x28x28 array. Implement K-means clustering on it for a few different values of K, and show results from the fit. Show the mean images for each class, and by selecting a few representative images for each class. You should explain how you selected these representative images. To render an image, use the numpy imshow function, which the distribution code gives an example of. Use squared norm as your distance metric. You should feel free to explore other metrics along with squared norm if you are interested in seeing the effects of using those. Also, your code should use the entire provided 6000-image dataset (which, by the way, is only 10% of the full MNIST set).

Are the results wildly different for different restarts and/or different K? Plot the K-means objective function as a function of iteration and verify that it never increases.

Finally, implement K-means++ and see if gives you more satisfying initializations (and final results) for K-means. Explain your findings.

As in past problem sets, please include your plots in this document. There may be tons of plots for this problem, so feel free to take up multiple pages, as long as it is organized.

Problem 4 (Calibration, 1pt)

Approximately how long did this homework take you to complete?

[1] That is, don't use a third-party machine learning implementation like `scikit-learn`; `numpy` and `PyTorch` are fine.