Machine Learning: Exercise Sheet 11

Dimensionality Reduction & Matrix Factorization

In-class Exercise

There is no in-class exer

Homework

t-SNE

Problem 1: Figure 1 shows a scatter plot of your two-dimensional data ($N = 13$ instances). You want to apply a non-linear dimensionality reduction technique based on neighbor graphs (e.g. T-SNE or UMAP). As a first step you compute the $N \times N$ weighted adjacency matrix representing the neighbor graph. Assume that the weights are computed as

$$p_{j|i} = \frac{\exp\left(-\|\mathbf{x}_i - \mathbf{x}_j\|^2 / 2\sigma^2\right)}{\sum_{k \neq i} \exp\left(-\|\mathbf{x}_i - \mathbf{x}_k\|^2 / 2\sigma^2\right)}$$

where $\boldsymbol{x}_i \in \mathbb{R}^2$ and you set $p_{i|i} = 0$. Finally, you obtain the similarity between instances i and j with $p_{ij} = \frac{p_{i|j} + p_{j|i}}{2}$.

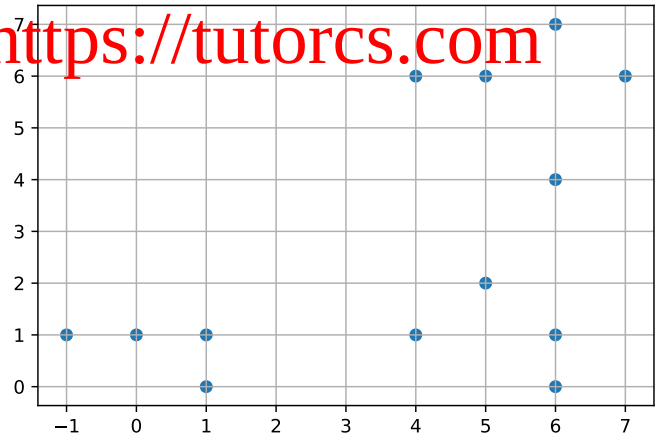
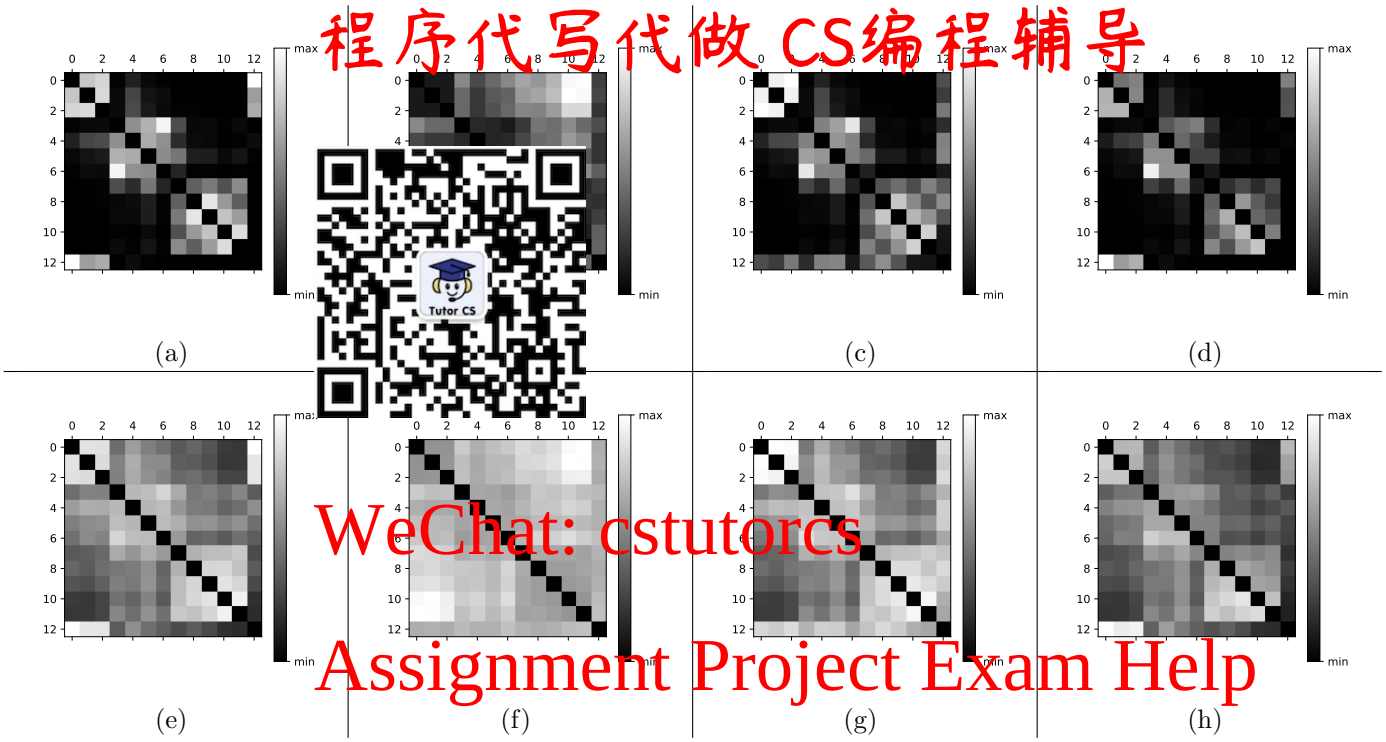


Figure 1: Scatter plot of the data

Which of the following neighbor graph plots (pixel in position i, j shows the value of p_{ij}) corresponds to the given dataset and the stated formula for $\sigma = 2$? What is your answer for $\sigma = 5$? *Justify your answers!*

Upload a single PDF file with your homework solution to Moodle by 19.01.2022, 11:59pm CET. We recommend to typeset your solution (using LaTeX or Word), but handwritten solutions are also accepted. If your handwritten solution is illegible, it won't be graded and you waive your right to dispute that.



(a) and (e) are correct for $\sigma = 2$ and $\sigma = 5$, respectively.

1. First column is correct.
2. Second column shows a distance instead of similarity.
3. Third column misses one instance in the lower left cluster and it is located at the center instead $(2.75, 3.5)$.
4. Fourth column shows an asymmetrical matrix.
5. Upper row $\sigma = 2$, lower row $\sigma = 5$.

Autoencoders

Problem 2: We train a linear autoencoder to D-dimensional data. The autoencoder has a single K-dimensional hidden layer, there are no biases, and all activation functions are identity ($\sigma(x) = x$).

- Why is it usually impossible to get zero reconstruction error in this setting if $K < D$?
- Under which conditions is this possible?

We have $f(\boldsymbol{x}) = \boldsymbol{X}\boldsymbol{W}_1\boldsymbol{W}_2$ where $\boldsymbol{X}$ is the data matrix and the dimensions of the weight matrices are $D \times K$ for $\boldsymbol{W}_1$ and $K \times D$ for $\boldsymbol{W}_2$.

The final multiplication $\boldsymbol{W}_2$ brings points from K-dimensions up into D-dimensions but the points will still all be in a K-dimensional linear subspace. Unless the data happen to lie exactly in a

K-dimensional linear subspace, they can't be exactly fitted.

Coding Exercise

Problem 3: Download `exercise_11_notebook.ipynb` and `exercise_11_matrix_factorizations.npy` from Moodle. Fill in the missing code and run the notebook. Convert the evaluated notebook to PDF and append it to your other solutions before uploading.