SLT coding exercise #1

Locally Linear Embedding

https://gitlab.vis.ethz.ch/vwegmayr/slt-coding-exercises

Due on Monday, March 6th, 2017

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Contents

The Model

The model section is intended to allow you to recapitulate the essential ingredients used in Locally Linear Embedding. Write down the *necessary* equations to specify Locally Linear Embedding and and shortly explain the variables that are involved. This section should only introduce the equations, their solution should be outlined in the implementation section.
Hard limit: One page

Locally linear embedding (LLM) is an unsupervised learning algorithm that computes low-dimensional neighbourhood preserving embeddings. Given N real-valued vectors x_i with the dimensionaly D. It is supposed that data point with its neighbourhoods lie on or close to a locally linear patch. We characterize the local goemetry of these patches by linear coefficients that reconstruct each data point from its neighbours. The reconstruction error is the sum of the squared distance between all the data points and their reconstructions:

$$E(W) = \sum_i (x_i - \sum_j w_{ij} x_j)^2, \tag{1}$$

whereas the weights w_{ij} is the contribution of the j-th data point to the i-th reconstruction with the constraint $\sum\limits_j w_{ij} = 1$.
With the fixed weights each high dimensional observation vector x_i is mapped to a low dimensional vector y_i with the dimensionality $d << D$. We choose the coordinates y_i to minimize the embedding cost function:

$$E(y_1, ...y_N) = \sum_i (y_i - \sum_j w_{ij} y_j)^2, \tag{2}$$

with the constraints $\sum\limits_i y_i = 0$ and $\sum_i y_i y_i^T = 1$.

The Questions

This is the core section of your report, which contains the tasks for this exercise and your respective solutions. Make sure you present your results in an illustrative way by making use of graphics, plots, tables, etc. so that a reader can understand the results with a single glance. Check that your graphics have enough resolution or are vector graphics. Consider the use of GIFs when appropriate.
Hard limit: Two pages

(a) Get the data

For this exercise we will work with the MNIST data set. In order to learn more about it and download it, go to http://yann.lecun.com/exdb/mnist/.

(b) Locally linear embedding

Implement the LLE algorithm and apply it to the MNIST data set. Provide descriptive visualizations for 2D & 3D embedding spaces. Is it possible to see clusters?

(c) Cluster structure

Investigate the cluster structure of the data. Can you observe block structures in the M matrix (use matrix plots)? Also plot the singular values of M. Do you notice something? Can you think of ways to determine the optimal embedding dimension?

(d) Nearest Neighbors

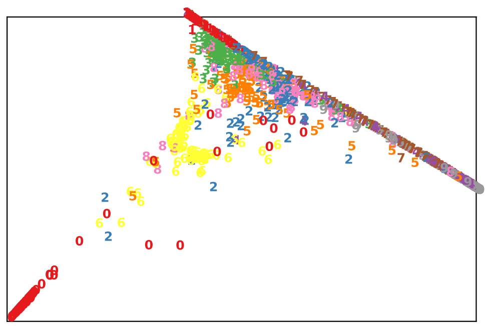
Investigate the influence of the choice of how many nearest neighbors you take into account. Additionally, try different metrics to find the nearest neighbors (we are dealing with images!).

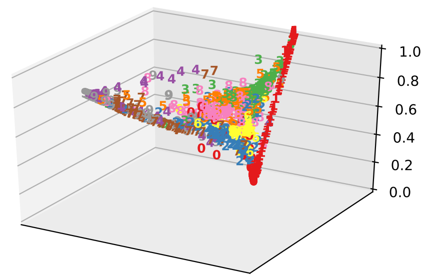
(e) Linear manifold interpolation

Assume you pick some point in the embedding space. How can you map it back to the original (high dimensional) space? Investigate how well this works for points within and outside the manifold (does it depend on the dimensionality of the embedding space?) Try things like linearly interpolating between two embedding vectors and plot the sequence of images along that line. What happens if you do that in the original space?

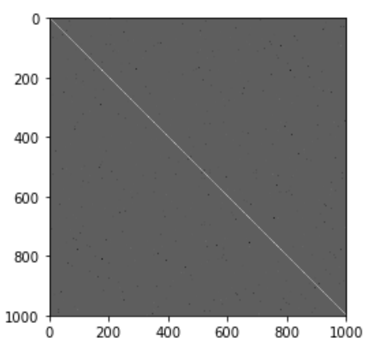
The Questions continued on next page...

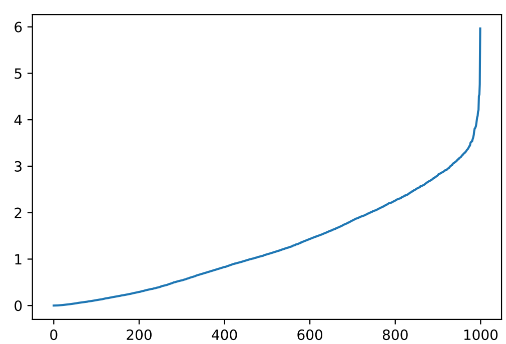
(b) Locally linear embedding: the figures below show the results of locally linear embedding applied to the mnist dataset. The large dimensional data are mapped to 2D and 3D space respectively. Fur the purpose of simplification, only the first thousand digit images of the ten thousand test images are used. The weights are found with five neighbourhoods, which are determined using k-d tree. We can observe clusters in both of the images, although the edges among the clusters can not be determined clearly. This is caused by the fact that compression of the data leads to information loss.



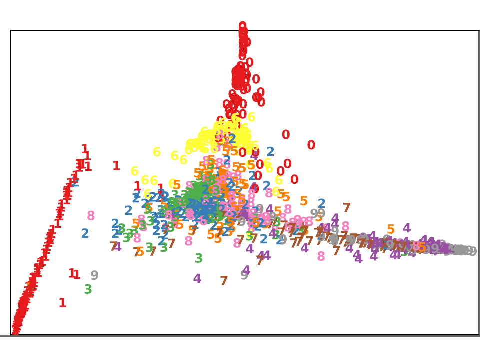


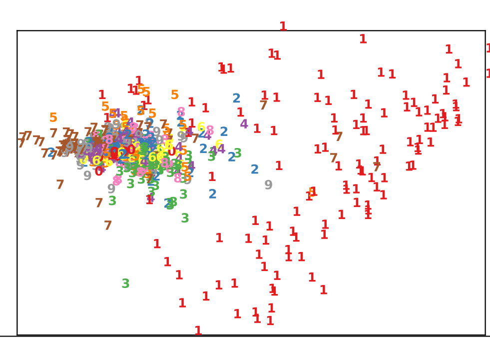
(c) Cluster structure: The figures below show the M matrix in gray value of the 2D embedding using thousand data with five neighbours and the plot of its eigenvalues. We can observe that the M matrix is a diagonal matrix, the off-diagonal elements are close to zero.
We can observe an increase of eigenvalues, where the increase is small in the beginning (0-900) and large in the end (900-1000). The optimal reconstruction is using eigenvectors of the M matrix with the smallest $d+1$ eigenvalues discard the first eigenvector with the eigenvalue zero. The optimal dimension d can be chosen such that the increase of the eigenvalues from the first to the $(d+1)$th is as slow as possible. We discard the eigenvalues after 900, since they increase dramatically and lead to large embedding error.





(d) Nearest Neighbors





The figures above show the results of 2D embedding using 10 neighbours (left) and 20 neighbours (right) respectively. Compared with the figure in the question (b) with 5 neighbours, we can observe that the number of the neighours influence the results in a dramatic way. We would expect that we can achieve a better performance, e.g. a clearer clustering, of embedding with increasing number of neighbours. However, it can not be observed here clearly.

The Implementation

In the implementation section you give a concise insight to the practical aspects of this coding exercise. It mainly mentions the optimization methods used to solve the model equations. Did you encounter numerical or efficiency problems? If yes, how did you solve them? Provide the link to your git branch of this coding exercise.
Hard limit: One page

With the Lagrange multiplier

Your Page

Your page gives you space to include ideas, observations and results which do not fall into the categories provided by us. You can also use it as an appendix to include things which did not have space in the other sections.
No page limit.

Your Answer
YOUR GIT BRANCH