

ISYE 6740, Summer 2020, Homework 2

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1. Order of faces using ISOMAP (30 points)

The objective of this question is to reproduce the ISOMAP algorithm results that we have seen discussed in lecture as an exercise. The file `isomap.mat` (or `isomap.dat`) contains 698 images, corresponding to different poses of the same face. Each image is given as a 64×64 luminosity map, hence represented as a vector in \mathbb{R}^{4096} . This vector is stored as a row in the file. [This is one of the datasets used in the original paper for ISOMAP, J.B. Tenenbaum, V. de Silva, and J.C. Langford, Science 290 (2000) 2319-2323.] In this question, you are expected to implement the ISOMAP algorithm by coding it up yourself.

- (a) (10 points) Choose the Euclidean distance between images (i.e., in this case a distance in \mathbb{R}^{4096}). Construct a similarity graph with vertices corresponding to the images, and tune the threshold ϵ so that each node has at least 100 neighbors (this approach corresponds to the so-called ϵ -Isomap). Visualize the similarity graph (you can visualize the graph using various graph visualization packages, and illustrate a few images corresponds to nodes at different parts of the graph; you can be a bit creative here).
- (b) (10 points) Implement the ISOMAP algorithm and apply it to this graph to obtain a $d = 2$ -dimensional embedding. Present a plot of this embedding. Find three points that are “close” to each other in the embedding space, and show what they look like. Do you see any visual similarity among them?
- (c) (10 points) Now choose ℓ_1 distance (or Manhattan distance) between images (recall the definition from “Clustering” lecture)). Repeat the steps above. Again construct a similarity graph with vertices corresponding to the images, and tune the threshold ϵ so that each node has at least 100 neighbors. Implement the ISOMAP algorithm and apply it to this graph to obtain a $d = 2$ -dimensional embedding. Present a plot of this embedding. Do you see any difference by choosing a different similarity measure, by comparing results in Part (a)(b) and Part (c)?

2. Density estimation: Psychological experiments. (30 points)

The data set `n90pol.csv` contains information on 90 university students who participated in a psychological experiment designed to look for relationships between the size of different regions of the brain and political views. The variables `amygdala` and `acc` indicate the volume of two particular brain regions known to be involved in emotions and decision-making, the amygdala and the anterior cingulate cortex; more exactly, these are residuals from the predicted volume, after adjusting for height, sex, and similar body-type variables. The variable `orientation` gives the students' locations on a five-point scale from 1 (very conservative) to 5 (very liberal).

- (a) (10 points) Form 2-dimensional histogram for the pairs of variables (`amygdala`, `acc`). Decide on a suitable number of bins so you can see the shape of the distribution clearly.
- (b) (10 points) Now implement kernel-density-estimation (KDE) to estimate the 2-dimensional with a two-dimensional density function of (`amygdala`, `acc`). Use a simple multi-dimensional Gaussian kernel, for

$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in \mathbb{R}^2,$$

where x_1 and x_2 are the two dimensions respectively

$$K(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(x_1^2 + x_2^2)}{2}}.$$

Recall in this case, the kernel density estimator (KDE) for a density is given by

$$p(x) = \frac{1}{m} \sum_{i=1}^m \frac{1}{h} K\left(\frac{x^i - x}{h}\right),$$

where x^i are two-dimensional vectors, $h > 0$ is the kernel bandwidth. Set an appropriate h so you can see the shape of the distribution clearly. Plot of contour plot (like the ones in slides) for your estimated density.

- (c) (10 points) Plot the condition distribution of the volume of the `amygdala` as a function of political `orientation`: $p(\text{amygdala} | \text{orientation} = a)$, $a = 1, \dots, 5$. Do the same for the volume of the `acc`. Plot $p(\text{acc} | \text{orientation} = a)$, $a = 1, \dots, 5$. You may either use histogram or KDE to achieve the goal. You can refer to the supplementary notes in Canvas on conditional expectation helpful.

3. Implementing EM algorithm for MNIST dataset. (40 points)

Implement the EM algorithm for fitting a Gaussian mixture model for the MNIST dataset. We reduce the dataset to be only two cases, of digits “2” and “6” only. Thus, you will fit GMM with $C = 2$. Use the data file `data.mat` or `data.dat` on Canvas. True label of the data are also provided in `label.mat` and `label.dat`

The matrix `images` is of size 784-by-1990, i.e., there are totally 1990 images, and each column of the matrix corresponds to one image of size 28-by-28 pixels (the image is vectorized; the original image can be recovered by map the vector into a matrix.)

You may find the tips in the supplementary notes useful, which explains how to evaluate the density of a multi-variate normal distribution. In this homework question, follow the low-rank approximation (with $r = 100$) to address the numerical issues.

- (a) (5 points) Select from data one raw image of “2” and “6” and visualize them, respectively.
- (b) (10 points) Use random Gaussian vector with zero mean as random initial means, and two identity matrices I as initial covariance matrices for the clusters. Plot the log-likelihood function versus the number of iterations to show your algorithm is converging.
- (c) (5 points points) Report, the fitting GMM model when EM has terminated in your algorithms, including the weights for each component and the mean vectors (please reformat the vectors into 28-by-28 images and show these images in your submission). Ideally, you should be able to see these means corresponds to “average” images. No need to report the covariance matrices.
- (d) (10 points) Use the p_{ic} to infer the labels of the images, and compare with the true labels. Report the mis-classification rate for digits “2” and “6” respectively. Perform K -means clustering with $K = 2$ (you may call a package or use the code from your previous homework). Find out the miss classification rate for digits “2” and “6” respectively, and compare with GMM. Which one achieves the better performance?
- (e) (10 points) Now first PCA to reduce the dimensionality of the data before applying to EM. We will put all “6” and “2” digits together, to project the original data into 5-dimensional vectors. Now implement EM algorithm for the projected data (with 5-dimensions). Compare the mis-classification rate of the EM algorithm using the original data (results from Part (b)-(c)), and try to explain what may cause the difference in their performance.