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

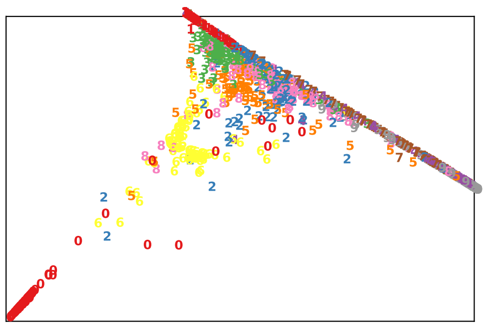
Investigate the influence of the choice of how many nearest neighbors you take into account. Additionally, try different metrics to find the nearest neighbors (we are dealing with images!).

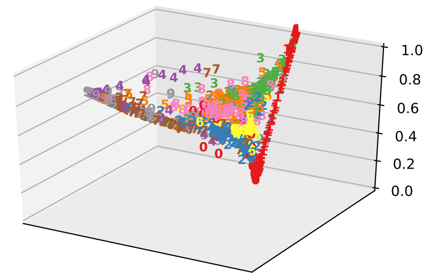
## (e) Linear manifold interpolation

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. . . 

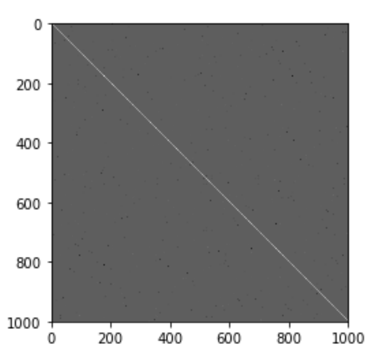
(b) Locally linear embedding: the figures below show the results of locally linear embedding applied to the mnist dataset. The large dimensional data are mapped to 2D and 3D space respectively. Fur the purpose of simplification, only the first thousand digit images of the ten thousand test images are used. The weights are found with five neighbourhoods, which are determined using ckd tree. We can observe clusters in both of the images.

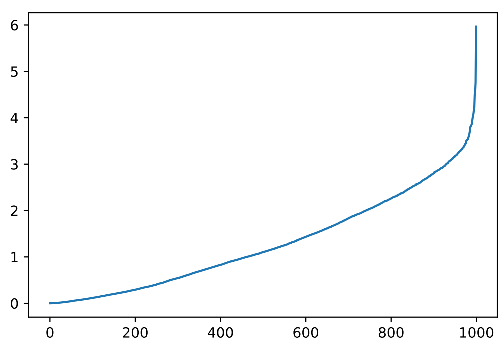




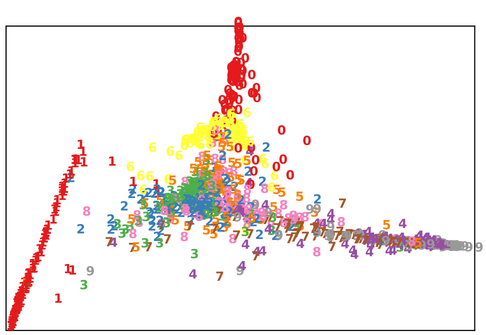

(c) Cluster structure: The figures below show the M matrix in gray value of the 2D embedding using thousand data with five neighbours and the plot of its eigenvalues. We can observe that the M matrix is a diagonal matrix, the off-diagonal elements are close to zero.

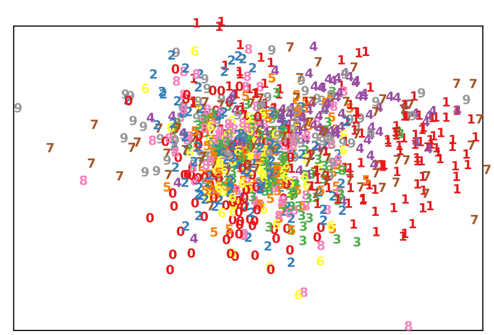
We can observe an increase of eigenvalues, where the increase is small in the beginning (0-900) and large in the end (900-1000). The optimal reconstruction is using eigenvectors of the M matrix with the smallest $d+1$ eigenvalues discard the first eigenvector with the eigenvalue zero. The optimal dimension $d$ 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.



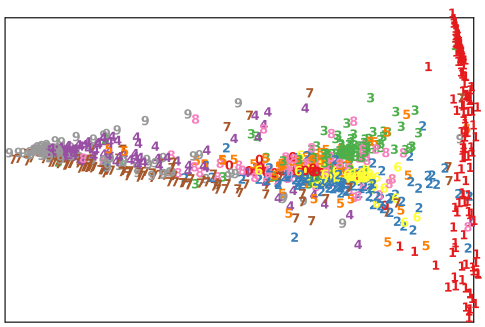



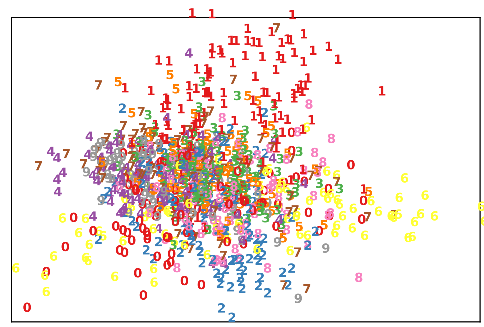

(d) Nearest Neighbors



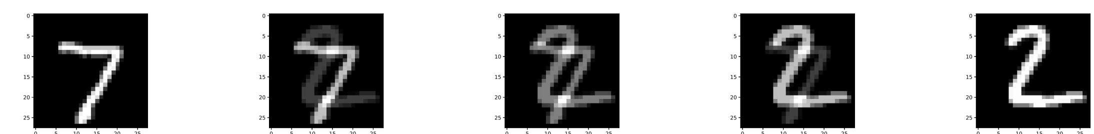


The figures above show the results of 2D embedding using 10 neighbours (left) and 50 neighbours (right) respectively. Compared with the figure in the question (b) with 5 neighbours, we can observe that the number of the neighours influence the results in a dramatic way. The increase of the number of neighbours does not lead to a better clustering. If we use too much neighbours, we may include points that do not belong to the cluster of the point. The distance metric used here is the usual Euclidean distance.
The figures below shows the results of the embedding using the sum-of-absolute-values Manhattan distance. In our case, the Manhattan distance leads to a better result, especially in the case using 50 neighbours.

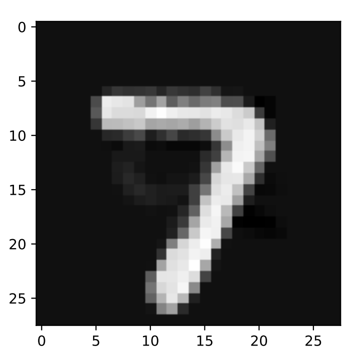


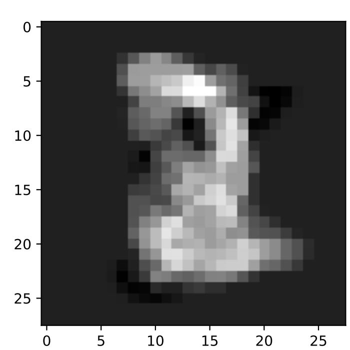


(e) Linear manifold interpolation: The figure below shows the linear interpolation applied to the orignal space. The first image is the first data point in the mnist test dataset and the fifth image is the second data point. The three images between are interpolated images.



For reconstruction we first compute the k nearest neighbours of the chosen points and then use the equation (3) to find the optimal weights. In the orignal space we weight the neighbour images with the weights we compute before. The sum is the mapping of the chosen point in the embedding space to the original space.
The figure below on the left side is the reconstructed image using point within the manifold (the first image above), whereas the figure on the right side use point outside the manifold (the forth image above). This method works well for points within the manifold, but not very well for points outside the manifold. The higher the dimensionality of the embedding space, the better will be the result of backwards mapping.





# 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

The first step to implement locally linear embedding is to compute the neighbors of each data point. We can use different approaches for finding the nearest neighbours, e.g. ball tree, ckd tree.
The second step is to compute the weight matrix W with the weights $w_{ij}$ that minimize the reconstruction error with the contraint $\sum_j w_{ij} = 1$. Using the Lagrange multiplier we can find that the optimal weight is

$$w_{ij} = \frac{\sum_k C^{(i)-1}_{jk}}{\sum_{lk} C^{(i)-1}_{lk}}, \tag{3}$$

whereas $C^{(i)}$ is the covariance matrix with the elements $C^{(i)}_{jk} = (x_i - x_j)^T(x_i - x_k)$. For each data $X_i$ we compute the matrix $C^{(i)}$ and its inverse in order to compute the weights.
The third step is to compute the d-dimensional vectors $y_i$ which minimize the embedding error by its bottom nonzero eigenvectors. The equation of the embedding error can be rewritten into

$$E(y_1, ..., y_N) = \sum_k u_k^T M u_k, \tag{4}$$

whereas $M = (I - W)^T(I - W)$ and $u_k = (y_{1k}...y_{Nk})$ for $k = 1, ..., d$. The vector $u$s are found computing the eigenvectors of the matrix M with the smallest $d + 1$ eigenvalues and discarding the first eigenvector associated with the eigenvalue 0.
During my implementation the computation of inverse C matrix is very inefficient. The more neighbours we use, the slower is the computation, as a high dimensional matrix with the dimensionality equal to the number of neighbours needs to be invert. For the implementation I have used the package numpy and scipy.
The link of my coding exercise: https://gitlab.vis.ethz.ch/vwegmayr/slt-coding-exercises/tree/16-930-687/1_locally_linear_embedding.

# 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
https://gitlab.vis.ethz.ch/vwegmayr/slt-coding-exercises/tree/16-930-687/1_locally_linear_embedding